Supplementary Information

Diastereoselective synthesis of a bicyclic β-lactam with penicillin G-like spectrum of activity by carbonylation of an acyclic diaminocarbene

Tim Schulz,[a] Christian Färber,[a] Michael Leibold,[a] Clemens Bruhn,[a] Pascal Prochnow,[b] Julia E. Bandow,[b] Tanja Schneider,[c] Timo Porsch,[d] Max C. Holthausen*[d] and Ulrich Siemeling*[a]

[a] Institute of Chemistry, University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel, Germany. E-mail: siemeling@uni-kassel.de

[b] Biology of Microorganisms, Ruhr University Bochum, Universitätsstr. 150, D-44801 Bochum, Germany

[c] *Pharmaceutical Microbiology, University of Bonn, Meckenheimer Allee 168, D-53115 Bonn, Germany.*

[d] Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe-Universität Frankfurt, Max-von-Laue-Str. 7, D-60438 Frankfurt am Main, Germany. E-mail: max.holthausen@chemie.uni-frankfurt.de

1. Experimental Section

General

All reactions were carried out in an inert atmosphere by applying standard Schlenk or glovebox techniques. Lithium diisopropylamide (LDA) was prepared by reaction of *n*-butyllithium with diisopropylamine in hexane, isolated by filtration, washed with hexane and dried *in vacuo*. NMR spectra were recorded at 298 K in $CDCl_3$ solution with a Varian Unity Inova 500 MHz NMR spectrometer operating at 500.1 MHz for ^1H. Signal assignments were made with the help of 2D NMR experiments (HSQC, HMBC and HH-COSY). Mass spectra were obtained with a quadrupole ion-trap spectrometer Finnigan LCQ^{DECA} (ThermoQuest, San José, USA). High-resolution mass spectra (HRMS) were measured with a time-of-flight mass spectrometer micrOTOF (Bruker Daltonics, Bremen, Germany) using an Apollo^{TM} "ion funnel" ESI ion source. Mass calibration was performed immediately prior to the measurement with ESI Tune Mix Standard (Agilent, Waldbronn, Germany).

Synthesis of *cis*-4b

The starting material diisopropylamino-*cis*-2,6-dimethylpiperidinocarbene (**1b**) may be obtained in 63% yield from the corresponding formamidinium salt.[S1] It is more convenient, however, to use **1b** generated *in situ*, since this has no detrimental effect on the overall yield.

A solution of the formamidinium salt [**1b**H][PF_6] (900 mg, 2.4 mmol) in THF (20 mL) placed in a thick-walled Rotaflo® ampoule (100 mL) was cooled to –80 °C. A solution of LDA (322 mg, 3.0 mmol) in THF (6 mL) cooled to –80 °C was added. After 10 min the mixture was allowed to warm to room temperature and stirred for a further 30 min. The resulting light yellow solution of **1b** was degassed by 3 freeze-pump-thaw cycles. After the last cycle, carbon monoxide was introduced into the vessel. The ampoule was connected to a CO-filled balloon in order to maintain a slight positive pressure of carbon monoxide. After 3 h volatile components were removed *in vacuo* and the crude product was extracted with toluene (3 × 15 mL). The solvent was removed *in vacuo* to afford the product as viscous oil. Yield: 388 mg (63%).

^{1}H NMR: δ = 4.09 (1H, m, O=C-N-C*H*Me), 3.87 (1H, s, *i*Pr_2NC*H*), 3.13 (2H, sept, $^3J_{HH}$ = 6.7 Hz, C*H*Me_2), 1.80 – 1.46 (6H, m, CH_2), 1.26 (3H, s, *i*Pr_2N-CH-C*Me*), 1.18 (3H, d, $^3J_{HH}$ = 6.9 Hz, O=C-N-CH*Me*), 1.12 (6H, d, $^3J_{HH}$ = 6.9 Hz, CH*Me*$_2$), 1.00 (6H, d, $^3J_{HH}$ = 5.5 Hz, CH*Me*$_2$).

^{13}C NMR: δ = 168.9 (C=O), 76.8 (*i*Pr_2N*C*), 61.1 (*i*Pr_2N-CH-*C*Me), 47.8 (br., *C*HMe_2), 42.7 (O=C-N-*C*HMe), 35.4 (CH_2), 30.4 (CH_2), 23.8 CH*Me*$_2$, 21.9 CH*Me*$_2$, 21.0 (*i*Pr_2N-CH-C*Me*), 19.7 (O=C-N-CH*Me*), 16.7 (CH_2).

IR (ATR): ν(CO) = 1739 (s) cm^{-1}.

MS/APCI(+): *m*/*z* (%) = 253.1 (100) $[M + H]^+$.

HRMS/ESI(+): *m*/*z* = 275.208603 $[M + Na]^+$, calcd. for $[C_{15}H_{28}N_2NaO]^+$ 275.209385.

Synthesis of [*cis*-4bH]Cl

A solution of *cis*-**4b** (90 mg, 0.4 mmol) in diethyl ether (10 mL) was cooled to 0 °C. 2M HCl in diethyl ether (0.3 mL, 0.6 mmol) was added. After 10 min the colourless precipitate was filtered off and washed with diethyl ether (2 × 5 mL). Yield: 65 mg (63%). Crystals suitable for an X-ray diffraction study were obtained by layering a chloroform solution of [*cis*-**4b**H]Cl with hexane.

^{1}H NMR: δ = 11.0 (1H, br. s, NH), 4.17 (1H, sept, $^3J_{HH}$ = 6.1 Hz, NC*H*), 4.10 (1H, br. m, NC*H*), 4.03 (1H, br. m, NC*H*) 3.94 (1H, s, *i*Pr_2HN-C*H*), 1.93 (3H, s, *i*Pr_2HN-CH-C*Me*), 1.84 – 1.30 (18H, m, 3 CH_2 and 4 Me), 1.24 (3H, d, $^3J_{HH}$ = 7.0 Hz, Me).

^{13}C NMR: δ = 159.5 (C=O), 72.4 (*i*Pr_2HN*C*), 59.9 (*i*Pr_2HN-CH-*C*Me), 57.1 (*C*HMe_2), 55.9 (*C*HMe_2), 43.9 (O=C-N-*C*HMe), 36.7 (CH_2), 29.8 (CH_2), 22.9 (CH_2), 20.8 (Me), 19.5 (Me), 19.2 (Me), 18.6 (Me), 16.1 (Me), 15.6 (Me).

IR (ATR): ν(CO) = 1745 (s) cm^{-1}.

HRMS/ESI(+): *m*/*z* = 253.226905 $[M – Cl]^+$, calcd. for $[C_{15}H_{29}N_2O]^+$ 253.227440.

X-ray Structure Analysis

The diffraction experiment was carried out by mounting a single-crystal on a glass fibre and all geometric and intensity data were taken from this sample. Data collection using Mo-K_α radiation (λ = 0.71073 Å) was made on a Stoe IPDS2 diffractometer equipped with a 2-circle goniometer and an area detector. Absorption correction was done by integration using X-red.[S2] The data sets were corrected for Lorentz and polarisation effects. The structures were solved by direct methods (SHELXS 97) and refined using alternating cycles of least squares refinements against F^2 (SHELXL 97).[S3] All non-hydrogen atoms were found in difference Fourier maps and were refined with anisotropic displacement parameters. H atoms were placed in constrained positions according to the riding model with the 1.2 fold isotropic displacement parameters. Graphical representations were made using ORTEP-3 win.[S4]

Crystal data for [*cis*-**4b**H]Cl·$CHCl_3$: $C_{16}H_{30}Cl_4N_2O$, M = 408.22, triclinic, a = 7.0484(6) b = 10.8646(9), c = 14.7271(14) Å, α = 90.854(7), β = 99.683(7), γ = 105.453(7)°, U = 1069.40(16) $Å^3$, T = 120(2) K, space group P -1 (no. 2), Z = 2, 8101 reflections measured, 3779 unique (R_{int} = 0.0728) which were used in all calculations. The final $wR(F^2)$ was 0.1574 (all data), the final $R1(F)$ was 0.0522 [$I > 2\sigma(I)$].

Determination of the Minimal Inhibitory Concentrations (MICs)

The MICs against bacterial strains were determined in a microtiter plate assay according to the Clinical and Laboratory Standards Institute (CLSI) guidelines[S5] as described previously.[S6] The Gram-positive strains used were *Bacillus subtilis* DSM 402, *Staphylococcus aureus* DSM 20231 (type strain), and *Staphylococcus aureus* ATCC 43300 (MRSA), the Gram-negative strains were *Escherichia coli* DSM 30083, *Acinetobacter baumannii* DSM 30007, and *Pseudomonas aeruginosa* DSM 50071. In brief, 5×10^5 cells mL^{-1} in Mueller Hinton broth (BD Diagnostics) were exposed to different compound concentrations ranging from 512 µg mL^{-1} to 0.5 µg mL^{-1} prepared by serial twofold dilution in final assay volumes of 200 µL. The lowest concentration that inhibited visible bacterial growth after incubation at 37 °C for 18 h was recorded as MIC. Experiments were performed with identical results in two independent experiments. The results are collected in Table S1.

Table S1 Minimal inhibitory concentrations

	Gram-negative			Gram-positive		
	E. coli	*A. baumannii*	*P. aeruginosa*	*B. subtilis* 168	*S. aureus* (type strain)	*S. aureus* (MRSA)
4a	no activity	no activity	no activity	256 µg mL^{-1}	256 µg mL^{-1}	256 µg mL^{-1}
cis-**4b**	no activity	no activity	no activity	128 µg mL^{-1}	64 – 128 µg mL^{-1}	128 µg mL^{-1}
penicillin G	64 µg mL^{-1}	no activity	no activity	8 µg mL^{-1}	0.5 µg mL^{-1}	16 µg mL^{-1}
amoxicillin	64 µg mL^{-1}	no activity	no activity	2 – 4 µg mL^{-1}	2 µg mL^{-1}	48 µg mL^{-1}

2. Computational Section

2.1 Computational Details

All structure optimisations and frequency calculations were performed with the Gaussian09 program package[S7] employing the B97-D functional, which includes empirical dispersion corrections,[S8] in combination with the SVP[S9] basis set (B97-D/SVP). For improved computational efficiency, the resolution-of-the-identity (RI) approximation[S10, S11] was used in these calculations employing the corresponding SVPfit auxiliary basis set.[S12, S13] All stationary points localised were characterised as minima or first order saddle points by eigenvalue analysis of computed Hessian matrices. Connectivities between minima and transition states implied in the Figures and Schemes were validated by intrinsic-reaction-coordinate (IRC) following calculations.[S14] Unscaled zero-point vibrational energies, as well as thermal and entropic corrections were obtained from Hessians computed at the RI-B97-D/SVP level using standard procedures implemented in Gaussian09. Subsequent single-point calculations were performed with the ORCA program package[S15] employing the B2GP-PLYP[S16] double-hybrid functional in combination with the def2-QZVP[S17] basis set. For the SCF part the RI-JK algorithm and for the MP2 part the RI algorithm were used as implemented in ORCA[S18] in combination with the appropriate def2-QZVP/jk and def2-QZVP/c auxiliary basis sets,[S19, S20] respectively. Empirical dispersion[S21, S22] and free-energy corrections were added and relative energies discussed in the text refer to Gibbs free energy differences at 298.15 K obtained at the B2GP-PLYP-D/def2-QZVP//B97-D/SVP level of theory.

Additional structure optimisations and frequency calculations were performed within the SMD solvent model,[S23] employing toluene as solvent. Following ref. S24 we extracted SMD free energy of solvation contributions for a number of decisive elementary steps and added these increments to the free energies obtained at the B2GP-PLYP-D/def2-QZVP//B97-D/SVP level of DFT (given in green colour in Fig. S2 below).

DFT methods have successfully been used to compute conformer energy differences dominated by anomeric effects.[S25] We further note a recent benchmark study,[S26] in which Grimme and Goerigk have shown that the B2GP-PLYP-D/def2-QZVP level of double-hybrid DFT provides an accurate description of relative conformer energies.

