Disodium Salts of Pseudoephedrine-Derived Myers Enolates: 
Stereoselectivity and Mechanism of Alkylation

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Chart 1. Substrates and aggregates
Part 1  Alkylation reactions

Synthesis of 29: alkylation with BnBr

Alkylation carried out with NaDA from glovebox:
Solid sodium diisopropylamide (NaDA, 61.6 mg, 0.25 mmol) was dissolved in 300 μL of tetrahydrofuran (THF) at 0 °C. 150 μL of the NaDA solution was added to a dry 5 mL Kimble vial equipped with a magnetic stir bar and 26.3 mg (0.10 mmol) of 33 at −78 °C in a dry ice acetone bath. The mixture was stirred at −78 °C for 20 min to dissolve. 50 μL of BnBr (0.20 mmol, 4.0 M in THF) was then added to the reaction mixture. The reaction was stirred at −78 °C for 10 min. Saturated aqueous ammonium chloride solution (0.2 mL) was added, and the resulting biphasic mixture was partitioned between water (0.2 mL) and ethyl acetate (2 mL). The aqueous layer was separated and extracted further with three 1 mL portions of ethyl acetate. The combined organic layers were dried over anhydrous magnesium sulfate and then concentrated. Purification of the residue by flash column chromatography (50 % ethyl acetate in hexanes) afforded 26 mg (73%) of product 29 as a white crystalline solid whose spectral properties were found to be in accordance with those previously reported.

Synthesis of 30: alkylation with MeI

Alkylation carried out with NaDA from glovebox:
Reaction was carried out according to synthesis of 29. Enolization of 33 (26.3 mg) with NaDA (1.67 M, 150 μL) and addition of MeI (4 M, 50 μL, 4 equiv) followed by stirring at −78 °C for 30 min afforded product. Purification of the product by flash chromatography (50 % ethyl acetate in hexanes) afforded 23.6 mg (85%) of product 30 as a white crystalline solid whose spectral properties were found to be in accordance with those previously reported.
**Part 2  Enolate aging**

![Chemical structure](image)

**Figure 1.** $^1$H NMR spectra of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ with varying aging time. (a) aged at $-80 \, ^\circ C$ for 1 day, (b) aged at $-80 \, ^\circ C$ for 7 days, and (c) aged at $-80 \, ^\circ C$ for 14 days. The disodium enolates decompose even at $-80 \, ^\circ C$ after 2 weeks.
Figure 2. $^{13}$C{${}^1$H} NMR spectra of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ with varying aging time. (a) aged at $-80$ °C for 1 day, (b) aged at $-80$ °C for 7 days, and (c) aged at $-80$ °C for 14 days. The disodium enolates decompose even at $-80$ °C after 2 weeks.
Figure 3. $^1$H NMR spectra of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ with varying aging temperature and time. (a) aged at $-80^\circ$C for 2 h, (b) aged at $-55^\circ$C for 30 min, (c) aged at $-30^\circ$C for 30 min, (d) aged at 0 $^\circ$C for 30 min, and (e) aged at 20 $^\circ$C for 30 min. The disodium enolates decompose at above $-30^\circ$C.
Figure 4. $^{13}\text{C}$ $^{1}\text{H}$ NMR spectra of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ with varying aging temperature and time. (a) aged at $-80$ °C for 2 h, (b) aged at $-55$ °C for 30 min, (c) aged at $-30$ °C for 30 min, (d) aged at 0 °C for 30 min, and (e) aged at 20 °C for 30 min. The disodium enolates decompose at above $-30$ °C.
Figure 5. $^{13}$C$\{$$^1$$H$\}$ NMR for a solution of 0.25 M 1 in neat THF with 0.50 M NaDA (2 equiv) at −80 °C with different aging time, (a) aged at −80 °C for 12 h; (b) aged at 0 °C for 5 min; (c) aged at 0 °C for 20 min; (d) aged at 20 °C for 10 min; and (e) aged at 20°C for 30 min.
Figure 6. $^{13}\text{C}\{^1\text{H}\}$ NMR for a solution of 0.25 M 1 in neat THF with 0.625 M NaDA (2.5 equiv) at –80 °C with different aging time, (a) aged at –80 °C for 12 h; (b) aged at 0 °C for 10 min; (c) aged at 20 °C for 20 min; (d) aged at 20 °C for 50 min; and (e) aged at 20°C for 90 min.
Part 3 Aggregate characterization

\[ A:B = 3:1 \]

