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SUPPLEMENTARY INFORMATION FILE

BASE-CATALYZED C-ALKYLATION OF POTASSIUM ENOLATES WITH STYRENES VIA A METAL-ENE REACTION: A MECHANISTIC STUDY

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1. GENERAL EXPERIMENTAL INFORMATION

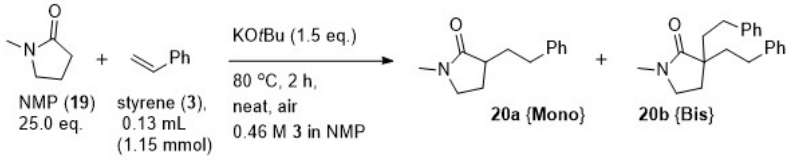
Unless specified otherwise, reactions were prepared in a glovebox supplied by Miwa Manufacturing Co., Ltd. and were carried out under an inert (N_2) atmosphere. Anhydrous solvents and reagents (*N,N*-dimethylacetamide, *N*-methylpyrrolidinone, cyclohexanone, α-tetralone) were degassed via 3x freeze/pump/thaw cycles and stored over 4Å molecular sieves (which had been activated by microwave heating, 10x 1 min at 700 W) in the glovebox. Cryogenic conditions (-78 °C) were achieved using dry ice/acetone baths. Temperatures of 0 °C were obtained by means of a variable temperature (VT) probe inside an NMR spectrometer or a temperature controller within a UV-vis spectrometer. 'Room temperature' (rt) indicates temperatures in the range of 20-25 °C. For purposes of thin layer chromatography (TLC), Silica gel 60N Aluminium plates were used, with UV light ($\lambda = 254$ and 365 nm) used for visualisation and/or cerium molybdate stain as the developing agent. Purification was achieved by column chromatography, using Silica gel 60N, particle size 100-210 μm (KANTO CHEMICAL CO., INC.). In some cases, purification was achieved by preparative gel permeation chromatography (GPC), using a LC908-C60 (Japan Analytical Industry CO., Ltd) instrument fitted with a combination of JAIGEL 1H-40 and JAIGEL 2H-40 columns, using $CHCl_3$ as eluent (Flow rate = 4.7 ml/min) and following by a UV detector ($\lambda = 254$ nm). Removal of solvents (*in vacuo*) was achieved using rotary evaporators.

For NMR spectroscopy, chloroform-d (D, 99.8% + 0.05v/v% TMS, Cambridge Isotope Laboratories), DMSO-d_6 (D, 99%, Cambridge Isotope Laboratories) and NMP-d_9 (D, 99.0%, Cambridge Isotope Laboratories) were used. NMR data were collected either using a Bruker Avance 500 instrument using 500 MHz and 126 MHz for ^{1}H and ^{13}C NMR, respectively, or on a Bruker Avance 400 instrument using 400 MHz and 101 MHz for ^{1}H and ^{13}C NMR, respectively. Kinetic NMR studies were conducted on the former 500 MHz instrument using a VT probe, set between 273 - 373 K (0 - 100 °C). Fourier Transformations of the data were carried out using Topspin (Bruker). Peak picking, integration and multiplicity were obtained using an NMR software by Hiroshi Nakamura (Emeritus Professor, University of Hokkaido). Reference values for residual solvents were taken as δ = 7.27 ($CDCl_3$) and 2.50 ppm (DMSO-d_6) for ^{1}H NMR; δ = 77.00 ppm ($CDCl_3$) and 39.5 ppm (DMSO-d_6) for ^{13}C NMR. Multiplicities for coupled signals were denoted as: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br. = broad, apt. = apparent and dd = double doublet *etc.* Coupling constants (*J*) are given in Hz and are uncorrected. Where appropriate, COSY, DEPT, HSQC and HMBC experiments were carried out to aid assignment. Infrared spectra were recorded on a PerkinElmer Spectrum 2000 FTIR as a thin film cast on a KBr disc.

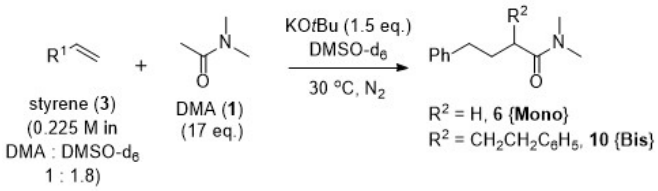
Matrix-Assisted Laser Desorption/Ionization High Resolution Mass Spectrometry (MALDI-HRMS) analyses were carried out on a JMS-S3000 spiralTOF from JEOL (Toyko, Japan) (resolution ($m/\Delta m$) = 45000). The matrix was either [3-(4-*tert*-Butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB) or 2,4,6-trihydroxyacetophenone (THAP) and $CHCl_3$ was used for dissolution. Electrospray ionization mass spectrometry (ESI-MS) and MS/MS analyses were carried out on a LC-MS8030 from Shimadzu (Kyoto, Japan) equipped with an electrospray ion source in infusion mode (samples directly injected to the source at 5 μL/min). UV-visible absorption measurements were performed using a JASCO V-760

spectrophotometer with a JASCO ETCR-762 temperature control unit. EPR spectroscopy was performed at the University of Tsukuba, Japan using a JEOL RESONANCE JES-FA200 X-band ESR spectrometer, fitted with a TEO11 cylindrical-type cavity. In order to successfully tune the instrument for high-polarity aprotic solvents (DMA, NMP, DMSO-d_6), Wilmad Quartz capillary tubes (i.d. 1 mm) were filled with reaction mixture and placed inside sealed Quartz EPR tubes (i.d. 3.5 mm) which were then placed inside the instrument cavity. All solvents and reagents were purchased from Wako Pure Chemical Industries, Tokyo Chemical Industry or Sigma Aldrich and used as supplied or purified using standard techniques.[1]

2. EXPERIMENTAL PROCEDURES



Procedure A: An oven-dried reaction vessel equipped with a stirrer bar was charged with KO*t*Bu (193 mg, 1.72 mmol, 1.5 eq.), 'amide' (2.50 mL, 25.0 eq.) and styrene (0.13 mL, 1.15 mmol, 1.0 eq.). A pale yellow color developed. The reaction vessel was sealed under ambient air/moisture and stirred at 80 °C for 2 h. A pale brown color developed after heating. After cooling to rt, the reaction mixture was quenched with H_2O (~1 mL) and washed into a separatory funnel with EtOAc (20 mL) and H_2O (10 mL). The layers were separated and the aqueous layer extracted with further EtOAc (3 x 20 mL). The combined organic layers were dried ($MgSO_4$), filtered and concentrated *in vacuo* to yield a colorless oil. Purification by column chromatography (25 - 75% EtOAc/Hexane) gave the desired products**.** Yields of compounds **6**, **10**, **20a** and **20b** are consistent with that previously reported.[2]



Procedure B: An oven-dried NMR tube containing 1,3,5-trimethoxybenzene (19.3 mg, 1.0 eq.) was taken inside a glovebox (under N_2) and was charged with KO*t*Bu (19.3 mg, 0.17 mmol, 1.5 eq.), DMSO-d_6 (0.33 mL) and 'K enolate precursor' (0.18 mL, ca. 15 - 17 eq.) and mixed until fully dissolved. The tube was sealed before removing from the glovebox. In the case of reactions at or below 30 °C, the NMR tube was placed inside the NMR spectrometer's VT probe set at the desired temperature and locked/tuned/shimmed. The sample was removed from the spectrometer, cap quickly removed, styrene (13 μL, 0.115 mmol, 1.0 eq.) quickly added via syringe and cap replaced (briefly exposing the sample to air). The sample was quickly inverted a couple of times to mix before quickly placing inside the spectrometer, locking and scanning over time. In the case of reactions above 30 °C, a 'blank' sample containing only DMSO-d_6 and 'K enolate precursor' was locked/tuned/shimmed at the desired temperature. Styrene was added (as per **Procedure A**) to the desired sample of interest at room temperature, the resulting sample was quickly inverted a couple of times to mix before quickly substituting it for the 'blank' sample inside the VT probe. For the purposes of these experiments, the experiment time was deemed to begin after addition and quick mixing of the styrene. 'K enolate precursor' refers to: DMA (**1**), DMP (**18**), NMP (**19**) or NMP-d_9 (**19-d_9**).

Alternatively, different styrenes (0.115 mmol, 1.0 eq.) were used (see Section 4.1.).

Alternatively, 18-crown-6 (45.6 mg, 1.5 eq.) was used as an additive and was added to the sample during its preparation (after addition of base and before addition of solvent) inside the glovebox.

Alternatively, the sample was prepared under ambient air/moisture conditions (see Section 4.3.5.).

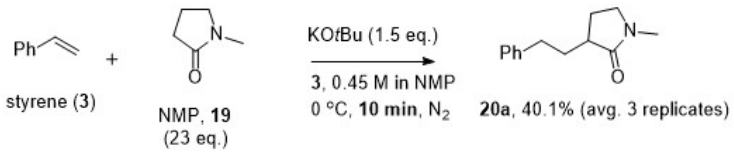
Alternatively, KO*t*Bu (3.2 mg, 25 mol%) was used (see Section 4.1.7. and Section 4.3.4.)

Alternatively, NaO*t*Bu (16.5 mg, 1.5 eq.) was used (see Section 4.3.6.)

Alternatively, cyclohexanone (36 μL, 0.345 mmol, 3.0 eq.) or α-tetralone (46 μL, 0.345 mmol, 3.0 eq.) were employed as the 'K enolate precursor' in DMSO-d_6 (0.48 mL), using KO*t*Bu (5.2 mg, 40 mol%) to mimic the conditions employed by Knochel (see Section 4.4.).[3] However, conditions here were more dilute (**3**, 0.24 M in DMSO-d_6) than conditions used by Knochel (**3**, 0.80 M in DMSO).[3]

In some cases, the reactions were quenched by addition of H_2O (ca. 0.5 mL) and shaken, before work up and purification by column chromatography (as per **Procedure A**) to obtain isolated products (see Section 7).

In all cases, by the time the first scan was taken (ca. 1-2 min after addition of styrene), the temperature of the VT probe had stabilized at the desired temperature (the internal temperature of the sample was assumed to be identical due to the small sample volume and high surface-area-to-volume ratio of the NMR tube). Scans were acquired every 10s (or with a adjusted longer delay as deemed necessary) for as long as deemed necessary for the reaction to complete (8 min - 21 h).



Procedure C: An oven-dried NMR tube containing 1,3,5-trimethoxybenzene (33.4 mg, 1.0 eq.) was taken inside a glovebox (under N_2) and was charged with KO*t*Bu (33.4 mg, 0.17 mmol, 1.5 eq.) and 'K enolate precursor' (0.45 mL, ca. 23 - 25 eq.) and mixed until fully dissolved. The tube was sealed before removing from the glovebox. The NMR tube was pre-cooled/brought to the desired temperature by the NMR spectrometer's VT probe. Styrene (23 μL, 0.199 mmol, 1.0 eq.) was added (as per **Procedure A**). The sample was quickly inverted a couple of times to mix before quickly placing inside the VT probe. For the purposes of these experiments, the experiment time was deemed to begin after addition and quick mixing of the styrene. After the desired time period, the reaction was quenched by addition of H_2O (ca. 0.5 mL) and shaken, before work up and purification by column chromatography (as per **Procedure A**) to obtain isolated products (see Section 7).

Procedure D: Conducted according to a literature procedure.[3] An oven-dried reaction vessel was charged with *tert*-butoxide (90 mg, 0.8 mmol) and anhydrous DMSO (2.5 mL) in a glovebox (under N_2) and was stirred. A dark brown color developed. Then, α-tetralone (546 μL {600 mg}, 4.0 mmol) and styrene (232 μL {210 mg}, 2.0 mmol) were added. The reaction vessel was sealed before removing from the glovebox, then stirred vigorously at 40 °C for 15 h. Water (3 mL) and $CHCl_3$ (25 mL) were added and the resulting solution washed with brine (3 x 25 mL), dried ($MgSO_4$), filtered and concentrated *in vacuo*. Following addition of 1,3,5-trimethoxybenzene (33.6 mg, 10 mol%), ^1H NMR

revealed an 85.5% yield of **28a** and an 11.3% of **28b**. Purification by column chromatography ($CHCl_3$) failed to separate **28a** and **28b**. Purification by GPC ($CHCl_3$), using a decreased flow rate of 1.7 mL/min overnight, afforded **28a** and **28b**.

Alternatively, cyclohexanone (415 μL {393 mg}, 4.0 mmol) was used instead of α-tetralone. NMR quantification was impossible due to overlapping peaks of **26a** and **26b**. Purification by GPC as above afforded **26a** (72%) and **26b** (11%).

3. NMR Quantification Methods

3.1. NMR Quantification Method by use of an Internal Standard in $CDCl_3$

For reactions of *N*,*N*-dimethylacetamide (DMA, **1**), the yields of monoadduct **6** and bisadduct **10** were quantified as previously described (and used to plot NMR kinetic profiles shown in Section 4.1.).[2] For the reaction of *N*-methyl-2-pyrrolidinone (NMP, **19**) in Figure S1 (Scheme 5, A of main manuscript), conducted according to **Procedure C**, the yields of monoadduct **20a** and bisadduct **20b** were quantified as described below.

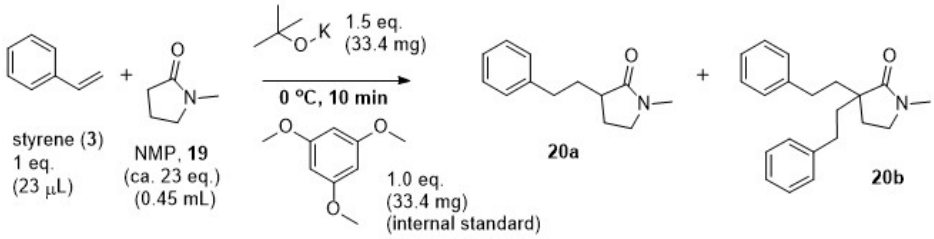


Figure S1. KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and styrene (0.45 M in NMP) at 0 °C for 10 minutes.

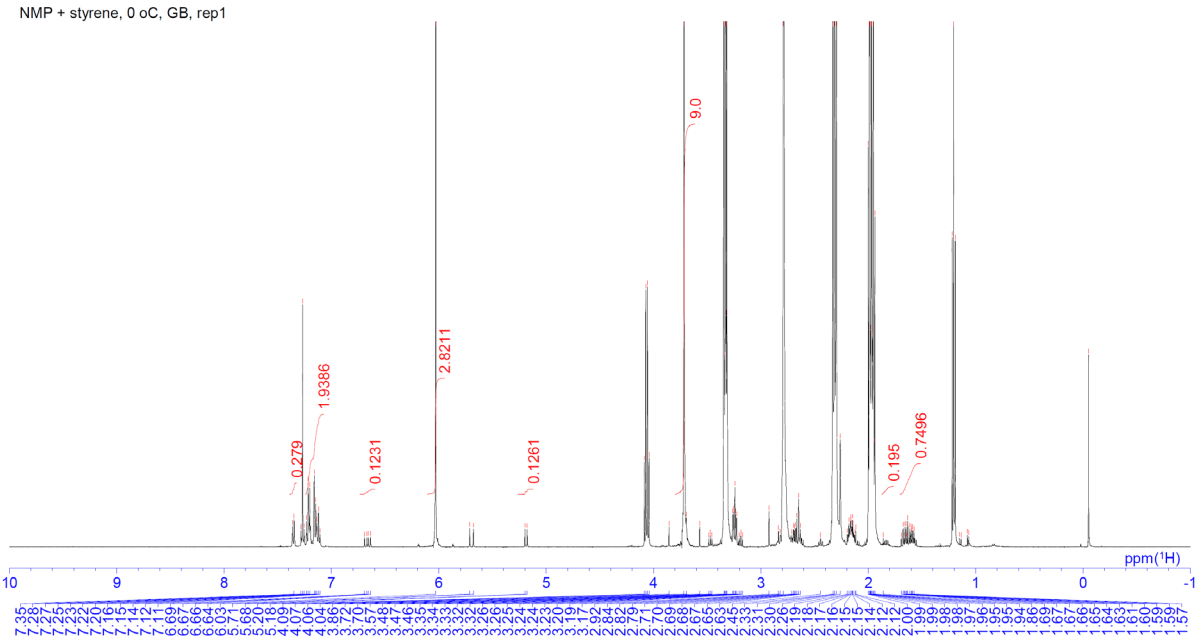


Figure S2. ^1H NMR ($CDCl_3$) spectra for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and styrene (0.45 M in NMP) at 0 °C after 10 minutes in the presence of 1,3,5-trimethoxybenzene (100 mol%). The ^1H NMR ($CDCl_3$) spectra for authentic monoadduct **20a** was previously reported and is shown in Section 6.[2]

After calibrating the spectrum to $CDCl_3$ (7.27 ppm), the integration of the peak at 3.70 ppm (1,3,5-trimethoxybenzene ArO-C**H**$_3$ protons) was set to 9 units. The integration of the unobstructed peak at 1.70 - 1.55 ppm (m, 2H) revealed a 37.5% yield of monoadduct **20a** according to the following calculation:

$$\frac{0.7496}{2} \times 100 = 37.5\%$$

For the spectrum in Figure S2, peaks for the bisadduct **20b** could not be observed, so the yield was calculated by subtracting the contribution of **20a** (setting the peak at 6.10 ppm to 3 units, then using the aromatic : aliphatic integration ratio is 1 : 1.063 as determined by the 1,3,5-trimethoxybenzene Ar**H** protons vs ArO-C**H**$_3$ protons to arrive at a value of 0.7972 / 1.063 = 0.7500 units for 2x Ar**H** of **20a**) and subtracting the contribution of the residual styrene (1 x ArH) from the combined integration of aromatic peaks from 7.40 - 7.10 ppm (monoadduct **20a** Ar**H** x 5 + bisadduct **20b** Ar**H** x 10 + styrene Ar**H** x H) by the following calculation (the additional 'x 2' reflects that 2 eq. styrenes are needed to form 1 molecule of **20b**):

$$\left(\frac{2.6731 - \left(\left(\frac{(0.1309 + 0.1340)}{2} \right) \times 5 \right) - \left(0.7497 \times \frac{1}{2} \times 5 \right)}{10} \right) \times 100 \times 2 \ = 2.7\%$$

Two replicates of this reaction gave 39.0% (4.2% bisadduct) and 43.7% (4.8% bisadduct). Therefore, the average monoadduct **20a** yield is 40.1% (average bisadduct **20b** yield is 3.9%).

For the reaction in Figure S3, conducted according to **Procedure C**, the yield of monoadduct **20a** was quantified as described below.

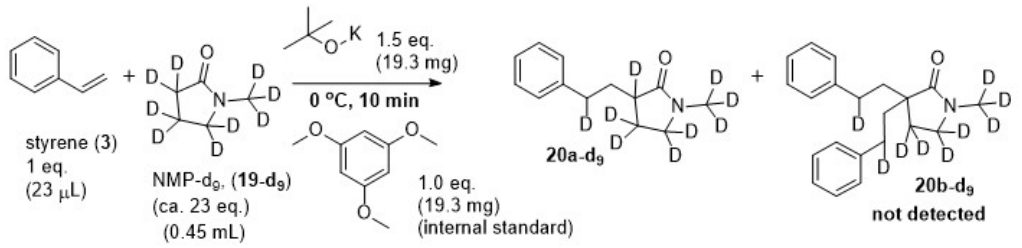


Figure S3. KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone-d$_9$ (NMP-d$_9$, **19-d$_9$**) and styrene (0.45 M in NMP-d$_9$) at 0 °C for 10 minutes.

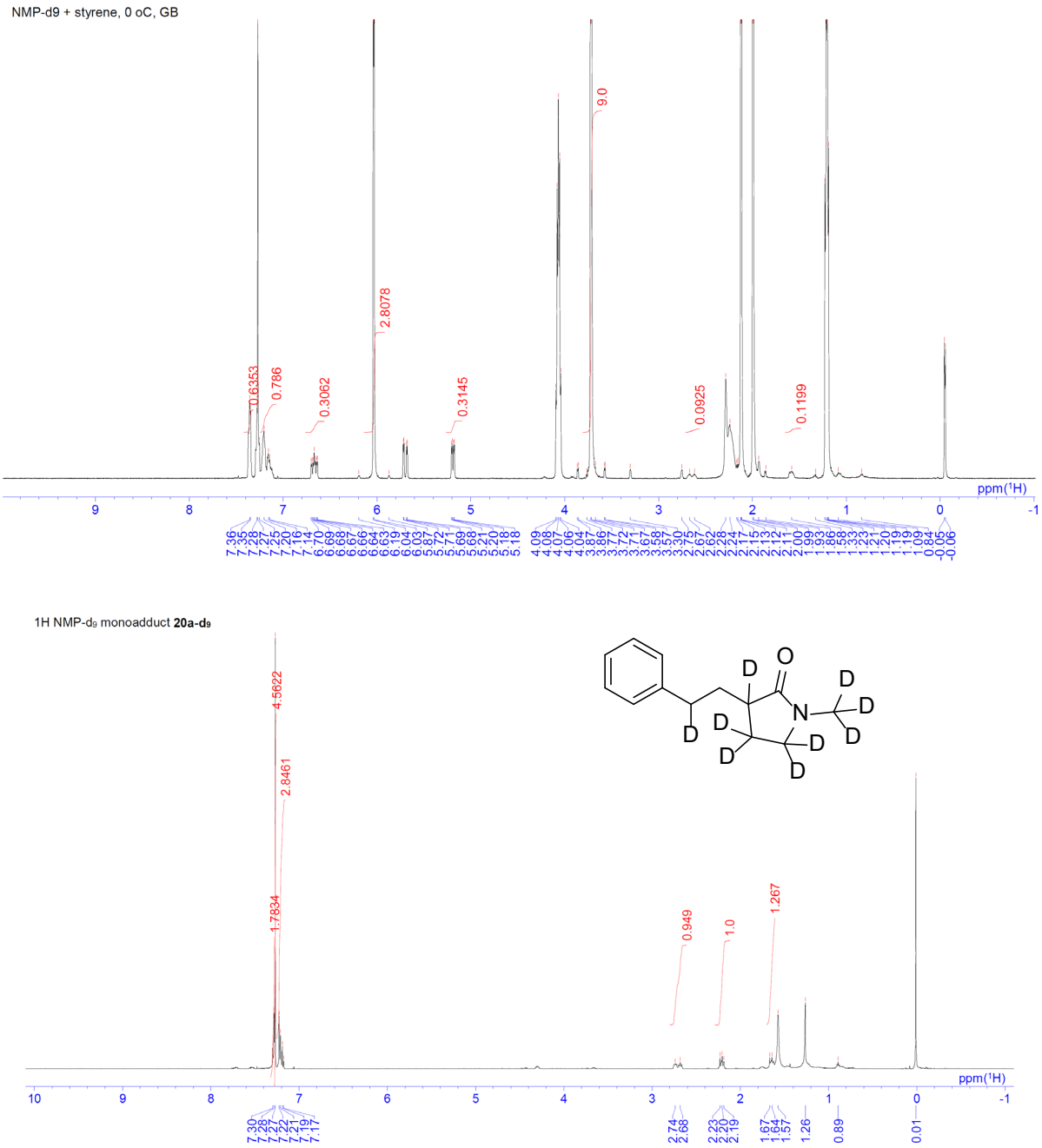


Figure S4. Top: ^{1}H NMR ($CDCl_3$) spectrum for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone-d_9 and styrene (0.45 M in NMP-d_9) at 0 °C after 10 minutes in the presence of 1,3,5-trimethoxybenzene (100 mol%). Bottom: ^{1}H NMR ($CDCl_3$) spectrum for isolated monoadduct **20a-d$_9$**.

After calibrating the spectrum to $CDCl_3$, the integration of the peak at 3.70 ppm (1,3,5-trimethoxybenzene ArO-C**H**$_3$ protons) was set to 9 units. The integrations of the unobstructed peaks at 1.58 ppm (m, 1H) and 2.65 ppm (m, 1H) revealed a 10.6% yield of monoadduct **20a-d$_9$** according to the following calculation:

$$\frac{(0.0925 + 0.1199)}{2} \times 100 = 10.6\%$$

No bisadduct **20b** was detected by ^{1}H NMR. Based on the yield comparisons after a fixed reaction time, the Kinetic Isotope Effect (KIE) *for formation of monoadduct **20a*** can be calculated as follows:

$$KIE = \frac{k_H}{k_D} = \frac{40.1\%}{10.6\%} = 3.78$$

3.2. NMR Quantification Method by use of an Internal Standard in DMSO-d_6

For reactions conducted in an NMR tube according to **Procedure B**, and followed over time by ^{1}H NMR in DMSO-d_6, the concentrations/yields of styrene starting material and combined monoadduct **20a** and bisadduct **20b** were quantified as described below:

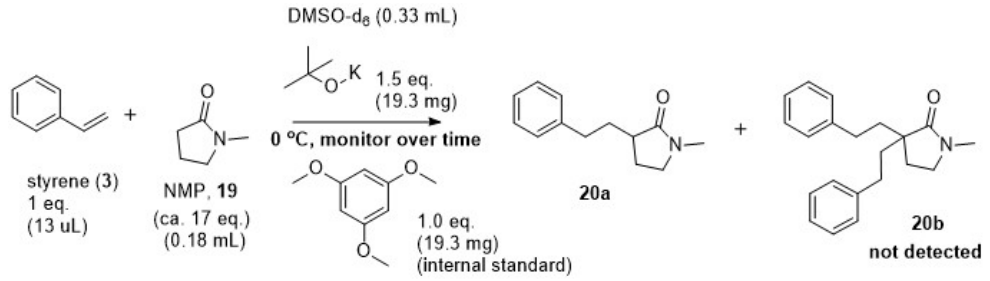
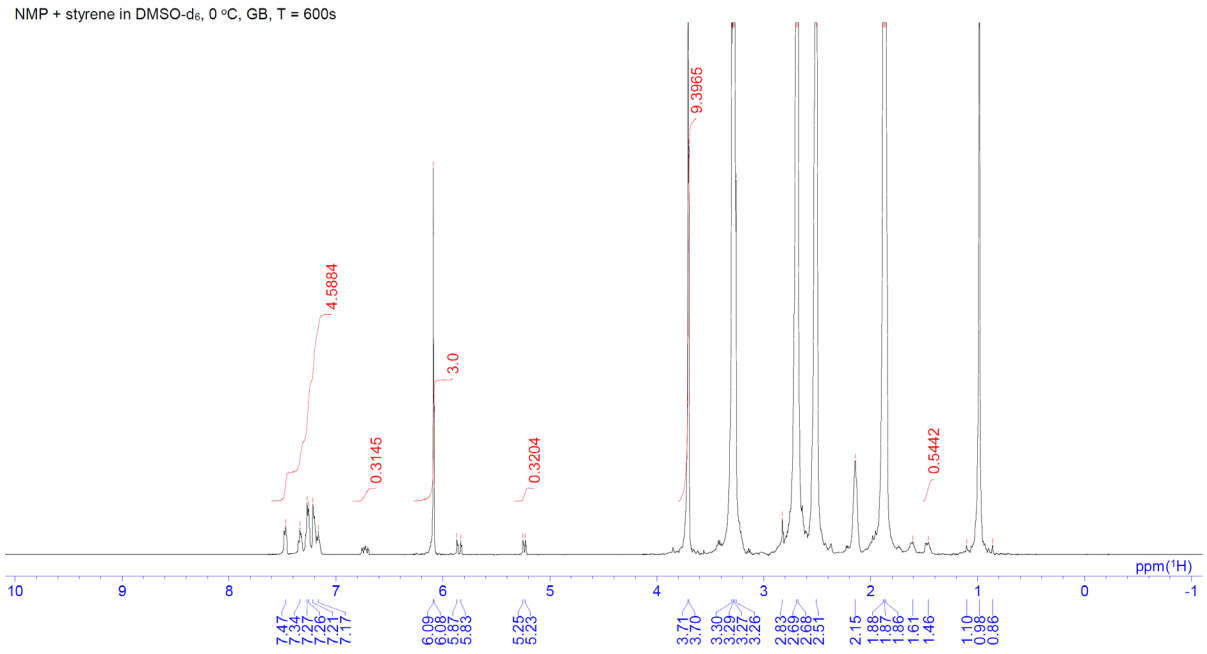


Figure S5. KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and styrene (0.225 M in NMP : DMSO-d_6 1 : 1.8) at 0 °C.



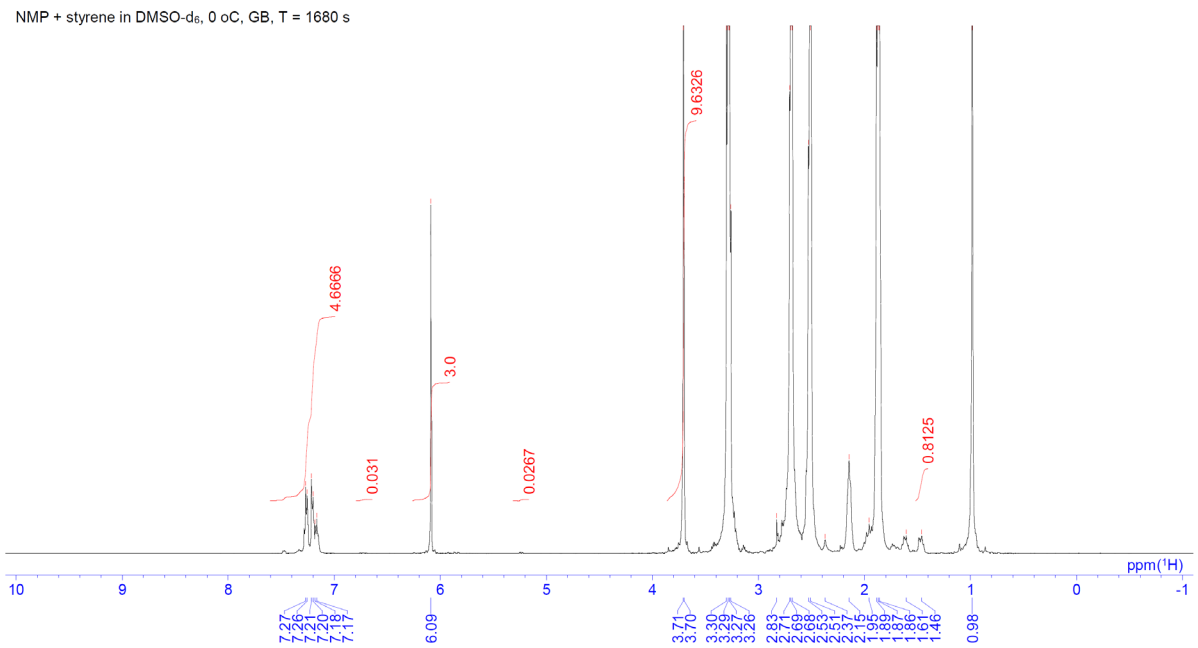


Figure S6. Top: ^{1}H NMR ($CDCl_3$) spectrum for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and styrene (0.225 M in NMP : DMSO-d_6 1 : 1.8) at 0 °C after 10 minutes in the presence of 1,3,5-trimethoxybenzene (100 mol%). The ^{1}H NMR ($CDCl_3$) spectra for authentic monoadduct **20a** was previously reported and is shown in Section 6.[2] Bottom: Same spectrum after 1680 s (reaction deemed complete).

For the spectrum in Figure S6 (top), the integration of the peak at 6.10 ppm (1,3,5-trimethoxybenzene 3x Ar**H** protons) was set to 3 units. The integrations of the unobstructed peaks at 5.25 ppm (d, 1H) and 6.72 ppm (dd, 1H) revealed a 31.7% yield of styrene starting material according to the following calculation:

$$\frac{(0.3145 + 0.3204)}{2} \times 100 = 31.7\%$$

The average integration of a styrene 1x Ar**H** peak and the integration of combined peaks from 7.46 - 7.18 ppm (styrene 5x Ar**H** protons + monoadduct **20a** 5x Ar**H** protons + bisadduct **20b** 10x Ar**H** protons) was used to *estimate* a 60.0% yield of combined products (combined monoadduct **20a** + bisadduct **20b**). *This calculation assumes only monoadduct **20a** is formed and hence fundamentally overestimates the yield of combined monoadduct **20a** + bisadduct **20b**.*

$$\frac{\left(4.5884 - \left(\left(\frac{(0.3145 + 0.3204)}{2}\right) \times 5\right)\right)}{5} \times 100 = 60.0\%$$

If the integration of the peak at 3.71 ppm (1,3,5-trimethoxybenzene 3x C**H**$_3$ groups) is set to 9 units, the integration of the unobstructed aliphatic peak at 1.52 - 1.39 ppm (m, assumed 1H of **20a** based on previously reported data in $CDCl_3$[2]) revealed a 52.1% yield of monoadduct **20a** according to the following calculation:

$$0.5213 \times 100 = 52.1\%$$

For the spectrum in Figure S6 (top), peaks for the bisadduct could not be observed, so the yield was calculated by subtracting the contribution of **20a** (setting the peak at 6.10 ppm to 3 units, then using the aromatic : aliphatic integration ratio is 1 : 1.044 as determined by the 1,3,5-trimethoxybenzene Ar**H** protons vs ArO-C**H**$_3$ protons to arrive at a value of 0.5442 / 1.044 = 0.5213 units for 1x Ar**H** of **20a**) and subtracting the contribution of the residual styrene from the combined integration of aromatic peaks from 7.46 - 7.18 ppm by the following calculation (the additional 'x 2' reflects that 2 eq. styrenes are needed to form 1 molecule of **20b**):

$$\frac{\left(4.5884 - (0.5213 \times 5) - \left(\left(\frac{(0.3145 + 0.3204)}{2}\right) \times 5\right)\right)}{10} \times 2 \times 100 = 7.9\%$$

For the spectrum in Figure S6 (bottom), at which time the reaction was deemed complete, the yields of **20a** and **20b** were 75.9% and 14.5%, respectively.