2.2 Reaction Pathways

Reaction pathways investigated for the carbonylation of diaminocarbene **1b** are depicted in Fig. S1. Starting from the axial isomer, ketene formation represents an exergonic step with a moderate activation barrier comparable with those previously found for related carbenes,[S27] whereas the alternative route via the equatorial isomer is kinetically significantly disfavoured. The resulting ketene $\mathbf{2b_{ax}}$ is, however, only slightly more stable than the conformer $\mathbf{2b_{eq}}$, and we thus investigated subsequent reaction steps for both ketene conformers.

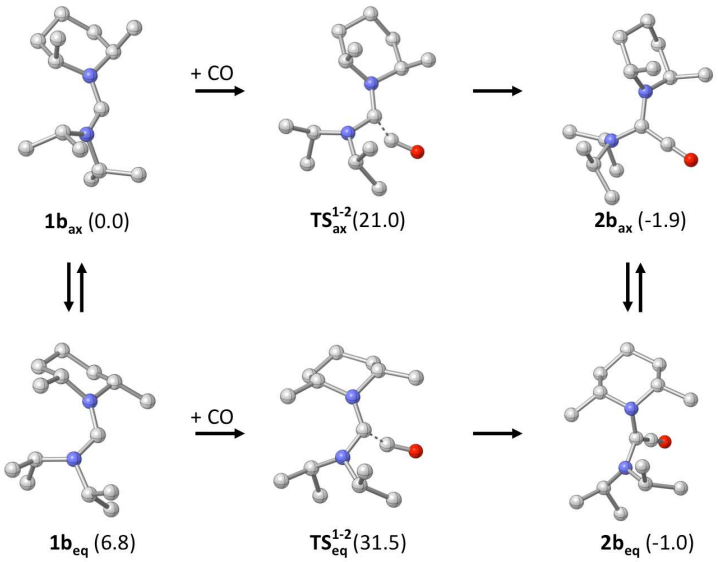

Fig. S1 Carbonylation of **1b** (ΔG(298K) in kcal mol^{-1}; B2GP-PLYP-D/def2-QZVP//B97-D/SVP).

Fig. S2 displays all pathways studied for the reactivity of **2b$_{ax}$**, including side reactions not reported in the main text, *viz.* the formation of β-lactam *trans*-**4b$_{ax}$** via the transient carbene **3b$_{ax/c}$** as well as the competing intermolecular reaction of **2b$_{ax}$** with residual diaminocarbene **1b$_{ax}$** leading to the betainic oxoallyl species **5$_{ax}$**. In previous work we have established similar reaction paths for related species.[S27, S28] Owing to the unsymmetrical nature of the ketene **2b$_{ax}$**, two different intramolecular pathways exist. Piperidyl migration to form **3b$_{ax}$** has a lower barrier and represents a more exergonic step than migration of the *i*Pr$_2$N substituent. However, the barrier for the competing intermolecular carbene addition leading to **5$_{ax}$** is only slightly higher (21.3 *vs.* 22.1 kcal mol^{-1}). We have therefore repeated the B97-D calculations for the axial pathways including solvent contributions evaluated by means of the SMD model[S23] and relative free energies are shown in green colour in Fig. S2. While hardly any changes in relative energies are seen between the gas-phase and the solvent-corrected data for most species, we find an increase of the barrier to oxyallyl formation by 4.0 kcal mol^{-1} and a lowering of the barriers leading to β-lactam formation by about 2 kcal mol^{-1}. Hence, although the solvent effects recovered within the SMD model do not lead to drastic changes of relative energies within the computed reaction pathways, they operate in opposite directions for the rate-limiting steps of the oxyallyl path and the β-lactam paths, respectively. Within the solvent model, the latter path leading to **3b$_{ax}$** is kinetically clearly favoured ($\Delta G^{\ddagger}$ = 19 kcal mol^{-1}) over the former one leading to **5$_{ax}$** ($\Delta G^{\ddagger}$ = 26 kcal mol^{-1}), which is fully in line with experimental observation.

We have identified two different conformers of the transient carbene resulting from the piperidyl migration (**3b$_{ax}$** and **3b$_{ax/c}$**). Upon subsequent C–H bond activation and ring clo-

sure, they give rise to the formation of two different β-lactam diastereomers (*cis*-**4**$_{ax}$ and *trans*-**4**$_{ax}$, respectively). The barrier for the formation of *cis*-**4**$_{ax}$ (16.9 kcal mol^{-1}) is substantially lower than that leading to *trans*-**4**$_{ax}$ (22.0 kcal mol^{-1}). The latter barrier competes in height with the preceding barrier to form **3b**$_{ax}$ and thus becomes kinetically discriminative, whereas the former one is readily surmountable under the reaction conditions. This picture is fully in line with the experimental observation of exclusive formation of *cis*-**4b**$_{ax}$.

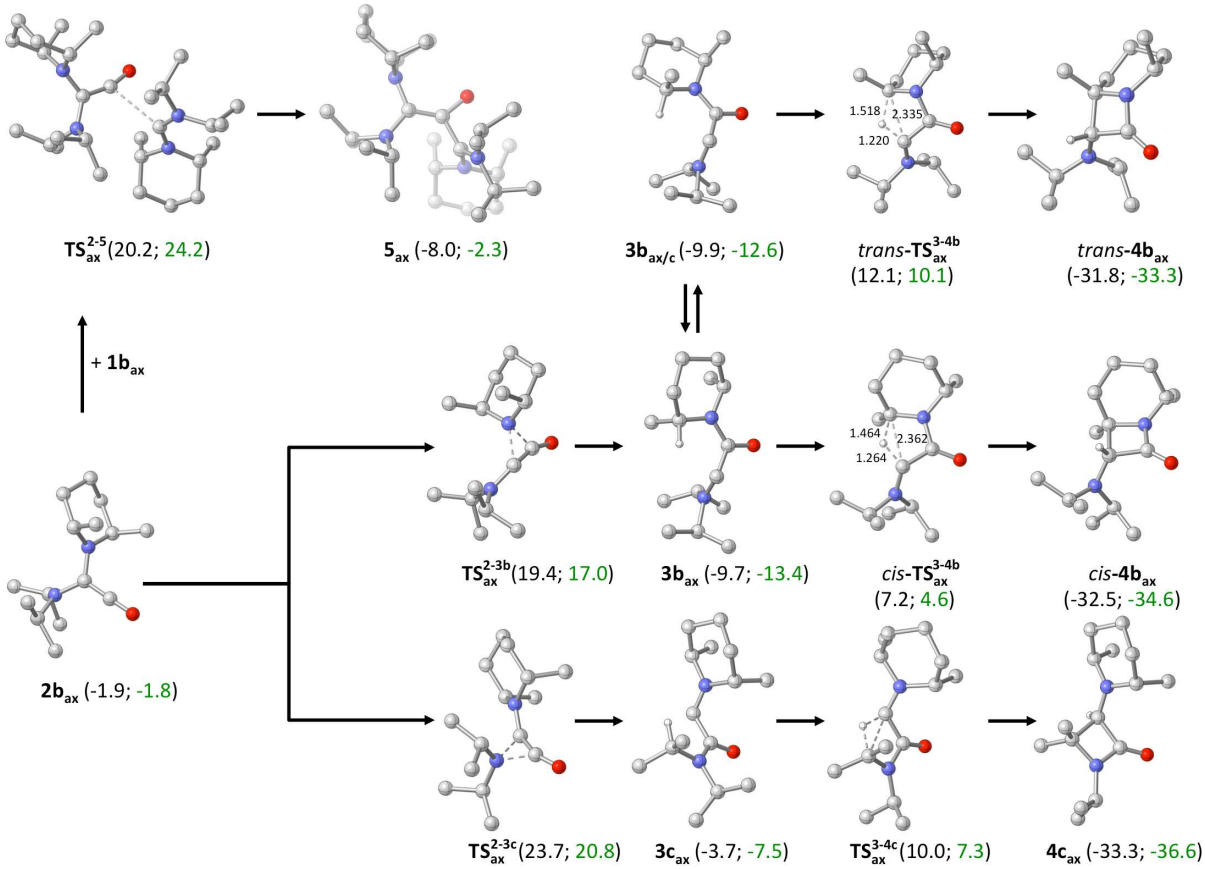

Fig. S2 Computed reaction pathways for **2b**$_{ax}$ (ΔG(298K) in kcal mol^{-1}; atomic distances in Å; black: B2GP-PLYP-D/def2-QZVP//B97-D/SVP; relative free energies corrected for solvent effects (B2GP-PLYP-D/def2-QZVP//B97-D/SVP + ΔG_{solv}) given in green.

The analogous reaction pathways studied commencing from the slightly less stable conformer **2b**$_{eq}$ are shown in Fig. S3. Despite systematic searches, we were unable in this case to localise a transition structure for the intermolecular reaction with another carbene unit corresponding to the formation of **5**$_{ax}$ above. The formation of **3b**$_{eq}$ has a barrier height (20.1 kcal mol^{-1}) comparable to that calculated for the corresponding formation of **3b**$_{ax}$. Subsequently, essentially barrierless conformational changes are necessary to bring the C–H bond either in 2- or in 6-position of the piperidyl group sufficiently close to the $C_{carbene}$ atom to allow for reactive interactions. Starting from the twisted boat conformers **3b**$_{eq/b}$ and **3b**$_{eq/bc}$, C–H bond activation is possible. The kinetically favoured product *cis*-**4b**$_{eq/b}$ can easily isomerise to the more stable *cis*-**4b**$_{ax}$, which connects both the axial and the equatorial pathways on the

product side. Due to the conformational flexibility of the piperidyl ring the reactions occurring along the two kinetically favoured pathways (Fig. S2 and S3) converge to the formation of the same product, *viz.* the thermodynamically most stable species *cis*-**4b**$_{ax}$.

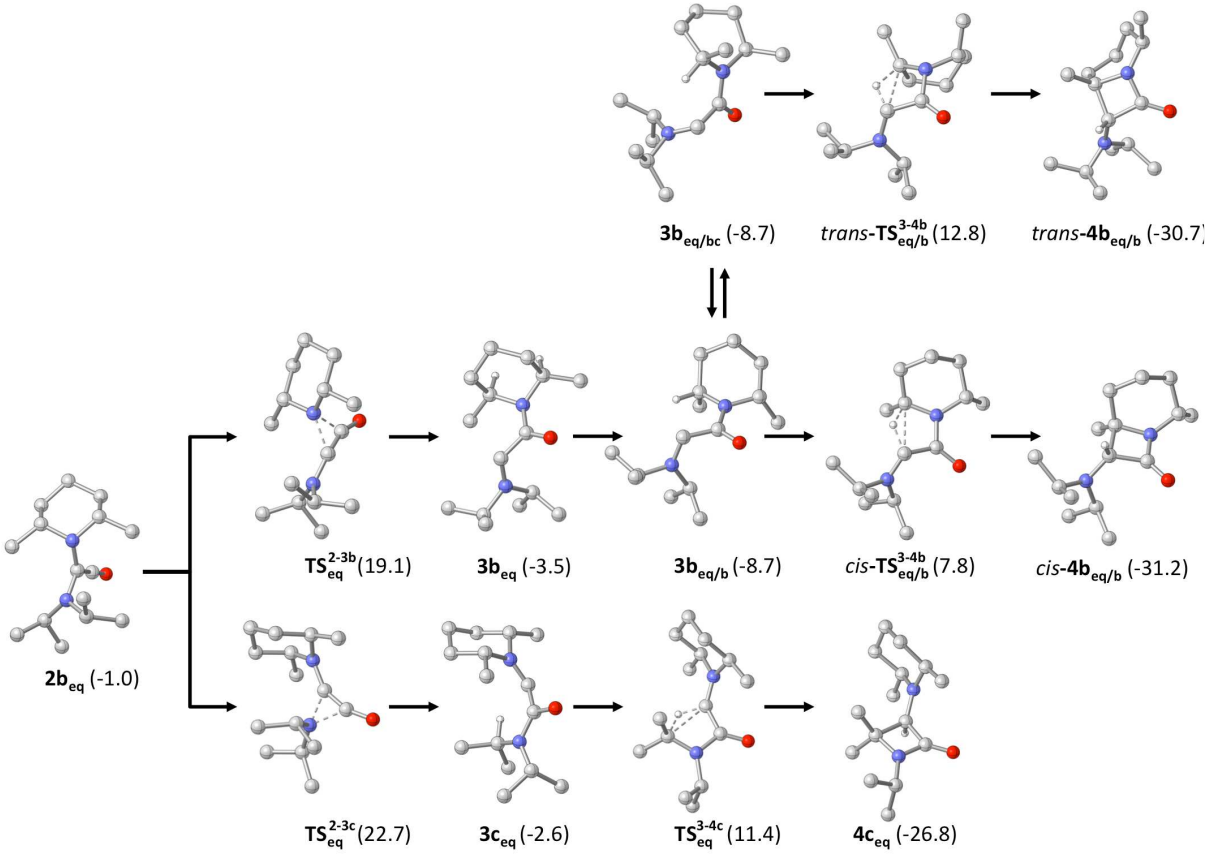

Fig. S3 Computed reaction pathways for **2b**$_{eq}$ (ΔG(298K) in kcal mol^{-1}; B2GP-PLYP-D/def2-QZVP//B97-D/SVP).