\textbf{Figure 7.} Partial $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for 0.25 M solutions of 3:1 8 (A) and 15 (B) in 12.3 M THF at −80 °C with different relaxation delay (A) 1 s, qualitative; (B) 60 s, quantitative. The region shown corresponds to quaternary enolate carbon. For the qualitative spectrum $A_4:AB_3:A_2B_2=22:54:24$; For the quantitative spectrum $A_4:AB_3:A_2B_2=25:50:25$. Longer relaxation does not improve integration of spectra obviously.
Figure 8. Partial $^{13}$C{¹H} NMR spectra for 0.25 M solutions of 8 (A) and 15 (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. The combination of 8 vs 15 gives clear resolution. There are three heteroaggregate species corresponding to tetramer assignment. Peaks between 166.5 ppm and 165.0 ppm are resulting from decomposition of enolate 15.
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Figure 13. Partial $^{13}$C\{H\} NMR spectra for 0.25 M solutions of 8 (A) and 15 (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. There are three heteroaggregate species corresponding to tetramer assignment.
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Figure 15. Partial $^{13}$C{H} NMR spectra for 0.25 M solutions of 8 (A) and 17 (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. Enolate B is reluctant to mix, probably owing to different bulkiness between Me and t-Bu group.
Figure 16. Partial $^{13}$C($^1$H) NMR spectra for 0.25 M solutions of 8 (A) and 32 (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. The phenyl ring on enolate B maybe metalated by NaDA.
Figure 17. Partial $^{13}$C{$^1$H} NMR spectra for 0.25 M solutions of 14 (A) and 15 (B) in 12.3 M THF at $-80^\circ$C. The region shown corresponds to quaternary enolate carbon. Heteroaggregate A$_2$B$_2$ are difficult to resolve. There are three heteroaggregate species corresponding to tetramer assignment.
Figure 18. Partial $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for 0.25 M solutions of 14 (A) and 16 (B) with 0.625 M NaDA in 12.3 M THF at $-80^\circ$C. The region shown corresponds to quaternary enolate carbon. Heteroaggregates do not resolve owing to overlap between species.
**Figure 19.** Partial $^{13}\text{C}^{1}\text{H}$ NMR spectra for 0.25 M solutions of 14 (A) and 17 (B) in 12.3 M THF at $-80^\circ\text{C}$. The region shown corresponds to quaternary enolate carbon. Enolate B is reluctant to mix, probably owing to different bulkiness between $n$-Bu and $t$-Bu group.
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Figure 23. Partial $^{13}$C($^1$H) NMR spectra for 0.25 M solutions of 16 (A) and 17 (B) in 12.3 M THF at −80 °C. The region shown corresponds to quaternary enolate carbon. Enolate B is reluctant to mix, probably owing to different bulkiness between Bn and t-Bu group.
**Figure 24.** Partial $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of a solution of 0.25 M 1 in 12.3 M THF at –80 °C with varying NaDA concentrations. (a) only NaDA and no substrate available, (b) 0.625 M NaDA (2.5 equiv), (c) 0.94 M NaDA (3.8 equiv), and (d) 1.25 M NaDA (5.0 equiv). No NaDA-mixed aggregate was observed.
Figure 25. Partial $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of a solution of 0.25 M 1 in 12.3 M THF at –80 °C with varying NaDA concentrations. (a) only NaDA and no substrate available, (b) 0.625 M NaDA (2.5 equiv), (c) 0.94 M NaDA (3.8 equiv), and (d) 1.25 M NaDA (5.0 equiv). No NaDA-mixed aggregate was observed.
Figure 26. Partial $^{13}$C {$^1$H} NMR spectra of a solution of 0.30 M 1 in 12.3 M THF at –80 °C with 0.70 M NaDA or NaHMDS. (a) 0.625 M NaDA, (b) 0.625 M NaHMDS and aged at –80 °C for 3 h, and (c) 0.625 M NaHMDS and aged at –80 °C for 29 h. NaHMDS is not basic enough to quantitatively form enolate.
Figure 27. Partial $^{13}$C-{$^1$H} NMR spectra for 1:1 ratio of 0.25 M solution of 8 and 14 in 12.3 M THF at −80 °C. Formation of heteroaggregates is slow at −78 °C (t$_{1/2}$ > 5h).
Figure 28. Partial $^{13}$C{$^1$H} NMR spectra for 1:1 ratio of 0.25 M solutions of 8 and 15 in 12.3 M THF at $–80$ °C. Formation of heteroaggregates is slow at $–78$ °C ($t_{1/2} > 5$ h).
Figure 29. Plot of percent homoaggregate and percent heteroaggregate in 0.25 M solutions of 8 and 15 in neat THF at –80 °C versus time. T_{1/2} is approximate 5 h.
Figure 30. $^1$H NMR spectra at −80 °C for (A) 0.25 M 8; (B) 0.10 M 8 reacted with 10M n-BuI at −60 °C for 30 min; (C) 0.25 M 22; (D) 0.25 M 31; (E) 0.25 M solutions of 1:1 22:31. The $^1$H NMR spectra of alkoxides are not simple.
Figure 31. Partial $^{13}$C{$^1$H} NMR spectra at –80 °C for (A) 0.25 M 8; (B) 0.25 M 22; (C) 0.25 M 31; (D) 0.25 M solutions of 1:1 22:31. $^{13}$C NMR spectra of alkoxides are not simple.
**2D NMR analysis of 8 homoaggregates:** A sample prepared from 0.70 M NaDA, 0.30 M 1 in 12.3 M THF-d8, after aging at –80 °C for 18 h, was studied by standard 2D NMR techniques. All chemical shifts were assigned using high-field indirect-resolution 2D HSQC, COSY and HMBC experiments.