For the reaction in Figure S7, conducted according to **Procedure B**, the concentrations/yields of styrene starting material and combined monoadduct **20a** and bisadduct **20b** were quantified as described below:

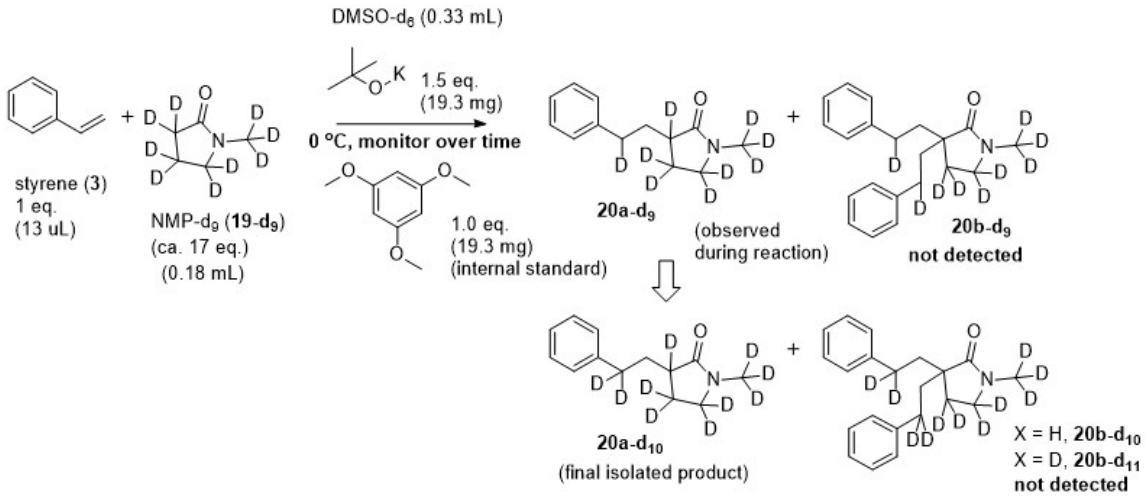


Figure S7. KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone-d$_9$ and styrene (0.225 M in NMP-d$_9$: DMSO-d$_6$ 1 : 1.8) at 0 °C.

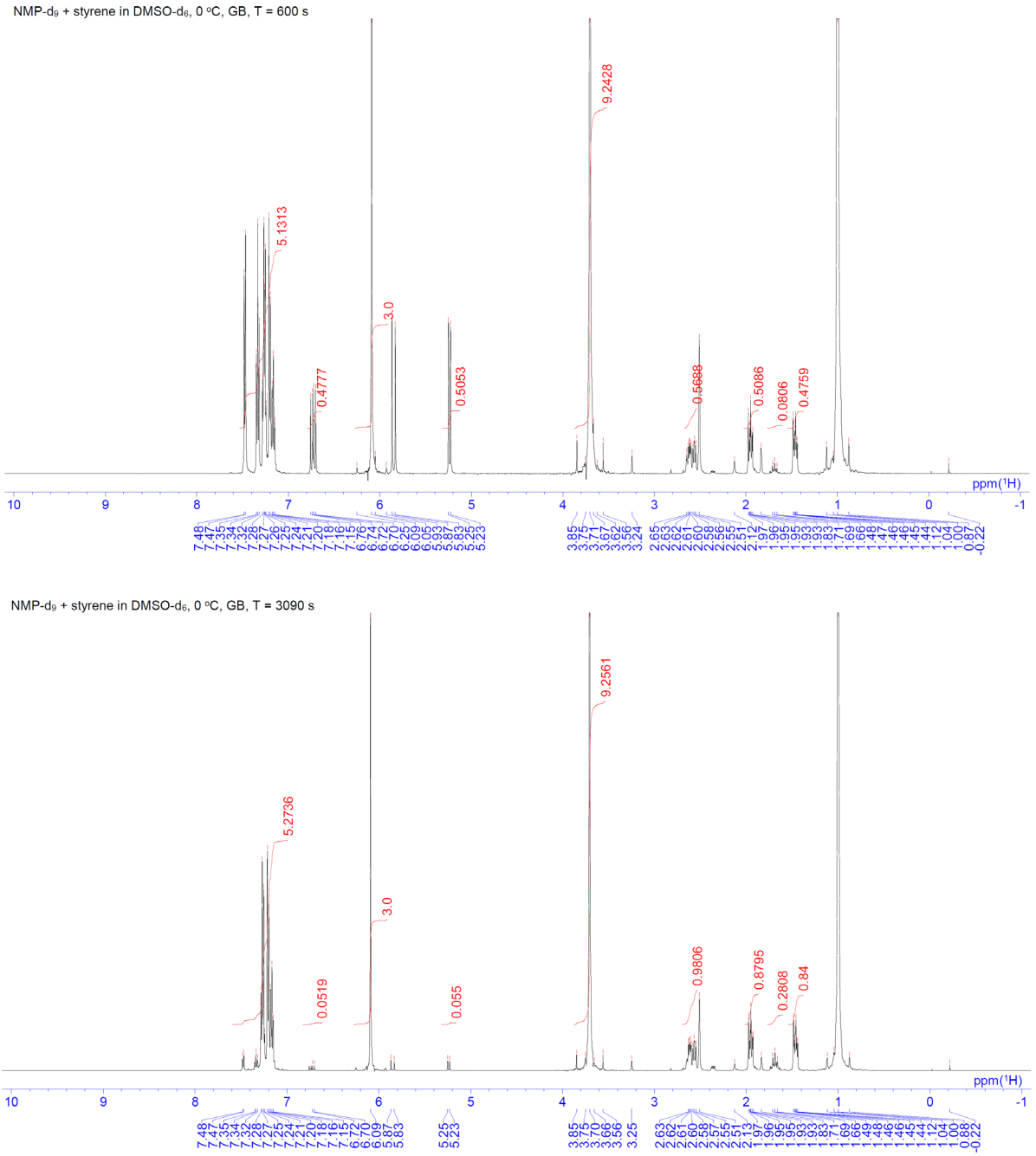


Figure S8. Top: ^{1}H NMR ($CDCl_3$) spectrum for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone-d_9 and styrene (0.225 M in NMP-d_9 : DMSO-d_6 1 : 1.8) at 0 °C after 10 minutes in the presence of 1,3,5-trimethoxybenzene (100 mol%). The ^{1}H NMR ($CDCl_3$) spectra for authentic monoadduct **20a-d_9** and **20a-d_{10}** are shown in Section 6.[2] Bottom: Same spectrum after 3090 s (reaction deemed complete).

For the spectrum in Figure S8 (top), the integration of the peak at 6.09 ppm (1,3,5-trimethoxybenzene 3x Ar**H** protons) was set to 3 units. The integrations of the unobstructed peaks at 5.25 ppm (d, 1H) and 6.72 ppm (dd, 1H) revealed a 49.2% yield of styrene starting material according to the following calculation:

$$\frac{(0.4777 + 0.5053)}{2} \times 100 = 49.2\%$$

The spectrum in Figure S8 (top) reveals monoadduct **20a-d$_9$** as the main product. The average integration of a styrene 1x Ar**H** peak and the integration of combined peaks from 7.60 - 7.00 ppm (styrene 5x Ar**H** protons + monoadduct ***20a-d$_9$*** 5x Ar**H** protons) was used to *estimate* a 53.5% yield of products (combined monoadduct ***20a-d$_9$*** + bisadduct ***20b-d$_9$***). *This calculation assumes only monoadduct **20a-d$_9$** is formed and hence fundamentally overestimates the yield of combined monoadduct **20a-d$_9$** + bisadduct **20b-d$_9$**.*

$$\frac{5.1313 - \left(\left(\frac{(0.4777 + 0.5053)}{2}\right) \times 5\right)}{5} \times 100 = 53.5\%$$

If the integration of the peak at 3.71 ppm (1,3,5-trimethoxybenzene 3x C**H**$_3$ groups) is set to 9 units, the integrations of the unobstructed aliphatic peaks at 1.97 - 1.93 ppm (m, 1H) and 1.48 - 1.44 ppm (m, 1H) revealed a 49.1% yield of monoadduct **20a-d$_9$** according to the following calculation:

$$\frac{(0.4962 + 0.4634)}{2} \times 100 = 48.0\%$$

The spectrum in Figure S8 (top) reveals peaks of monoadduct **20b-d$_9$** as the minor product (the peak at 1.73 - 1.64 ppm corresponds to the previously reported data for **20b**).[2] If the integration of the peak at 3.71 ppm (1,3,5-trimethoxybenzene 3x C**H**$_3$ groups) is set to 9 units, the integrations of the unobstructed aliphatic peak at 1.73 - 1.64 ppm (m, 4H) revealed a 3.9% yield of bisadduct **20b-d$_9$** according to the following calculation (the additional 'x 2' reflects that 2 eq. styrenes are needed to form 1 molecule of **20b-d$_9$**):

$$\frac{0.0785}{4} \times 2 \times 100 = 3.9\%$$

The sum of **20a-d$_9$** and **20b-d$_9$** yields calculated from the aliphatic region (48.0% + 3.9% = 51.9%) corresponds well to the yield of combined products calculated from the aromatic region (53.5%), validating the calculation method for the aromatic region. For the spectrum in Figure S8 (bottom), at which time the reaction was deemed complete, the yields of **20a-d$_9$** and **20b-d$_{10}$** were 83.6% and 13.7%, respectively.

The methods above were applied to calculate the concentration of styrene and estimate the concentration of combined products in the NMR tube reactions over time (see Figure S9). Based on the rate constants *for the conversion of styrene*, the Kinetic Isotope Effect (KIE) *for the conversion of styrene* can be calculated as follows:

$$KIE = \frac{k_H}{k_D} = \frac{2.02 \times 10^{-3}}{8.99 \times 10^{-4}} = 2.25$$

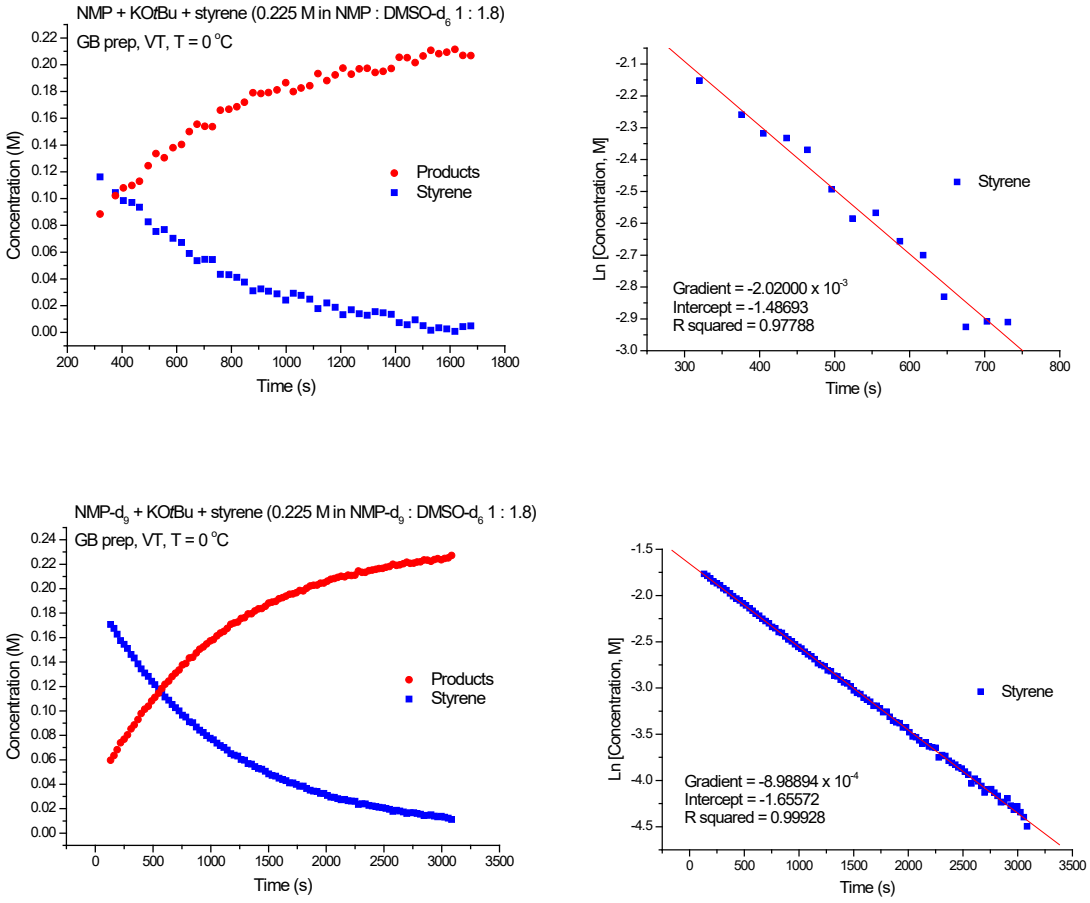


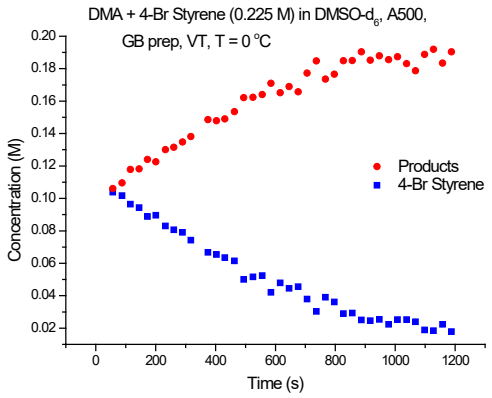
Figure S9. Concentration of styrene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and styrene (0.225 M in NMP : DMSO-d_6 1 : 1.8) at 0 °C (top) and for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone-d_9 and styrene (0.225 M in NMP-d_9 : DMSO-d_6 1 : 1.8) at 0 °C (bottom).

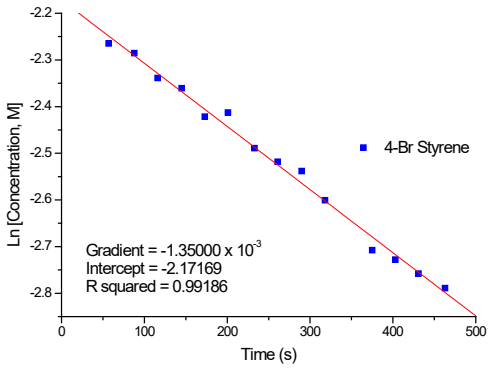
4. NMR KINETIC PROFILES

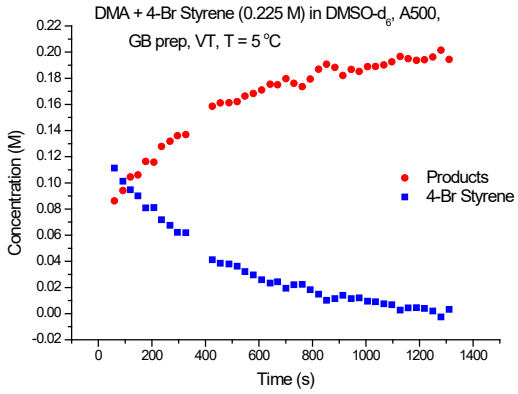
4.1. REACTION PROFILES FOR *N,N*-DIMETHYLACETAMIDE (DMA, 1) WITH VARIOUS STYRENES

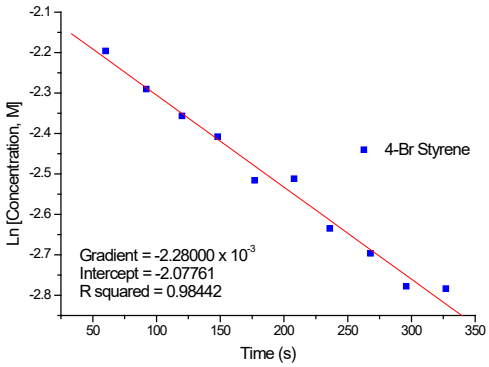
All reactions were conducted according to **Procedure B**. The kinetics of some reactions (4-bromostyrene, 4-methylstyrene and 4-vinylanisole) were too fast or too slow to measure at 30 °C. For purposes of comparison of rate constants at 30 °C, the rate constants of these reactions at higher or lower temperatures were acquired and Arrhenius plots were extrapolated to determine the calculated rate constants at 30 °C.

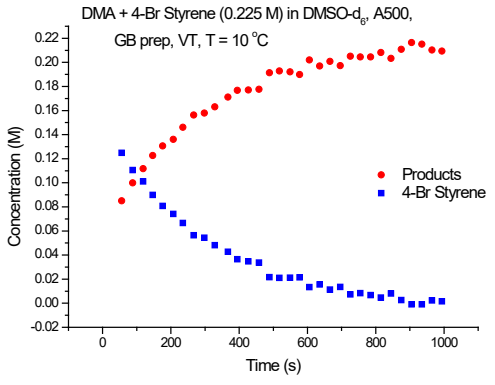
4.1.1. 4-Bromostyrene Reaction with DMA at various temperatures

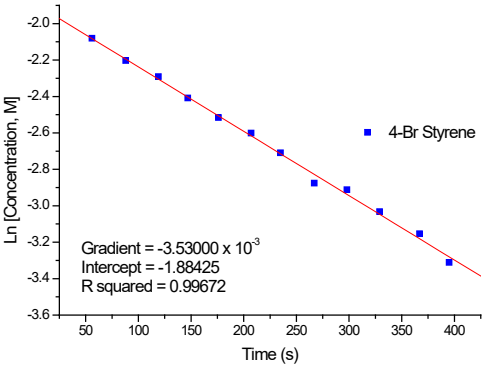












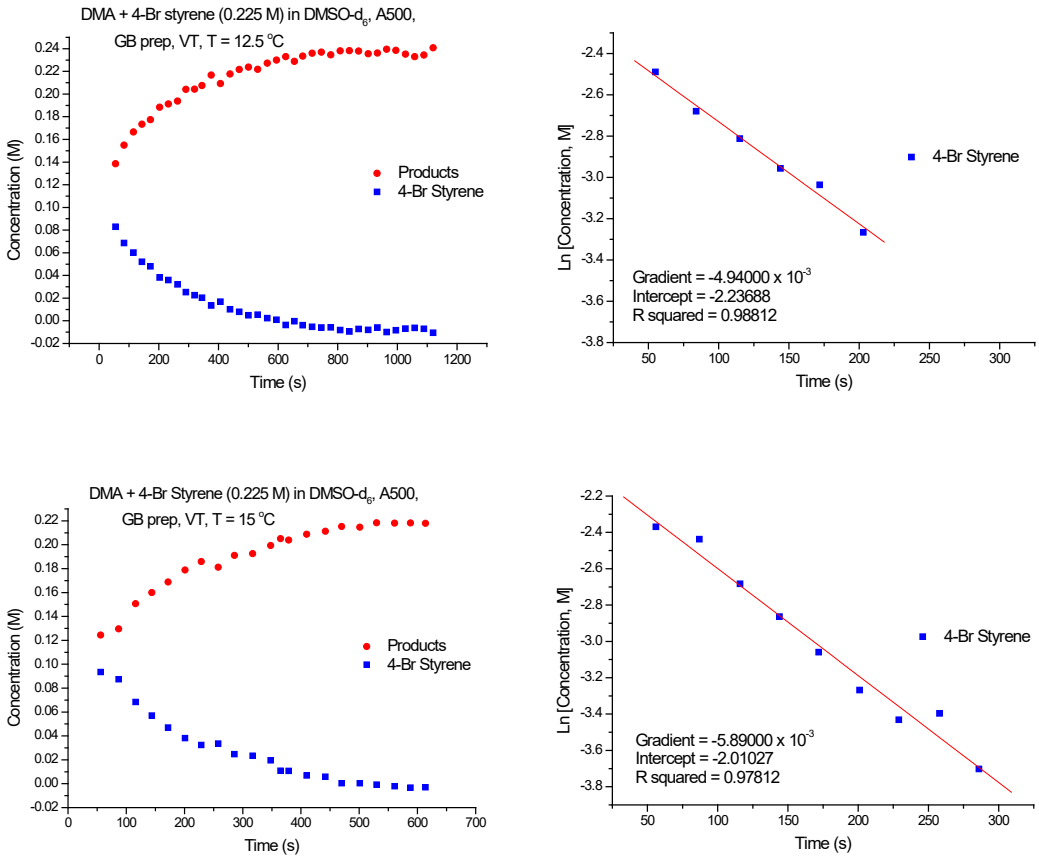


Figure S10. Concentrations of 4-bromostyrene and estimated concentrations of combined products over time for the KO*t*Bu-catalyzed reaction of *N,N*-dimethylacetamide and 4-bromostyrene (0.225 M in DMA : DMSO-d_6 1 : 1.8) at various temperatures.

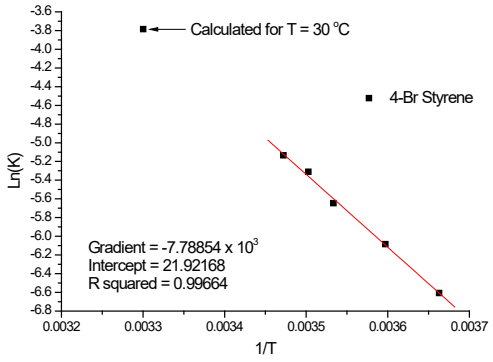


Figure S11. Arrhenius plot for 4-bromostyrene extrapolated to predict the rate constant at 30 °C.

Calculated rate constant for 4-bromostyrene conversion at 30 °C = 2.273 x 10^{-2} s^{-1}.

4.1.2. 4-Fluorostyrene reaction with DMA at 30 °C

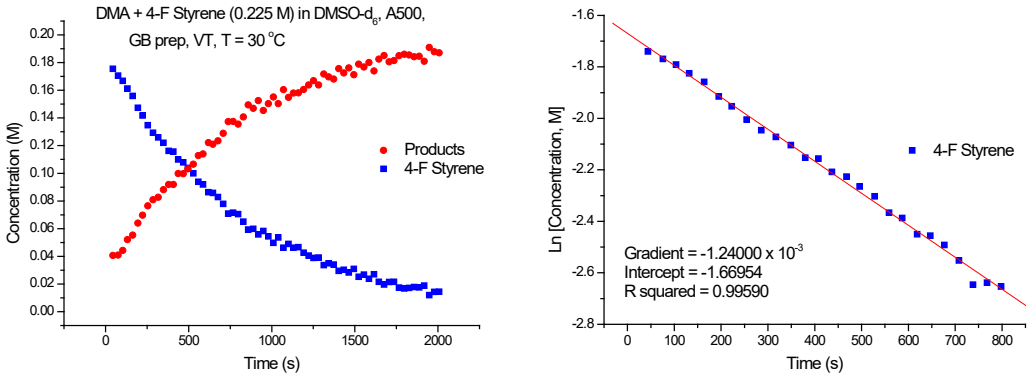


Figure S12. Concentration of 4-fluorostyrene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of *N,N*-dimethylacetamide and 4-fluorostyrene (0.225 M in DMA : DMSO-d_6 1 : 1.8) at 30 °C.

4.1.3. 2-Vinylnaphthalene reaction with DMA at 30 °C

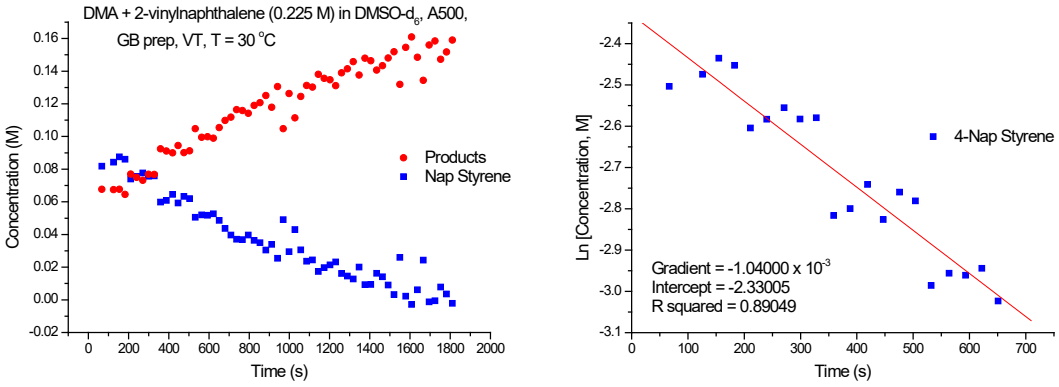


Figure S13. Concentration of 2-vinylnaphthalene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of *N,N*-dimethylacetamide and 2-vinylnaphthalene (0.225 M in DMA : DMSO-d_6 1 : 1.8) at 30 °C.

4.1.4. Styrene reaction with DMA at 30 °C

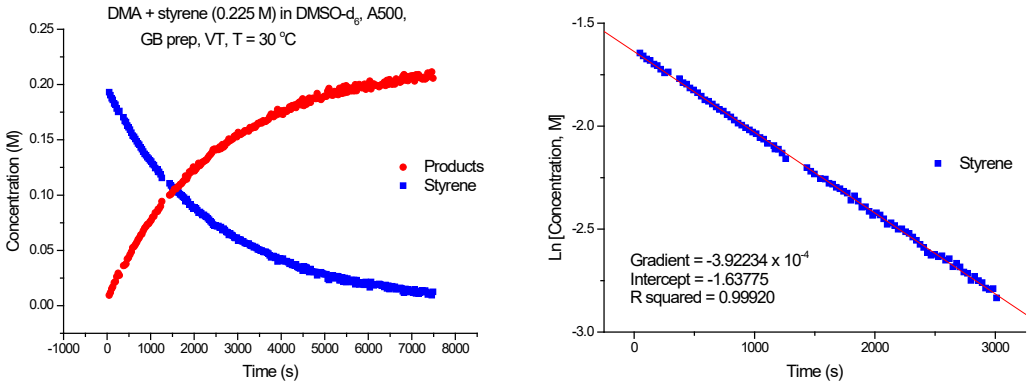
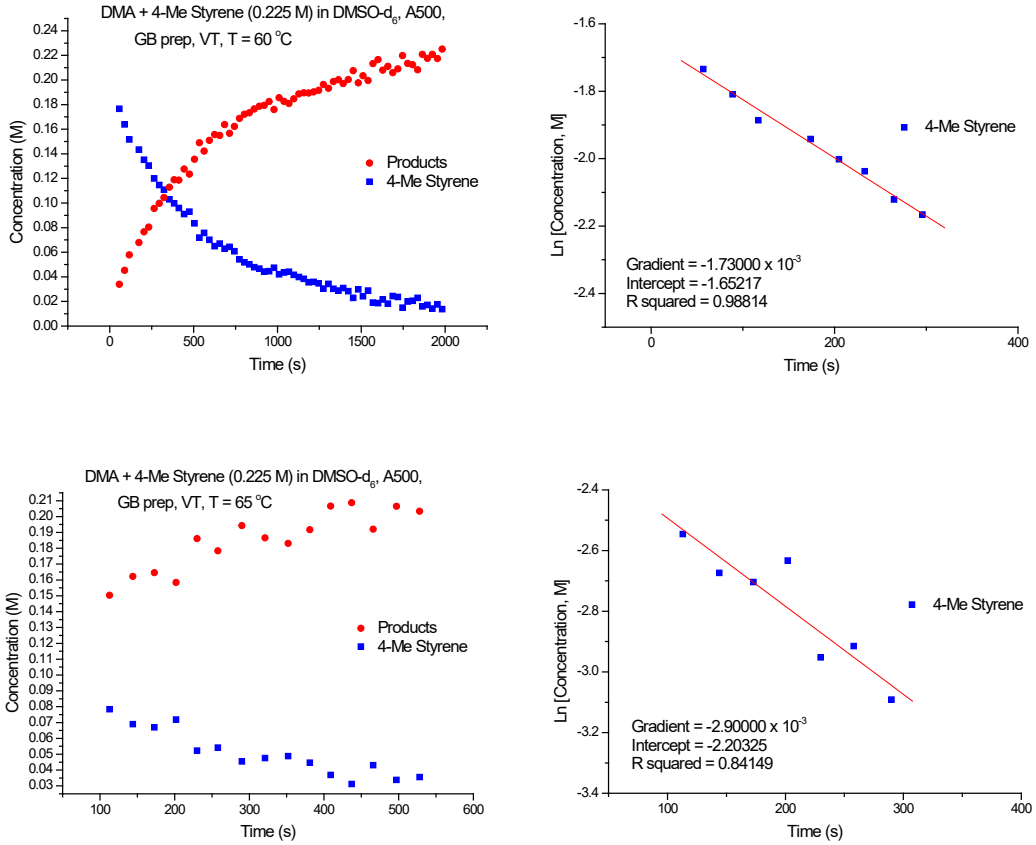


Figure S14. Concentration of styrene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of *N,N*-dimethylacetamide and styrene (0.225 M in DMA : DMSO-d_6 1 : 1.8) at 30 °C.

4.1.5. 4-Methylstyrene reaction with DMA at various temperatures



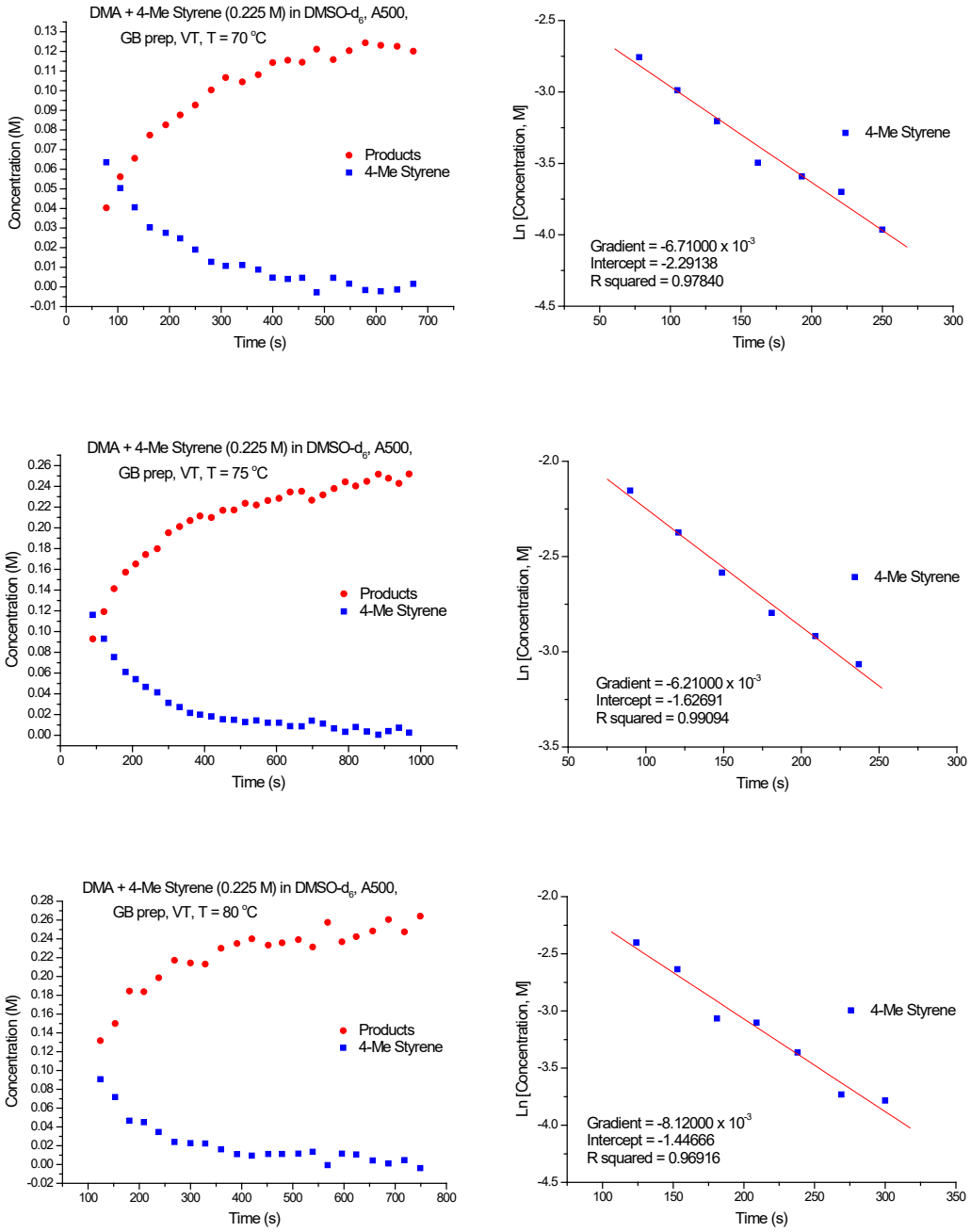


Figure S15. Concentrations of 4-methylstyrene and estimated concentrations of combined products over time for the KO*t*Bu-catalyzed reaction of *N,N*-dimethylacetamide and 4-methylstyrene (0.225 M in DMA : DMSO-d_6 1 : 1.8) at various temperatures.