In conclusion, our computational results agree well with the experimentally observed diastereoselective formation of *cis*-**4b**$_{ax}$ in the reaction of **1b** with CO.

3. References

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4. Optimised Structures (Cartesian coordinates in Å obtained at the RI-B97-D/SVP level of DFT)

$1b_{ax}$

C	-0.503809	0.549681	0.182245
N	0.329564	-0.471375	0.475910
C	0.401756	-0.793714	1.938914
H	1.144961	-1.605139	2.045441
C	1.040693	-1.444081	-0.410631
H	0.738867	-1.210863	-1.437876
C	0.928635	0.405641	2.739885
H	0.219839	1.248335	2.646547
H	1.042283	0.134474	3.807868
H	1.911865	0.730613	2.348470
C	-0.945789	-1.297499	2.475597
H	-1.261146	-2.217196	1.948849
H	-0.874681	-1.516491	3.558561
H	-1.707873	-0.515139	2.305882
C	0.569884	-2.894041	-0.176222
H	-0.529300	-2.964092	-0.266995
H	1.029397	-3.553011	-0.937940
H	0.862175	-3.277558	0.818414
C	2.568258	-1.316649	-0.299671
H	2.907946	-1.548918	0.727878
H	3.072233	-2.019868	-0.991788
H	2.896197	-0.287860	-0.540568
N	-0.563806	1.136687	-1.037983
C	0.410964	1.064148	-2.171305
H	1.318096	0.603040	-1.756345
C	0.842571	2.479914	-2.623969
H	1.505641	2.377236	-3.505698
H	1.441963	2.935842	-1.811256
C	-0.350114	3.395005	-2.926541
H	-0.936270	2.991085	-3.775841
H	0.002941	4.399164	-3.231131
C	-1.227152	3.483164	-1.671026
H	-2.115291	4.121111	-1.845236
H	-0.637816	3.950423	-0.856767
C	-1.696504	2.094268	-1.191087
H	-2.086467	2.193153	-0.164430
C	-2.832008	1.518995	-2.056755
H	-3.086964	0.500160	-1.711120
H	-3.730941	2.157862	-1.958387
H	-2.573163	1.469780	-3.129346
C	-0.072828	0.214179	-3.364448
H	0.786302	-0.049274	-4.011980
H	-0.556440	-0.719066	-3.023276
H	-0.803675	0.761901	-3.983850

$1b_{eq}$

C	-0.193029	-0.910396	0.098672
N	-1.327522	-0.176390	0.072550
N	0.888902	-0.577575	0.835324
C	-2.446987	-0.809322	-0.697903
H	-3.258183	-0.060469	-0.749729
C	-2.983697	-2.027619	0.065700
H	-3.320598	-1.737422	1.079557
H	-3.835408	-2.485079	-0.474737
H	-2.172092	-2.772439	0.165658
C	-2.047896	-1.170900	-2.137487
H	-1.225563	-1.907151	-2.114383
H	-2.916380	-1.599787	-2.674020
H	-1.700120	-0.276322	-2.685906
C	-1.478529	1.288095	0.301714
H	-0.560132	1.614414	0.801229

C	-1.524634	2.052922	-1.037132
H	-2.425898	1.794628	-1.623377
H	-1.547156	3.143095	-0.844288
H	-0.633203	1.819144	-1.647476
C	-2.683622	1.647760	1.186364
H	-3.637115	1.457458	0.658889
H	-2.683171	1.060758	2.120563
H	-2.657375	2.724048	1.446620
C	2.194709	-1.175368	0.416167
C	3.112837	-0.006112	-0.016387
H	2.651308	-1.649901	1.314345
C	2.095654	-2.238424	-0.675975
C	3.320008	1.029927	1.104810
H	4.091100	-0.410694	-0.342384
H	2.641386	0.472841	-0.899089
C	1.984096	1.492904	1.718673
H	3.926135	0.562752	1.908463
H	3.899145	1.896182	0.729735
C	1.126402	0.261442	2.068967
H	2.167674	2.097225	2.630526
H	1.432279	2.136744	1.004306
H	1.782604	-0.391241	2.680467
C	-0.093864	0.531191	2.964080
H	3.112324	-2.647139	-0.846050
H	1.411506	-3.050813	-0.380784
H	1.711372	-1.807642	-1.616916
H	0.228073	0.492213	4.021326
H	-0.544740	1.523339	2.801559
H	-0.872707	-0.235108	2.810572

CO

C	0.000000	0.000000	0.130400
O	0.000000	0.000000	1.269600

$2b_{ax}$

N	-1.406132	1.627717	-1.711250
C	-0.335266	0.674672	-2.045009
C	-2.302951	2.094473	-2.702159
C	-0.821895	-0.723057	-2.490567
C	-1.870995	1.755153	-0.318382
C	-0.746033	2.210254	0.628438
N	-2.521317	3.488985	-2.835250
C	0.615591	1.276082	-3.093501
C	-2.585665	0.496104	0.209018
C	-3.007607	1.267955	-3.487849
O	-3.607519	0.556486	-4.221122
H	0.241370	0.534706	-1.111639
H	-2.608121	2.580331	-0.347926
H	-3.037367	0.686689	1.202378
H	-3.389688	0.190120	-0.487127
H	-1.874299	-0.345396	0.315394
H	-1.165410	2.453492	1.623329
H	0.014549	1.419263	0.776401
H	-0.244486	3.107973	0.222039
H	1.424011	0.563117	-3.344068
H	0.056434	1.504285	-4.020618
H	1.067244	2.212954	-2.718466
H	0.033986	-1.423358	-2.555028
H	-1.556964	-1.136694	-1.778220
H	-1.292639	-0.678997	-3.490196
C	-3.860982	4.054537	-2.602861
C	-3.726089	5.490429	-2.045457
C	-4.810185	4.014403	-3.822490
H	-4.313703	3.419053	-1.816854
C	-2.809566	6.354583	-2.926786
H	-4.732589	5.943316	-1.956727
H	-3.292026	5.433593	-1.027438

C	-1.424257	5.698208	-3.027159
H	-3.250696	6.463400	-3.937272
H	-2.722026	7.374835	-2.506093
C	-1.504251	4.254887	-3.574073
H	-0.746352	6.293605	-3.669173
H	-0.977075	5.659634	-2.013977
C	-1.679416	4.207149	-5.106473
H	-0.544157	3.761128	-3.337356
H	-5.831668	4.309704	-3.512519
H	-4.484226	4.708060	-4.617570
H	-4.861418	2.998009	-4.251178
H	-1.838381	3.163459	-5.437283
H	-2.540960	4.811075	-5.443403
H	-0.771497	4.595199	-5.608499

2b$_{eq}$

N	-1.336060	1.729385	-1.501974
C	-1.255660	0.485107	-2.297077
C	-2.406786	2.634327	-1.749965
C	-2.564771	-0.326118	-2.282236
C	-0.668640	1.735957	-0.186221
C	0.862031	1.627679	-0.326076
N	-2.367500	3.554994	-2.838954
C	-0.769684	0.779590	-3.728078
C	-1.210375	0.665410	0.784071
C	-3.452668	2.557092	-0.916946
O	-4.395179	2.452386	-0.206343
H	-0.483601	-0.141077	-1.811441
H	-0.899910	2.723817	0.252548
H	-0.719786	0.754589	1.772653
H	-2.301204	0.775816	0.925294
H	-1.009256	-0.353006	0.399561
H	1.343096	1.727902	0.665784
H	1.158546	0.645519	-0.741487
H	1.249150	2.418644	-0.992052
H	-0.696713	-0.156049	-4.316819
H	-1.461784	1.472859	-4.235073
H	0.224773	1.262317	-3.699328
H	-2.431662	-1.282476	-2.823688
H	-2.874018	-0.548880	-1.244826
H	-3.378173	0.237089	-2.770048
C	-3.572201	3.742994	-3.684867
C	-4.563776	4.756645	-3.062915
H	-3.190175	4.201824	-4.623071
C	-4.275228	2.435840	-4.058589
C	-3.871792	6.089288	-2.730512
H	-5.405326	4.923577	-3.764136
H	-4.995409	4.313443	-2.143847
C	-2.588688	5.860092	-1.914718
H	-3.600446	6.598064	-3.679305
H	-4.565921	6.763344	-2.191643
C	-1.666582	4.847429	-2.628078
H	-2.051528	6.816158	-1.755652
H	-2.834969	5.452073	-0.911903
H	-1.469900	5.238926	-3.649942
C	-0.320615	4.693473	-1.920615
H	-5.058265	2.652414	-4.808824
H	-3.566964	1.707792	-4.489804
H	-4.761851	1.972145	-3.182179
H	0.222074	5.656679	-1.954441
H	-0.461766	4.419897	-0.860581
H	0.288971	3.910299	-2.402605

3b$_{ax}$

C	-3.614720	-1.054588	-0.151586
C	-2.484248	-0.250127	-0.805033
N	-1.772938	0.566107	0.244463

C	-0.619221	0.274419	0.778161
C	0.020596	-1.004787	0.432213
C	-2.949199	0.599766	-1.995821
C	-2.531611	1.756335	0.775717
C	-2.700140	1.654317	2.295396
C	-1.825072	3.048164	0.349349
O	-0.440178	-2.043089	0.940067
H	-1.728189	-0.963464	-1.173977
H	-3.533603	1.724412	0.312873
H	-3.332850	-0.071719	-2.786994
H	-3.765308	1.294095	-1.723283
H	-2.113135	1.188489	-2.415340
H	-4.101440	-1.701267	-0.906725
H	-3.194371	-1.688127	0.648947
H	-4.388013	-0.385796	0.273494
H	-3.284062	2.518176	2.665682
H	-3.227391	0.721505	2.568222
H	-1.706386	1.645400	2.777606
H	-2.376437	3.929804	0.726837
H	-0.802726	3.054240	0.771438
H	-1.755285	3.119270	-0.752192
N	1.181899	-0.973189	-0.317501
C	1.883870	-2.241645	-0.589052
C	1.577886	0.277129	-0.985279
C	3.410844	-2.021535	-0.600575
C	1.366815	-2.928225	-1.868670
H	1.628138	-2.901872	0.257575
C	3.112743	0.436421	-0.979289
H	1.151368	1.089190	-0.360516
C	3.819939	-0.831441	-1.482904
H	3.902361	-2.954981	-0.936159
H	3.746483	-1.825007	0.436924
H	3.384680	1.317374	-1.592055
H	3.440815	0.638816	0.059188
H	4.917963	-0.693559	-1.460737
H	3.543781	-1.027413	-2.538129
C	0.979996	0.422113	-2.399491
H	1.806997	-3.940121	-1.958439
H	0.267818	-3.032555	-1.816224
H	1.626370	-2.360100	-2.780113
H	1.122412	1.456852	-2.766894
H	1.457502	-0.265121	-3.120590
H	-0.101664	0.202766	-2.381244