**Experimental:** 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for 1H observation using a 5 mm Varian inverse-detect probe head with Z-axis pulsed field-gradient. Sample temperature was maintained at –80 °C as calibrated with a neat methanol sample. 1H and 13C chemical shifts were referenced to the residual downfield THF-d7 resonance at 3.58 ppm and 67.57 ppm, respectively. 2D experiments were acquired using standard pulse sequences supplied in VnmrJ 3.2A (Agilent Inc.) and processed and analyzed in MestReNova 11.0.3 (Mestrelab Research S.L.).

**Determination of the 3D aggregate structure:** The 3D structure of the aggregate was derived from 2D ROESY (reported as H–H correlations). However, with only one subunit, it is hard to differentiate between inter- or intra- subunit nOe correlations. Therefore, 2D NMR of heteroaggregates was carried out.
Table 1. $^1$H and $^{13}$C chemical shifts and assignments for enolate 8 at –80 °C.

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$^1$HSQC correlations were omitted from the table. $^2$Important correlations that allowed determination of subunit arrangement are marked in red.
Figure 32. $^1$H NMR spectrum of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ at –80 °C. Labels indicate assignments by 2D NMR.
**Figure 33.** Full-display HSQC spectrum of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ at -80 °C. $^{13}$C decoupler was turned off.
Figure 34. Expansion of the HSQC spectrum of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ at $-80 \, ^\circ\text{C}$. $^{13}\text{C}$ decoupler was turned off.
Figure 35. Expansion of the HSQC spectrum of a solution of 0.30 M 8 in 12.3 M THF-\(d_8\) at –80 °C. \(^{13}\)C decoupler was turned off.
**Figure 36.** Full-display HMBC spectrum of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ at –80 °C.
Figure 37. Expansion of the HMBC spectrum of a solution of 0.30 M 8 in 12.3 M THF-\textit{d}_8 at $-80$ °C.
Figure 38. Expansion of the HMBC spectrum of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ at -80 °C.
Figure 39. Full-display COSY spectrum of a solution of 0.30 M 8 in 12.3 M THF-d$_8$ at –80 °C.
Figure 40. Expansion of the COSY spectrum of a solution of 0.30 M \( \text{8} \) in 12.3 M THF-\( \text{d}_8 \) at –80 °C.
Figure 41. Expansion of the COSY spectrum of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ at $-80 \degree C$. 
Figure 42. Full-display ROESY spectrum of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ at –80 °C.
Figure 43. Expansion of the ROESY spectrum of a solution of 0.30 M 8 in 12.3 M THF-$d_8$ at $-80 \, ^\circ$C.
2D NMR analysis of heteroaggregate 18: A sample prepared from 0.70 M NaDA, 0.255 M 1 and 0.045 M 34 in 12.3 M THF-$d_8$, after aging at –80 °C for 18 h, was studied by standard 2D NMR techniques. All chemical shifts were assigned using high-field indirect-resolution 2D HSQC, COSY and HMBC experiments.