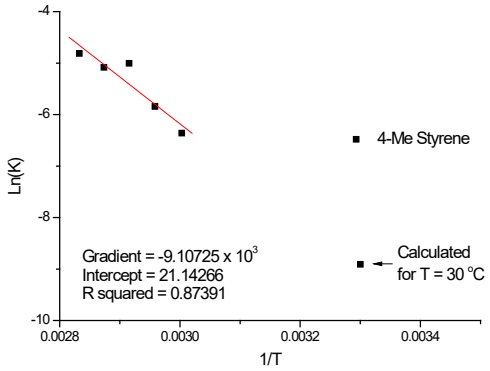
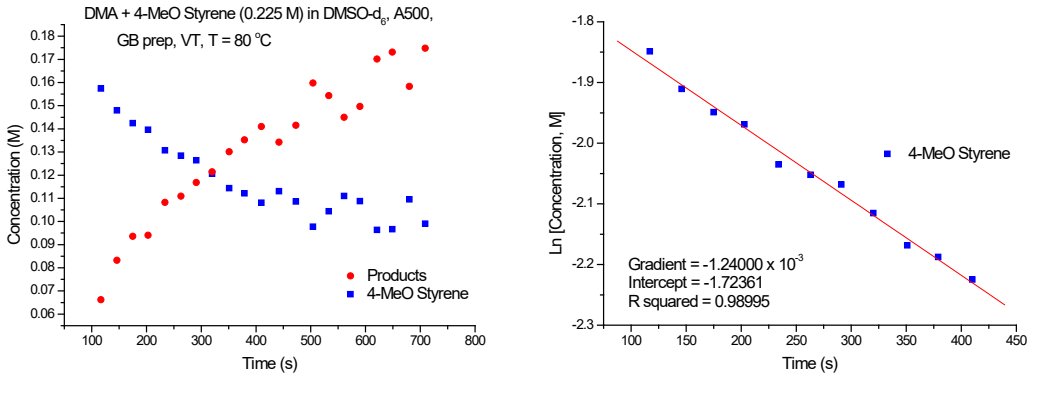


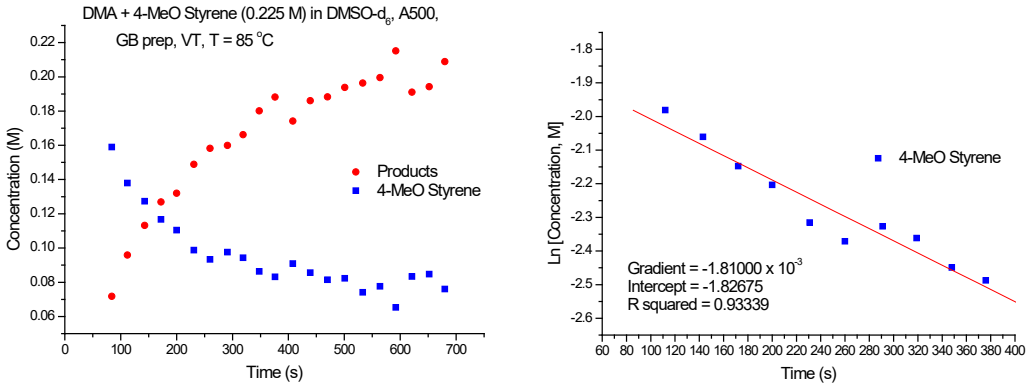
Figure S16. Arrhenius plot for 4-methylstyrene extrapolated to predict the rate constant at 30 °C.

Calculated rate constant for 4-methylstyrene conversion at 30 °C = 0.135 x 10^{-2} s^{-1}.

4.1.6. 4-Vinylanisole reaction with DMA at various temperatures



V



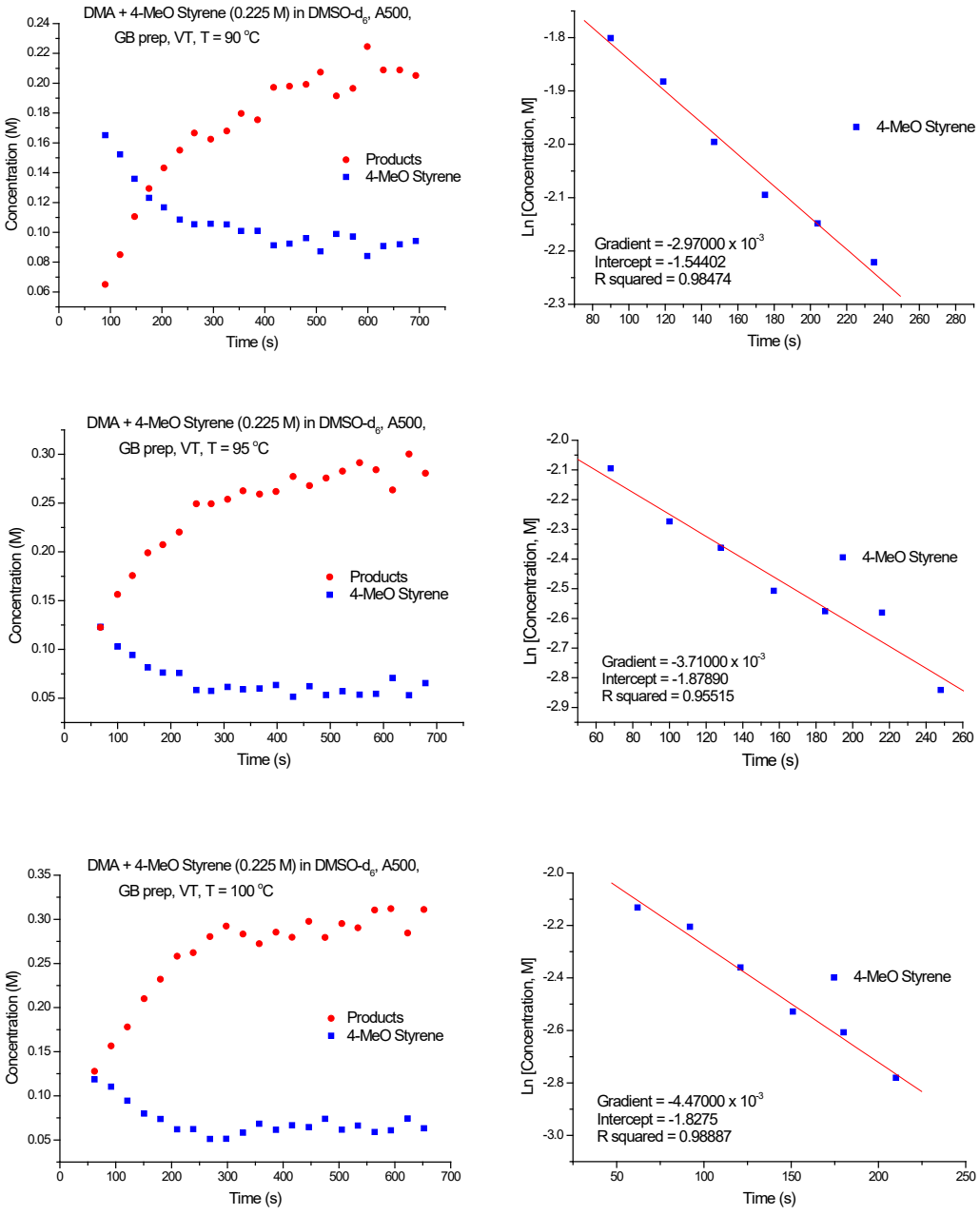


Figure S17. Concentrations of 4-vinylanisole and estimated concentrations of combined products over time for the KO*t*Bu-catalyzed reaction of *N,N*-dimethylacetamide and 4-vinylanisole (0.225 M in DMA : DMSO-d_6 1 : 1.8) at various temperatures.

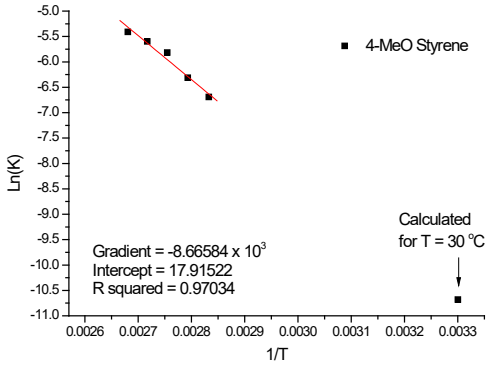


Figure S18. Arrhenius plot for 4-vinylanisole extrapolated to predict the rate constant at 30 °C.

Calculated rate constant for 4-vinylanisole conversion at 30 °C = 2.295 x 10^{-5} s^{-1}.

4.1.7. Styrene reaction with DMA at 30 °C in presence of catalytic (25 mol%) KO*t*Bu

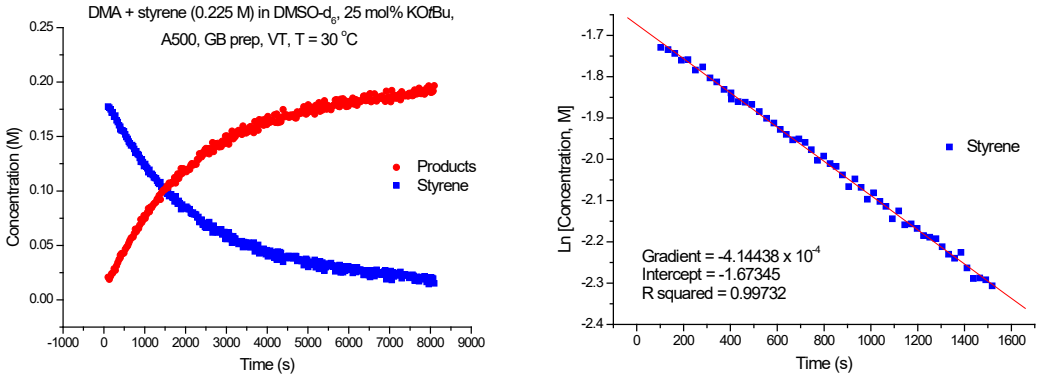


Figure S19. Concentration of styrene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed (25 mol% loading) reaction of *N,N*-dimethylacetamide and styrene (0.225 M in DMA : DMSO-d_6 1 : 1.8) at 30 °C.

4.2. Reaction Profile for *N*,*N*-dimethylpropionamide (DMP, 18) with Styrene

The reaction was conducted according to **Procedure B** at 30 °C.

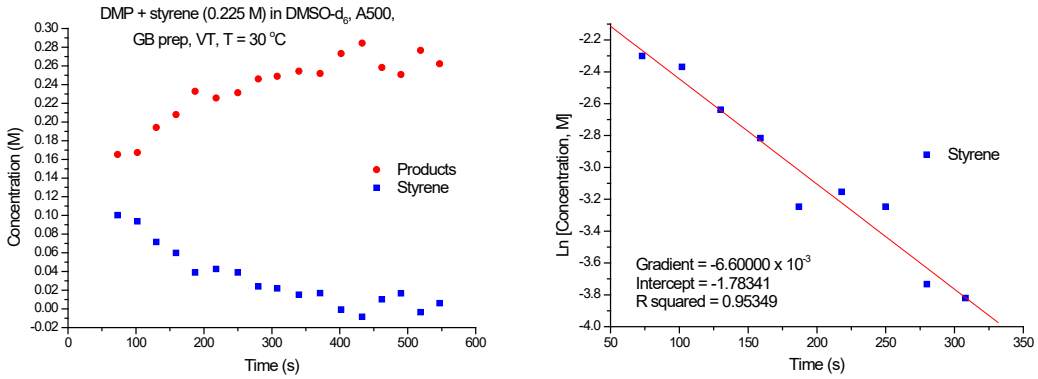
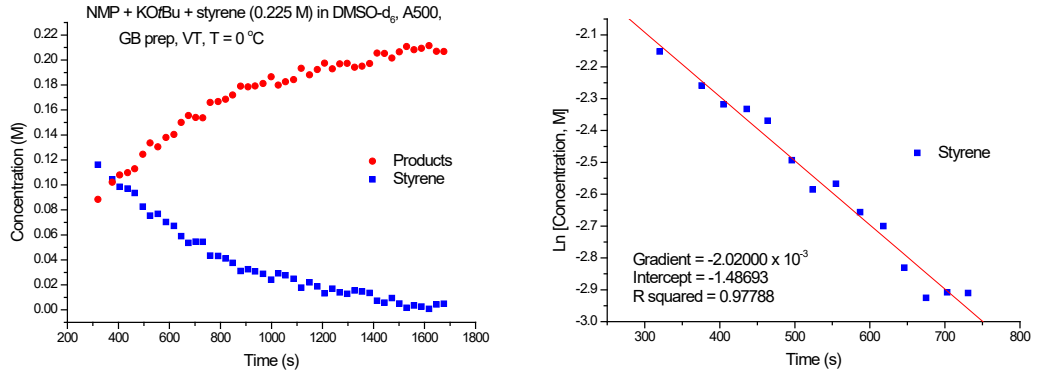


Figure S20. Concentration of styrene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of *N*,*N*-dimethylpropionamide and styrene (0.225 M in DMP : DMSO-d_6 1 : 1.8) at 30 °C.

4.3. Reaction Profiles for *N*-methyl-2-pyrrolidinone (NMP, 19) with Various Styrenes under Various Conditions

4.3.1. Styrene reaction with NMP at various temperatures

The reactions were conducted according to **Procedure B**.



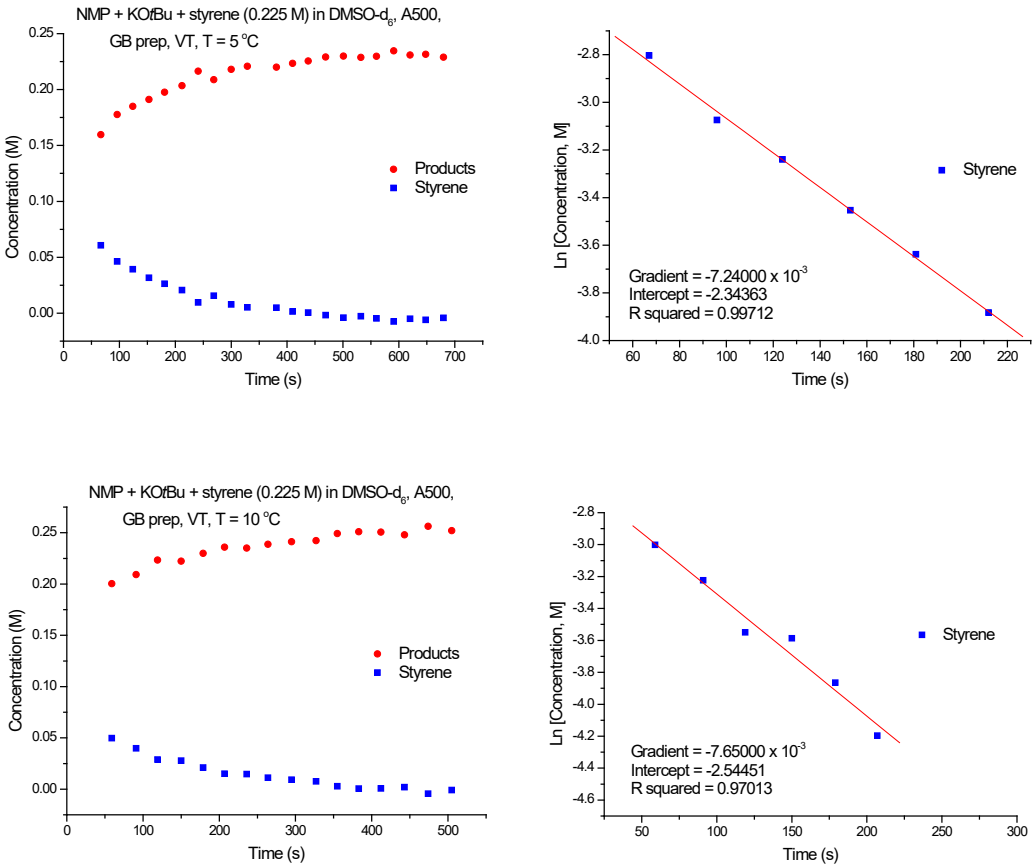


Figure S21. Concentrations of styrene and estimated concentrations of combined products over time for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and styrene (0.225 M in NMP : DMSO-d_6 1 : 1.8) at various temperatures.

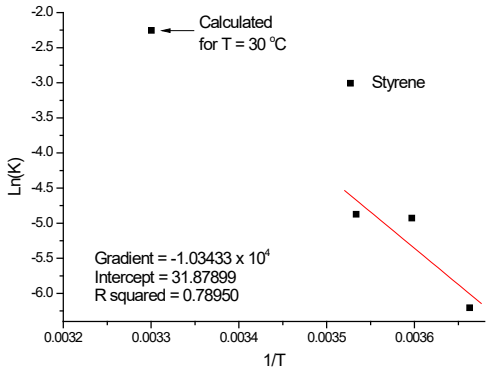


Figure S22. Arrhenius plot for styrene in the presence of NMP extrapolated to predict the rate constant at 30 °C.

Calculated rate constant for styrene conversion in the presence of NMP at 30 °C = 1.050 x 10^{-1} s^{-1}.

4.3.2. 4-Fluorostyrene reaction with NMP at 0 °C

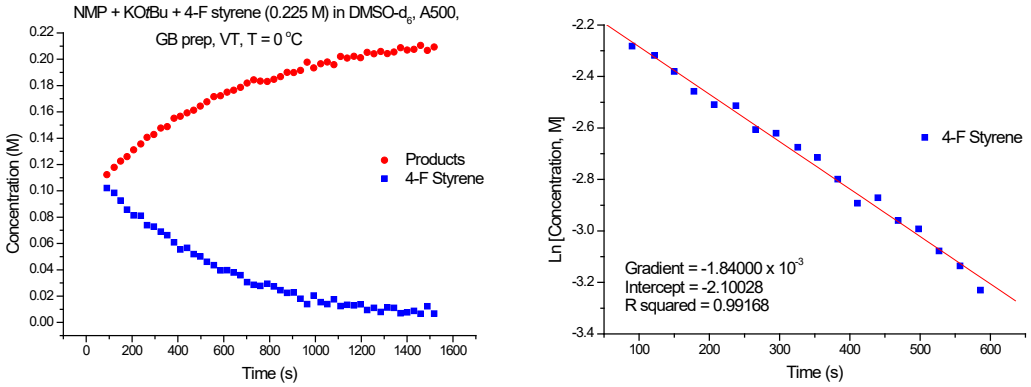


Figure S23. Concentration of 4-fluorostyrene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and 4-fluorostyrene (0.225 M in NMP : DMSO-d_6 1 : 1.8) at 0 °C.

4.3.3. 4-Vinylanisole reactions with NMP at 0 °C

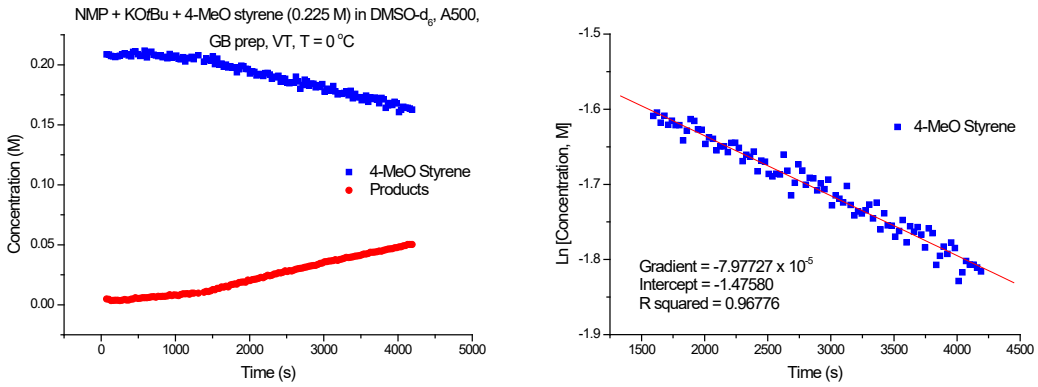
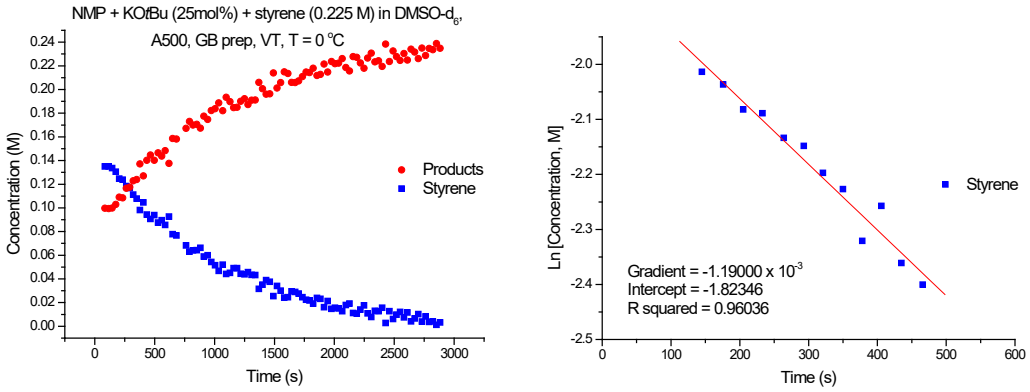


Figure S24. Concentration of 4-vinylanisole and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and 4-vinylanisole (0.225 M in NMP : DMSO-d_6 1 : 1.8) at 0 °C.

4.3.4. Styrene reaction with NMP at 0 °C in presence of catalytic (25 mol%) KO*t*Bu



4.3.5. Styrene reaction with NMP under ambient air/moisture at 25 °C

This reaction was conducted in a 400 MHz NMR instrument at room temperature (25 °C). The temperature was not controlled explicitly with a VT probe. This experiment shows a higher temperature was required for successful reaction when preparation was done under ambient air/moisture.

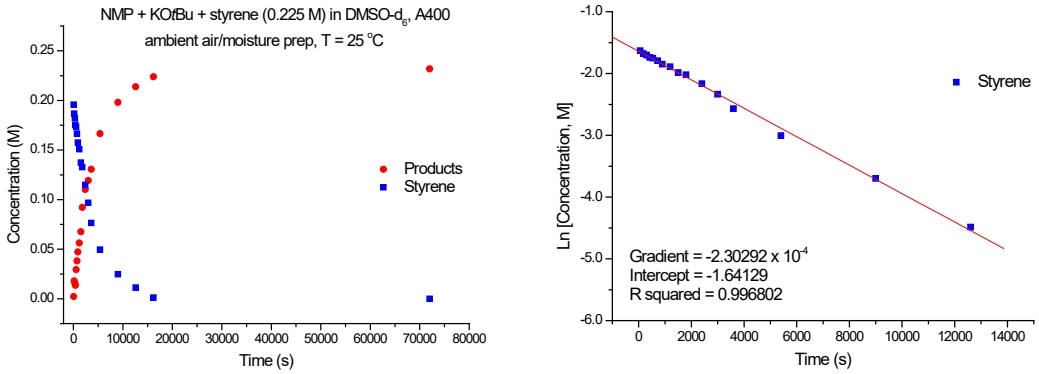


Figure S25. Concentration of styrene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and styrene (0.225 M in NMP : DMSO-d_6 1 : 1.8) at 25 °C prepared under ambient air/moisture.

4.3.6. Styrene reaction with NMP using NaO*t*Bu at 80 °C

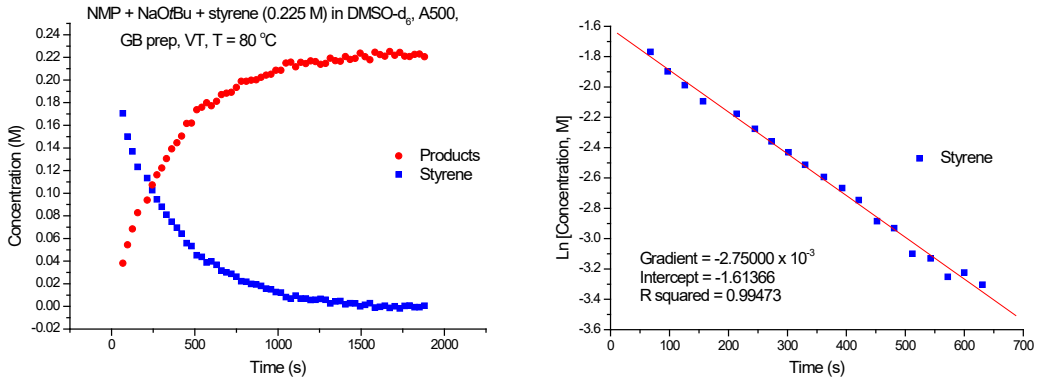


Figure S26. Concentration of styrene and estimated concentration of combined products over time for the NaO*t*Bu-catalyzed reaction of *N*-methyl-2-pyrrolidinone and styrene (0.225 M in NMP : DMSO-d_6 1 : 1.8) at 80 °C.

4.4. Reaction Profiles for Cyclohexanone (25) and α-Tetralone (27) with Styrene

4.4.1. Styrene reaction with cyclohexanone using KO*t*Bu at 40 °C

The reactions were conducted according to a modified **Procedure B** designed to mimic conditions reported in the literature[3] (see details in Section 2) at 40 °C.

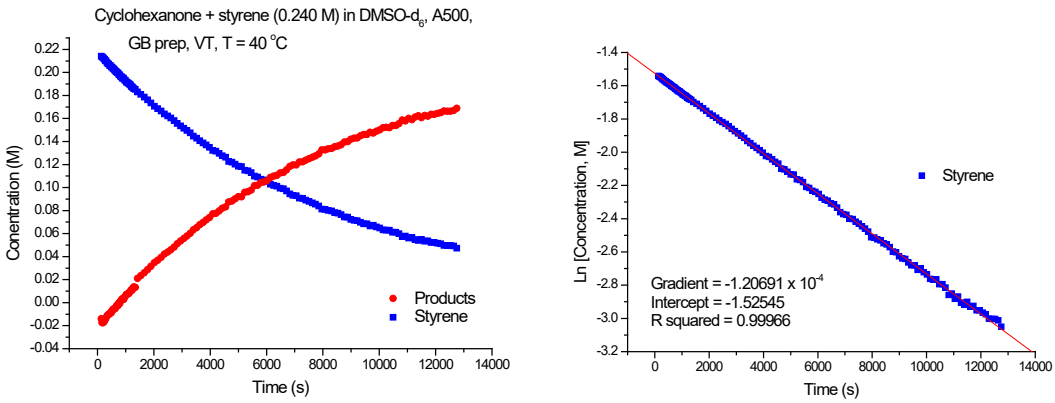


Figure S27. Concentration of styrene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of cyclohexanone and styrene (0.240 M in DMSO-d_6) at 40 °C.

4.4.2. Styrene reaction with α-tetralone using KO*t*Bu at 40 °C

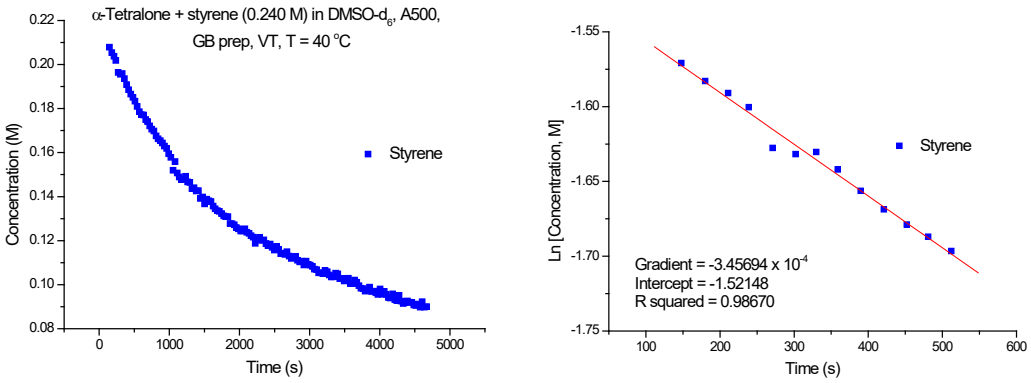


Figure S28. Concentration of styrene and estimated concentration of combined products over time for the KO*t*Bu-catalyzed reaction of α-tetralone and styrene (0.240 M in DMSO-d_6) at 40 °C.

5. UV-Vis Studies

5.1. Studies of reactions in DMSO-d_6 solvent

In the case of either DMA (**1**) or NMP (**19**) in DMSO-d_6 in the presence of KO*t*Bu (0.35 M in amide : DMSO-d_6 1 : 1.8) as per **Procedure B**, the resulting solutions were a very pale yellow color before addition of styrene (Figure S29).



Figure S29. Samples freshly prepared according to **Procedure B**. Left: DMA + KO*t*Bu (1.5 eq.). Right: NMP + KO*t*Bu (1.5 eq.).

In the case of DMA (**1**) in DMSO-d_6 and following addition of various styrenes and exposure to temperatures necessary for reactivity for the kinetic studies, colors were observed in the reaction mixtures (Figure S30). In the case of styrene (**3**), the development of blue/purple color was followed by UV-vis spectroscopy, see Figure S31. The same color, but paler, occurred in the reaction using catalytic (25 mol%) KO*t*Bu (Figure S32).

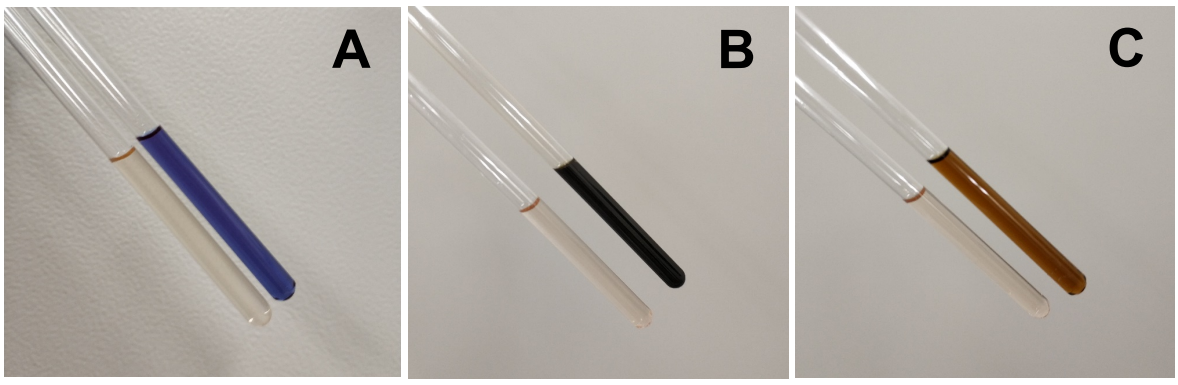


Figure S30. All samples prepared according to **Procedure B**. **A**, Left: DMA + KO*t*Bu (1.5 eq.), freshly-prepared sample. Right: DMA + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.), 2 h after styrene addition and held at 30 °C. **B**, Left: DMA + KO*t*Bu (1.5 eq.). Right: DMA + KO*t*Bu (1.5 eq.) + 4-bromostyrene (1.0 eq.), 1 h after styrene addition and held at 30 °C. **C**, Left: DMA + KO*t*Bu (1.5 eq.). Right: DMA + KO*t*Bu (1.5 eq.) + 4-methylstyrene (1.0 eq.), 1 h after styrene addition and held at 80 °C.

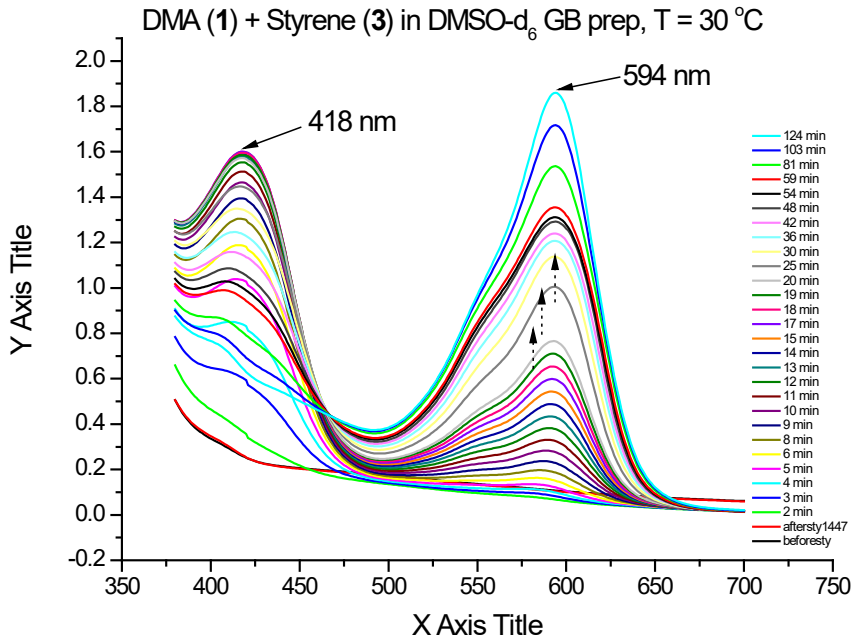


Figure S31. UV-vis spectrum over time (2 h) for reaction of DMA + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.) in DMSO-d_6 solvent at 30 °C.



Figure S32. Sample prepared according to **Procedure B**. DMA + KO*t*Bu (0.25 eq.) + styrene (1.0 eq.), 1 h after styrene addition and held at 30 °C.

In the case of NMP (**19**) in DMSO-d_6 and following addition of various styrenes and exposure to temperatures necessary for reactivity (0 °C was sufficient in all cases) for the kinetic studies, colors were observed in the reaction mixtures (Figure S33). In the case of styrene (**3**), the development of a pale yellow color was followed by UV-vis spectroscopy, see Figure S34. The same color, but paler, occurred in the reaction using catalytic (25 mol%) KO*t*Bu (Figure S35, left). A red color (Figure S35, right) was observed in the presence of 18-crown-6 (1.5 eq.).