3b$_{ax/c}$

C	3.095806	-1.968339	0.063833
C	2.056526	-0.983488	0.613472
N	1.859740	0.154116	-0.353474
C	0.802609	0.341730	-1.096195
C	-0.237352	-0.697837	-1.101419
C	2.373841	-0.479490	2.028159
C	3.022442	1.101825	-0.500806
C	3.514149	1.118054	-1.952224
C	2.620479	2.493510	0.001023
O	-0.056931	-1.674388	-1.848633
H	1.082870	-1.500011	0.652203
H	3.833079	0.710240	0.139232
H	2.398506	-1.339579	2.723647
H	3.357306	0.023613	2.082082
H	1.597772	0.227031	2.377304
H	3.191878	-2.833032	0.747907
H	2.770573	-2.330845	-0.927314
H	4.092276	-1.495502	-0.029605
H	4.380094	1.799801	-2.050461
H	3.818480	0.104750	-2.273550
H	2.697120	1.461448	-2.612062
H	3.465169	3.199831	-0.106035

H	1.764370	2.857465	-0.597012
H	2.321020	2.460013	1.065539
N	-1.394500	-0.502118	-0.367030
C	-1.589699	0.750140	0.390749
C	-2.526433	-1.424155	-0.600007
C	-2.399496	0.478406	1.675876
C	-2.189805	1.882522	-0.465817
C	-3.320899	-1.637414	0.704413
H	-0.583864	1.084605	0.705238
C	-3.686403	-0.310404	1.386999
H	-2.623035	1.444944	2.167028
H	-1.770130	-0.112218	2.372026
H	-4.226922	-2.230499	0.475343
H	-2.702292	-2.236149	1.402846
H	-4.242237	-0.496902	2.325890
H	-4.353769	0.282765	0.731212
C	-3.412795	-0.987839	-1.782172
H	-2.781528	-0.791265	-2.666901
H	-4.123126	-1.799015	-2.033769
H	-3.998562	-0.079678	-1.554435
H	-2.133057	2.839838	0.087672
H	-1.612698	1.981559	-1.402286
H	-3.248877	1.694271	-0.714574
H	-2.061491	-2.383042	-0.887468

cis-**4b**$_{ax}$

C	2.836058	-1.494709	0.794439
C	1.862821	-0.410341	1.301630
N	1.383776	0.493697	0.244536
C	0.151506	0.187129	-0.405596
C	-0.418639	-1.271404	-0.437803
C	2.454302	0.370746	2.489311
C	2.368032	1.290971	-0.499504
C	2.802220	0.667637	-1.846052
C	1.858909	2.731149	-0.696345
O	-0.045395	-2.356919	-0.839196
H	0.963088	-0.930547	1.680115
H	3.267231	1.342428	0.141285
H	2.713691	-0.322161	3.312518
H	3.382201	0.902188	2.201473
H	1.730104	1.117603	2.862641
H	3.102661	-2.189154	1.615013
H	2.366634	-2.071921	-0.021542
H	3.772858	-1.035360	0.423786
H	3.619799	1.260238	-2.300704
H	3.149151	-0.370463	-1.706012
H	1.962544	0.652455	-2.567717
H	2.608758	3.349016	-1.227412
H	0.930323	2.733244	-1.300920
H	1.633203	3.197952	0.280479
N	-1.592452	-0.864422	0.157442
C	-2.928360	-1.444240	0.171036
C	-1.252324	0.573334	0.255913
C	-3.851675	-0.553062	-0.700979
C	-3.451260	-1.611312	1.608882
H	-2.829772	-2.443074	-0.295166
C	-2.215499	1.393410	-0.625797
H	0.163203	0.570313	-1.442388
C	-3.676395	0.949620	-0.392255
H	-4.904778	-0.860720	-0.553699
H	-3.601119	-0.726739	-1.766295
H	-2.092408	2.475822	-0.427882
H	-1.962379	1.218784	-1.691859
H	-4.360172	1.542543	-1.029345
H	-3.964427	1.154427	0.658245
C	-1.158904	1.119200	1.679897
H	-0.657234	0.398228	2.347352

H	-0.563475	2.050997	1.669994
H	-2.160735	1.341163	2.093115
H	-4.437851	-2.112604	1.602830
H	-2.747389	-2.219774	2.205599
H	-3.565665	-0.629985	2.105634

trans-**4b**$_{ax}$

C	2.927761	-1.820804	0.109932
C	1.813976	-1.001490	0.793040
N	1.475310	0.240585	0.079868
C	0.366438	0.267088	-0.817558
C	-0.234392	-1.063320	-1.384353
C	2.134877	-0.735068	2.275939
C	2.525561	1.249740	-0.106701
C	3.221789	1.191153	-1.485648
C	1.980920	2.662845	0.175862
O	0.200426	-2.094811	-1.859676
H	0.902095	-1.625495	0.772011
H	3.295941	1.035613	0.656503
H	2.281487	-1.690895	2.814626
H	3.065459	-0.146342	2.389626
H	1.312227	-0.173617	2.756319
H	3.090907	-2.774447	0.648942
H	2.636942	-2.048108	-0.930469
H	3.884714	-1.263913	0.113061
H	4.063765	1.909443	-1.524189
H	3.608493	0.177538	-1.687485
H	2.520248	1.459783	-2.299208
H	2.783673	3.421056	0.095344
H	1.193086	2.925871	-0.556712
H	1.538378	2.710777	1.188309
N	-1.515489	-0.662341	-1.076918
C	-1.123514	0.547247	-0.309946
C	-2.724768	-1.450926	-0.876606
C	-1.383515	0.325511	1.189286
C	-1.752189	1.843551	-0.824146
C	-2.945889	-1.610325	0.651951
H	0.574455	0.953224	-1.660091
C	-2.791214	-0.272056	1.406438
H	-1.263724	1.277333	1.740501
H	-0.632906	-0.377509	1.590887
H	-3.944953	-2.050141	0.836861
H	-2.192091	-2.324405	1.039238
H	-2.970835	-0.431843	2.486719
H	-3.562938	0.444435	1.060102
C	-3.936442	-0.829188	-1.590295
H	-3.715381	-0.675900	-2.662336
H	-4.815839	-1.494555	-1.499425
H	-4.199929	0.149471	-1.148210
H	-1.242318	2.712042	-0.365169
H	-1.652162	1.910433	-1.923836
H	-2.826869	1.905799	-0.568893
H	-2.510326	-2.441376	-1.321191

3c$_{ax}$

C	-0.405764	0.706957	1.681868
C	0.444342	-0.474993	1.453960
N	1.453614	-0.426677	0.504470
C	1.526248	0.737459	-0.397594
C	2.751207	1.642625	-0.155635
O	0.267895	-1.441025	2.217302
C	2.295859	-1.635905	0.373784
C	3.756569	-1.355323	-0.002608
C	1.648257	-2.674541	-0.564471
C	1.356600	0.372247	-1.882750
H	0.652377	1.357128	-0.123368
H	2.293946	-2.082646	1.384104

H	1.295529	1.297160	-2.487540
H	2.211265	-0.219563	-2.257650
H	0.433144	-0.214092	-2.042964
H	2.595907	2.610447	-0.670582
H	2.864785	1.837771	0.925884
H	3.686389	1.202627	-0.540721
H	4.317854	-2.307877	0.031831
H	3.854543	-0.946657	-1.025047
H	4.226417	-0.649422	0.704791
H	2.216328	-3.624430	-0.528278
H	0.614691	-2.880170	-0.231696
H	1.628482	-2.325102	-1.612734
N	-1.600518	0.708749	1.141465
C	-2.112601	-0.361583	0.203396
C	-2.564695	1.774417	1.577786
C	-2.952780	0.245166	-0.937204
H	-1.202954	-0.796033	-0.244827
C	-3.384206	2.315727	0.390264
C	-3.437489	1.286478	2.743783
H	-1.911649	2.576054	1.961473
C	-4.044692	1.191447	-0.420537
H	-3.384761	-0.585211	-1.528694
H	-2.280235	0.813077	-1.611366
H	-4.137482	3.026484	0.780427
H	-2.709322	2.887438	-0.278205
H	-4.619766	1.612224	-1.266999
H	-4.763602	0.634758	0.211506
C	-2.829725	-1.487487	0.965119
H	-2.972528	-2.344644	0.279135
H	-2.206222	-1.813579	1.814791
H	-3.824626	-1.180903	1.332316
H	-3.962207	2.151726	3.191189
H	-4.199332	0.555862	2.422677
H	-2.799938	0.819754	3.516224

4c$_{ax}$

C	-0.060574	0.010417	-0.452773
C	-0.738223	-1.233407	0.199154
N	-1.802361	-0.481882	0.630405
C	-1.292693	0.830480	0.166119
C	-2.184221	1.527440	-0.865307
O	-0.503050	-2.424255	0.296363
C	-3.057858	-0.925538	1.221770
C	-4.180076	-1.036349	0.170713
C	-3.466173	-0.031863	2.403103
C	-0.866883	1.777965	1.288767
H	-0.203330	-0.067710	-1.551122
H	-2.835467	-1.943878	1.597436
H	-0.196895	2.553901	0.874106
H	-1.740255	2.269972	1.754875
H	-0.307144	1.231065	2.067360
H	-1.650732	2.397889	-1.293658
H	-2.447538	0.835553	-1.687302
H	-3.121558	1.898559	-0.407245
H	-5.084464	-1.486262	0.623452
H	-4.451391	-0.039796	-0.223825
H	-3.856286	-1.672990	-0.673015
H	-4.374750	-0.436289	2.887375
H	-2.658583	0.025250	3.155268
H	-3.693076	0.994333	2.056740
N	1.275171	0.404406	-0.147571
C	1.998294	-0.239602	0.959014
C	2.023549	1.068952	-1.221491
C	3.027940	0.751176	1.545468
H	1.242404	-0.433999	1.743895
C	3.079061	2.023712	-0.621704
C	2.631323	0.101846	-2.263478

H	1.288679	1.701168	-1.758903
C	3.937374	1.332804	0.450432
H	3.625761	0.238149	2.323229
H	2.480387	1.582138	2.033015
H	3.711413	2.427506	-1.436123
H	2.549952	2.877526	-0.153664
H	4.655897	2.052945	0.887203
H	4.537427	0.523499	-0.009935
C	2.645064	-1.601561	0.613595
H	2.978021	-2.100047	1.545201
H	1.911167	-2.256506	0.115278
H	3.529478	-1.482585	-0.037501
H	2.969934	0.661241	-3.157650
H	3.497647	-0.444532	-1.852736
H	1.879217	-0.644330	-2.582348