**Experimental:** 2D NMR spectra were acquired on a 500 MHz Varian INOVA spectrometer operating at 499.92 MHz for $^1$H observation using a 5 mm Varian inverse-detect probe head with Z-axis pulsed field-gradient. Sample temperature was maintained at –80 °C as calibrated with a neat methanol sample. $^1$H and $^{13}$C chemical shifts were referenced to the residual downfield THF-$d_7$ resonance at 3.58 ppm and 67.57 ppm, respectively. 2D experiments were acquired using standard pulse sequences supplied in VnmrJ 3.2A (Agilent Inc.) and processed and analyzed in MestReNova 11.0.3 (Mestrelab Research S.L.).

**Determination of the 3D aggregate structure:** The 3D structure of the aggregate was derived from 2D ROESY (reported as H–H correlations) and HSQC-NOESY (reported as C–H correlations) experiments. The enolate is in the Z configuration based on the strong nOe correlation between H-12 and C-13, between H-12' and C-13', between H-12" and C-13", between H-12''' and C-13'''. Reciprocal C-12 and H-13 (C-12' and H-13', C-12" and H-13", C-12''' and H-13'''') correlation is also observed. The starting point for solving the structure is correlations between C-5 and H-14'' (also between C-5''' and H-15). This correlation indicates the alkoxide part (C-5) of the red subunit is close to the enolate part (H-14'') of the blue subunit. Similarly, the alkoxide part (C-5'''') of the blue subunit is close to the enolate part (H-15) of the red subunit (Figure 42). The bottom face of the aggregate should be similar to the top face. There are two ways to assemble the bottom face (Figure 43-A and Figure 43-B). The right-hand structure will require close proximity of the two enolate parts from top to bottom face. However, such correlations are not available. The final structure is the left-hand structure. Black subunits are from homoaggregates 8.
**Figure 44.** Illustration of blue and red subunits.

**Figure 45.** Two possible structures of heteroaggregates.
Table 2. $^1$H and $^{13}$C chemical shifts and assignments for heteroaggregate 18 at −80 °C.