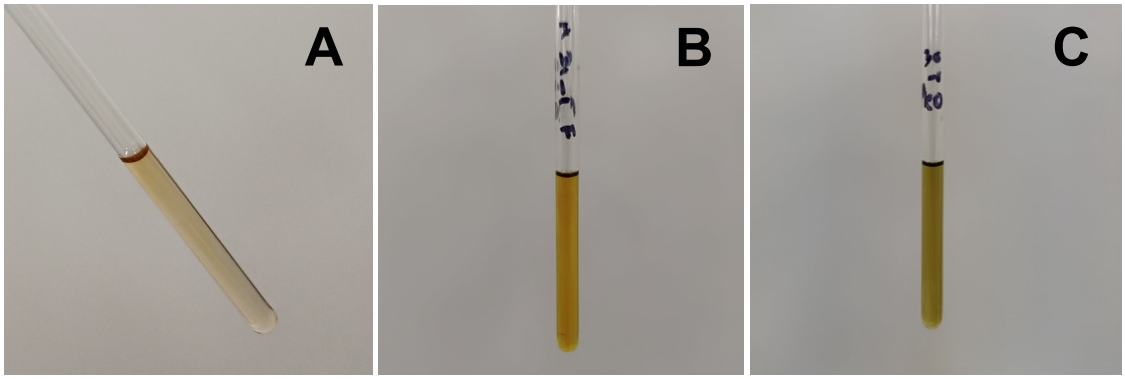


Figure S33. All samples prepared according to **Procedure B**. **A**, Left: NMP + KO*t*Bu + styrene (1.0 eq.), 2 h after styrene addition and held at 0 °C. **B**, NMP + KO*t*Bu (1.5 eq.) + 4-fluorostyrene (1.0 eq.), 1 h after styrene addition and held at 0 °C. **C**, NMP + KO*t*Bu (1.5 eq.) + 4-vinylanisole (1.0 eq.), 2.5 h after styrene addition and held at 0 °C.

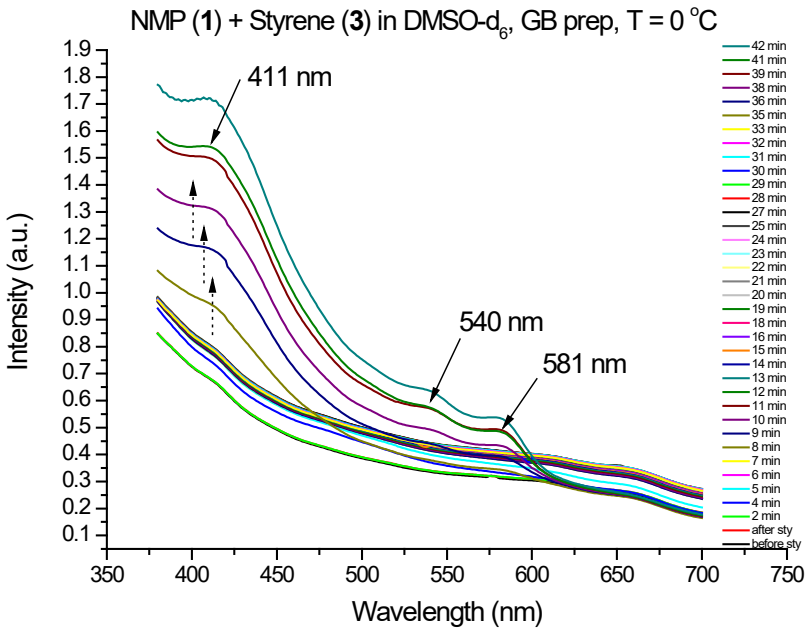


Figure S34. UV-vis spectrum over time (45 min) for reaction of NMP + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.) in DMSO-d_6 solvent at 0 °C.



Figure S35. Samples prepared according to **Procedure B**. Left: NMP + KO*t*Bu (0.25 eq.) + styrene (1.0 eq.), 1.5 h after styrene addition and held at 0 °C. Middle: NMP + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.), 2 h after styrene addition and held at 0 °C. Right: NMP + KO*t*Bu (1.5 eq.) + 18-crown-6 (1.5 eq.) + styrene (1.0 eq.), 1.5 h after styrene addition and held at 0 °C.

5.2. Studies of reactions in amide as solvent

In the case of DMA (**1**) in the presence of KO*t*Bu (0.35 M in DMA) as per **Procedure C**, the resulting solution was a very pale yellow color before addition of styrene (Figure S36, left). In the case of NMP (**19**) in the presence of KO*t*Bu (0.35 M in NMP) as per **Procedure C**, the resulting solution was a pale red color before addition of styrene (Figure S36, right).

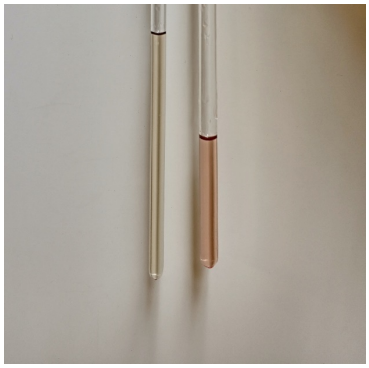


Figure S36. Samples freshly prepared according to **Procedure C**. Left: DMA + KO*t*Bu (1.5 eq.). Right: NMP + KO*t*Bu (1.5 eq.).

In the case of DMA (**1**) and following addition of styrene at a temperature of 30 °C, a pale yellow color developed and darkened over time (Figure S37, **B** and Figure S38) and was followed by UV-vis spectroscopy, see Figure S39. In the case of NMP (**19**) and following addition of styrene at a temperature of 0 °C, a red/purple color developed (Figure S37, **C** and Figure S40) and was followed by UV-vis spectroscopy, see Figure S41.

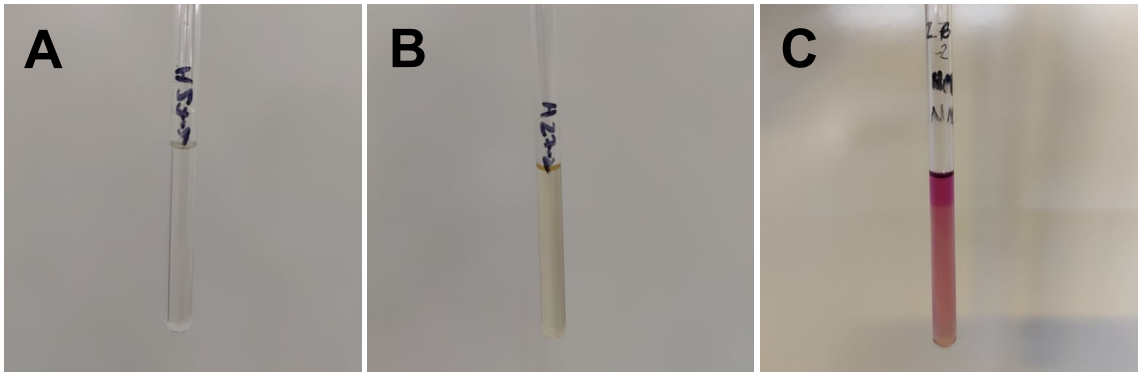


Figure S37. All samples prepared according to **Procedure C**. **A**, DMA + KO*t*Bu (0.25 eq.), freshly prepared sample. **B**, DMA + KO*t*Bu (0.25 eq.) + styrene (1.0 eq.), 2 h after styrene addition and held at 30 °C. **C**, NMP + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.), 1 h after styrene addition and held at 0 °C.

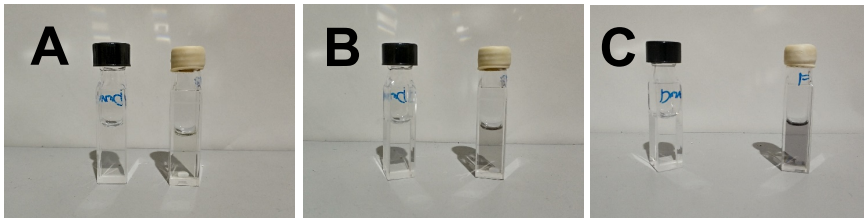


Figure S38. A, Left: *N*,*N*-dimethylacetamide (DMA, 1) only. Right: DMA + KO*t*Bu (1.5 eq.), freshly-prepared sample. **B**, Left: DMA only. Right: DMA + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.), 2 h after styrene addition and at 30 °C. **C**, Left: DMA only. Right: DMA + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.), 3 d after styrene addition and at rt.

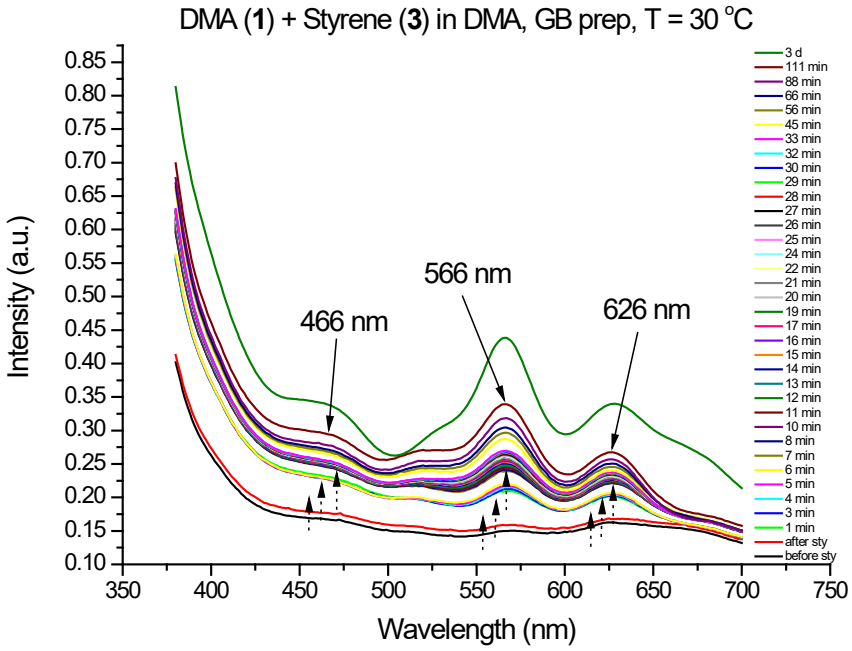


Figure S39. UV-vis spectrum over time (2 h) for reaction of DMA + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.) in DMA solvent at 30 °C.

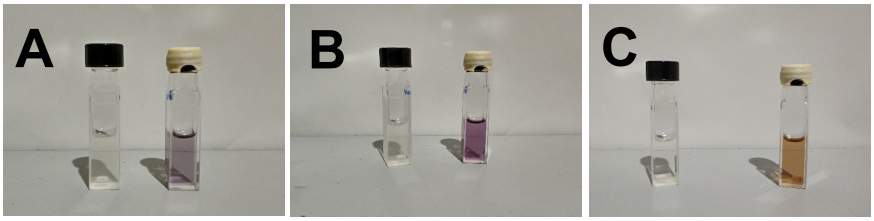


Figure S40. A, Left: *N*-methyl-2-pyrrolidinone (NMP, 19) only. Right: NMP + KO*t*Bu (1.5 eq.), freshly prepared sample. **B**, Left: NMP only. Right: NMP + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.), 1 h after styrene addition and at 0 °C. **C**, Left: NMP only. Right: NMP + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.), 3 d after styrene addition and at rt.

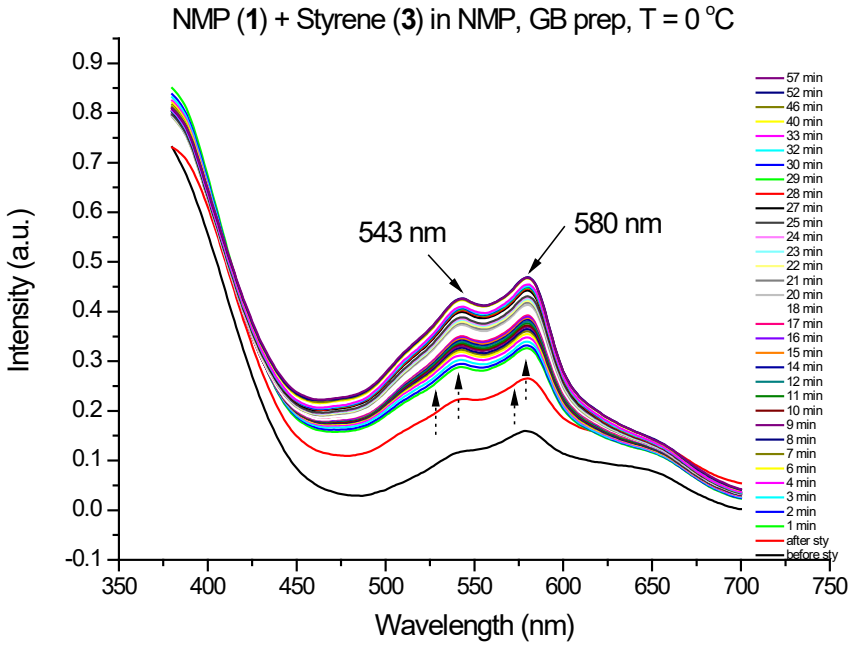


Figure S41. UV-vis spectrum over time (1 h) for reaction of NMP + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.) in NMP solvent at 0 °C

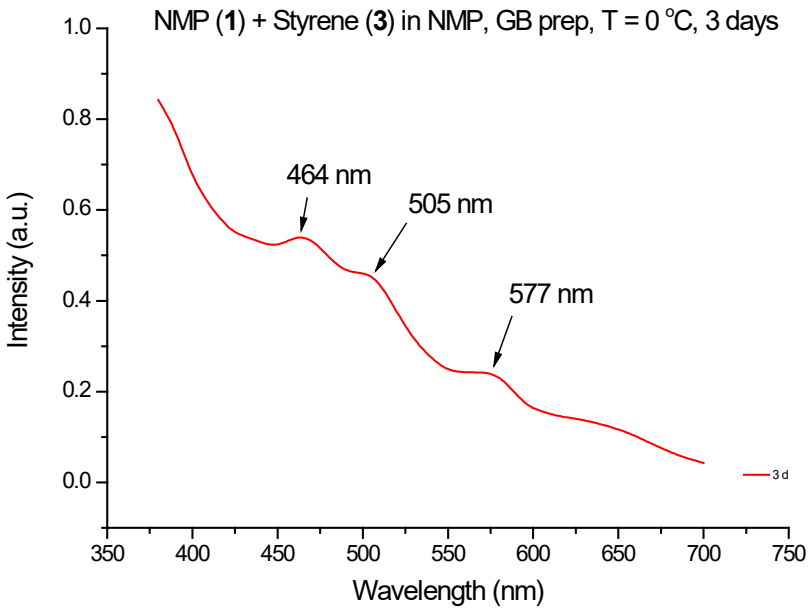


Figure S42. UV-vis spectrum over time for reaction of NMP + KO*t*Bu (1.5 eq.) + styrene (1.0 eq.) in NMP solvent at 0 °C, then left at rt over 3 days and re-measured.

5.3. Identity of Colored Species

For DMA and NMP, faint colors are observed even before styrene addition (Figures S29, S36), which we attribute to small concentrations of K enolate species (e.g. **2**, see main manuscript). Strong colors develop upon styrene addition (Figures S30, S33, S38, S40) and depend on the nature of the styrene. We propose these colors arise from an *alkylpotassium* species (a K enolate or K benzylate) and are *unlikely to originate from a radical species* due to the reaction proceeding successfully in air or when TEMPO is present as previously reported.[2] Radical addition to styrenes would be expected to initiate polymerization but mass balance is excellent in many of these amide CAKES reactions.[2]

The peaks in the visible part of the spectrum are inconsistent with the previously-reported UV-vis spectrum of benzylpotassium,[4] Computation suggests that the benzylpotassium (Figure S45) is not a persistent species and rapidly proceeds to deprotonate HO*t*Bu or the K enolate precursor, yet the colors are persistent until exposed to air/moisture.

Therefore, we conclude that a product K enolate species is the most likely responsible for this second stronger color. Since the color depends on the nature of the styrene (Figure S30, S33), we propose that either the monoadduct K enolate or bisadduct K enolate (e.g. **7** or the K enolate resulting from deprotonation of **10**, see main manuscript) is responsible. Co-ordinating additive 18-crown-6 results in a stronger initial (red/purple) color (even before products are observed) as previously reported,[2] and stronger colors develop when 18-crown-6 is present compared to when it is absent (Figure S35). Here, the role of 18-crown-6 is likely to promote the concentration of colored K enolate species, which is plausible given that computational studies find the deprotonation step energetically favourable in this case (see Figure 12 of main manuscript).

6. EPR STUDIES

In order to investigate whether or not the aforementioned coloured species was radical in nature, it was analyzed by EPR spectroscopy. According to a modified **Procedure A**, four samples were prepared for EPR analysis:

Sample **A**: An oven-dried vial containing a stirrer bar was charged with KO*t*Bu (19.3 mg, 0.17 mmol, 1.5 eq.), DMSO-d_6 (0.33 mL) and DMA (**1**) (0.18 mL, ca. 17 eq.) inside a glovebox and mixed until fully dissolved at rt. Styrene (13 μL, 0.115 mmol, 1.0 eq.) was added via syringe at rt. After stirring overnight at rt in the glovebox, an aliquot of the solution was transferred into a Wilmad Quartz EPR capillary tube which was placed inside an EPR tube. The EPR tube was sealed in the glovebox and analyzed by EPR spectroscopy. Sample **A** gave a blue/purple colour (Figure S43).

Sample **B**: Sample **A** was repeated substituting DMA (**1**) for NMP (**19**). Reaction **B** gave a yellow colour.

Sample **C**: Sample **A** was repeated using DMA (**1**) (0.51 mL) and no DMSO-d_6. Reaction **C** gave a pale purple colour.

Sample **D**: Sample **B** was repeated using NMP (**19**) (0.51 mL) and no DMSO-d_6. Reaction **C** gave a yellow colour.

As control experiments:

Sample **E**: Sample **A** was repeated but no solution added (EPR tube containing Wilmad Quartz EPR capillary tube only).

Sample **F**: Sample **C** was repeated but no styrene added.

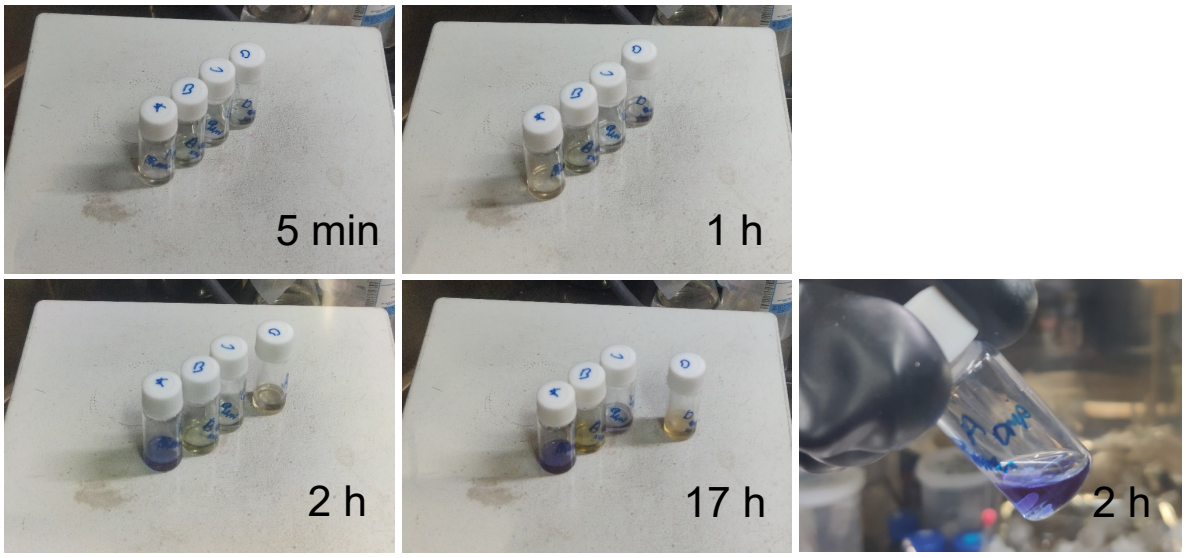


Figure S43. Coloured species observed during reactions of DMA (**1**) or NMP (**19**) with KO*t*Bu/styrene with or without DMSO-d_6 co-solvent.

1906052jb44a2
$g_{//}$ = 2.00174 $g_{\perp}$ = 2.00054

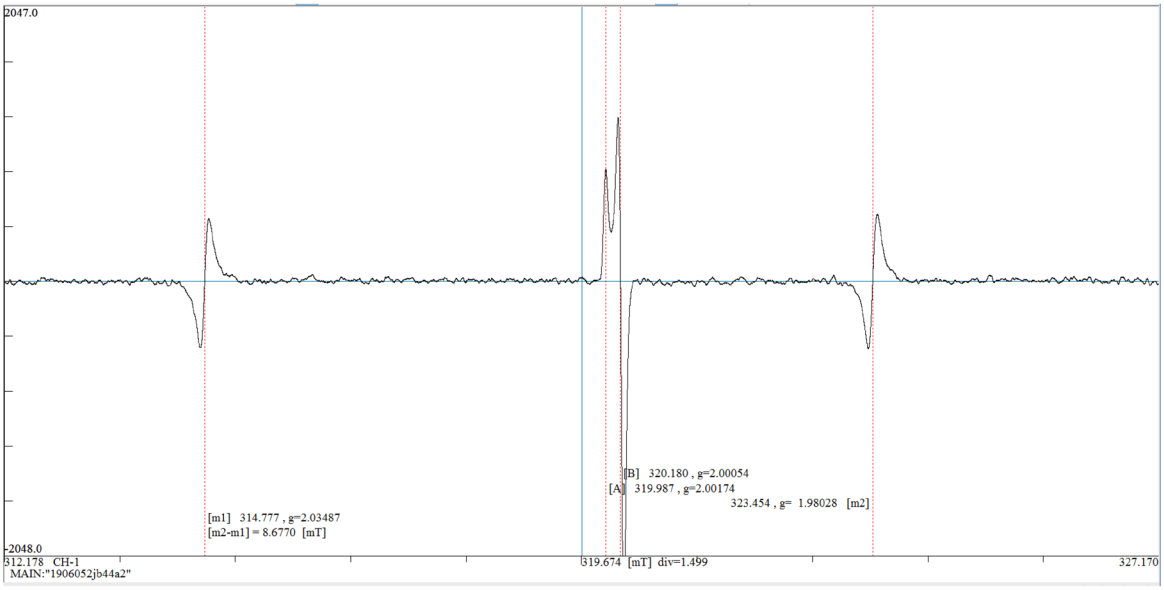


Figure S44. EPR spectrum of Sample **A**.

1906052jb44b
g_A= 2.00174 g_B= 2.00054

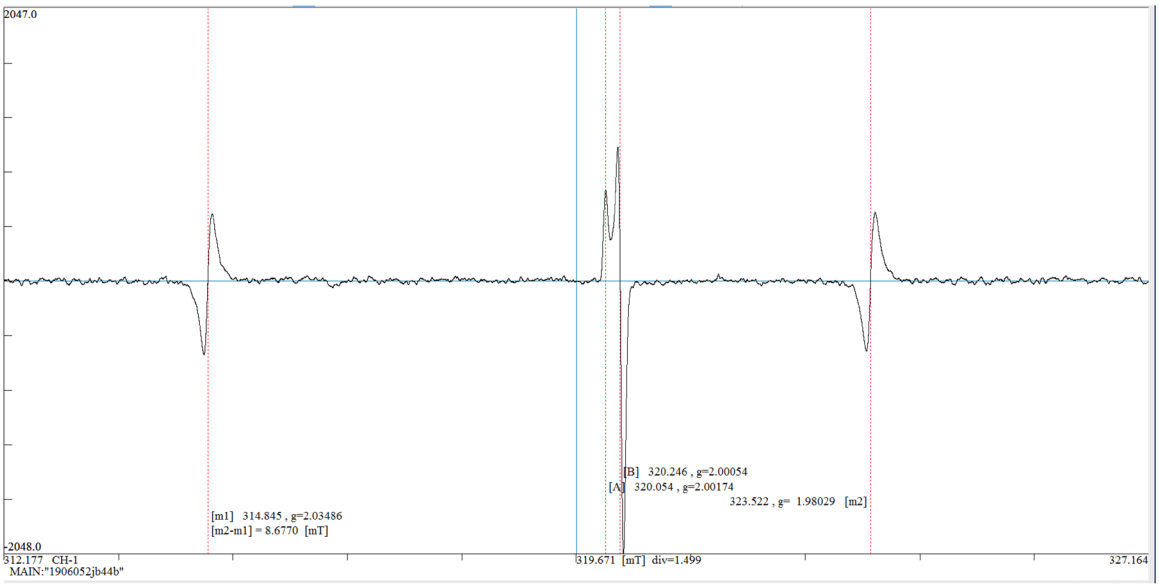


Figure S45. EPR spectrum of Sample **B**.

1906052jb44c
g_A= 2.00173 g_B= 2.00054

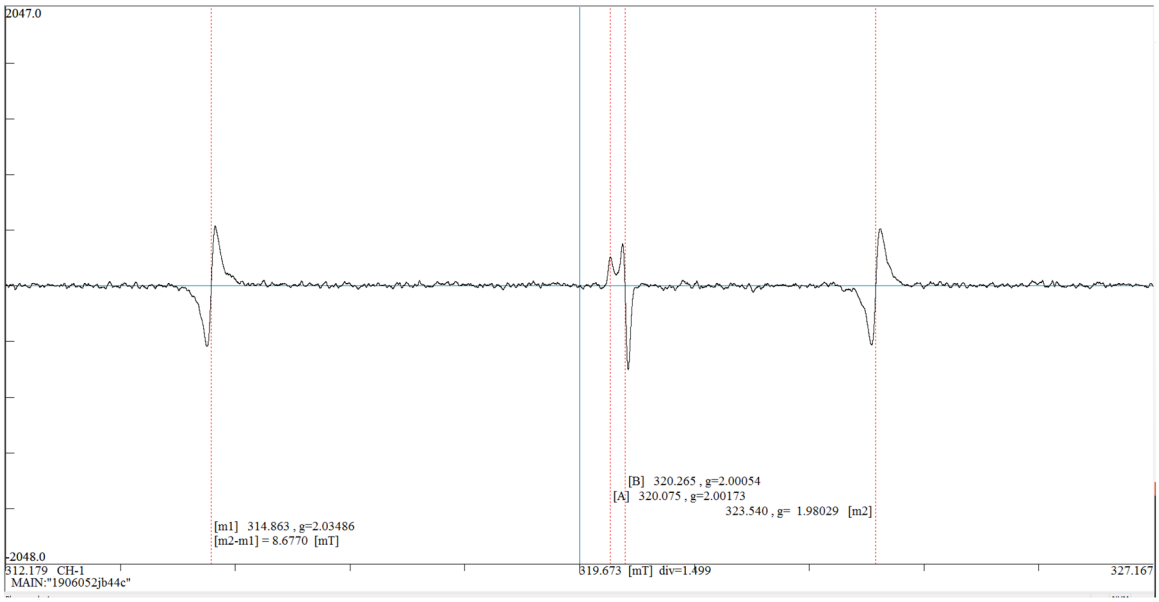


Figure S46. EPR spectrum of Sample **C**.

1906052jb44d
g_A= 2.00175 g_B= 2.00054

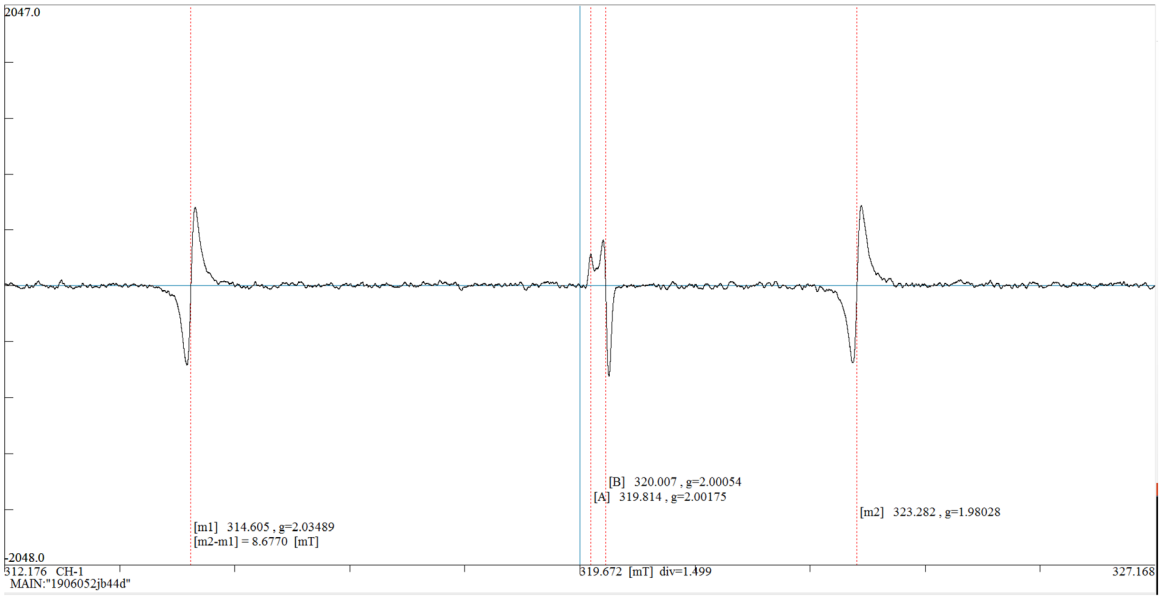


Figure S47. EPR spectrum of Sample **D**.

190711capillary_tube
g_A= 2.00173 g_B= 2.00054

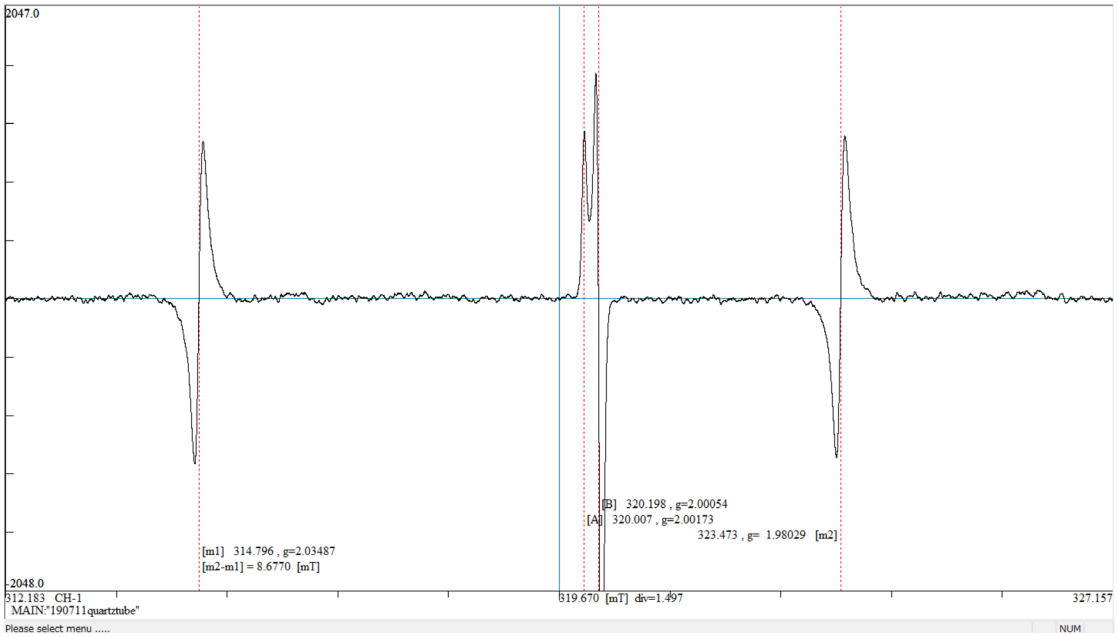


Figure S48. EPR spectrum of Sample **E**.

190711capillary_tube+solution
g_A= 2.00173 g_B= 2.00054

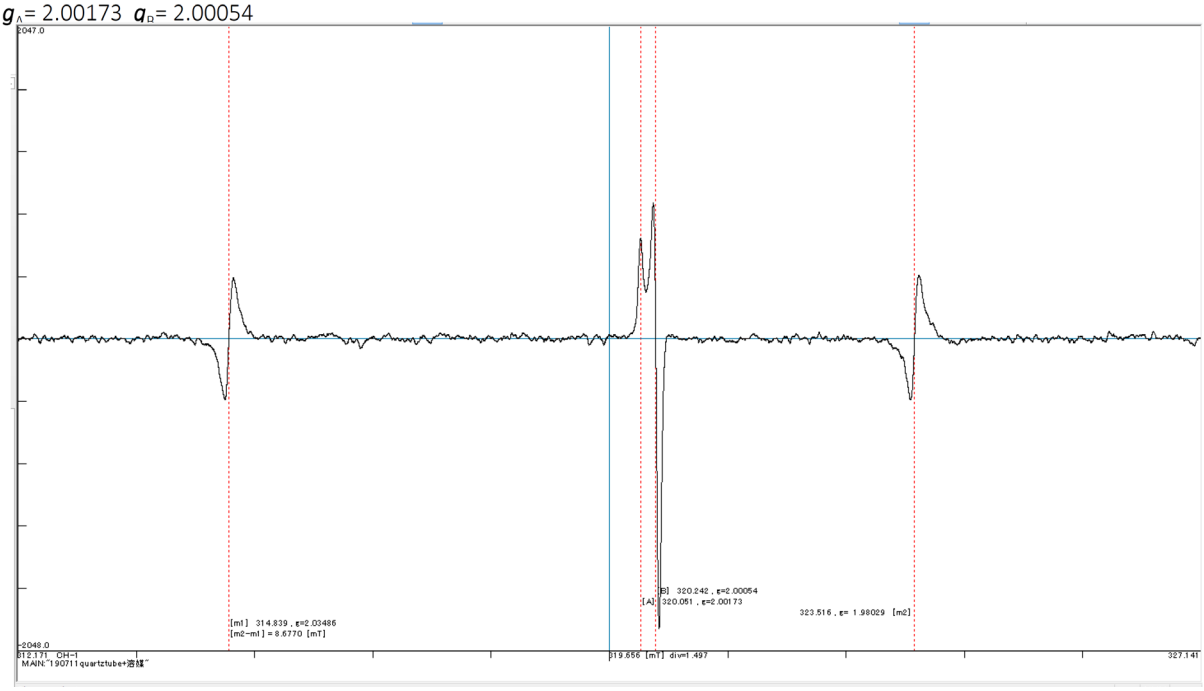
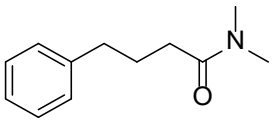


Figure S49. EPR spectrum of Sample **E**.