5_{ax}

N	1.954364	1.370537	-0.319047
C	1.175357	2.495634	-0.928568
C	1.358106	0.136803	-0.288126
C	-0.095768	-0.000587	-0.681619
O	0.010258	-0.034832	-1.979276
C	-1.200010	-0.050037	0.145529
N	-1.067988	0.110593	1.570198
C	-0.433208	1.305380	2.143376
H	0.022488	1.834840	1.295354
H	0.122809	2.187516	-0.823294
C	-1.881525	-0.694520	2.496677
H	-1.484858	-0.476886	3.506741
C	3.362963	1.572587	0.125439
H	3.713218	0.579207	0.435908
C	0.704811	0.921862	3.112797
H	1.185366	1.823199	3.540370
H	0.322390	0.327225	3.963915
H	1.469296	0.319520	2.588998
C	-1.399895	2.302434	2.822669
H	-2.209625	2.597411	2.130190
H	-1.860069	1.864097	3.728189
H	-0.851785	3.215301	3.129612
C	-3.387451	-0.339559	2.551209
H	-3.540576	0.751398	2.580265
H	-3.906667	-0.730661	1.665011
H	-3.842835	-0.781656	3.460381
C	-1.707658	-2.207152	2.276854
H	-0.680354	-2.535802	2.517605
H	-2.408570	-2.771882	2.920671
H	-1.919433	-2.467663	1.226105
C	1.454036	2.634616	-2.436226
H	0.668274	3.274951	-2.879336
H	2.432339	3.106641	-2.637223
H	1.392477	1.645215	-2.916484
C	1.302864	3.841391	-0.206232
H	0.546745	4.521298	-0.640226
H	1.105095	3.752971	0.875905
H	2.291756	4.310466	-0.355079
C	3.504733	2.433088	1.400882
H	2.741493	2.162478	2.144820
H	4.500557	2.226347	1.836851
H	3.447896	3.514863	1.204305
C	4.292384	2.097865	-0.982446
H	4.077397	3.158039	-1.204486
H	5.341813	2.029719	-0.639084
H	4.187429	1.526649	-1.921640
C	-3.220410	1.116483	-0.572477
C	-2.950744	-1.330424	-1.167580
C	-4.754732	0.930856	-0.493186
H	-2.927550	1.738195	0.296433

C	-4.475791	-1.529703	-0.981655
H	-2.429991	-2.196287	-0.716858
C	-5.249448	-0.249974	-1.344569
H	-5.250734	1.871626	-0.804358
H	-5.033541	0.746328	0.560834
H	-4.812079	-2.375895	-1.612365
H	-4.689587	-1.799393	0.071121
H	-6.336728	-0.398792	-1.192630
H	-5.108189	-0.025397	-2.419905
N	-2.518388	-0.161079	-0.385869
C	-2.789584	1.884376	-1.846518
H	-1.696634	1.809210	-1.981522
H	-3.259976	1.458747	-2.751425
H	-3.087710	2.950644	-1.776637
C	-2.603721	-1.347426	-2.677216
H	-1.543344	-1.091502	-2.826024
H	-2.818310	-2.354963	-3.087884
H	-3.214169	-0.619933	-3.241909
C	1.386537	-2.141668	0.546307
C	3.249144	-1.337070	-0.990038
C	2.437942	-2.901632	1.381375
H	0.678063	-1.661237	1.237295
C	4.275594	-2.144163	-0.174243
H	3.711435	-0.388149	-1.285083
C	3.633760	-3.354041	0.526566
H	1.947027	-3.769165	1.862582
H	2.799771	-2.233706	2.188781
H	5.096224	-2.464991	-0.844375
H	4.715629	-1.476407	0.594448
H	4.383948	-3.870164	1.155517
H	3.296346	-4.086845	-0.231617
N	2.076834	-1.005861	-0.127253
C	2.815148	-2.008967	-2.308085
H	1.910534	-1.502747	-2.691001
H	3.634582	-1.910356	-3.045688
H	2.598230	-3.082392	-2.184286
C	0.577811	-3.073147	-0.377398
H	1.205908	-3.851064	-0.845305
H	-0.188896	-3.583150	0.232692
H	0.072398	-2.497525	-1.168148

3b$_{eq}$

C	-3.704516	-1.040337	0.217606
C	-2.690279	-0.276118	-0.641787
N	-1.791524	0.548723	0.239597
C	-0.552171	0.258348	0.529219
C	-0.020907	-1.051735	0.144009
C	-3.337474	0.563520	-1.752380
C	-2.431045	1.736010	0.910490
C	-2.366004	1.582462	2.434190
C	-1.778158	3.033800	0.422944
O	-0.359090	-1.967891	0.917056
H	-2.021711	-1.008428	-1.125364
H	-3.492717	1.735657	0.606642
H	-3.875808	-0.109663	-2.445960
H	-4.070870	1.290409	-1.356302
H	-2.571416	1.115704	-2.327339
H	-4.333101	-1.686196	-0.424992
H	-3.164679	-1.670644	0.946013
H	-4.373039	-0.344427	0.760069
H	-2.857199	2.445597	2.922270
H	-2.871838	0.653131	2.754566
H	-1.309272	1.530313	2.752871
H	-2.261108	3.906624	0.901015
H	-0.706086	3.024959	0.693211
H	-1.866347	3.137187	-0.674529
N	0.858336	-1.224341	-0.920450

C	1.721914	-2.445766	-0.938711
C	1.614210	-0.066501	-1.478370
C	2.872053	-2.229694	0.067596
H	2.163275	-2.450982	-1.955825
C	0.996051	-3.788424	-0.782812
C	2.771939	0.270516	-0.512234
C	0.771048	1.150609	-1.873187
C	3.676281	-0.960956	-0.289435
H	3.538666	-3.114567	0.074266
H	2.422803	-2.142481	1.075850
H	3.366979	1.113225	-0.917046
H	2.321261	0.605347	0.442711
H	4.426398	-0.746302	0.496463
H	4.240654	-1.156148	-1.225717
H	2.058598	-0.451494	-2.417723
H	1.384905	1.812924	-2.512603
H	-0.121800	0.838847	-2.446321
H	0.446125	1.730459	-0.992624
H	1.681423	-4.592566	-1.115592
H	0.690073	-3.973021	0.257624
H	0.092975	-3.815599	-1.420784

$3b_{eq/b}$

C	2.851703	-2.134705	0.025179
C	1.981204	-1.048068	0.668314
N	1.919879	0.159377	-0.231056
C	0.892718	0.519227	-0.951388
C	-0.272477	-0.379943	-1.000685
C	2.413232	-0.681347	2.095298
C	3.197633	0.950520	-0.353265
C	3.664953	0.984803	-1.812203
C	2.997692	2.352519	0.233591
O	-0.207578	-1.381974	-1.734426
H	0.946398	-1.426276	0.716476
H	3.957905	0.417358	0.244339
H	2.315038	-1.572963	2.743070
H	3.466635	-0.348118	2.142060
H	1.773050	0.120273	2.507726
H	2.854623	-3.039684	0.662393
H	2.440121	-2.394369	-0.966016
H	3.899133	-1.795557	-0.090308
H	4.612824	1.550215	-1.891148
H	3.825831	-0.040063	-2.194565
H	2.891197	1.470632	-2.433526
H	3.933310	2.937637	0.156184
H	2.200237	2.869147	-0.332237
H	2.701011	2.299767	1.298127
N	-1.418357	-0.010713	-0.327771
C	-2.622683	-0.853702	-0.471877
C	-1.434795	1.178954	0.531870
C	-3.889414	-0.034189	-0.150291
C	-2.519359	-2.143823	0.357312
H	-2.657606	-1.142188	-1.539802
C	-2.624899	2.124768	0.165385
H	-0.493700	1.716514	0.304316
C	-3.725408	1.408142	-0.646103
H	-4.077391	-0.033215	0.943113
H	-4.756355	-0.532856	-0.622395
C	-1.407337	0.805105	2.026632
H	-0.556563	0.131662	2.239768
H	-1.303432	1.715346	2.648769
H	-2.339818	0.292020	2.326706
H	-3.417590	-2.772273	0.199173
H	-1.629586	-2.716568	0.041706
H	-2.441918	-1.911408	1.436314
H	-3.445008	1.383104	-1.717575
H	-4.676324	1.968787	-0.571546

H	-2.244685	2.990664	-0.407591
H	-3.061315	2.525573	1.101118

3b$_{eq/bc}$

C	3.011778	-0.676932	1.535498
C	1.727758	0.032740	1.088671
N	1.676410	0.121985	-0.413987
C	0.857176	-0.537850	-1.188176
C	-0.008163	-1.550654	-0.559641
C	1.523933	1.406762	1.742127
C	2.708600	1.016403	-1.052412
C	3.611064	0.201742	-1.985641
C	2.013945	2.178866	-1.770356
O	0.483832	-2.666548	-0.320468
H	0.874396	-0.606308	1.370710
H	3.327614	1.421875	-0.232357
H	1.466325	1.284546	2.840299
H	2.357604	2.100040	1.524159
H	0.581758	1.869364	1.393631
H	3.012527	-0.791758	2.636233
H	3.058689	-1.678243	1.072028
H	3.913708	-0.101510	1.252283
H	4.375591	0.858820	-2.441629
H	4.121222	-0.607033	-1.430350
H	2.996069	-0.256016	-2.781396
H	2.763538	2.842717	-2.240780
H	1.347070	1.771141	-2.552522
H	1.407993	2.775177	-1.062293
N	-1.339581	-1.253751	-0.352901
C	-2.219326	-2.302053	0.201125
C	-1.884229	0.083190	-0.622547
C	-3.369581	-1.656527	1.006977
H	-1.586629	-2.871542	0.908969
C	-2.703409	-3.284657	-0.875286
C	-2.487573	0.696695	0.681686
H	-1.028338	0.706378	-0.938141
C	-2.873779	-0.387007	1.715100
H	-3.749966	-2.400222	1.731708
H	-4.215333	-1.402113	0.337582
H	-1.761262	1.397763	1.135514
H	-3.380735	1.294278	0.414348
H	-3.637582	0.006402	2.412257
H	-1.986714	-0.651809	2.325090
C	-2.875255	0.070097	-1.802223
H	-2.392875	-0.373123	-2.692330
H	-3.782453	-0.513912	-1.564647
H	-3.188942	1.104034	-2.043767
H	-3.309175	-4.088849	-0.412938
H	-3.323623	-2.770489	-1.632554
H	-1.830356	-3.742275	-1.372863

cis-**4b$_{eq/b}$**

C	2.954899	-1.858336	-0.124996
C	2.102590	-1.007166	0.839233
N	1.663363	0.274865	0.265972
C	0.383773	0.334741	-0.362003
C	-0.330041	-0.934169	-0.916335
C	2.805676	-0.809574	2.194694
C	2.683108	1.239367	-0.167198
C	3.019338	1.173878	-1.674748
C	2.285010	2.668531	0.246824
O	-0.084194	-1.799860	-1.734407
H	1.176935	-1.577617	1.042678
H	3.604293	0.979230	0.385594
H	3.037014	-1.790153	2.652863
H	3.763533	-0.266019	2.078639
H	2.162767	-0.232824	2.884684

H	3.181137	-2.843713	0.327173
H	2.407730	-2.018924	-1.070651
H	3.918473	-1.357969	-0.341342
H	3.862371	1.851383	-1.912574
H	3.290834	0.147091	-1.973303
H	2.154997	1.491127	-2.289970
H	3.070554	3.397301	-0.031878
H	1.348916	2.969855	-0.263470
H	2.112704	2.720400	1.337903
N	-1.455095	-0.689690	-0.154679
C	-2.837401	-1.049519	-0.455001
C	-0.953895	0.554490	0.485341
C	-3.668506	0.254193	-0.634908
C	-3.437991	-1.992648	0.597408
H	-2.786261	-1.583116	-1.425099
C	-1.799879	1.788568	0.069230
H	0.394721	1.082644	-1.176704
C	-2.781949	1.438712	-1.066217
H	-4.158616	0.514431	0.326153
H	-4.477099	0.068043	-1.366334
C	-0.769526	0.455723	1.997091
H	-0.214763	-0.457423	2.271033
H	-0.195412	1.330414	2.357393
H	-1.751009	0.444437	2.509097
H	-4.481060	-2.253086	0.331619
H	-2.847015	-2.924240	0.667667
H	-3.445528	-1.504390	1.591226
H	-2.226245	1.171163	-1.988085
H	-3.406881	2.318509	-1.309941
H	-1.126181	2.617810	-0.223939
H	-2.388204	2.148504	0.937038

trans-**4b**$_{eq/b}$

C	2.854556	-0.667499	1.392941
C	1.537425	0.120082	1.232695
N	1.194554	0.417472	-0.168092
C	0.322533	-0.461123	-0.877478
C	0.062872	-1.919855	-0.379326
C	1.539463	1.388220	2.106967
C	2.126634	1.232301	-0.959720
C	3.106759	0.411858	-1.829283
C	1.360005	2.258331	-1.814779
O	0.733619	-2.845187	0.036654
H	0.725567	-0.525449	1.611917
H	2.733117	1.798517	-0.229516
H	1.705197	1.117365	3.167181
H	2.351034	2.082521	1.814565
H	0.578231	1.928052	2.024354
H	3.019913	-0.927952	2.456562
H	2.809680	-1.599814	0.803924
H	3.716873	-0.059593	1.057198
H	3.844946	1.080248	-2.313720
H	3.647629	-0.332323	-1.219989
H	2.571092	-0.127851	-2.634274
H	2.059559	2.914004	-2.368310
H	0.721784	1.741721	-2.558104
H	0.707658	2.883004	-1.176660
N	-1.300911	-1.770500	-0.510463
C	-2.356710	-2.512951	0.171573
C	-1.272050	-0.311158	-0.785045
C	-3.128334	-1.532490	1.098521
H	-1.821570	-3.254194	0.798662
C	-3.279561	-3.256443	-0.804198
C	-1.790056	0.506123	0.424640
H	0.604628	-0.492410	-1.946440
C	-2.210830	-0.401285	1.600669
H	-3.567383	-2.102069	1.939189