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<th>Atom</th>
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1HSQC correlations were omitted from the assignment table. 2Important correlations that allowed determination of subunit arrangement are marked in red. 3Not determined.
Figure 46. $^1$H NMR spectrum for 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at –80 °C. Labels indicate assignments by 2D NMR.
Figure 47. Full display HSQC spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-\(d_8\) at –80 °C. \(^{13}\)C decoupler was turned off.
Figure 48. Expansion of the HSQC spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at −80 °C. $^{13}$C decoupler was turned off.
**Figure 49.** Expansion of the HSQC spectrum 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at $-80 \, ^\circ C$. $^{13}C$ decoupler was turned off.
Figure 50. Full display HMBC spectrum for 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at –80 °C.
Figure 51. Expansion of the HMBC spectrum for 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at –80 °C.
Figure 52. Full display COSY spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at –80 °C.
Figure 53. Expansion of the COSY spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at $-80$ °C.
Figure 54. Expansion of the COSY spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at –80 °C.
Figure 55. Full display HSQC-NOESY spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at –80 °C.
**Figure 56.** Expansion of the HSQC-NOESY spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at −80 °C.
Figure 57. Expansion of the HSQC-NOESY spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-\textit{d}$_8$ at –80 °C.
Figure 58. Full display NOESY spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at –80 ºC.
Figure 59. Full display ROESY spectrum of 0.30 M solutions of 85:15 8 and 15 in 12.3 M THF-$d_8$ at –80 °C.
Figure 60. IR spectra in neat THF at −78 °C (A) 0.040 M substrate 1; (B) 0.040 M enolate 8; (C) 0.040 M product.
Figure 61. $^1$H NMR spectra for reaction of 0.10 M 1 and 0.25 M NaDA in 12.3 M THF-$d_8$ with 0.40 M $n$-BuI at –60 °C. Reaction of enolate can be followed on NMR with clear disappearance of starting material.
**Figure 62.** Plot of disappearance of enolate 8 carried out using 0.10 M I, 0.25 M NaDA, and 0.40 M n-Bul at –60 °C.
Figure 63. $^1$H NMR spectra for reaction of 0.10 M 1 and 0.25 M NaDA in 12.3 M THF-$d_8$ with 1.0 M i-BuI at $-50 \, ^\circ\text{C}$. Reaction of enolate can be followed on NMR with clear disappearance of starting material.
Figure 64. Plot of disappearance of enolate 8 carried out using 0.10 M 1, 0.25 M NaDA, and 1.0 M i-Bul at –50 °C.
Figure 65. Plot of initial rate versus n-Bul concentrations for alkylation of 0.10 M 8 in neat tetrahydrofuran-\textit{d}_8 (THF-\textit{d}_8) at −80 °C. The curve depicts an unweighted least-squares fit to the function \( f(x) = ax^n \) such that \( a = (3.1 \pm 1.2) \times 10^{-3} \), \( n = 0.97 \pm 0.08 \).
Figure 66. Plot of initial rate versus enolate 8 concentrations for alkylation of 0.493 M n-Bul in neat tetrahydrofuran-\textit{d}_8 (THF-\textit{d}_8) at −80 °C. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^n$ such that $a = (3.9 \pm 0.087) \times 10^{-3}$, $n = 0.29 \pm 0.014$. Inset demonstrates plot of log(initial rate) vs log[enolate]. The curve depicts an unweighted least-squares fit to the function $f(x) = ax + b$ such that $a = 0.29 \pm 0.013$, $b = 2.4 \pm 0.011$.

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Figure 67. Plot of initial rate versus THF-$d_8$ concentrations for alkylation of 0.050 M 8 and 0.203 M $n$-BuI in hexanes cosolvent at $-80 \, ^\circ\text{C}$. The curve depicts an unweighted least-squares fit to the function $f(x) = ax^n$ such that $a = (1.1 \pm 2.2) \times 10^{-6}$, $n = 3.0 \pm 0.85$.

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Part 5  Crystal Structure Data

Owing to the low resolution of the crystal, only coordinates (xyz) are presented.

Samples for X-ray spectroscopy were prepared from 0.30 M (R,R)-1 and 0.70 M NaDA in neat THF, aged at 20 °C for 20 min, cooled back down to −80 °C, crystal formed. The crystals were redissolved at 20 °C with vigorous shaking, slowly cooled back to −20 °C and left at −20 °C for 3 days until crystals grew. Owing to the low quality of the crystal, only coordinates (xyz) are presented. Samples for single crystal X-ray diffraction were prepared from 0.30 M (R,R)-1 and 0.70 M NaDA in neat THF, aged at 20 °C for 20 min, cooled back down to −80 °C, crystal formed. Unit cell parameters: a = 16.6515(6) Å, b = 15.3595(8) Å, c = 30.4861(10) Å, α = 90°, β = 92.594(3)°, γ = 90°, V = 7789.1(6) Å³, space group = I2.

Table 3. Geometric coordinates for crystal structure 22

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S-86
Part 6. Computations

Geometries are optimized at the M06-2X level of theory using the 6-31G(d) basis set for tetramer computation and 6-311+G(2d,p) basis set for the other computations. Energies are defined as follows: G is the sum of electronic and thermal free energies calculated at the M06-2X level of theory (T = 195 K). \( G_{SP} \) is derived from an M062X SP calculation corresponding to the DFT-optimized geometry and includes a thermal correction from the DFT calculation.