The same EPR signal was observed from every sample including Sample **E** (Figures S44-S49). Its shape and g-factors are typical of an F-centre (trapped electron). That no signals related to organic radical species were observed in these coloured samples supports the conclusion from a previous study[2] employing radical scavengers; that a radical mechanism is unlikely in amide CAKES reactions.

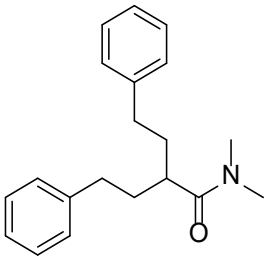
7. ^{1}H NMR, ^{13}C NMR SPECTRA AND HRMS-MALDI LISTED DATA

***N*,*N*-dimethyl-4-phenylbutanamide (6)**



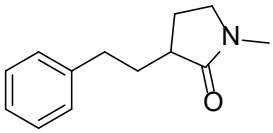
Prepared according to **Procedure A**. Colorless oil (150.0 mg, 68%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 - 7.26 (m, 2H), 7.23 - 7.16 (m, 3H), 2.95 (s, 6H), 2.69 (t, *J* = 7.5 Hz, 2H), 2.32 (t, *J* = 7.5 Hz, 2H), 1.99 (quint, *J* = 7.5 Hz, 2H); ^{1}H NMR data are consistent with that previously reported by us.[2]

***N*,*N*-dimethyl-2-phenethyl-4-phenylbutanamide (10)**



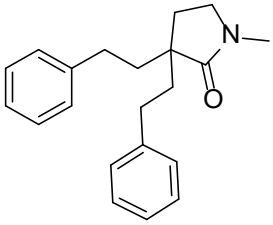
Prepared according to **Procedure A** and isolated from the reaction above. Colorless oil (30.0 mg, 18%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 - 7.22 (m, 4H), 7.18 (t, *J* = 7.5 Hz, 2H), 7.11 (d, *J* = 7.5 Hz, 4H), 2.97 (s, 3H), 2.71 (s, 3H), 2.66 - 2.51 (m, 5H), 2.06 - 1.99 (m, 2H), 1.83 - 1.77 (m, 2H); ^{1}H NMR data are consistent with that previously reported by us.[2]

***N*-methyl-3-phenethylpyrrolidin-2-one (20a)**



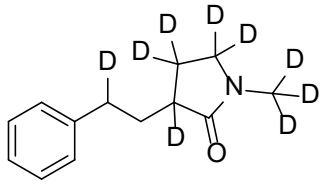
Prepared according to **Procedure A.** Colorless oil (204.0 mg, 87%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 - 7.27 (m, 2H), 7.23 - 7.18 (m, 3H), 3.34 - 3.28 (m, 2H), 2.86 (s, 3H), 2.80 - 2.67 (m, 2H), 2.43 - 2.37 (m, 1H), 2.28 - 2.18 (m, 2H), 1.75 - 1.65 (m, 2H); ^{1}H NMR data are consistent with that previously reported by us.[2]

***N*-methyl-3,3-diphenethylpyrrolidin-2-one (20b)**



Prepared according to **Procedure A** and isolated from the reaction above. Colorless oil (26.0 mg, 15%); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 - 7.25 (m, 4H), 7.24 - 7.14 (m, 6H), 3.35 (t, *J* = 7.5 Hz, 2H), 2.90 (s, 3H), 2.72 - 2.62 (m, 2H), 2.60 - 2.51 (m, 2H), 2.07 (t, *J* = 7.1 Hz, 2H), 1.94 - 1.82 (m, 4H); ^{1}H NMR data are consistent with that previously reported by us.[2]

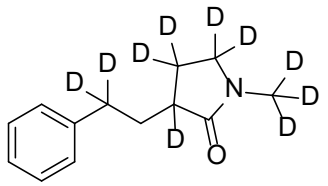
***N*-methyl-3-phenethylpyrrolidin-2-one-d$_9$ (20a-d$_9$)**



Prepared according to **Procedure C.** Colorless oil (2.5 mg, 6%); IR ν_{max} (neat) 3436, 3084 - 2854 (C-H), 2211 - 2072 (C-D), 1675 (C=O), 1604, 1582, 1496, 1450, 1423, 1260, 1217 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$)* δ 7.32 - 7.27 (m, 2H), 7.25 - 7.17 (m, 3H), 2.78 - 2.65 (m, 1H), 2.26 - 2.17 (m, 1H), 1.70 - 1.61 (m, 1H); ^{2}H NMR (77 MHz, $CDCl_3$) δ 3.28 (s, 2D), 2.82 (br. s, 4D), 2.38 (s, 1D), 2.18 (s, 1D), 1.68 (s, 1D); ^{13}C NMR (126 MHz, $CDCl_3$)* δ 176.6, 141.6, 128.5, 128.4, 125.9, 40.4 (apt. t, *J* = 20.1 Hz), 33.1 (apt. t, *J* = 19.4 Hz), 33.0;** HRMS (MALDI, DCTB as matrix with sodium trifluoroacetate) *m/z* calculated for $C_{13}H_8D_9NONa$ ([M+Na]$^+$), 235.1767; Found 235.1772; HRMS (MALDI, DCTB as matrix without sodium trifluoroacetate) *m/z* calculated for $C_{13}H_9D_9NO$ ([M+H]$^+$), 213.1948; Found 213.1947.

*A peak was observed at 1.26 ppm (^{1}H) and 29.7 ppm (^{13}C) which is 'grease'. **Due to coupling with ^{2}H atoms, the remaining 3x ^{13}C environments could not be observed.

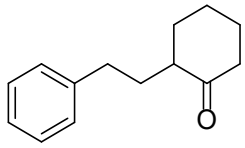
***N*-methyl-3-phenethylpyrrolidin-2-one-d$_9$ (20a-d$_{10}$)**



Prepared according to a modified **Procedure B**; following the kinetic study, the reaction was left for ca. two weeks before quenching, work up and purification. Colorless oil (17.6 mg, 41%); IR ν_{max} (neat) 3476, 3083 - 2854 (C-H), 2206 - 2071 (C-D), 1679 (C=O), 1605, 1496, 1447, 1416, 1259 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$)* δ 7.30 - 7.27 (m, 2H), 7.25 - 7.17 (m, 3H), 2.21 (d, *J* = 13.7 Hz, 1H), 1.75 - 1.65 (d, *J* = 13.7 Hz, 1H); ^{2}H NMR (77 MHz, $CDCl_3$) δ 3.28 (s, 2D), 2.82 (s, 3D), 2.73 (s, 1D), 2.68 (s, 1D), 2.38 (s, 1D), 2.18 (s, 1D), 1.68 (s, 1D); ^{13}C NMR (126 MHz, $CDCl_3$)* δ 176.6, 141.6, 128.5, 128.3, 125.9, 46.7 (apt. t, *J* = 21.6 Hz), 40.4 (apt. t, *J* = 20.0 Hz), 32.9, 32.5 (apt. t, *J* = 19.4 Hz), 29.0 (apt. t, *J* = 20.9 Hz), 24.0 (apt. t, *J* = 20.1 Hz); HRMS (MALDI, DCTB as matrix with sodium trifluoroacetate) *m/z* calculated for $C_{13}H_7D_{10}NONa$ ([M+Na]$^+$), 236.1830; Found 236.1830; HRMS (MALDI, without sodium trifluoroacetate) *m/z* calculated for $C_{13}H_8D_{10}NO$ ([M+H]$^+$), 214.2011; Found 214.2024.

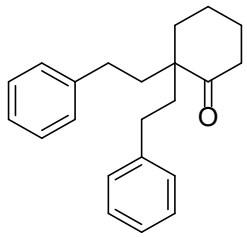
*A peak was observed at 1.26 ppm (^{1}H) and 29.7 ppm (^{13}C) which is 'grease'.

2-phenylethyl-3,4-dihydronapthalen-1(2*H*)-one (26a)



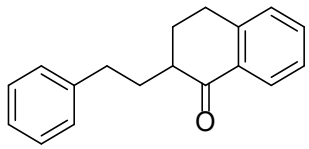
Prepared according to Procedure D. Colorless oil (292 mg, 72%); IR ν_{max} (neat) 3085 - 2860 (C-H), 1708 (C=O), 1603, 1496, 1451, 1371, 1338, 1312, 1227, 1206 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 - 7.27 (m, 2H), 7.20 - 7.17 (m, 2H), 2.66 - 2.60 (m, 2H), 2.42 - 2.38 (m, 1H), 2.33 - 2.27 (m, 2H), 2.19 - 2.11 (m, 2H), 2.07 - 2.03 (m, 1H), 1.88 - 1.86 (m, 1H), 1.74 - 1.61 (m, 2H), 1.53 - 1.41 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.2, 128.4, 128.3, 125.8, 49.9, 42.1, 34.0, 33.2, 31.2, 28.0, 24.9; HRMS (MALDI, THAP as matrix with sodium trifluoroacetate) *m/z* calculated for $C_{14}H_{18}ONa$ ([M+Na]$^{+}$), 225.1250; Found 225.1228; ^{1}H and ^{13}C NMR data are consistent with the literature.[3] The remaining 1x ^{13}C (C=O) environment could not be observed.

2-phenylethyl-3,4-dihydronapthalen-1(2*H*)-one (26b)



Prepared according to Procedure D. Colorless oil (68 mg, 22%); IR ν_{max} (neat) 3085 - 2861 (C-H), 1705 (C=O), 1603, 1496, 1455, 1372, 1336, 1313, 1219 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 - 7.16 (m, 10H), 2.67 - 2.57 (m, 2H), 2.19 - 2.13 (m, 2H), 2.05 - 1.99 (m, 2H), 1.91 - 1.80 (m, 4H), 1.50 - 1.46 (m, 1H), 1.41 - 1.36 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 142.5, 142.4, 128.4 (2 x C), 128.3 (2 x C), 125.7, 125.7, 51.7, 39.2, 37.0, 36.5, 30.1, 27.1, 20.8; HRMS (MALDI, THAP as matrix with sodium trifluoroacetate) *m/z* calculated for $C_{13}H_7D_{10}NONa$ ([M+Na]$^{+}$), 329.1876; Found 329.1858; ^{1}H and ^{13}C NMR data are consistent with the literature.[5] The remaining 1x ^{13}C (C=O) environment could not be observed.

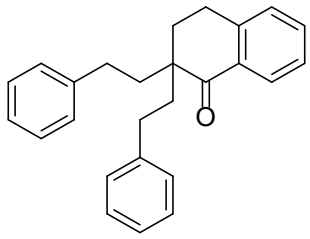
2-phenylethyl-3,4-dihydronapthalen-1(2*H*)-one (28a)



Prepared according to Procedure D. Colorless oil (363 mg, 73%); IR ν_{max} (neat) 3065 - 2844 (C-H), 1682 (C=O), 1602, 1497, 1456, 1434, 1362, 1282, 1217 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.05 (dd, *J*

= 7.9, 1.1 Hz, 1H), 7.47 (td, *J* = 7.5, 1.5 Hz, 1H), 7.33 - 7.19 (m, 7H), 3.06 - 2.97 (m, 2H), 2.85 - 2.72 (m, 2H), 2.56 - 2.50 (m, 1H), 2.38 - 2.28 (m, 2H), 2.01 - 1.93 (m, 2H), 1.85 - 1.78 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.1, 143.8, 142.0, 133.1, 132.6, 128.6, 128.5, 128.4, 127.4, 126.6, 125.8, 46.8, 33.2, 31.3, 28.5, 28.4; HRMS (MALDI, THAP as matrix with sodium trifluoroacetate) *m/z* calculated for $C_{18}H_{18}ONa$ ([M+Na]$^+$), 273.1250; Found 273.1227; ^{1}H and ^{13}C NMR data are consistent with the literature.[3]

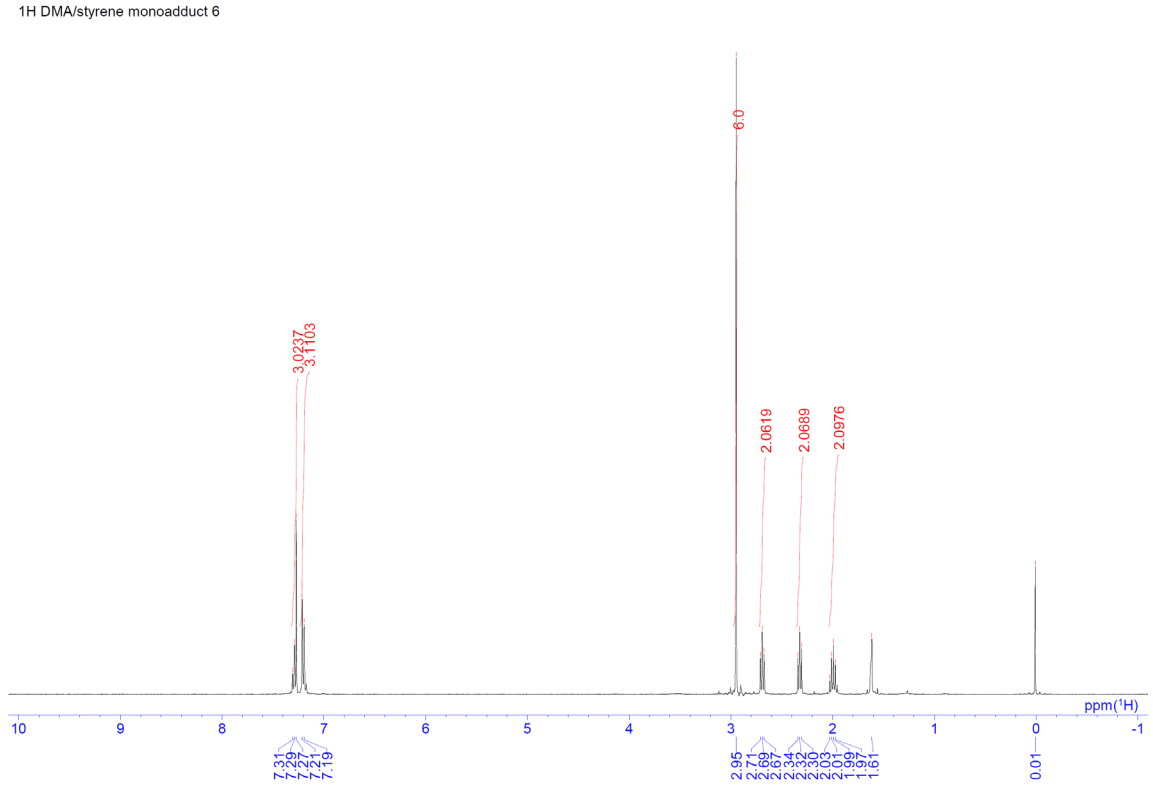
2,2-diphenethyl-3,4-dihydronapthalen-1(2*H*)-one (28b).



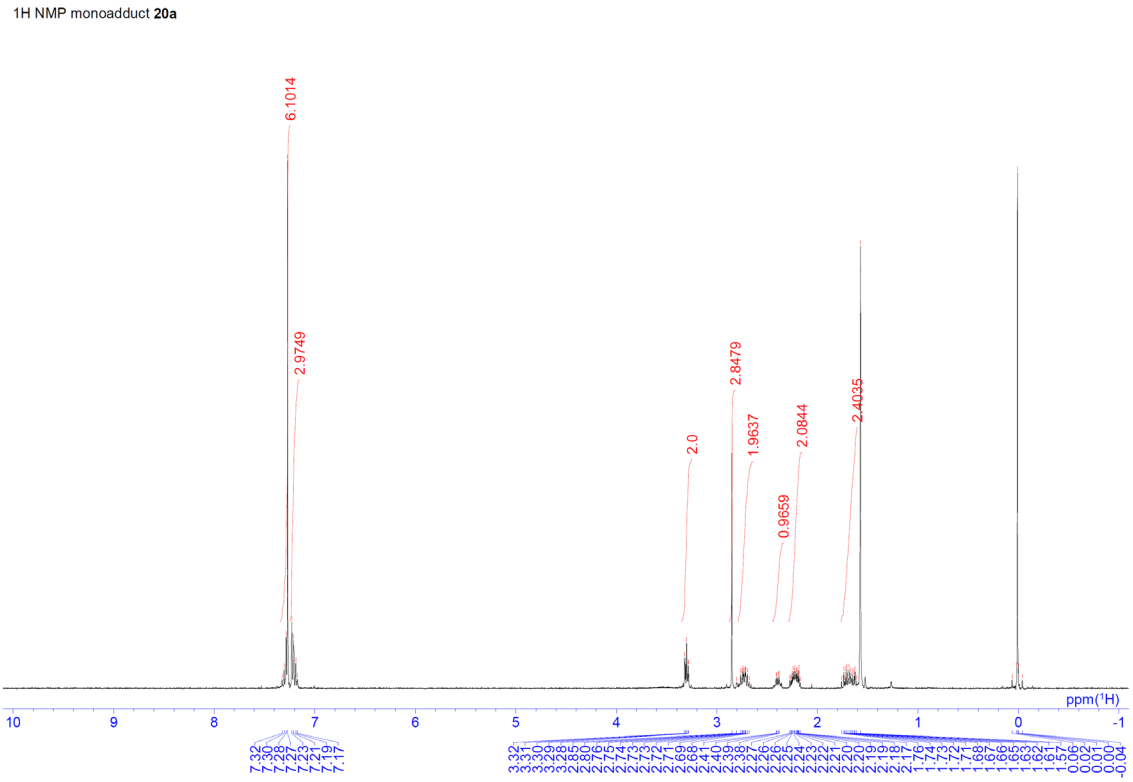
Prepared according to Procedure D. Colorless oil (31 mg, 9%); IR ν_{max} (neat) 3065 - 2862 (C-H), 1705 (C=O), 1603, 1496, 1455, 1372, 1336, 1313, 1219 cm^{-1}; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (d, *J* = 8.0, 1H), 7.48 (t, *J* = 7.5, 1H), 7.35 - 7.17 (m, 12H), 3.07 (t, *J* = 6.4, 2H), 2.67 - 2.60 (m, 4H), 2.26 - 2.23 (m, 2H), 2.13 - 2.07 (m, 2H), 1.96 - 1.90 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 200.1, 142.9, 142.4 133.1, 132.0, 128.7, 128.4 (2 x C), 128.1, 126.7, 125.8, 48.0, 36.7, 31.1, 30.4, 25.1; HRMS (MALDI, THAP as matrix with sodium trifluoroacetate) *m/z* calculated for $C_{26}H_{26}ONa$ ([M+Na]$^+$), 377.1876; Found 377.1868.

8. ^{1}H NMR, ^{13}C NMR Spectra for Novel Compounds

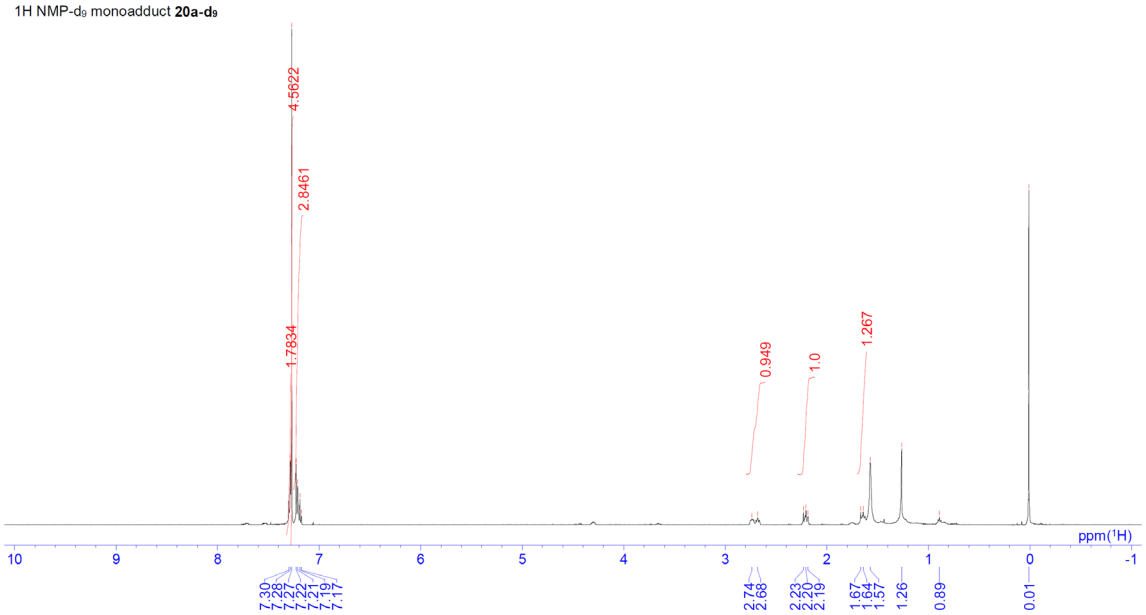
^{1}H NMR (400 MHz, $CDCl_3$) – *N*,*N*-dimethyl-4-phenylbutanamide (**6**)



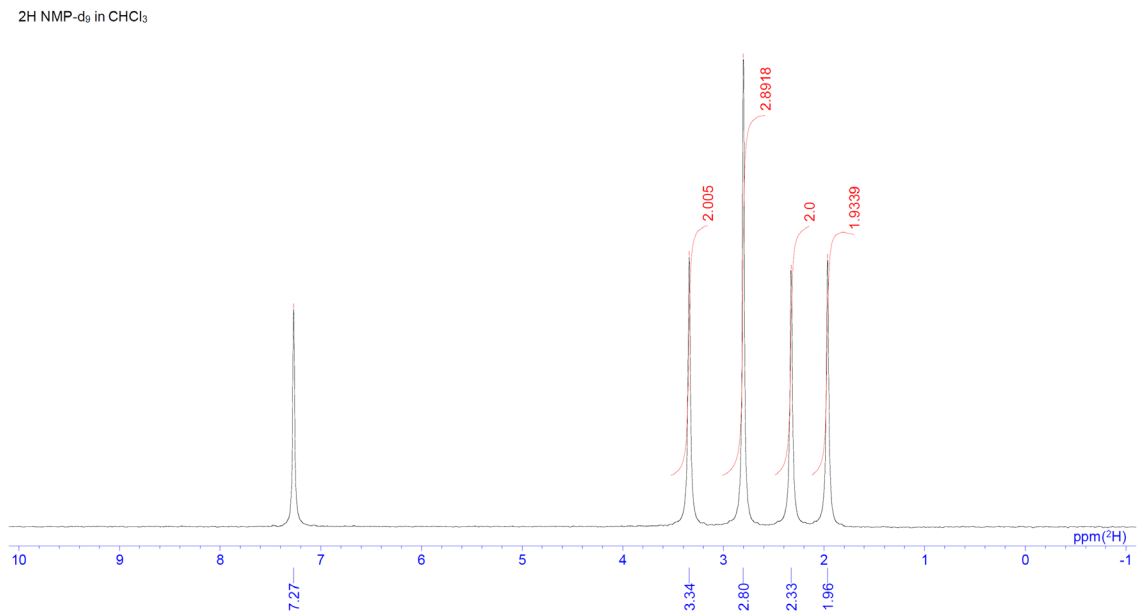
^{1}H NMR (400 MHz, $CDCl_3$) – *N*-methyl-3-phenethylpyrrolidin-2-one (**20a**)



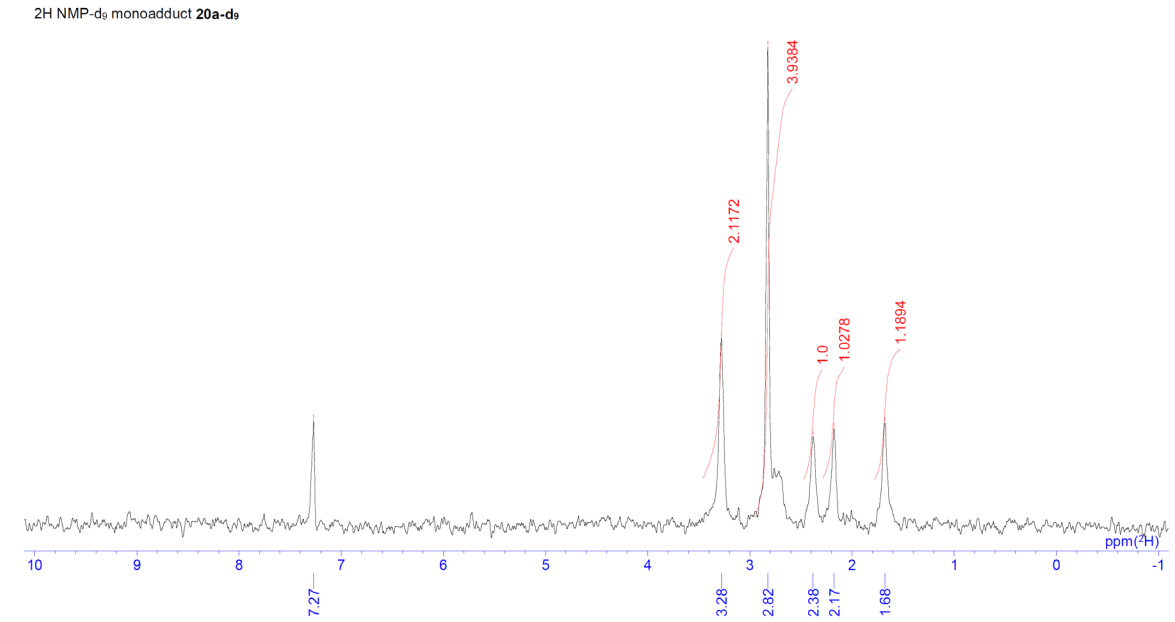
^{1}H NMR (500 MHz, $CDCl_3$) – *N*-methyl-3-phenethylpyrrolidin-2-one-d_9 (**20a-d_9**)



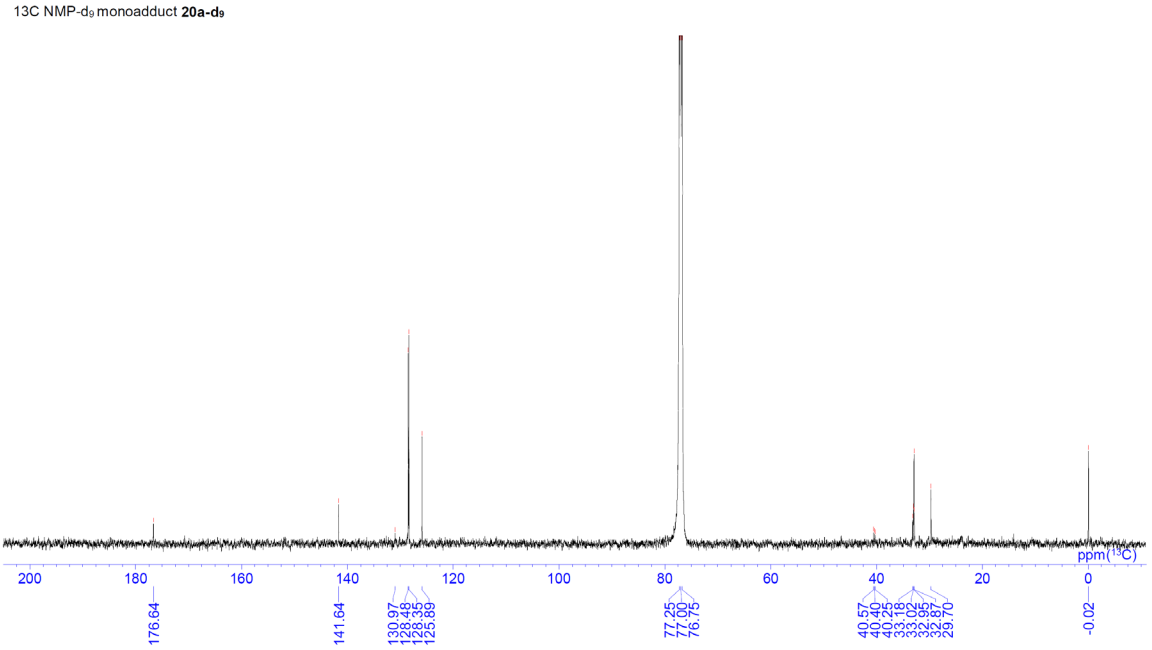
^{2}H NMR (77 MHz, $CHCl_3$) – *N*-methyl-2-pyrrolidinone-d_9 (**19-d_9**)



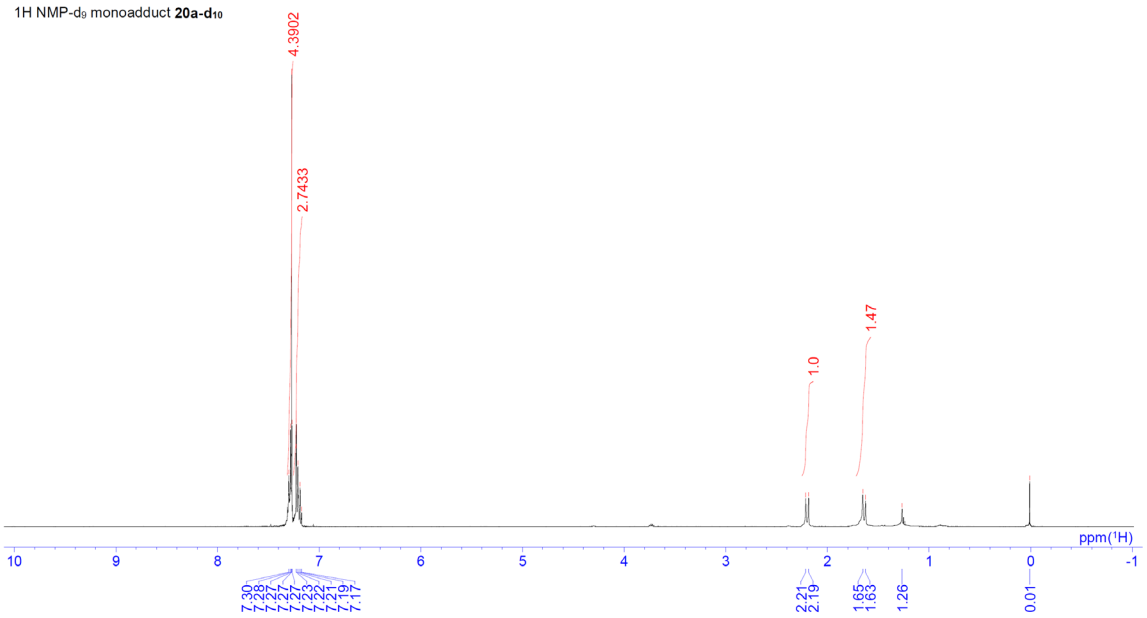
^{2}H NMR (77 MHz, $CHCl_3$) – *N*-methyl-3-phenethylpyrrolidin-2-one-d_9 (**20a-d_9**)



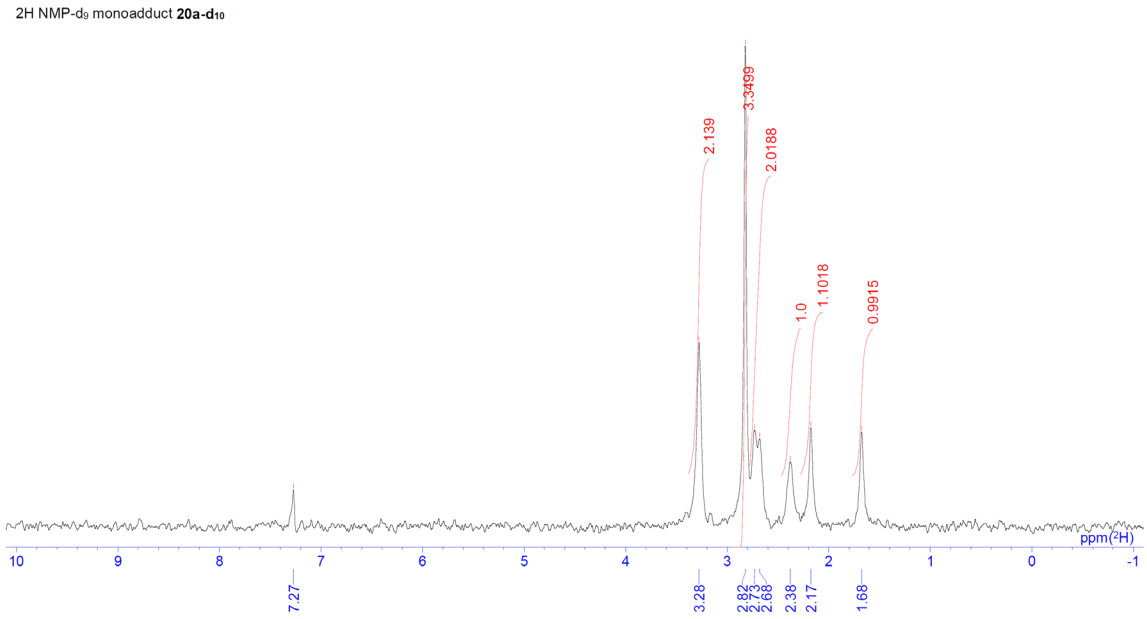
^{13}C NMR (126 MHz, $CDCl_3$) – *N*-methyl-3-phenethylpyrrolidin-2-one-d_9 (**20a-d_9**)