H	-3.973757	-1.083869	0.536463
H	-1.006688	1.225314	0.729043
H	-2.673024	1.098260	0.114413
H	-2.726944	0.202502	2.370730
H	-1.319546	-0.845173	2.087327
C	-1.955235	0.080154	-2.095359
H	-1.565687	-0.527556	-2.934313
H	-3.051063	-0.068535	-2.033005
H	-1.769031	1.149890	-2.312699
H	-4.058525	-3.814480	-0.249128
H	-3.783083	-2.538422	-1.479934
H	-2.702200	-3.971058	-1.419101

3c$_{eq}$

C	-0.470417	0.425444	1.512814
C	0.396399	-0.732845	1.328468
N	1.277936	-0.734998	0.249959
C	1.232255	0.397473	-0.687327
C	2.563125	1.158982	-0.807410
O	0.422398	-1.586292	2.232988
C	2.328694	-1.772458	0.250737
C	3.584116	-1.346056	1.037623
C	2.669708	-2.298778	-1.150409
C	0.650685	0.040724	-2.069937
H	0.522791	1.109125	-0.212427
H	1.880155	-2.608385	0.817518
H	0.395307	0.967223	-2.620385
H	1.368579	-0.530108	-2.684051
H	-0.267154	-0.564342	-1.960971
H	2.413704	2.065446	-1.424628
H	2.924950	1.466582	0.189614
H	3.344250	0.546228	-1.292495
H	4.252820	-2.218191	1.175728
H	4.154589	-0.556726	0.516278
H	3.287710	-0.977263	2.035818
H	3.364455	-3.154024	-1.052035
H	1.763573	-2.646126	-1.679382
H	3.168148	-1.535616	-1.775955
N	-1.752023	0.470995	1.304330
C	-2.657052	-0.503501	0.569685
C	-2.528105	1.708305	1.691521
C	-3.113375	0.170078	-0.742441
C	-2.059356	-1.886137	0.327858
C	-2.972708	2.422249	0.399966
H	-3.435160	1.338012	2.213257
C	-1.753965	2.625606	2.630741
C	-3.828626	1.505048	-0.486059
H	-3.775042	-0.529508	-1.289069
H	-2.215434	0.331556	-1.370905
H	-3.529974	3.340276	0.667574
H	-2.057447	2.737684	-0.142181
H	-4.072143	2.003780	-1.444012
H	-4.791301	1.304516	0.027680
H	-3.544198	-0.613610	1.226192
H	-2.847838	-2.523394	-0.114224
H	-1.215304	-1.841372	-0.382191
H	-1.697395	-2.341078	1.263056
H	-2.424326	3.446653	2.950180
H	-1.398571	2.073139	3.517827
H	-0.868765	3.048523	2.125380

4c$_{eq}$

C	-0.116402	-0.187155	-0.406030
C	-0.937640	-1.343277	0.242637
N	-1.871593	-0.462661	0.733627
C	-1.221757	0.784583	0.270973
C	-2.041803	1.578942	-0.752815

O	-0.892926	-2.558067	0.265937
C	-3.184951	-0.767932	1.287179
C	-4.282460	-0.786461	0.204570
C	-3.535692	0.176058	2.446134
C	-0.735806	1.695850	1.397159
H	-0.396642	-0.238113	-1.473377
H	-3.078456	-1.798652	1.679574
H	-0.241709	1.116851	2.194169
H	-0.012652	2.431398	0.999502
H	-1.580383	2.251973	1.844446
H	-1.421054	2.389453	-1.181543
H	-2.385308	0.925419	-1.576265
H	-2.929200	2.046423	-0.284184
H	-5.235698	-1.150021	0.634357
H	-4.454088	0.225726	-0.205803
H	-3.992921	-1.459876	-0.622886
H	-4.490391	-0.133385	2.911280
H	-2.745253	0.165843	3.218504
H	-3.655808	1.214629	2.083494
N	1.298444	-0.068844	-0.338900
C	2.139739	-0.335554	0.843438
C	2.029794	0.702722	-1.361131
C	2.680834	0.969354	1.482896
C	1.515936	-1.254283	1.896343
C	2.480253	2.071891	-0.798686
H	2.963159	0.129863	-1.569476
C	1.299268	0.864475	-2.697718
C	3.365373	1.871500	0.442413
H	3.400727	0.699939	2.281234
H	1.847795	1.510512	1.965077
H	3.033679	2.634325	-1.577151
H	1.575147	2.660545	-0.543785
H	3.643718	2.844780	0.892122
H	4.309892	1.386995	0.117187
H	3.035613	-0.868418	0.447176
H	2.260827	-1.425124	2.695440
H	0.622119	-0.799745	2.360945
H	1.221849	-2.224026	1.464362
H	1.981969	1.353011	-3.416752
H	0.997614	-0.112567	-3.119285
H	0.398980	1.500380	-2.598796

TS1-2$_{ax}$

N	-1.446105	1.639882	-1.903304
C	-0.884364	0.358647	-2.408214
C	-2.535398	2.142667	-2.563947
C	-1.895436	-0.792478	-2.530760
C	-1.085625	2.011121	-0.505679
C	0.408620	2.337046	-0.343380
N	-2.738360	3.490063	-2.596619
C	-0.166510	0.609972	-3.744582
C	-1.548824	0.927289	0.485684
C	-4.181126	1.240064	-1.970211
O	-4.875456	0.577134	-2.638351
H	-0.119961	0.052189	-1.671312
H	-1.681622	2.908435	-0.268974
H	-1.396216	1.279102	1.523953
H	-2.623796	0.718144	0.333343
H	-0.977544	-0.011406	0.357773
H	0.617124	2.693524	0.683674
H	1.028500	1.437191	-0.517222
H	0.731720	3.114634	-1.060628
H	0.307152	-0.318229	-4.118906
H	-0.901957	0.959751	-4.494153
H	0.613108	1.386519	-3.630279
H	-1.360816	-1.718677	-2.816149
H	-2.419946	-0.969813	-1.576094

H	-2.649355	-0.571871	-3.305294
C	-3.936913	3.919956	-3.372861
C	-4.472256	5.277191	-2.875083
C	-3.707046	3.885951	-4.895207
H	-4.718938	3.174178	-3.154146
C	-3.378389	6.350040	-2.818272
H	-5.306197	5.585693	-3.533904
H	-4.889132	5.139342	-1.857724
C	-2.256978	5.854160	-1.897064
H	-2.979861	6.545051	-3.833379
H	-3.790477	7.307186	-2.445647
C	-1.671773	4.505459	-2.359647
H	-1.431535	6.590008	-1.835602
H	-2.665246	5.729145	-0.874130
C	-0.744740	4.648344	-3.584717
H	-1.041001	4.144926	-1.542123
H	-4.682258	3.928867	-5.416797
H	-3.096689	4.735144	-5.250473
H	-3.203136	2.941717	-5.169760
H	-0.404273	3.652627	-3.918119
H	-1.243720	5.150031	-4.430536
H	0.140998	5.250805	-3.305066

TS1-2$_{eq}$

N	-1.370342	1.693228	-1.819929
C	-1.106422	0.262748	-2.153886
C	-2.428437	2.265696	-2.490633
C	-2.313346	-0.681866	-2.040530
C	-0.830079	2.157062	-0.513478
C	0.704987	2.050308	-0.412176
N	-2.448893	3.551730	-2.904757
C	-0.476586	0.182963	-3.554491
C	-1.484066	1.412996	0.667112
C	-4.030147	1.840097	-1.412513
O	-4.919758	1.126122	-1.660370
H	-0.350988	-0.086147	-1.427554
H	-1.128886	3.211745	-0.425999
H	-1.122114	1.836393	1.623964
H	-2.583239	1.513971	0.627862
H	-1.220392	0.338852	0.649291
H	1.061752	2.613541	0.471408
H	1.021096	0.998778	-0.277951
H	1.206683	2.449241	-1.309026
H	-0.208965	-0.861456	-3.807826
H	-1.201741	0.554423	-4.303824
H	0.434311	0.808576	-3.611223
H	-1.982713	-1.716353	-2.254224
H	-2.753132	-0.658570	-1.028753
H	-3.096432	-0.407449	-2.767553
C	-3.679632	4.035288	-3.611678
C	-4.541107	4.838024	-2.607532
H	-3.314536	4.758893	-4.370730
C	-4.444620	2.962837	-4.391054
C	-3.738178	5.993877	-1.971532
H	-5.431220	5.238434	-3.131070
H	-4.904896	4.152045	-1.820786
C	-2.356014	5.539265	-1.453474
H	-3.574280	6.777159	-2.740941
H	-4.322911	6.462538	-1.156567
C	-1.616336	4.758957	-2.558014
H	-1.753869	6.416313	-1.142628
H	-2.471455	4.883227	-0.566973
H	-1.683078	5.379333	-3.471761
C	-0.110217	4.551491	-2.345880
H	-5.162023	3.476428	-5.060227
H	-3.744104	2.371901	-5.007629
H	-5.005649	2.270610	-3.747756

H	0.423165	5.430797	-2.752597
H	0.175058	4.464531	-1.286887
H	0.239698	3.652708	-2.879907

TS2-3b$_{ax}$

C	-3.625866	-1.076115	1.112379
C	-2.506287	-1.033803	0.057027
N	-1.689352	0.201715	0.171915
C	-0.403007	0.163181	0.565387
C	0.472898	-0.674358	1.168209
C	-3.058010	-1.235367	-1.364897
C	-2.370792	1.506342	-0.007089
C	-2.463197	2.270130	1.323745
C	-1.690463	2.350079	-1.094108
O	0.978660	-1.371754	2.019535
H	-1.806842	-1.861554	0.274242
H	-3.396947	1.275411	-0.348983
H	-3.615557	-2.189756	-1.427741
H	-3.756059	-0.421767	-1.641482
H	-2.238788	-1.257203	-2.105277
H	-4.174787	-2.035274	1.050849
H	-3.203712	-0.973869	2.128849
H	-4.354820	-0.258777	0.951383
H	-2.970724	3.244501	1.185881
H	-3.020343	1.682083	2.075748
H	-1.443098	2.452247	1.712453
H	-2.248245	3.290910	-1.263079
H	-0.663541	2.606572	-0.775107
H	-1.632547	1.793653	-2.048425
N	0.966495	-0.325077	-0.320741
C	0.928003	-1.504501	-1.225059
C	2.111542	0.615296	-0.446496
C	2.263158	-2.277019	-1.129975
C	0.530510	-1.146760	-2.668569
H	0.126224	-2.147135	-0.815012
C	3.430411	-0.183301	-0.335134
H	2.017885	1.272409	0.436993
C	3.474983	-1.351127	-1.337886
H	2.262851	-3.101779	-1.869896
H	2.321762	-2.723739	-0.119705
H	4.286892	0.502109	-0.488550
H	3.498825	-0.588493	0.692148
H	4.413136	-1.924314	-1.211362
H	3.481902	-0.960845	-2.375238
C	2.055471	1.507615	-1.698238
H	0.193709	-2.061104	-3.192866
H	-0.294443	-0.413337	-2.672392
H	1.372623	-0.723192	-3.241268
H	2.735415	2.369364	-1.558374
H	2.377518	0.974999	-2.609084
H	1.034242	1.890790	-1.860890

cis-**TS3-4b$_{ax}$**

C	3.190877	-1.579999	0.911287
C	2.120507	-0.548243	1.295496
N	1.642185	0.175142	0.081502
C	0.438465	0.002203	-0.452608
C	-0.452686	-1.115006	-0.106709
C	2.583865	0.421477	2.394542
C	2.603723	1.093574	-0.594481
C	2.854548	0.651136	-2.042553
C	2.110958	2.545554	-0.504363
O	-0.165193	-2.317467	-0.060141
H	1.246299	-1.105332	1.669877
H	3.555671	1.014679	-0.039514
H	2.842154	-0.151407	3.305416
H	3.483135	0.990214	2.091241