Table 4. Geometric coordinates and thermally corrected M062X energies for THF

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G &= -232.234012 \\
G_{SP} &= -232.3100352
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Table 5. Geometric coordinates and thermally corrected M062X energies for 19

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Table 6. Geometric coordinates and thermally corrected M062X energies for 20

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**Table 7.** Geometric coordinates and thermally corrected M062X energies for 35 (octagonal prism version of 21)

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Figure 68. Computation overview for resting state of tetrasolvated monomers.

resting state di-equatorial

two THF on N-Na

24a

[Diagram with reaction arrows and energy values]

resting state di-axial

Phenyl concave

Phenyl convex

+2.8 kcal/mol

+1.3 kcal/mol

+5.5 kcal/mol

-3.1 kcal/mol

+9.1 kcal/mol

+9.6 kcal/mol
Table 9. Geometric coordinates and thermally corrected M062X energies for resting state 24a

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G_{SP} &= -1964.367172
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Table 10. Geometric coordinates and thermally corrected M062X energies for resting state 24

![Diagram of molecular structure]

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\( G_{SP} = -1964.375154 \)

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S-104
Table 11. Geometric coordinates and thermally corrected M062X energies for resting state 24b

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\[ G_{SP} = -1964.371067 \]

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S-106
Table 12. Geometric coordinates and thermally corrected M062X energies for resting state 24c

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\[ G_{SP} = -1964.372211 \]

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Table 13. Geometric coordinates and thermally corrected M062X energies for resting state 25a

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Table 14. Geometric coordinates and thermally corrected M062X energies for resting state 25b

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S-112
Table 15. Geometric coordinates and thermally corrected M062X energies for resting state 25

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Table 16. Geometric coordinates and thermally corrected M062X energies for resting state 25c

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Figure 69. Computational overview for transition state of tetrasolvated monomers with pseudo-diaxial substituents
Table 17. Geometric coordinates and thermally corrected M062X energies for transition state 26

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### Table 20. Geometric coordinates and thermally corrected M062X energies for transition state 26c

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Table 21. Geometric coordinates and thermally corrected M062X energies for transition state 26d

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Table 23. Geometric coordinates and thermally corrected M062X energies for transition state 26f

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Table 24. Geometric coordinates and thermally corrected M062X energies for transition state 26g

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Figure 70. Computational overview for transition state of tetrasolvated monomers with pseudo-diequatorial substituents

- **major experimentally**
  - two THF on N-Na
    - $27a$: $\Delta G = -1.6 \text{ kcal/mol}$
    - $27a$ to $27b$: $\Delta G = 2.6 \text{ kcal/mol}$
    - $27c$: $\Delta G = 7.8 \text{ kcal/mol}$
    - $27c$ to $27b$: $\Delta G = 6.3 \text{ kcal/mol}$
    - $27c$ to $27d$: $\Delta G = 4.3 \text{ kcal/mol}$
    - $27d$: $\Delta G = 6.2 \text{ kcal/mol}$
    - $27d$ to $27f$: $\Delta G = 2.6 \text{ kcal/mol}$
    - $27f$: $\Delta G = 0.4 \text{ kcal/mol}$

- **minor experimentally**
  - one THF on N-Na
    - $27b$: $\Delta G = 3.6 \text{ kcal/mol}$
    - $27b$ to $27a$: $\Delta G = 7.7 \text{ kcal/mol}$
    - $27b$ to $27c$: $\Delta G = 1.5 \text{ kcal/mol}$
    - $27c$ to $27e$: $\Delta G = 2.6 \text{ kcal/mol}$
    - $27e$: $\Delta G = 4.3 \text{ kcal/mol}$

Phenyl concave and Phenyl convex
Table 25. Geometric coordinates and thermally corrected M062X energies for transition state 27a

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\[ \text{Gsp} = -4617.669169 \]

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Table 28. Geometric coordinates and thermally corrected M062X energies for transition state 27

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Table 29. Geometric coordinates and thermally corrected M062X energies for transition state 27d

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Table 30. Geometric coordinates and thermally corrected M062X energies for transition state 27e

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Table 31. Geometric coordinates and thermally corrected M062X energies for transition state 27f

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\[
G = -4614.754293 \\
G_{SP} = -4617.667687
\]
Figure 71. Computation overview for resting state of trisolvated monomers.

resting state di-equatorial

resting state di-axial

Phenyl concave

Phenyl convex

\[ 37a \] +0.6 kcal/mol

\[ 37c \] –2.5 kcal/mol

\[ 37b \] +4.6 kcal/mol

\[ 37d \] –6.5 kcal/mol
Table 33. Geometric coordinates and thermally corrected M062X energies for resting state 37a

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Table 34. Geometric coordinates and thermally corrected M062X energies for resting state 37b