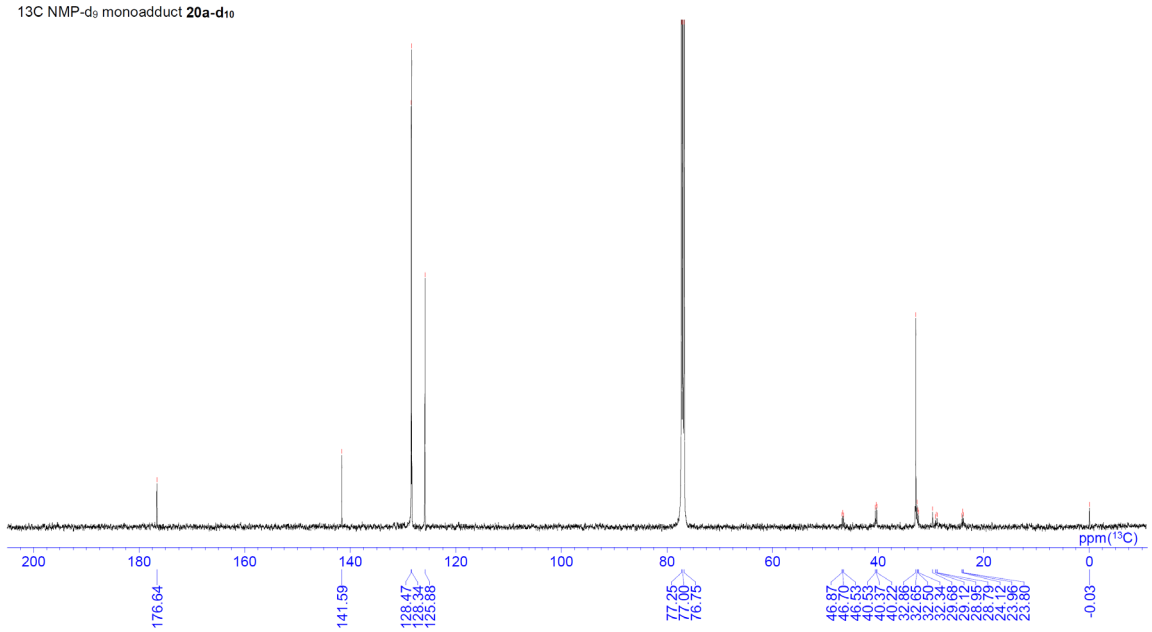
^{1}H NMR (500 MHz, $CDCl_3$) – *N*-methyl-3-phenethylpyrrolidin-2-one-d_{10} (**20a-d_{10}**)



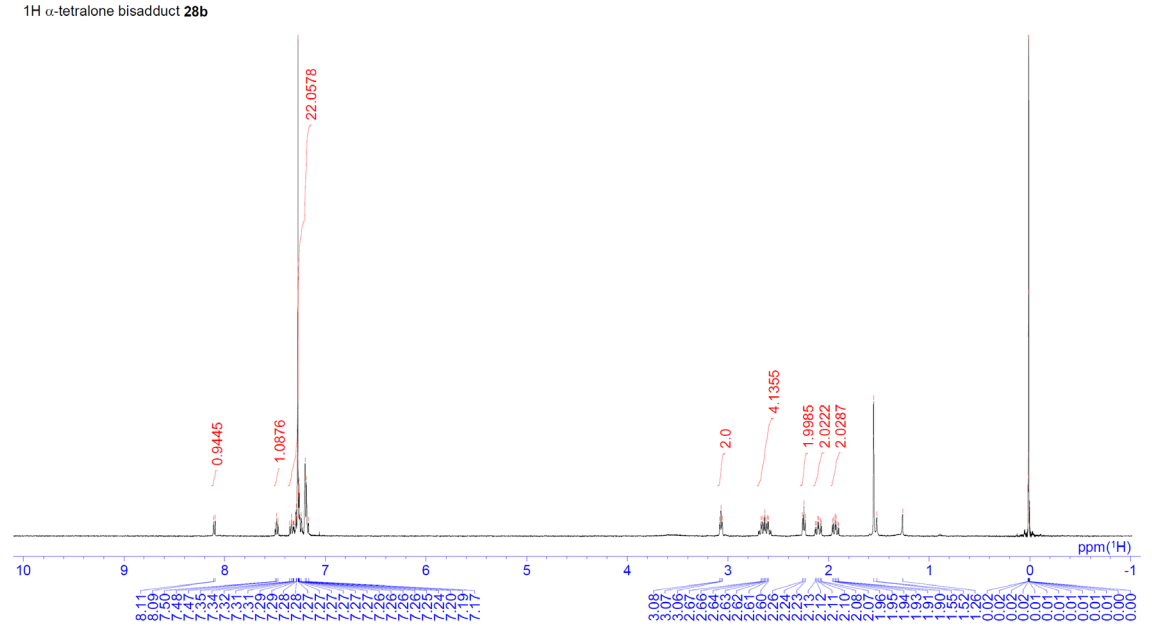
^{2}H NMR (77 MHz, $CHCl_3$) – *N*-methyl-3-phenethylpyrrolidin-2-one-d_{10} (**20a-d_{10}**)



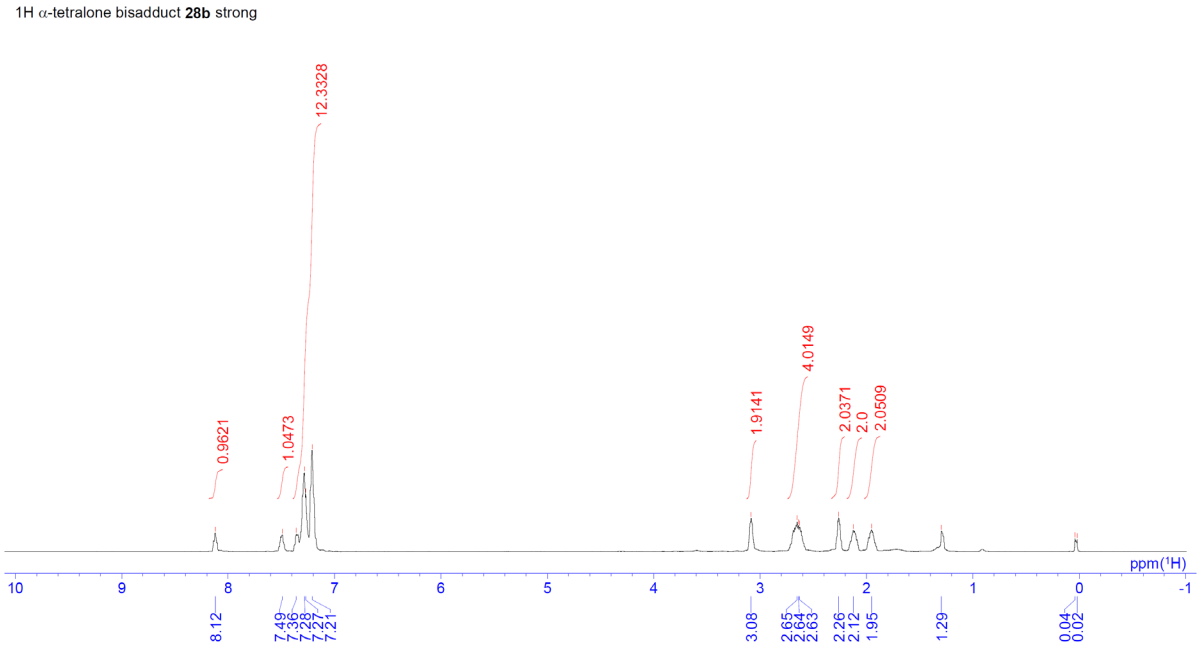
^{13}C NMR (126 MHz, $CDCl_3$) – *N*-methyl-3-phenethylpyrrolidin-2-one-d_{10} (**20a-d$_{10}$**)



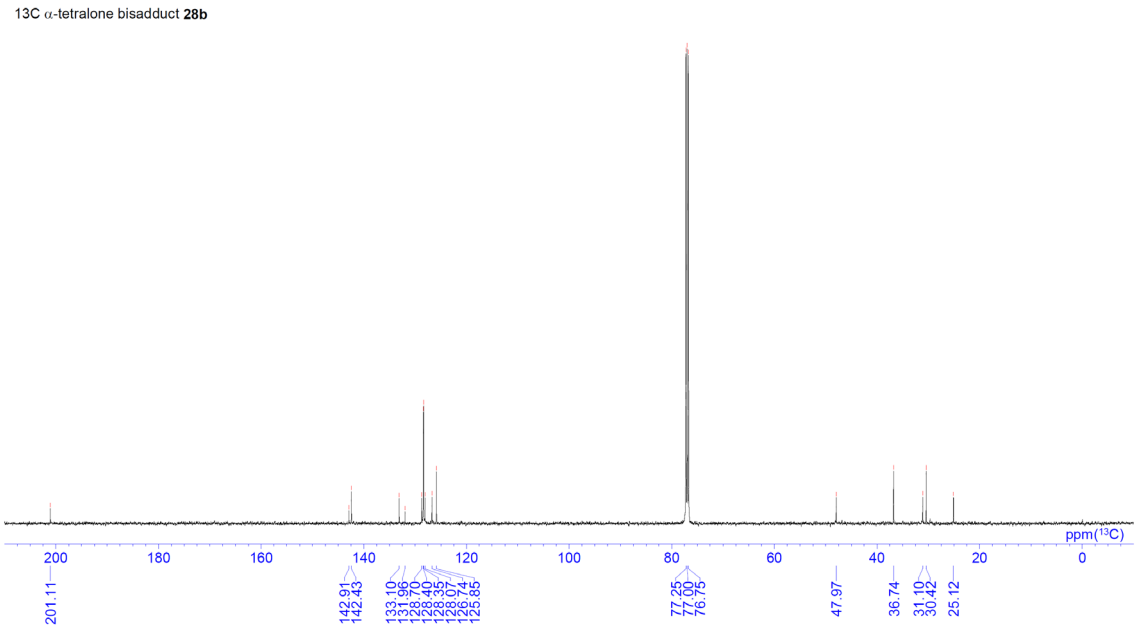
^{1}H NMR (500 MHz, $CDCl_3$) – 2,2-diphenethyl-3,4-dihydronapthalen-1(2*H*)-one (**28b**)



^{1}H NMR (500 MHz, $CDCl_3$) – 2,2-diphenethyl-3,4-dihydronapthalen-1(2*H*)-one (**28b**) {high conc.}



^{13}C NMR (126 MHz, $CDCl_3$) – 2,2-diphenethyl-3,4-dihydronapthalen-1(2*H*)-one (**28b**)



9. HRMS-MALDI AND ESI-MS STUDIES

9.1. SAMPLE PREPARATION PROCEDURES

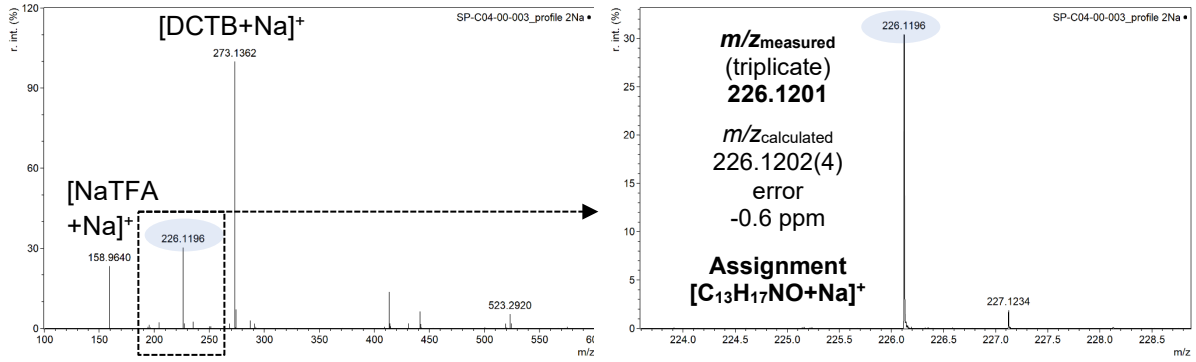
For HRMS-MALDI sample preparation: To each vial was added ca. 1-2 mg of sample (**20a**, **20a-d_9** or **20a-d_{10}**), followed by ca. 200 μL of $CHCl_3$. The resulting solution (ca. 0.5 μL) was deposited on the disposable MALDI target (Hudson Surface Technology, New Jersey, USA) to form a thin film which was left to air-dry (6 spots per sample). The matrix solution (ca. 0.5 μL) of ([3-(4-tert-Butylphenyl)-2-methyl-2-propenylidene]malononitrile, 'DCTB', ca. 10 mg mL in $CHCl_3$) was further deposited on top of the spots and left to air dry. Then, ca. 0.1 μL of a sodium trifluoroacetate solution, 'NaTFA' (ca. 1 mg mL NaTFA in $CHCl_3$) was added to half of the spots. NaTFA favours the formation of $[M+Na]^+$ adducts while DCTB (only) favours the formation of protonated species $[M+H]^+$. Additional aliquots of DCTB and NaTFA (only) were finally deposited around the sample spots for the sake of external calibration.
Accurate mass measurements were conducted using sodiated samples with $[DCTB+Na]^+$ and $[NaTFA+Na]^+$ as two internal calibrants bracketing the peaks of interest (peak intensity calibration was not deemed necessary for the purposes of this study). Samples without cationizing agent were calibrated externally using the DCTB+NaTFA spots. Resolution power is ~45,000 for each mass spectrum.
Alternatively, for samples containing **26a/26b** or **28a/28b**: To each vial was added ca. 1-2 mg of sample, followed by ca. 1 mL of $CHCl_3$ The resulting solution (ca. 1 μL) was deposited on the disposable MALDI target to form a thin film which was left to air-dry (4 spots per sample). The matrix solution (ca. 1 μL) of 2,4,6-trihydroxyacetophenone (THAP), ca. 20 mg/mL in THF, was deposited on top of the spots and left to air dry. Then, ca. 1 μL of NaFTA (ca. 1 mg/mL in THF) was added to the spots. Accurate mass measurements were conducted using sodiated samples with $[NaTFA+Na]^+$ and bis(2-ethylhexylphthalate (contaminant) as two internal calibrants bracketing the peaks of interest (peak intensity calibration was not deemed necessary for the purposes of this study). Resolution power is ~38,000 for each mass spectrum.

For ESI-MS sample preparation: Sample **20a** was recovered from the MALDI plate, diluted with MeOH (1/100) and the resulting solution directly infused into the ESI ion source with no other preparation. Regarding the vials prepared as mentioned above containing ca. 1-2 mg of sample (**20a-d_9** or **20a-d_{10}**), ca. 10 μL was taken, diluted with MeOH (1/100) and the resulting solution directly infused into the ESI ion source with no other preparation.

9.2. HRMS-MALDI Spectra and Analysis for D-Labelling Studies

HRMS-MALDI (Matrix: DCTB, Dissolution: $CHCl_3$, Method: Positive) and ESI-MS analysis – *N*-methyl-3-phenethylpyrrolidin-2-one (**20a**, *for comparison with deuterated species*)

With NaTFA



Without cationizing agent

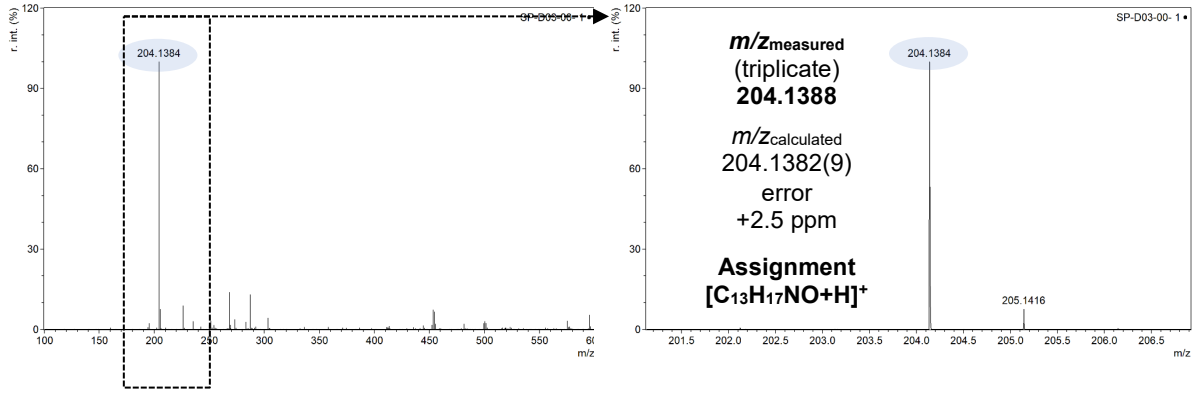
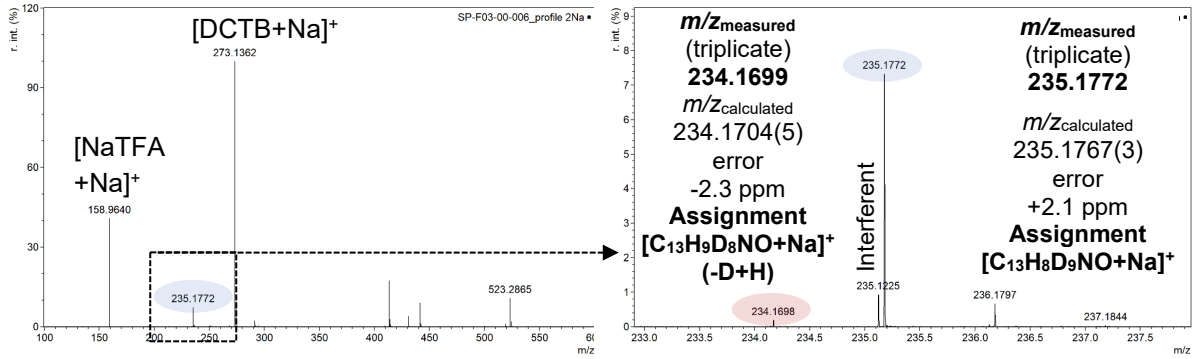


Figure S50. HRMS-MALDI analysis of **20a**.

No +● radical cation detected. Therefore, a -1 Da shift in the following samples **20a-d$_9$** and **20a-d$_{10}$** would suggest the replacement of D by H.

HRMS-MALDI (Matrix: DCTB, Dissolution: $CHCl_3$, Method: Positive) and ESI-MS analysis – *N*-methyl-3-phenethylpyrrolidin-2-one-d_9 (**20a-d_9**)

With NaTFA



Without cationizing agent

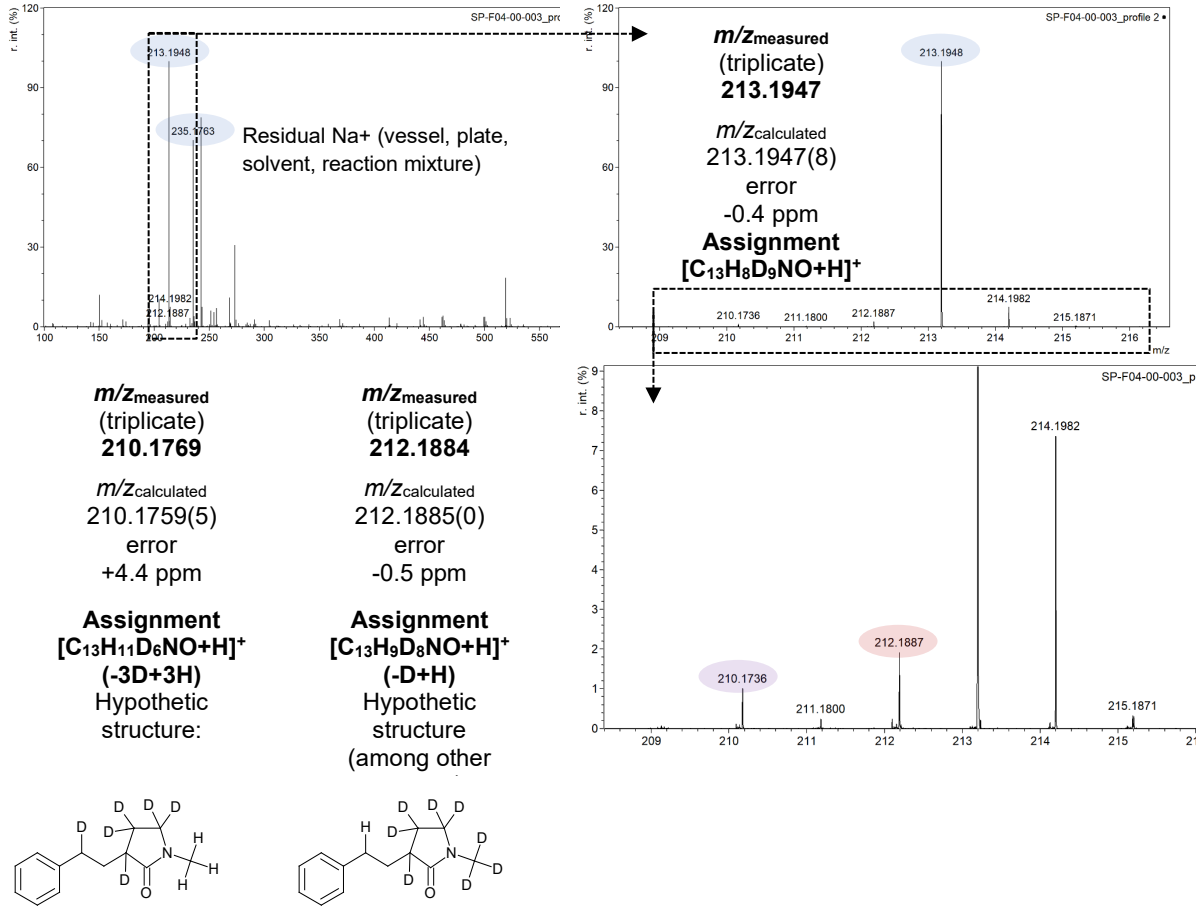
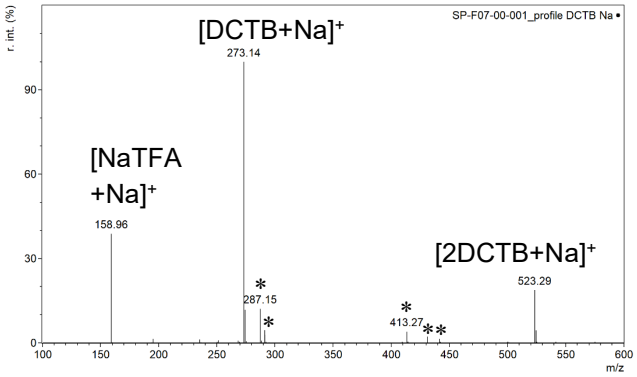


Figure S51. HRMS-MALDI analysis of **20a-d_9**.

Compound **20a-d_9** is **nearly fully deuterated** but two partially deuterated species are barely detected in the background noted (-D+H) and (-3D+3H). Their relative abundance varies with the spot and the laser fluence, but average abundances can be estimated from 6 measurements (3 spots, duplicated) at ~2.3% for (-D+H) and ~0.8% for (-3D+3H) considering the main fully deuterated compound at 100%. Since the compounds differ only by their number of neutrons, it is reasonable to assume their ionization behaviour is identical and thus the estimate of abundance by mass spectrometry is valid.

HRMS-MALDI (Matrix: DCTB, Dissolution: $CHCl_3$, Method: Positive) and ESI-MS analysis – *N*-methyl-3-phenethylpyrrolidin-2-one-d_{10} (**20a-d_{10}**)

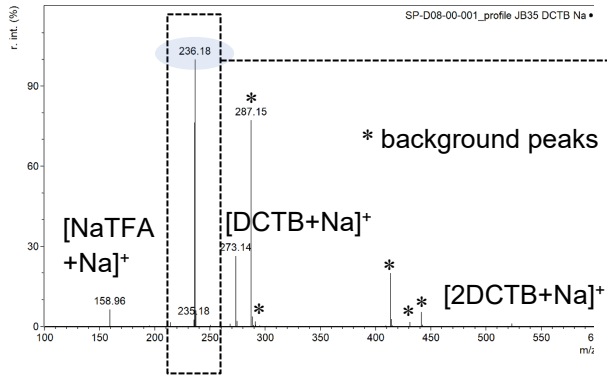
With NaTFA

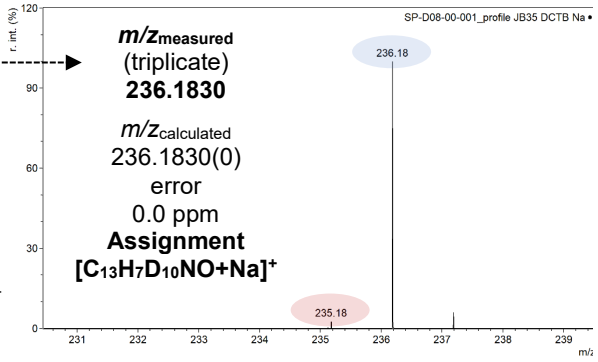


← DCTB+NaTFA (blank)

Only two species detected in the range 0-1000 (*m/z* 235 and m/z 236) in addition to several background peaks (seen with DCTB + sodium trifluoroacetate only).

↓ **20a-d_{10}**+DCTB+NaTFA





***m/z*measured**
(triplicate)
236.1830

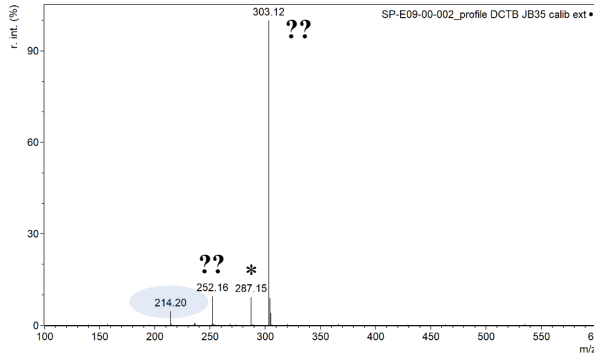
*m/z*calculated
236.1830(0)
error
0.0 ppm
Assignment
[$C_{13}H_7D_{10}NO$+Na]+

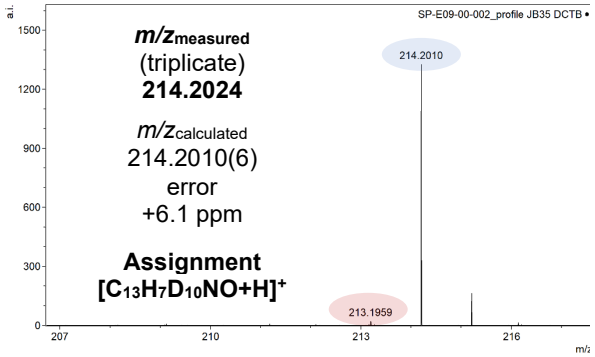
Assignment
[$C_{13}H_8D_9NO$+Na]+ =
20a-d_9

***m/z*measured**
(triplicate)
235.1770

*m/z*calculated
235.1767(3)
error
+1.2 ppm

Without cationizing agent





***m/z*measured**
(triplicate)
214.2024

*m/z*calculated
214.2010(6)
error
+6.1 ppm

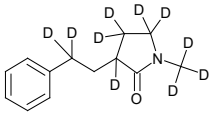
Assignment
[$C_{13}H_7D_{10}NO$+H]+

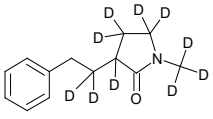
Assignment
[$C_{13}H_8D_9NO$+Na]+
= **20a-d_9**

***m/z*measured**
(triplicate)
213.1959

*m/z*calculated
213.1947(8)
error
+5.3 ppm

Possible isomeric shapes of **20a-d_{10}:**





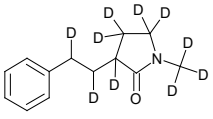


Figure S52. HRMS-MALDI analysis of **20a-d_{10}**.

9.3. ESI-MS SPECTRA AND ANALYSIS FOR D-LABELLING STUDIES

ESI-MS/MS, 20a

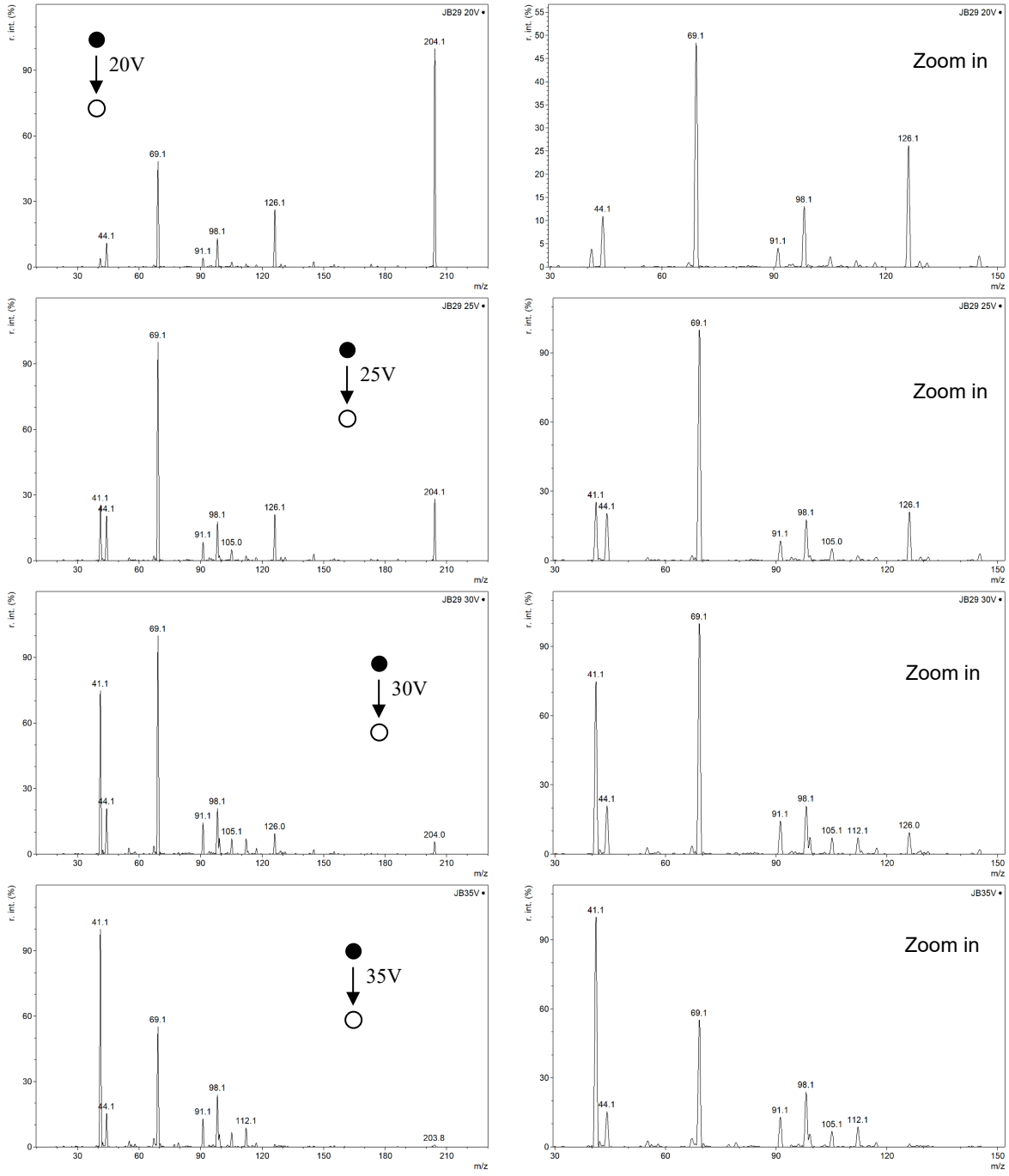
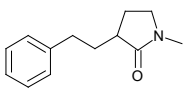


Figure S53. ESI-MS/MS fragmentation of **20a**.

Structure:



ESI-MS/MS, 20a-d_9 (analysis of main component)

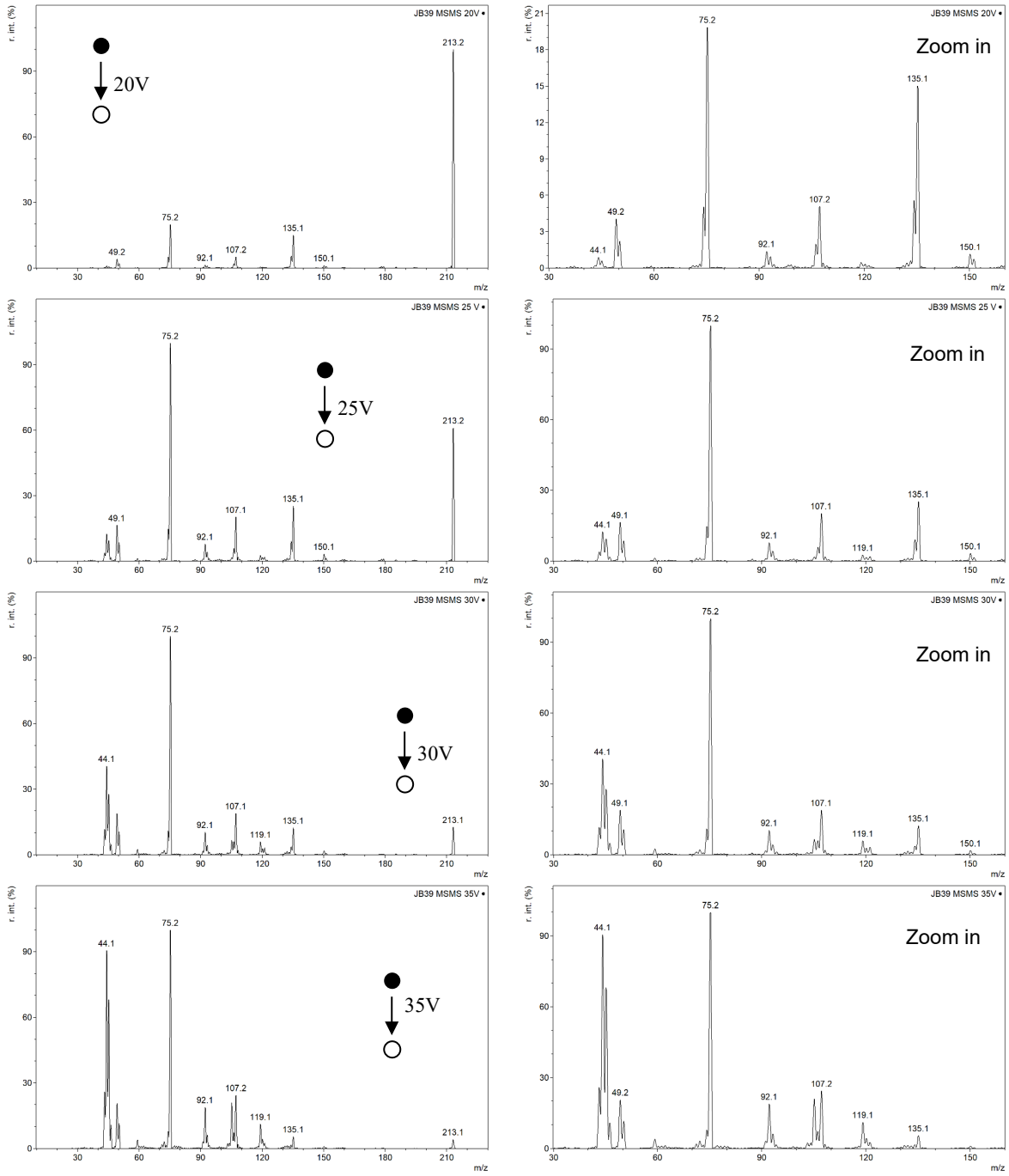


Figure S54. ESI-MS/MS fragmentation of **20a-d_9** (main component).