H	1.783678	1.140903	2.648256
H	3.518701	-2.136668	1.809695
H	2.762889	-2.293585	0.185541
H	4.081149	-1.092740	0.468375
H	3.585204	1.326445	-2.526820
H	3.247163	-0.381900	-2.070637
H	1.905910	0.676445	-2.609571
H	2.846399	3.230468	-0.966907
H	1.149936	2.652058	-1.041859
H	1.960311	2.845965	0.549202
N	-1.719322	-0.563593	0.070220
C	-2.962530	-1.339476	0.034054
C	-1.653987	0.849877	0.240226
C	-4.016625	-0.568407	-0.790514
C	-3.438399	-1.670902	1.460379
H	-2.712414	-2.288360	-0.474931
C	-2.728342	1.595429	-0.544800
H	-0.410925	0.935928	-0.528401
C	-4.105644	0.912288	-0.370959
H	-4.999483	-1.066794	-0.684823
H	-3.732894	-0.617430	-1.860595
H	-2.769841	2.654190	-0.226449
H	-2.469289	1.580135	-1.624636
H	-4.871107	1.435455	-0.976532
H	-4.423791	0.987449	0.688129
C	-1.365692	1.364172	1.642748
H	-0.667949	0.688805	2.169719
H	-0.917230	2.377573	1.609432
H	-2.296454	1.434352	2.248301
H	-4.339057	-2.314155	1.428760
H	-2.639513	-2.208189	2.003027
H	-3.687909	-0.750952	2.022334

trans-**TS3-4b**$_{ax}$

C	3.180808	-1.955070	0.267767
C	2.004382	-1.102085	0.765042
N	1.751365	0.029620	-0.170886
C	0.665991	0.136853	-0.936457
C	-0.270787	-0.970455	-1.175162
C	2.186420	-0.618385	2.213186
C	2.791793	1.092866	-0.260371
C	3.343338	1.197319	-1.689147
C	2.240227	2.433073	0.250105
O	0.007491	-2.146373	-1.428716
H	1.101873	-1.732044	0.721047
H	3.615266	0.781890	0.407075
H	2.280226	-1.493193	2.884702
H	3.099763	-0.005481	2.333089
H	1.317330	-0.017546	2.538914
H	3.336319	-2.815316	0.946108
H	2.954302	-2.335906	-0.743636
H	4.121242	-1.371125	0.237683
H	4.130768	1.973076	-1.739021
H	3.770395	0.230349	-2.012295
H	2.527194	1.465987	-2.384871
H	3.030288	3.206965	0.225102
H	1.405672	2.768535	-0.393804
H	1.869200	2.338208	1.287487
N	-1.559966	-0.428001	-1.087468
C	-1.482750	0.775180	-0.292255
C	-2.721670	-1.316023	-0.947739
C	-1.597916	0.472420	1.193721
C	-2.275167	1.971091	-0.787311
C	-2.921086	-1.615116	0.566044
H	-0.093344	1.085128	-0.818820
C	-2.905287	-0.337225	1.430868
H	-1.596350	1.402402	1.795201

H	-0.739174	-0.143681	1.525668
H	-3.866250	-2.173287	0.714303
H	-2.092455	-2.276196	0.889077
H	-2.998537	-0.604658	2.501777
H	-3.779012	0.297823	1.182140
C	-3.982305	-0.753382	-1.619667
H	-3.763821	-0.452593	-2.660565
H	-4.774517	-1.525776	-1.632125
H	-4.377593	0.126286	-1.080896
H	-1.878617	2.904952	-0.341019
H	-2.217665	2.049222	-1.888066
H	-3.347934	1.911905	-0.503761
H	-2.432216	-2.254818	-1.454032

TS2-3c$_{ax}$

C	-0.273333	0.491406	1.222777
C	0.669832	-0.162638	1.944531
N	1.225429	0.030600	0.472860
C	2.173709	1.153934	0.237454
C	3.564919	0.903378	0.852563
O	1.183772	-0.671901	2.918571
C	1.249553	-1.232680	-0.315541
C	2.647118	-1.844040	-0.492809
C	0.498758	-1.093169	-1.653696
C	2.250581	1.596278	-1.229989
H	1.714548	1.981361	0.808682
H	0.669635	-1.943513	0.304604
H	2.848827	2.524978	-1.296740
H	2.741512	0.834764	-1.863139
H	1.243535	1.799800	-1.637596
H	4.109959	1.864988	0.917271
H	3.459357	0.487988	1.870393
H	4.175421	0.211204	0.247202
H	2.545951	-2.840743	-0.963780
H	3.281799	-1.222955	-1.150123
H	3.150219	-1.962758	0.482391
H	0.311931	-2.098278	-2.078632
H	-0.470309	-0.589873	-1.494079
H	1.081667	-0.516735	-2.392273
N	-1.511923	0.312149	0.729624
C	-2.202627	-0.990205	0.944585
C	-2.294283	1.520428	0.357676
C	-3.268029	-1.243144	-0.141460
H	-1.416600	-1.758046	0.827837
C	-3.345587	1.188289	-0.720126
C	-2.906801	2.222302	1.583705
H	-1.557568	2.214585	-0.087012
C	-4.193822	-0.033853	-0.337959
H	-3.844142	-2.148783	0.129547
H	-2.754228	-1.453535	-1.100418
H	-3.980188	2.079804	-0.886544
H	-2.823680	0.971824	-1.674022
H	-4.941573	-0.246634	-1.125555
H	-4.757277	0.169600	0.593842
C	-2.762660	-1.120828	2.373343
H	-3.116622	-2.155399	2.547756
H	-1.971897	-0.893282	3.111323
H	-3.611263	-0.434242	2.542535
H	-3.309058	3.212385	1.293844
H	-3.731486	1.634648	2.025537
H	-2.128413	2.369204	2.354949

TS3-4c$_{ax}$

C	0.137676	-0.036463	-0.589133
C	-0.696700	-0.941006	0.214125
N	-1.856508	-0.233462	0.542896
C	-1.662998	1.164756	0.323327

C	-2.784346	1.914052	-0.372901
O	-0.464830	-2.125937	0.486297
C	-3.055297	-0.907485	1.053010
C	-4.143238	-1.089313	-0.022660
C	-3.591426	-0.216473	2.316129
C	-0.962995	1.941076	1.430459
H	-0.674876	0.928438	-0.714144
H	-2.687848	-1.914289	1.331656
H	-0.463556	2.844552	1.024887
H	-1.683499	2.280614	2.206391
H	-0.198366	1.313883	1.922464
H	-2.449127	2.933418	-0.644520
H	-3.107090	1.389336	-1.290571
H	-3.672289	2.027001	0.286109
H	-4.941204	-1.756072	0.357725
H	-4.607191	-0.124958	-0.299086
H	-3.710354	-1.546257	-0.931555
H	-4.440022	-0.791300	2.733164
H	-2.802905	-0.144715	3.087729
H	-3.952701	0.805179	2.091727
N	1.426145	0.192034	-0.340455
C	2.104350	-0.267062	0.912388
C	2.244555	0.823459	-1.414934
C	3.082942	0.806231	1.431562
H	1.295197	-0.381755	1.653260
C	3.224637	1.860964	-0.831074
C	2.935143	-0.227889	-2.299848
H	1.511721	1.355059	-2.047483
C	4.044175	1.291553	0.336925
H	3.636375	0.387558	2.294073
H	2.497652	1.672178	1.800724
H	3.881435	2.223599	-1.644805
H	2.642783	2.730307	-0.463991
H	4.728406	2.062875	0.738571
H	4.675927	0.451818	-0.013507
C	2.755977	-1.650061	0.742544
H	3.066557	-2.023386	1.737177
H	2.015912	-2.350225	0.320327
H	3.652734	-1.614469	0.099344
H	3.339733	0.261773	-3.206234
H	3.771190	-0.725522	-1.779497
H	2.203593	-0.996801	-2.607760

TS2-5$_{ax}$

N	2.000472	1.706747	0.255485
C	0.754340	2.534196	0.300122
C	1.759543	0.404645	-0.021739
C	-0.721495	-0.159857	-1.224593
O	-0.306863	0.234728	-2.265195
C	-1.568372	-0.551259	-0.244481
N	-1.131598	-1.259291	0.900452
C	-0.767433	-0.466727	2.091206
H	-0.472997	0.512614	1.683464
H	-0.020441	1.811190	0.013501
C	-1.630322	-2.627268	1.117839
H	-1.161681	-2.970174	2.060033
C	3.327759	2.376885	0.442750
H	3.969253	1.602401	0.893209
C	0.475587	-1.026805	2.806058
H	0.767419	-0.354284	3.636628
H	0.284807	-2.025710	3.244929
H	1.316736	-1.097447	2.097781
C	-1.913274	-0.250043	3.104724
H	-2.825370	0.120599	2.605340
H	-2.166935	-1.193425	3.625399
H	-1.607519	0.486410	3.874038
C	-3.162304	-2.761860	1.309788

H	-3.555263	-2.006414	2.008897
H	-3.696271	-2.648900	0.351024
H	-3.399620	-3.768561	1.708085
C	-1.157995	-3.573273	0.000686
H	-0.058603	-3.665816	-0.002588
H	-1.597247	-4.580879	0.130768
H	-1.475409	-3.180395	-0.984165
C	0.735856	3.646091	-0.758150
H	-0.266237	4.112570	-0.773683
H	1.473508	4.443132	-0.551941
H	0.935535	3.221912	-1.758674
C	0.347380	3.045620	1.698676
H	-0.744977	3.223081	1.698380
H	0.567448	2.285411	2.469526
H	0.836969	3.991415	1.985259
C	3.355168	3.523969	1.465339
H	2.959054	3.205618	2.444535
H	4.409163	3.832817	1.601353
H	2.790146	4.408220	1.125071
C	3.945250	2.828020	-0.895109
H	3.418644	3.713820	-1.290773
H	5.011018	3.095803	-0.754274
H	3.884353	2.027950	-1.651859
C	-3.128701	1.352228	0.113343
C	-3.821679	-0.589045	-1.368053
C	-4.583046	1.472639	0.620382
H	-2.460515	1.466398	0.985224
C	-5.268796	-0.457942	-0.839553
H	-3.566627	-1.663865	-1.417519
C	-5.593645	0.989031	-0.432253
H	-4.785297	2.521640	0.913488
H	-4.686909	0.844770	1.527496
H	-5.976478	-0.818291	-1.611712
H	-5.376230	-1.110618	0.048383
H	-6.624482	1.054559	-0.033634
H	-5.553532	1.648191	-1.322081
N	-2.887638	-0.014128	-0.385366
C	-2.763776	2.484333	-0.873183
H	-1.778114	2.301266	-1.332269
H	-3.505958	2.587028	-1.683625
H	-2.720235	3.450164	-0.332431
C	-3.694549	-0.044321	-2.810096
H	-2.643556	-0.048923	-3.144979
H	-4.283195	-0.683083	-3.497604
H	-4.080521	0.986607	-2.899100
C	2.047023	-1.918405	-0.433766
C	4.146445	-0.520899	-0.546511
C	2.806670	-2.973743	0.393773
H	1.044368	-1.799614	0.004320
C	4.891082	-1.596231	0.273921
H	4.521157	0.443744	-0.203106
C	4.306573	-3.000379	0.067520
H	2.342592	-3.963311	0.216104
H	2.676107	-2.737571	1.468270
H	5.965759	-1.568092	0.004564
H	4.811020	-1.328935	1.346850
H	4.834189	-3.733612	0.707559
H	4.461612	-3.323005	-0.980807
N	2.669546	-0.562600	-0.266576
C	4.470553	-0.596175	-2.052929
H	3.771351	0.031133	-2.633992
H	5.499971	-0.225124	-2.220512
H	4.415138	-1.622997	-2.447470
C	1.852633	-2.353710	-1.899276
H	2.759403	-2.795231	-2.348783
H	1.060722	-3.124944	-1.929919
H	1.523346	-1.502459	-2.516979