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Table 35. Geometric coordinates and thermally corrected M062X energies for resting state 37c

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G_{\text{SP}} &= -1732.052959
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O & 2.93609200 & -0.35383600 & -0.39753700 & \\
Na & 1.77943700 & -0.50145400 & 2.04954500 & \\
O & 3.29929900 & -1.80920400 & 3.07601200 & \\
C & 2.95112000 & -3.18668900 & 2.84510200 & \\
C & 3.98826700 & -3.68727200 & 1.85044800 & \\
C & 4.52621000 & -2.94933000 & 1.90344600 & \\
C & 4.92569000 & -1.59167200 & 2.78672300 & \\
O & 4.76929400 & -0.83636700 & 2.00134900 & \\
H & 5.18790100 & -0.50145400 & 2.04954500 & \\
H & 6.00362600 & -2.83303800 & 1.54217600 & \\
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H & 3.00726300 & -3.73317900 & 3.79660400 & \\
C & 1.93169000 & -3.20682900 & 2.45128900 & \\
O & -0.04162000 & 0.98279000 & 2.19209000 & \\
C & 0.24745700 & 2.34312000 & 1.84481600 & \\
C & -1.03770300 & 2.81613500 & 1.16316100 & \\
C & -2.14677600 & 2.03048500 & 1.90344600 & \\
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Table 36. Geometric coordinates and thermally corrected M062X energies for resting state 37d

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H  -0.46663300  1.08310900  -4.37680700  H  1.58866100  0.43384900  2.49649000
C  -0.03081800  -1.62445800  -3.58007400  H  1.80281700  -0.98039900  3.58330100
C  0.09094600  -3.11957900  -3.63291600  H  -0.84898300  0.20506000  2.59816500
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C  0.33483200  -2.47647300  1.89697500  H  -1.26064200  -2.34754200  -0.98305300
Figure 72. Computational overview for transition state of trisolvated monomers.

* major experimentally

* minor experimentally

![Diagram showing computational overview for transition state of trisolvated monomers.](image)
Table 37. Geometric coordinates and thermally corrected M062X energies for transition state 38a

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Table 38. Geometric coordinates and thermally corrected M062X energies for transition state 38b

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Table 39. Geometric coordinates and thermally corrected M062X energies for transition state 38c

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The coordinates are given in Angstroms (Å).
Table 40. Geometric coordinates and thermally corrected M062X energies for transition state 38d

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Table 41. Geometric coordinates and thermally corrected M062X energies for transition state 39a

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Table 42. Geometric coordinates and thermally corrected M062X energies for transition state 39b

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S-172
Table 43. Geometric coordinates and thermally corrected M062X energies for transition state 39c

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Table 44. Geometric coordinates and thermally corrected M062X energies for transition state 39d

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\text{C} & -2.64254800 & 1.09072700 & 1.39467900 & \text{H} & -0.59994500 & -2.97969700 & -2.90306400 \\
\text{C} & -1.79095600 & 2.40609000 & 1.48548700 & \text{O} & -4.18025200 & -1.18507600 & -1.84304300 \\
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\text{C} & -0.96696600 & 2.98067300 & -0.85110200 & \text{C} & -6.02295800 & -1.48572300 & -0.41273700 \\
\text{O} & -0.93879100 & 1.74946900 & -1.22856400 & \text{C} & -6.52392400 & -1.52202000 & -1.85812600 \\
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\[G_{SP} = -4385.349424\]
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Table 45. Geometric coordinates and single point M062X energy for transition state 26 with one THF

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Table 46. Geometric coordinates and single point M062X energy for transition state 26 with no Ph and Me group on the backbone

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G_{SP} = -4348.12457247
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Table 47. Geometric coordinates and single point M062X energy for transition state 27 with one THF

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Table 48. Geometric coordinates and single point M062X energy for transition state 27 with no Ph and Me group on the backbone

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Table 49. Optimized geometries at the M062X level of theory with 6-31G(d) basis set for forward and reverse IRC calculations of transition structures 26/27 at 195K with free energies (Hartrees), corrected M062X energies and cartesian coordinates (X, Y, Z). (Note: GSP includes single-point M062X corrections to M062X/6-31+G(2d,p) optimized structures.) The 2D representations below correspond to the transition state, which the IRC has been done.

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