Possible structures:



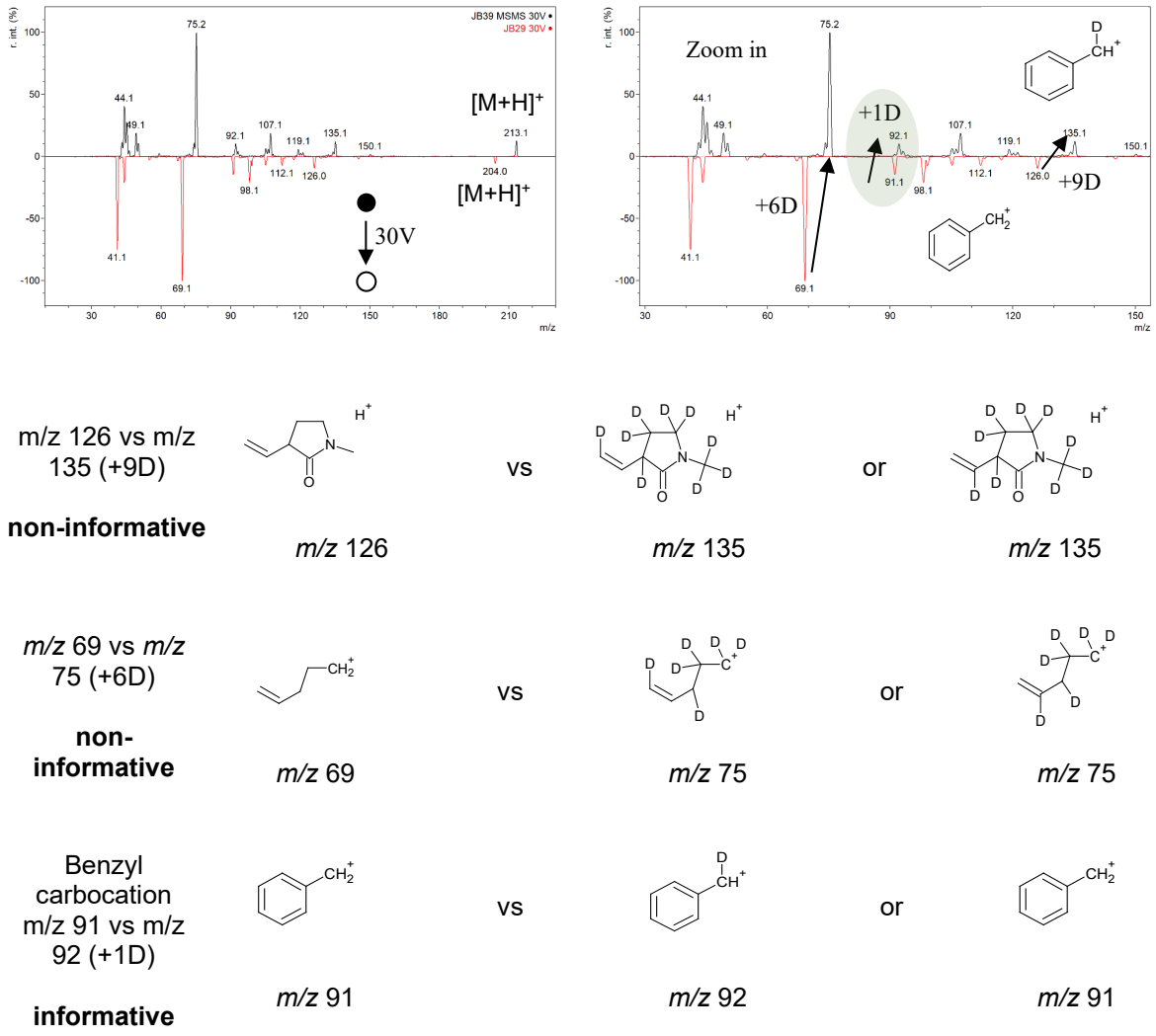
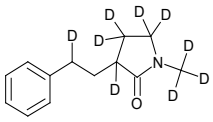
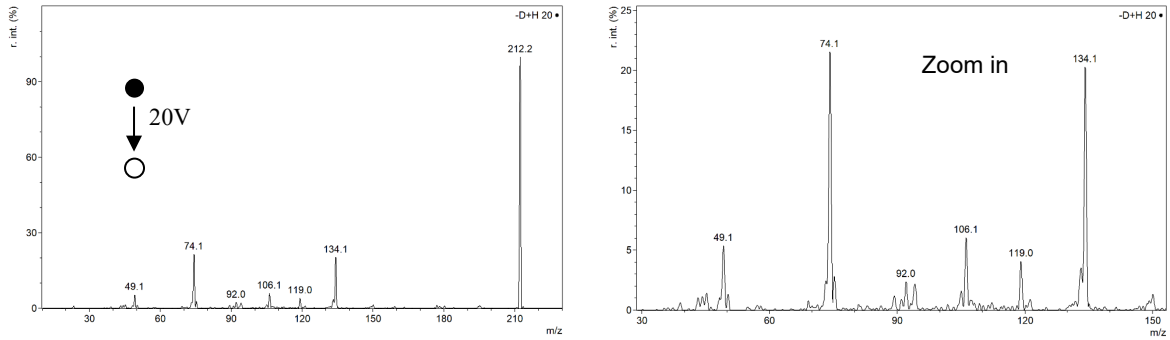


Figure S55. Comparison of the MS/MS fingerprints (top, black line: **20a-d$_9$ (main component)** $C_{13}H_8D_9NO$; bottom, red line: **20a** $C_{13}H_{17}NO$) and assignment of fragments.



Structure of **20a-d$_9$** hypothesized from *m/z* 92 fragment:

ESI-MS/MS, 20a-d$_9$ (analysis of minor component, 2.3% abundance)



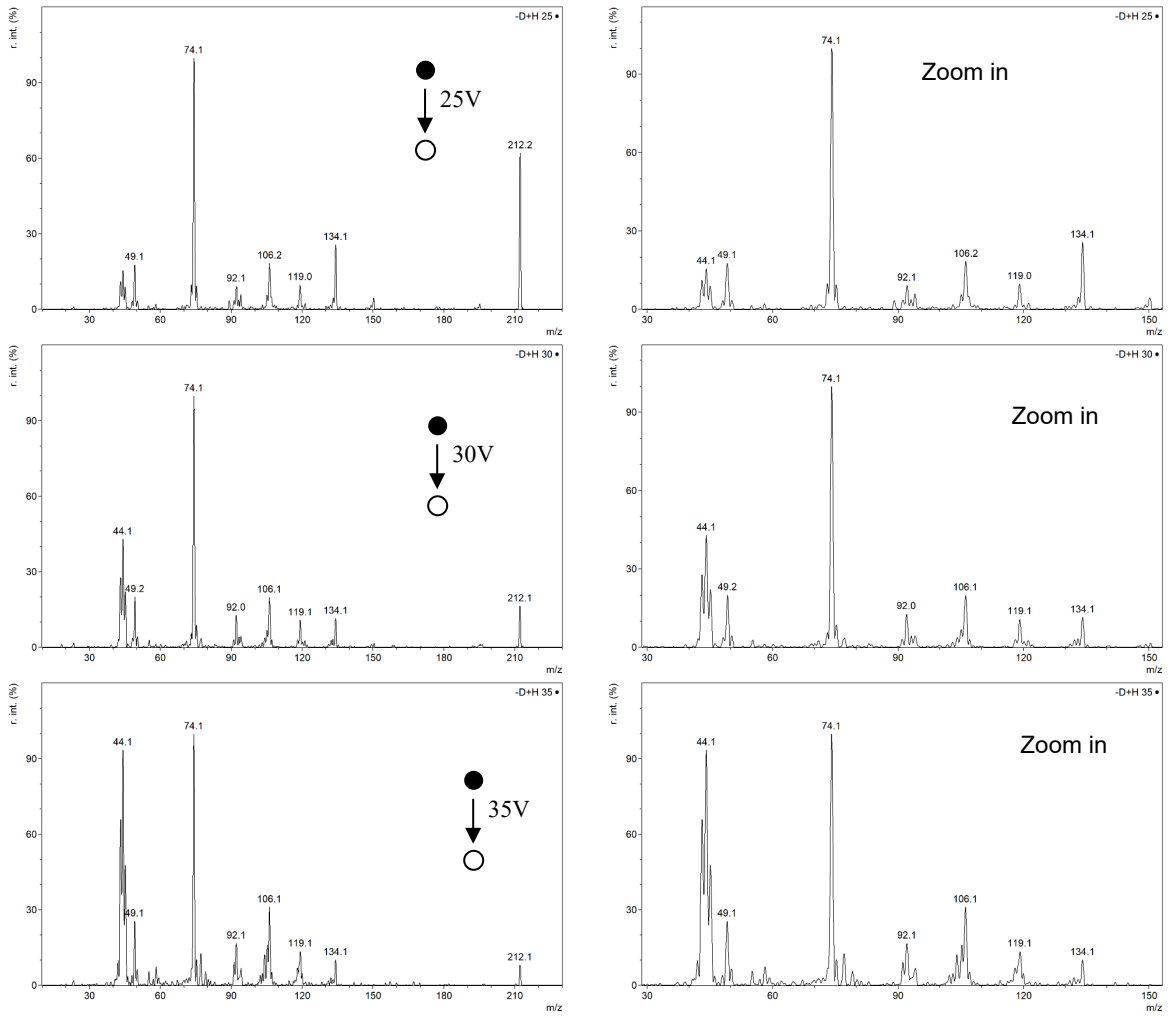


Figure S56. ESI-MS/MS fragmentation of **20a-d$_9$** (minor component).

Possible structures:



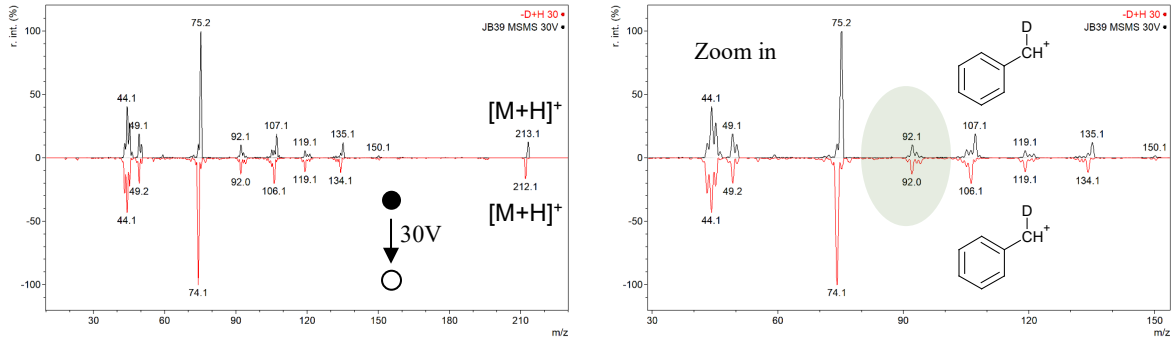
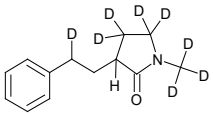


Figure S57. Comparison of the MS/MS fingerprints (top, black line: **20a-d$_9$** (main component) $C_{13}H_8D_9NO$; bottom, red line: **20a-d$_9$** (minor component) $C_{13}H_9D_8NO$).



Structure of the minor -D+H in **20a-d$_9$** hypothesized from *m/z* 92:

ESI-MS/MS, 20a-d$_{10}$ (analysis of main component)

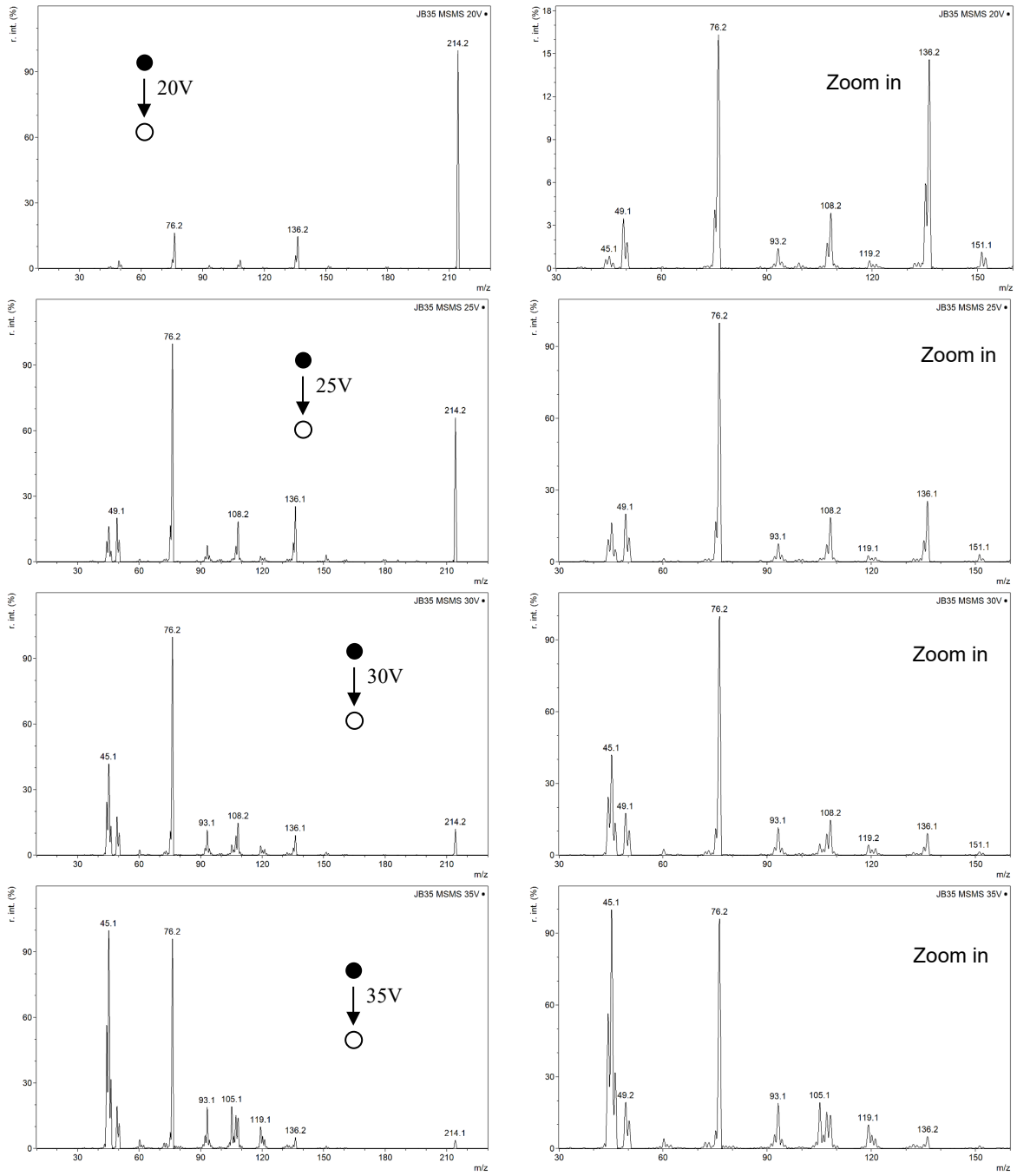
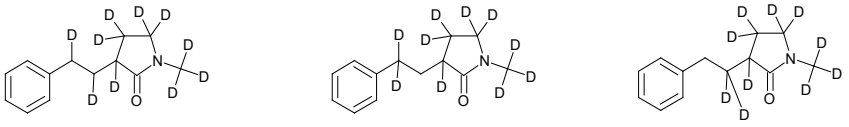


Figure S58. ESI-MS/MS fragmentation of **20a-d$_{10}$** (main component) and possible structures.

Possible structures:



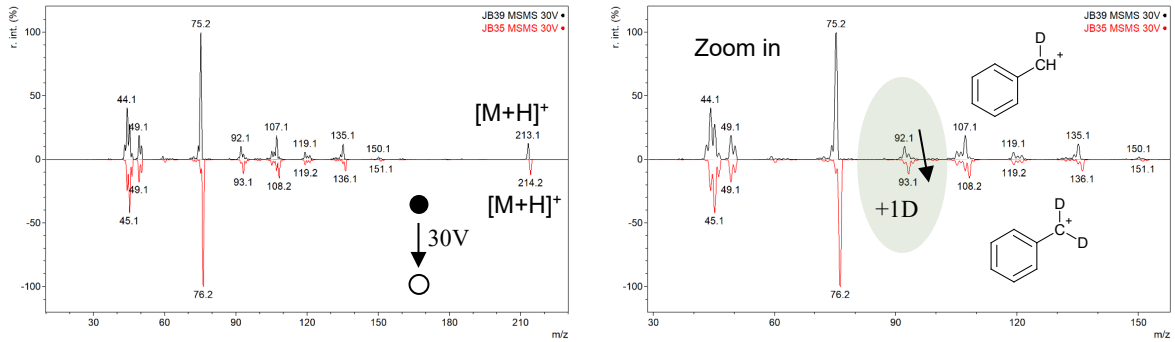
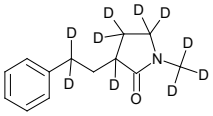


Figure S59. Comparison of the MS/MS fingerprints (top, black line: **20a-d$_9$** $C_{13}H_8D_9NO$; bottom, red line: **20a-d$_{10}$** $C_{13}H_7D_{10}NO$) and hypothesized structure.



Structure of **20a-d$_{10}$** hypothesized from *m/z* 93:

The structure of **20a-d$_9$** (2.3% abundance of the **20a-d$_{10}$**) in this reaction was assumed to be identical to that found above for the previous reaction where **20a-d$_9$** was the product. In this case, the possibility of **20a-d$_9$** having 2x D atoms at the benzylic position and 1x H atom α-to the amide cannot be excluded.

The structure **20a-d7** (<1.0% abundance), was assumed to be consistent with that found above the minor components of **20a-d6**. That is, an *N*-CH_3 group instead of an *N*-CD_3 group.

9.4. HRMS-MALDI Spectra and Analysis for the KO*t*Bu-catalyzed Reactions of cyclohexanone (25) or α-tetralone (27) with Styrene

The previously-described[3] reaction below was repeated in our hands according to **Procedure D**.

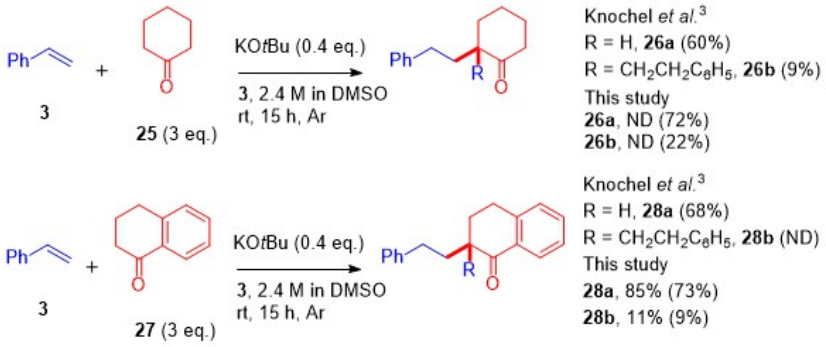
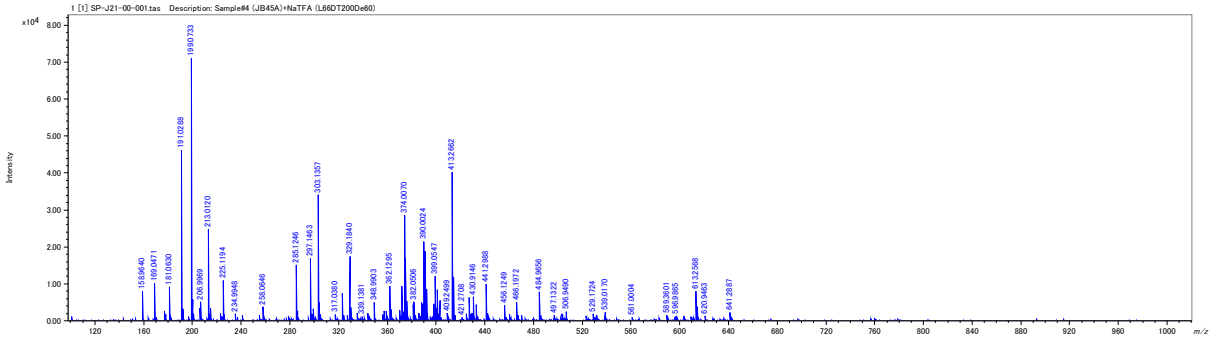


Figure S60. KO*t*Bu-catalyzed reaction of cyclohexanone or α-tetralone with styrene under previously reported conditions.[3] ND, not determined. Yields were determined by ^{1}H NMR by comparison to 1,3,5-trimethoxybenzene (1.0 eq.) as an internal standard. Isolated yields are in parenthesis.

Because the ratio of **26a** : **26b** could not be determined directly by ^{1}H NMR of the crude reaction products and the isolated yields were affected by purification, it was deemed useful to compare the ratios of **26a** : **26b** and **28a** : **28b** by mass spectroscopy. The ionization responses of monoadduct (e.g. **26a**) and bisadduct (e.g. **26b**) are unknown and their absolute ratio (e.g. **26a** : **26b**) cannot be inferred. Also, structures **26a** and **28a** likely ionize differently due to the extra aromatic present in **28a**. However, we reasoned that the ratios of **26a** : **26b** vs **28a** : **28b** should be comparable because regardless of the parent structure, the same structural difference (an extra CH_2CH_2Ph unit) occurs in each case.

After workup of the reaction of **25**, a sample of the crude reaction products was taken and analyzed by HRMS-MALDI.

Whole mass spectrum (example spectrum):



Expansion (*m/z* 100-500):

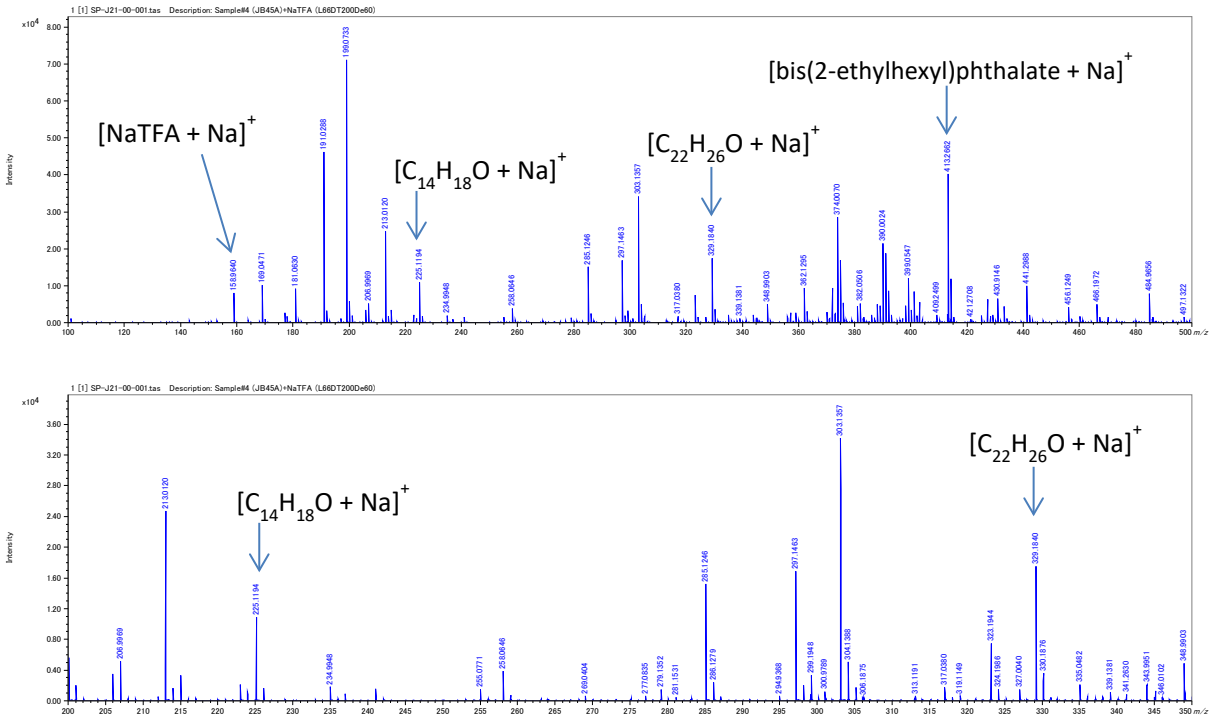
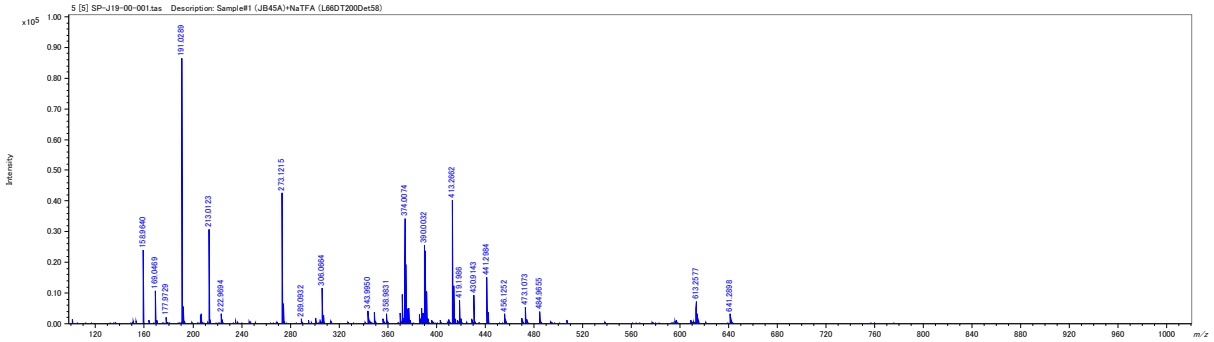


Figure S61. Mass spectrum of the reaction of **25** under previously reported conditions.[3]

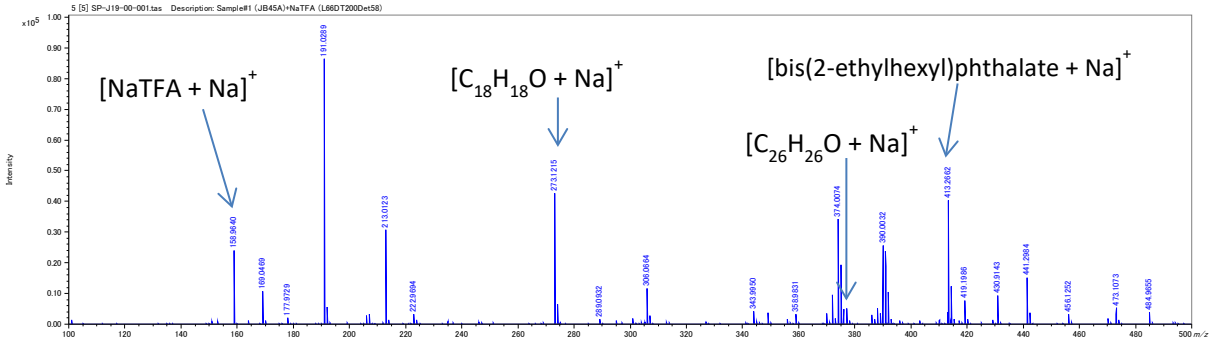
The analysis was repeated three times and the average ratio **26a** : **26b** = 1 : 1.81.

After workup of the reaction of **27**, a sample of the crude reaction products was taken and analyzed by HRMS-MALDI.

Whole mass spectrum (example spectrum):



Expansion (*m/z* 100-500):



Expansion (*m/z* 250-400):

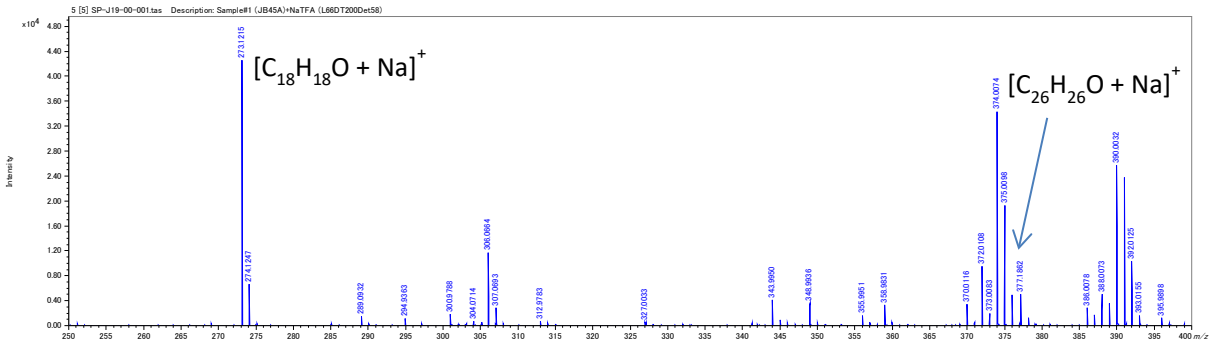


Figure S62. Mass spectrum of the reaction of **27** under previously reported conditions.[3]

The analysis was repeated three times and the average ratio **28a** : **28b** = 1 : 0.17. Therefore, the change in ratios from **26a** : **26b** to **28a** : **28b** supports that the bisadduct/monoadduct ratio is lower in the reaction of α-tetralone (**27**) which is in line with conclusions from computation. It is noted that this analysis is tentative and that the exact ionization responses would be necessary for firm conclusions about product composition to be drawn from the mass spectra.

10. COMPUTATIONAL INVESTIGATION

All calculations were performed using Density Functional Theory (DFT)[6,7] using the Gaussian09 software package.[8] All minima (reactants, intermediates, products) and maxima (transition states) were optimized using the UB3LYP functional with a 6-31+G(d,p) basis set on all atoms,[9] except bromine for which the Stuttgart/Dresden Effective Core Potential MWB28[10] and associated valence basis sets were used. Solvation was modelled implicitly using the Conductor-like Polarisable Continuum Model (CPCM)[14,15] for a solvent of *N*,*N*-dimethylacetamide, dimethyl sulfoxide or benzene, as specified. Frequency calculations were performed on all optimized structures in order to characterize minima (zero imaginary frequencies) and maxima (single imaginary frequency). All calculations were repeated (optimization and frequency) at the M06-2X functional with a 6-31++G(d,p) basis set on all atoms, except bromine which used the pseudopotential specified above. Solvation was modelled implicitly using the CPCM as specified above. This was deemed an acceptable working level of theory used by recent studies.[11-13] All profiles are plotted using the Gibbs free energy values. GaussView 5.0.9 was used for the visualisation of structures. Pictures are shown for UB3LYP/6-31+G(d,p) optimized structures.

10.1. REACTIONS OF *N*,*N*-DIMETHYLACETAMIDE (DMA, 1) WITH VARIOUS STYRENES

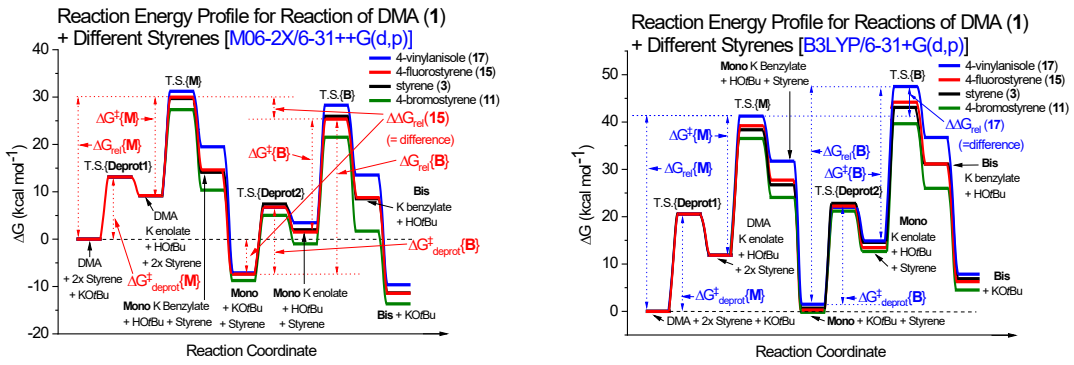


Figure S63. Left: M06-2X/6-31++G(d,p) computed reaction profile for KO*t*Bu-catalyzed reaction of DMA (**1**) with styrene (**3**, black line), 4-bromostyrene (**11**, green line), 4-fluorostyrene (**15**, red line) and 4-vinylanisole (**17**, blue line). The transition states for reactions of monoadduct K benzylates or bisadduct K benzylates with proton sources are not shown. Right: B3LYP/6-31+G(d,p) profile.