TS2-3b$_{eq}$

C	-3.764260	-1.028666	1.297211
C	-2.798899	-1.051215	0.098902
N	-1.830473	0.073358	0.174325
C	-0.551071	-0.112712	0.526011
C	0.374370	-0.915298	1.083558
C	-3.559898	-1.087124	-1.238499
C	-2.358780	1.452653	0.018769
C	-2.133457	2.289512	1.286843
C	-1.778513	2.116248	-1.241126
O	0.894865	-1.635147	1.915263
H	-2.186376	-1.964656	0.174003
H	-3.449994	1.353516	-0.126616
H	-4.175771	-2.004672	-1.298687
H	-4.240729	-0.220592	-1.338385
H	-2.862020	-1.074761	-2.095878
H	-4.441626	-1.903743	1.264274
H	-3.199444	-1.052949	2.247152
H	-4.390204	-0.115632	1.283578
H	-2.533238	3.313031	1.153842
H	-2.635137	1.819889	2.152898
H	-1.053951	2.354235	1.512942
H	-2.188294	3.136026	-1.374038
H	-0.678487	2.189264	-1.162881
H	-2.018844	1.518059	-2.139764
N	0.885001	-0.443343	-0.352290
C	1.076086	-1.511844	-1.382191
C	1.947578	0.607330	-0.437736
C	2.439692	-2.202620	-1.164882
H	1.100950	-0.988942	-2.363597
C	-0.066109	-2.526607	-1.396776
C	3.327620	-0.049844	-0.212061
C	1.738077	1.765666	0.537067
C	3.588592	-1.186986	-1.207884
H	2.575278	-2.983134	-1.939369
H	2.409658	-2.700605	-0.176714
H	4.111919	0.727972	-0.290696
H	3.343898	-0.444701	0.822375
H	4.554657	-1.681499	-0.988588
H	3.665019	-0.765258	-2.232314
H	1.908832	1.001191	-1.478197
H	2.551214	2.500766	0.387069
H	0.770116	2.264792	0.375188
H	1.769677	1.410364	1.582578
H	0.150781	-3.298194	-2.158320
H	-0.158182	-3.026465	-0.415555
H	-1.024823	-2.048452	-1.648333

cis-**TS3-4b$_{eq/b}$**

C	3.260855	-2.060811	-0.050810
C	2.304047	-1.153597	0.735619
N	1.892948	0.013467	-0.098432
C	0.671605	0.167775	-0.594697
C	-0.323536	-0.906407	-0.664139
C	2.871386	-0.712645	2.094618
C	2.941444	1.020490	-0.434455
C	3.148109	1.103572	-1.952911
C	2.593355	2.382729	0.183496
O	-0.163311	-2.044930	-1.124701
H	1.378883	-1.725905	0.914176
H	3.880223	0.661334	0.023817
H	3.073678	-1.605198	2.716744
H	3.823140	-0.159157	1.984562
H	2.151359	-0.067105	2.630364
H	3.532636	-2.942417	0.560290
H	2.760055	-2.405708	-0.972405

H	4.194963	-1.528577	-0.315673
H	3.939162	1.839603	-2.191680
H	3.440417	0.118120	-2.359706
H	2.205126	1.413581	-2.439516
H	3.393918	3.116606	-0.027319
H	1.648868	2.761873	-0.249940
H	2.468987	2.297494	1.279132
N	-1.533108	-0.368893	-0.214302
C	-2.827387	-0.902328	-0.665074
C	-1.316249	0.852533	0.484858
C	-3.888675	0.219078	-0.653475
C	-3.234707	-2.127947	0.165753
H	-2.670661	-1.234352	-1.710855
C	-2.305314	1.976263	0.155176
H	-0.109953	1.122885	-0.233140
C	-3.256151	1.579528	-0.988616
H	-4.355780	0.280536	0.351743
H	-4.691899	-0.047492	-1.365521
C	-0.918208	0.746613	1.950545
H	-0.231040	-0.103115	2.110902
H	-0.413768	1.674286	2.288654
H	-1.812509	0.599643	2.595401
H	-4.187822	-2.550455	-0.208758
H	-2.446431	-2.897878	0.093084
H	-3.369101	-1.843471	1.227879
H	-2.694377	1.504115	-1.941284
H	-4.032255	2.356422	-1.122916
H	-1.754970	2.908813	-0.088988
H	-2.910099	2.206031	1.059302

trans-**TS3-4b**$_{eq/b}$

C	3.068564	-0.626627	1.582332
C	1.729720	0.071172	1.299199
N	1.515531	0.181446	-0.172942
C	0.668840	-0.587081	-0.859327
C	0.004321	-1.762691	-0.277701
C	1.601047	1.423694	2.019001
C	2.383082	1.132024	-0.925607
C	3.217920	0.396805	-1.983582
C	1.537512	2.262190	-1.531425
O	0.524742	-2.668658	0.379202
H	0.928143	-0.587665	1.668519
H	3.077159	1.574449	-0.188875
H	1.676689	1.261810	3.111139
H	2.403651	2.128823	1.731990
H	0.626009	1.897012	1.802945
H	3.217897	-0.734806	2.673513
H	3.058409	-1.629885	1.121736
H	3.917718	-0.042178	1.177583
H	3.882365	1.110242	-2.506891
H	3.834858	-0.389630	-1.511677
H	2.550074	-0.083559	-2.721804
H	2.185868	2.989183	-2.055865
H	0.819341	1.847651	-2.263993
H	0.969986	2.794915	-0.745866
N	-1.348233	-1.665298	-0.631372
C	-2.364365	-2.462672	0.068699
C	-1.623829	-0.285245	-0.941438
C	-3.164081	-1.522420	1.019924
H	-1.780647	-3.173676	0.685818
C	-3.266670	-3.256719	-0.883717
C	-1.905181	0.564486	0.303747
H	-0.239646	-0.081938	-1.505633
C	-2.282988	-0.351607	1.499936
H	-3.549006	-2.110332	1.874347
H	-4.046728	-1.113484	0.485065
H	-1.038000	1.204477	0.571183

H	-2.747911	1.252930	0.089793
H	-2.799761	0.238310	2.280464
H	-1.364369	-0.763275	1.962477
C	-2.529814	-0.055831	-2.134963
H	-2.207627	-0.665967	-2.999394
H	-3.583249	-0.327707	-1.899201
H	-2.529674	1.012455	-2.427896
H	-3.985628	-3.870335	-0.306183
H	-3.843767	-2.575675	-1.537242
H	-2.661956	-3.926802	-1.522022

TS2-3c$_{eq}$

C	-0.274157	0.339132	1.535332
C	0.799035	-0.292078	2.040553
N	1.031839	0.022723	0.457728
C	1.870891	1.214112	0.153820
C	3.375422	0.902956	0.100615
O	1.527117	-0.822994	2.851619
C	1.048798	-1.207951	-0.380916
C	2.284478	-2.101797	-0.152047
C	0.795677	-0.953883	-1.874003
C	1.411283	2.019369	-1.075912
H	1.702873	1.859796	1.035001
H	0.178517	-1.776027	-0.010463
H	1.840490	3.037981	-1.019193
H	1.745473	1.569869	-2.026316
H	0.311816	2.111489	-1.098597
H	3.942942	1.853379	0.112574
H	3.678931	0.297937	0.972722
H	3.649653	0.363205	-0.824423
H	2.086808	-3.104404	-0.579182
H	3.184777	-1.698338	-0.646410
H	2.485349	-2.205740	0.927623
H	0.581385	-1.919557	-2.370189
H	-0.067452	-0.282622	-2.028106
H	1.679540	-0.513504	-2.368644
N	-1.605649	0.320221	1.388120
C	-2.412450	-0.926876	1.261743
C	-2.341017	1.509950	0.891847
C	-2.728434	-1.197859	-0.223831
C	-1.796346	-2.117337	1.994564
C	-2.638322	1.322809	-0.612572
H	-3.317300	1.512460	1.424391
C	-1.622797	2.821138	1.204377
C	-3.421460	0.020146	-0.865546
H	-3.371119	-2.096296	-0.311506
H	-1.780694	-1.417065	-0.752117
H	-3.206395	2.193690	-0.994467
H	-1.670935	1.295957	-1.152734
H	-3.563437	-0.142712	-1.951681
H	-4.433303	0.125290	-0.421892
H	-3.377164	-0.693095	1.762001
H	-2.529755	-2.944597	2.018243
H	-0.880354	-2.487755	1.502849
H	-1.529287	-1.843538	3.030862
H	-2.260953	3.669181	0.892248
H	-1.415511	2.903772	2.286428
H	-0.660269	2.885093	0.668489

TS3-4c$_{eq}$

C	0.103570	-0.207304	-0.400979
C	-0.843957	-1.045725	0.333127
N	-1.910171	-0.210046	0.704240
C	-1.580420	1.162816	0.510074
C	-2.578826	2.009415	-0.260599
O	-0.808438	-2.270657	0.490058
C	-3.206866	-0.771193	1.097731

C	-4.211875	-0.858623	-0.067363
C	-3.784891	-0.036524	2.316543
C	-0.900621	1.884909	1.663070
H	-0.587749	0.833834	-0.508570
H	-2.958992	-1.808537	1.396026
H	-0.236910	1.202212	2.220884
H	-0.298294	2.741198	1.297077
H	-1.651703	2.291956	2.375995
H	-2.135993	2.995220	-0.500838
H	-2.879264	1.514794	-1.202212
H	-3.498325	2.201169	0.333267
H	-5.090332	-1.459849	0.237781
H	-4.572907	0.140593	-0.372708
H	-3.742014	-1.348719	-0.939803
H	-4.707989	-0.540304	2.660666
H	-3.057506	-0.028046	3.149257
H	-4.044624	1.011021	2.070714
N	1.428609	-0.147640	-0.344556
C	2.316061	-0.398059	0.838799
C	2.185055	0.485853	-1.467518
C	2.860553	0.957632	1.346532
C	1.673733	-1.206474	1.961995
C	2.694987	1.868359	-1.010279
H	3.071674	-0.162909	-1.634839
C	1.385378	0.558220	-2.766766
C	3.580861	1.742974	0.239305
H	3.544607	0.769697	2.197040
H	2.003818	1.542829	1.733577
H	3.251077	2.347397	-1.839241
H	1.811352	2.503185	-0.793047
H	3.883014	2.742861	0.606610
H	4.511859	1.205832	-0.036579
H	3.174316	-0.977955	0.438195
H	2.442603	-1.392456	2.734811
H	0.844765	-0.648581	2.433452
H	1.270901	-2.162696	1.594495
H	2.057689	0.897791	-3.577327
H	0.967138	-0.429360	-3.030138