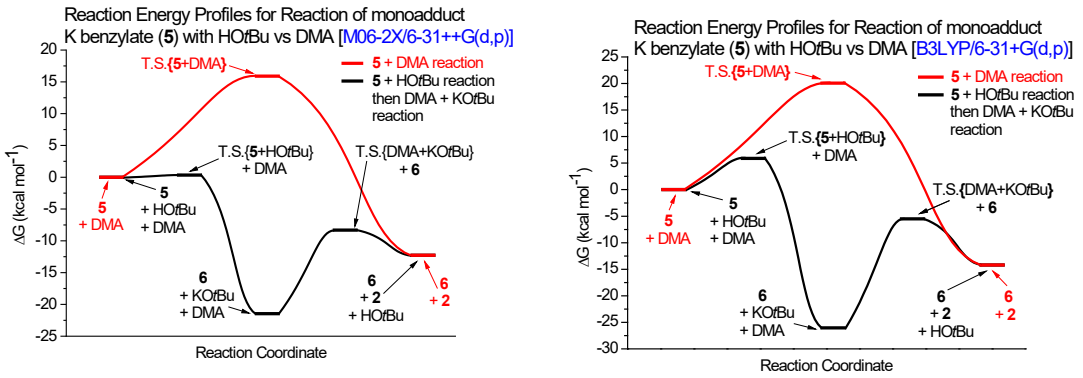


Figure S64. Left: M06-2X/6-31++G(d,p) computed reaction profile for reaction of DMA(**1**)/styrene monoadduct K benzylate (**5**) with HO*t*Bu affording **6** and KO*t*Bu, followed by deprotonation of DMA by KO*t*Bu to provide DMA K enol (**2**) (black line), vs reaction profile for the reaction of **5** with DMA to directly afford DMA K enol (**2**) (red line). Right: B3LYP/6-31+G(d,p) profile.

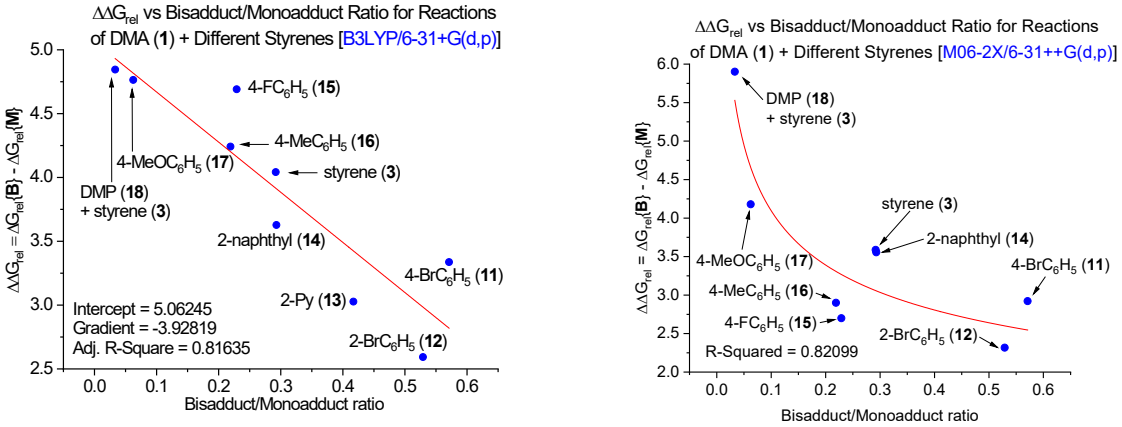
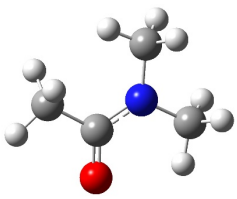


Figure S65. Comparison of B3LYP/6-31+G(d,p) and M06-2X/6-31++(d,p) methods for $\Delta\Delta G_{rel}$ vs Bisadduct/Monoadduct ratio.

10.1.1. XYZ Co-ordinates of starting materials, intermediates, products

***N,N*-Dimethylacetamide** (DMA, **1**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

15

-287.768153 [B3LYP/6-31+G(d,p)]

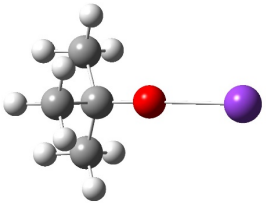
C	-0.72387200	-0.28658200	0.00000300
O	-1.07367300	-1.48168400	0.00004800
N	0.58802200	0.07717100	-0.00003300
C	1.63553600	-0.94008400	-0.00003000

H	2.26739800	-0.82909600	-0.88892500
H	2.26694000	-0.82962100	0.88926100
H	1.17901300	-1.92744800	-0.00042900
C	1.07476300	1.45370300	0.00003800
H	1.69189700	1.63265800	0.88833500
H	1.69173300	1.63281100	-0.88833900
H	0.25491200	2.16711800	0.00019000
C	-1.77546200	0.81158700	-0.00003300
H	-1.69474300	1.45085200	-0.88473800
H	-2.75481200	0.33350400	-0.00014200
H	-1.69489700	1.45075400	0.88475700

-287.620053 [M06-2X/6-31++G(d,p)]

C	-0.71530400	-0.29829100	-0.01276200
O	-1.05365500	-1.48758900	0.01258600
N	0.58653200	0.07885900	-0.07121100
C	1.63884700	-0.92183900	0.01430800
H	2.37491900	-0.74983400	-0.77599300
H	2.14581100	-0.85854400	0.98428500
H	1.20243100	-1.91114600	-0.10114600
C	1.03550400	1.46054900	0.01671900
H	1.28550600	1.72918000	1.05012000
H	1.93178500	1.57598500	-0.59761500
H	0.27945100	2.14748600	-0.35766500
C	-1.76131400	0.79741800	0.00827100
H	-1.73700200	1.38486000	-0.91369700
H	-2.73710000	0.32381900	0.10182700
H	-1.60869200	1.47986600	0.84846500

Potassium *tert*-butoxide, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

15

-832.974043 [B3LYP/6-31+G(d,p)]

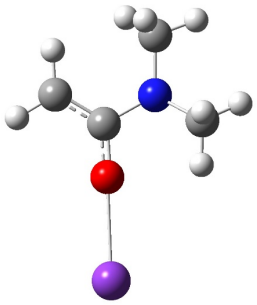
C	-1.67616000	1.41249600	0.36175500
C	-1.14228600	-0.00044200	-0.00180800
H	-1.28905800	1.71624500	1.34244800
H	-1.32896100	2.14382600	-0.37894800
H	-2.77367500	1.45854000	0.39841800
C	-1.73226900	-0.39720000	-1.38307800
C	-1.67863200	-1.00478200	1.05546800
H	-1.38422100	-1.39930700	-1.66363500
H	-2.83130400	-0.40300700	-1.39134000
H	-1.38938200	0.30640800	-2.15227400
H	-2.77621600	-1.02235400	1.10945700
H	-1.33260300	-2.01841200	0.81665400
H	-1.29293000	-0.74239800	2.04864100
O	0.24289800	-0.00973700	-0.03420500
K	2.72796100	-0.00116200	-0.00262200

-832.823346 [M06-2X/6-31++G(d,p)]

C	1.67130900	-1.30415300	-0.62051900

C	1.12645200	0.00015500	0.00013700
H	1.30769800	-2.16456900	-0.04611200
H	1.30484900	-1.40266400	-1.64929900
H	2.76831100	-1.33947600	-0.63925700
C	1.67736900	1.18683200	-0.81951300
C	1.68015500	0.11376800	1.43688600
H	1.31843000	2.12962200	-0.38965900
H	2.77452300	1.21316300	-0.84288800
H	1.31148100	1.12268900	-1.85122800
H	2.77738700	0.11412700	1.46928800
H	1.32126500	1.04152800	1.89807500
H	1.31757300	-0.72779800	2.03904600
O	-0.25130600	0.00332700	0.00267100
K	-2.69067200	0.00037600	0.00045900

***N*,*N*-Dimethylacetamide K enolate** (**2**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

15

-887.122050 [B3LYP/6-31+G(d,p)]

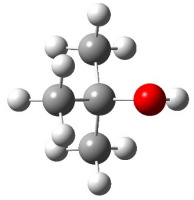
C	0.67368100	0.67294400	-0.03362600
N	1.56583300	-0.42228600	-0.27691500
C	1.14225300	-1.71969700	0.24169800
H	1.70201100	-2.51672900	-0.25911400
H	1.31820300	-1.81429300	1.33008600
H	0.07875400	-1.85837100	0.05321400
C	2.99677400	-0.20259900	-0.13324900
H	3.30147100	-0.00142100	0.91021700
H	3.53088300	-1.09516000	-0.47384600
H	3.31889500	0.63972100	-0.75014600
O	-0.58832000	0.38178500	-0.07954000
K	-3.05836700	-0.13554400	-0.02176600
C	1.17231100	1.94600200	0.19619800
H	2.22676300	2.17620400	0.26977000
H	0.46760500	2.76721300	0.28197700

-886.954597 [M06-2X/6-31++G(d,p)]

C	0.69901200	0.71433100	-0.02322600
N	1.46261700	-0.46241700	-0.30167500
C	0.94816100	-1.68072200	0.30613200
H	1.42851400	-2.54873500	-0.15475600
H	1.14742200	-1.71536800	1.39251300
H	-0.12695200	-1.74518200	0.14888200
C	2.90538400	-0.37239900	-0.19373800
H	3.24453600	-0.17337000	0.83821700
H	3.34470300	-1.31893400	-0.52057700
H	3.28623800	0.42156500	-0.83961500
O	-0.58111700	0.55251800	-0.04158200

K	-2.96665700	-0.12588100	-0.04380700
C	1.33446000	1.91544600	0.21279500
H	2.40802000	2.02660800	0.26377300
H	0.72251400	2.80198600	0.33651300

***tert*-Butanol**, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

15

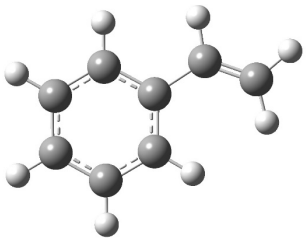
-233.601251 [B3LYP/6-31+G(d,p)]

C	0.67550400	1.26560200	-0.52886300
C	-0.00658900	-0.00000400	0.00965100
H	0.19823900	2.16108000	-0.11800800
H	1.73702200	1.28283200	-0.25483700
H	0.61052500	1.30895400	-1.62134400
C	0.67686700	-1.26480900	-0.52898700
C	-1.50081600	-0.00079500	-0.31991300
H	0.20072700	-2.16085300	-0.11806100
H	0.61170900	-1.30820600	-1.62145500
H	1.73847400	-1.28083600	-0.25522100
H	-1.65447300	-0.00056400	-1.40331900
H	-1.98512200	-0.88963200	0.09743300
H	-1.98614000	0.88724200	0.09795500
O	0.05866100	0.00000000	1.46007500
H	0.98996200	0.00001700	1.72492400

-233.474165 [M06-2X/6-31++G(d,p)]

C	0.67060300	1.25813000	-0.52791800
C	-0.00603700	0.00000000	0.01463600
H	0.19503500	2.15162100	-0.11259000
H	1.73271900	1.27173900	-0.25870700
H	0.59717500	1.29796700	-1.61904200
C	0.67084000	-1.25798500	-0.52795200
C	-1.49327700	-0.00013700	-0.31490300
H	0.19546600	-2.15158000	-0.11262700
H	0.59738700	-1.29781900	-1.61907400
H	1.73296900	-1.27139000	-0.25878000
H	-1.64401300	-0.00008800	-1.39796600
H	-1.97366100	-0.88920600	0.10469100
H	-1.97384400	0.88878200	0.10479700
O	0.06206200	-0.00000700	1.44909800
H	0.99149300	-0.00001600	1.71333900

Styrene (**3**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

16

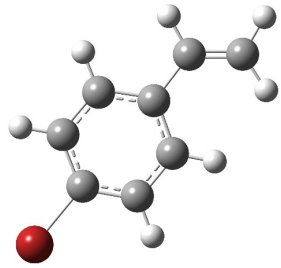
-309.575492 [B3LYP/6-31+G(d,p)]

C	-2.26930600	0.26209400	-0.00000600
C	-1.78359000	-1.04834400	-0.00000400
C	-0.40636200	-1.28422600	0.00000600
C	0.51580100	-0.22042700	-0.00000100
C	0.00937200	1.09486400	0.00000300
C	-1.36470900	1.33202700	0.00000600
H	-3.33884800	0.45050700	-0.00001000
H	-2.47420800	-1.88676200	-0.00000200
H	-0.03615200	-2.30645900	0.00002200
H	0.69124300	1.93963600	0.00001400
H	-1.73280700	2.35409300	0.00000200
C	1.95779400	-0.53100900	-0.00000500
H	2.18987300	-1.59569900	0.00000600
C	2.98244700	0.33673700	-0.00000300
H	2.84467700	1.41437600	-0.00001100
H	4.00753200	-0.01998300	0.00000700

-309.421947 [M06-2X/6-31++G(d,p)]

C	-2.25998100	0.26590200	-0.00000300
C	-1.78111000	-1.04279400	-0.00000200
C	-0.40739600	-1.28261400	0.00000100
C	0.51150900	-0.22449900	0.00000200
C	0.01545100	1.08861900	0.00000100
C	-1.35466600	1.33031800	-0.00000100
H	-3.32826500	0.45809300	-0.00000500
H	-2.47444100	-1.87817700	-0.00000200
H	-0.03809600	-2.30510300	0.00000200
H	0.70149200	1.93010000	0.00000200
H	-1.71944900	2.35291600	-0.00000200
C	1.95524300	-0.53645200	0.00000400
H	2.19162700	-1.59988500	0.00001000
C	2.96493700	0.34011600	-0.00000100
H	2.80981900	1.41514600	-0.00000900
H	3.99339400	-0.00466700	0.00000100

4-Bromostyrene (**11**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

16

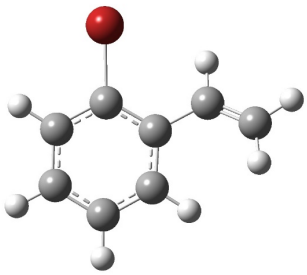
-2880.714673 [B3LYP/6-31+G(d,p)]

C	-1.31333800	1.37652400	0.00000700
C	-2.11868700	0.22343300	-0.00000900
C	-1.47688500	-1.03021600	-0.00000100
C	-0.08792300	-1.12851000	0.00000700
C	0.68062000	0.03816800	0.00003300
C	0.07979000	1.29515500	0.00002400
H	-1.78247300	2.35640800	0.00000500
H	-2.06043600	-1.94491500	-0.00001100
H	0.38990000	-2.10202300	-0.00000400
H	0.68165800	2.19715600	0.00002200
C	-3.58364600	0.38017000	0.00000300
H	-3.92753700	1.41376000	-0.00000800
C	-4.50936200	-0.59200000	0.00002400
H	-4.25804200	-1.64891700	0.00003900
H	-5.56644200	-0.34623100	0.00003500
Br	2.58571300	-0.09433100	-0.00001700

-2880.639190 [M06-2X/6-31++G(d,p)]

C	-1.30422300	1.37723900	0.00001900
C	-2.10509300	0.22798100	-0.00006300
C	-1.47183800	-1.02374700	0.00002000
C	-0.08602000	-1.12380500	0.00004300
C	0.68402100	0.03746900	0.00025600
C	0.08567100	1.29108800	0.00007200
H	-1.77344300	2.35740700	-0.00001400
H	-2.05813300	-1.93688700	-0.00001400
H	0.39561400	-2.09560300	0.00003100
H	0.69467700	2.18817700	0.00007100
C	-3.57284600	0.38329900	0.00002600
H	-3.92225200	1.41467800	0.00003700
C	-4.48041600	-0.59829400	0.00006800
H	-4.21002800	-1.65030500	0.00005100
H	-5.54009100	-0.36676900	0.00011000
Br	2.56908900	-0.09537400	-0.00008400

2-Bromostyrene (**12**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

16

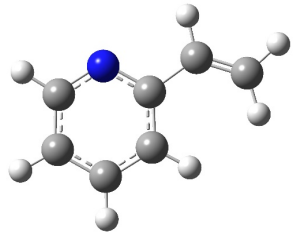
-2880.712786 [B3LYP/6-31+G(d,p)]

C	1.71532100	-2.13384700	0.06092100
C	0.35598200	-1.81833200	0.06527000
C	-0.04424200	-0.48404400	-0.00960300
C	0.88061600	0.57333400	-0.09905000
C	2.24574600	0.21723500	-0.10581400
C	2.66265700	-1.10856000	-0.02423200
H	2.02571600	-3.17247300	0.11718700
H	-0.38777200	-2.60457900	0.13025100
H	2.98758400	1.00376300	-0.19946100
H	3.72267700	-1.34224000	-0.03843800
C	0.45982100	1.98472400	-0.17174900
H	-0.54163600	2.15985000	-0.55501900
C	1.19474300	3.04333000	0.20162600
H	2.18847200	2.94851600	0.63042000
H	0.80392200	4.05037400	0.09555700
Br	-1.93208100	-0.13389300	0.00900800

-2880.638381 [M06-2X/6-31++G(d,p)]

C	1.76296500	-2.07901100	0.07622500
C	0.39798100	-1.80644900	0.07967000
C	-0.03594700	-0.48789000	-0.01847600
C	0.85607600	0.58714100	-0.12258100
C	2.22593800	0.27730800	-0.13076100
C	2.67892900	-1.03254500	-0.02854500
H	2.10596800	-3.10573200	0.14914300
H	-0.32708700	-2.60842900	0.16264900
H	2.94000000	1.08767000	-0.24089200
H	3.74450500	-1.23740000	-0.04218700
C	0.39619800	1.98653900	-0.22544600
H	-0.55499700	2.14789000	-0.72644500
C	1.06354900	3.03696800	0.26053200
H	1.99829000	2.92638200	0.80375600
H	0.67714400	4.04294300	0.13624000
Br	-1.90451300	-0.17559100	0.01183000

2-Vinylpyridine (**13**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

15

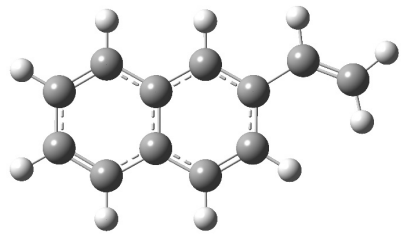
-325.626531 [B3LYP/6-31+G(d,p)]

C	-2.24412200	0.19997400	-0.00000200
C	-1.66739300	-1.07059000	-0.00000300
C	0.48371200	-0.21696100	0.00000000
C	-0.01470200	1.09912500	0.00000200
C	-1.39052800	1.30714100	0.00000100
H	-3.32285100	0.31479000	-0.00000400
H	-2.29518400	-1.95918200	-0.00000500
H	0.66446400	1.94452600	0.00000400
H	-1.79166500	2.31610700	0.00000200
C	1.92364900	-0.53983600	0.00000100
H	2.12928800	-1.60826500	0.00000400
C	2.94874400	0.32567600	0.00000000
H	2.81482000	1.40369800	-0.00000200
H	3.97282800	-0.03379500	0.00000200
N	-0.34398100	-1.28643500	0.00000000

-325.472034 [M06-2X/6-31++G(d,p)]

C	-2.23529400	0.20257300	-0.00000200
C	-1.66248800	-1.06631000	-0.00000300
C	0.47872500	-0.22045000	0.00000100
C	-0.00972900	1.09396500	0.00000200
C	-1.38215900	1.30497800	0.00000100
H	-3.31316700	0.31877700	-0.00000300
H	-2.29207400	-1.95260300	-0.00000400
H	0.67330000	1.93603400	0.00000400
H	-1.78097800	2.31448100	0.00000100
C	1.92104900	-0.54455400	0.00000200
H	2.12936300	-1.61227200	0.00000300
C	2.93184000	0.32899400	0.00000100
H	2.78128300	1.40458000	-0.00000100
H	3.95907400	-0.01935100	0.00000200
N	-0.34406600	-1.28354600	-0.00000100

2-Vinylnaphthalene (**14**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

22

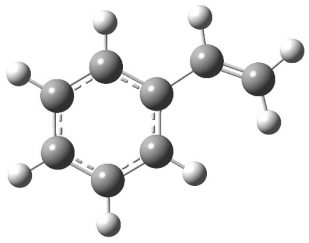
-463.185338 [B3LYP/6-31+G(d,p)]

C	3.07570400	-1.03729600	0.00000000
C	1.78128000	-1.51565600	-0.00000200
C	0.67498500	-0.61983300	-0.00000300
C	0.92733800	0.79130900	0.00000000
C	2.27120100	1.25321400	0.00000200
C	3.32367600	0.35944600	0.00000200
H	-0.85134900	-2.15090800	-0.00000800
H	3.91179500	-1.73050700	0.00000000
H	1.59036600	-2.58567500	-0.00000400
C	-0.66990300	-1.07834300	-0.00000600
C	-0.18806700	1.67879400	0.00000000
H	2.45844400	2.32395800	0.00000400
H	4.34700500	0.72318800	0.00000500
C	-1.47738300	1.20254300	0.00000000
C	-1.74642200	-0.20210300	-0.00000200
H	-0.00427300	2.75013000	-0.00000300
H	-2.30238000	1.90752600	-0.00000200
C	-3.11384600	-0.74749300	0.00000600
H	-3.16661800	-1.83582600	0.00003600
C	-4.26757000	-0.05927300	-0.00000300
H	-4.30899400	1.02609200	-0.00002000
H	-5.21994700	-0.57983100	0.00001100

-462.969057 [M06-2X/6-31++G(d,p)]

C	3.06743000	-1.03223400	-0.00000400
C	1.77916500	-1.51131800	-0.00000100
C	0.67442800	-0.61661700	0.00000100
C	0.92169400	0.78523300	0.00000000
C	2.26242000	1.25214700	-0.00000300
C	3.31236200	0.36428000	-0.00000500
H	-0.84783800	-2.15321600	0.00000500
H	3.90478000	-1.72290400	-0.00000600
H	1.58719000	-2.58103700	0.00000000
C	-0.66854800	-1.07988200	0.00000400
C	-0.19223600	1.67305100	0.00000200
H	2.44446300	2.32366400	-0.00000400
H	4.33441600	0.72974800	-0.00000800
C	-1.47575300	1.19595900	0.00000500
C	-1.73766200	-0.20767900	0.00000500
H	-0.00670400	2.74394700	0.00000300
H	-2.30372200	1.89750400	0.00000800
C	-3.10821200	-0.75186600	0.00000600
H	-3.16701500	-1.83953000	0.00002000
C	-4.24687000	-0.05031400	-0.00001000
H	-4.26941300	1.03531600	-0.00002600
H	-5.20545800	-0.55805100	-0.00000800

4-Fluorostyrene (**15**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

16

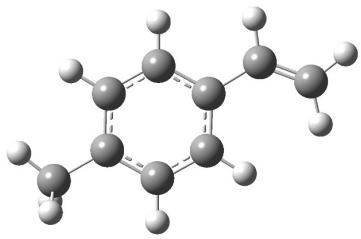
-408.826070 [B3LYP/6-31+G(d,p)]

C	-0.11795800	1.34164800	0.00000300
C	-0.97838900	0.22767400	-0.00000100
C	-0.39812500	-1.05691800	-0.00000700
C	0.98549900	-1.22600500	-0.00000800
C	1.79070200	-0.09170100	-0.00000400
C	1.27145900	1.19465700	0.00000100
H	-0.54119800	2.34219300	0.00000700
H	-1.02818400	-1.94025200	-0.00001200
H	1.43495100	-2.21306500	-0.00001300
H	1.93349700	2.05360600	0.00000400
C	-2.43529900	0.45521200	0.00000200
H	-2.72796300	1.50460500	-0.00001100
C	-3.40817900	-0.46986800	0.00001700
H	-3.20985100	-1.53798900	0.00002900
H	-4.45178900	-0.17189800	0.00001400
F	3.14803000	-0.25393200	-0.00000400

-408.643017 [M06-2X/6-31++G(d,p)]

C	-0.11580600	1.34037600	0.00000200
C	-0.97175500	0.23066200	-0.00000100
C	-0.39989000	-1.05141100	-0.00000700
C	0.97975700	-1.22294100	-0.00000700
C	1.78607700	-0.09266600	-0.00000300
C	1.26990200	1.19167600	0.00000200
H	-0.53999600	2.34063000	0.00000600
H	-1.03336400	-1.93244500	-0.00001100
H	1.43058300	-2.20928700	-0.00001200
H	1.93640400	2.04686300	0.00000500
C	-2.43075900	0.45868000	0.00000100
H	-2.72725900	1.50678700	-0.00000900
C	-3.38870300	-0.47389400	0.00001600
H	-3.17412700	-1.53863200	0.00002800
H	-4.43476800	-0.18700800	0.00001600
F	3.12995500	-0.25664500	-0.00000400

4-Methylstyrene (**16**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

19

-348.873606 [B3LYP/6-31+G(d,p)]

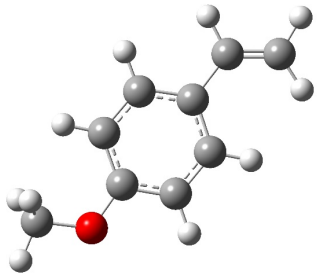
C	1.80134200	-0.07294300	-0.00026200
C	1.20821600	1.19599200	-0.00021800
C	-0.18186100	1.34306000	-0.00006600
C	-1.03545400	0.22650400	-0.00000800
C	-0.43647800	-1.05023000	-0.00015200
C	0.94797200	-1.19257500	-0.00030700
H	1.83777400	2.08230100	-0.00033000

H	-0.61218000	2.34160600	-0.00008300
H	-1.05651100	-1.94168900	-0.00024200
H	1.37876500	-2.19116700	-0.00053100
C	-2.49382800	0.43872700	0.00009700
H	-2.79755500	1.48543600	0.00009200
C	-3.45887100	-0.49557500	0.00022800
H	-3.24894700	-1.56158400	0.00025700
H	-4.50561100	-0.20834900	0.00032100
C	3.30185900	-0.24563200	0.00039500
H	3.63680400	-0.79819800	0.88604500
H	3.63610300	-0.81276500	-0.87618200
H	3.81399000	0.72044700	-0.00758400

-348.696178 [M06-2X/6-31++G(d,p)]

C	-1.79255800	-0.07159800	-0.00110600
C	-1.20608000	1.19490100	-0.00058600
C	0.18112700	1.34278900	0.00014100
C	1.02900900	0.22965700	0.00042000
C	0.43821500	-1.04483000	-0.00027200
C	-0.94280000	-1.18843600	-0.00097500
H	-1.83872300	2.07875100	-0.00111600
H	0.61311800	2.34065300	0.00028800
H	1.06119700	-1.93425000	-0.00058600
H	-1.37611300	-2.18600300	-0.00196000
C	2.48976600	0.44131500	-0.00006600
H	2.79832800	1.48633000	-0.00113000
C	3.43850000	-0.50142200	0.00066200
H	3.21092000	-1.56354600	0.00168800
H	4.48795600	-0.22686200	0.00019300
C	-3.28920900	-0.25019600	0.00109000
H	-3.61196900	-0.84843500	-0.85648500
H	-3.61828600	-0.77282800	0.90483700
H	-3.80224500	0.71309800	-0.04158100

4-Vinylanisole (**17**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

20

-424.078000 [B3LYP/6-31+G(d,p)]

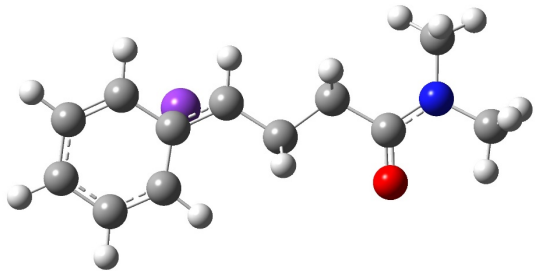
C	-0.50833700	-1.27859100	-0.00010100
C	-1.45175800	-0.23897700	-0.00008500
C	-0.95746500	1.08411700	-0.00017000
C	0.40523600	1.34533400	-0.00015100
C	1.33236300	0.28657300	-0.00007500
C	0.86926000	-1.03450500	-0.00008000
H	-0.85443700	-2.30923500	-0.00007000
H	-1.64692300	1.92270200	-0.00022300
H	0.77598600	2.36575600	-0.00019100
H	1.55687700	-1.87142000	-0.00010500

C	-2.88631100	-0.56879500	-0.00007600
H	-3.10222500	-1.63713400	-0.00034700
C	-3.92680800	0.28168000	0.00031700
H	-3.80745800	1.36166700	0.00068300
H	-4.94564400	-0.09254600	0.00035000
O	2.64941000	0.64792400	0.00003700
C	3.64132200	-0.38300500	0.00022000
H	4.60229100	0.13117000	0.00048100
H	3.56041800	-1.00871300	0.89594000
H	3.56081700	-1.00862400	-0.89560200

-423.877273 [M06-2X/6-31++G(d,p)]

C	-0.50037000	-1.27692700	-0.00005600
C	-1.44021500	-0.24347400	-0.00008400
C	-0.95697000	1.07791200	-0.00009700
C	0.40129600	1.34361500	-0.00005400
C	1.32846800	0.29001900	-0.00000500
C	0.87446900	-1.02945200	-0.00001200
H	-0.84552800	-2.30786900	-0.00006100
H	-1.65076300	1.91309200	-0.00015900
H	0.77268700	2.36350600	-0.00007000
H	1.56537600	-1.86369200	0.00001400
C	-2.87691500	-0.57434100	-0.00009800
H	-3.09756700	-1.64138600	-0.00035600
C	-3.90133300	0.28609200	0.00019300
H	-3.76277900	1.36350100	0.00048900
H	-4.92417000	-0.07473300	0.00014500
O	2.63810200	0.65188700	0.00003200
C	3.60925600	-0.38404100	0.00010700
H	4.57834500	0.11247000	0.00016400
H	3.51668100	-1.00819100	0.89526400
H	3.51679700	-1.00821600	-0.89504500

Styrene/DMA monoadduct K benzylate (**5**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-1196.673842 [B3LYP/6-31+G(d,p)]

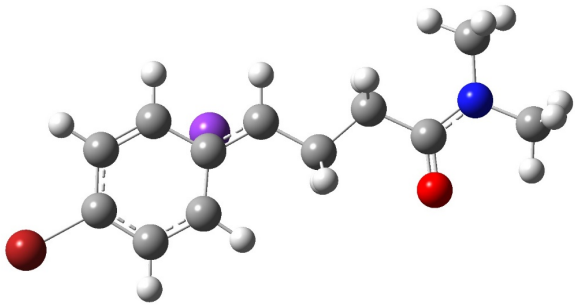
C	-4.73639300	-1.07178700	0.06629200
C	-4.37897500	-0.24030400	1.15294100
C	-3.06090600	0.10546100	1.40598300
C	-1.95792400	-0.35316900	0.58036800
C	-2.36088100	-1.21459900	-0.51671700
C	-3.69449500	-1.54628700	-0.74941400
H	-5.77161200	-1.33866800	-0.12384600
H	-5.15639500	0.14016000	1.81492400
H	-2.83280200	0.74616000	2.25774800
H	-1.59754700	-1.61921900	-1.17677100
H	-3.92844200	-2.19802700	-1.59111500

C	-0.63523300	0.04959300	0.79680200
H	-0.41303700	0.61465100	1.70297900
C	0.53334500	-0.50748600	0.01759100
H	0.43349100	-0.32623100	-1.06572400
H	0.60858100	-1.60847800	0.10000900
C	1.86275700	0.09444900	0.48273200
H	1.81613500	1.18897300	0.39398700
H	1.99997600	-0.10906400	1.55274200
C	3.08584700	-0.40943500	-0.27960300
O	2.97246000	-1.17826400	-1.25134300
C	5.52694500	-0.49547100	-0.47976000
H	6.09076300	-1.10542300	0.23743400
H	5.25788200	-1.10802600	-1.33765500
H	6.16579900	0.33203800	-0.80707700
C	4.52872400	0.86360000	1.31758700
H	3.66461000	1.49121400	1.52587000
H	4.75047300	0.25697000	2.20575800
H	5.38332900	1.51979900	1.12984600
N	4.31177600	0.02597100	0.14012000
K	-2.03737800	2.14316300	-1.08200100

-1196.368680 [M06-2X/6-31++G(d,p)]

C	-4.51610600	-0.53776500	0.77069000
C	-4.15150800	0.81958500	0.92674500
C	-2.83375400	1.22927100	0.91220300
C	-1.72906600	0.30336300	0.72079300
C	-2.13599700	-1.08993400	0.63611800
C	-3.47148400	-1.47006200	0.65604600
H	-5.55444000	-0.84916600	0.78594900
H	-4.92973600	1.57008800	1.05498300
H	-2.60095500	2.28702100	1.02406600
H	-1.37077900	-1.85524100	0.53758300
H	-3.70999400	-2.52934000	0.57057300
C	-0.41565100	0.71513700	0.58920300
H	-0.18372700	1.77514900	0.68499700
C	0.72365500	-0.24837000	0.39397100
H	0.56104600	-0.90126300	-0.47956600
H	0.83538200	-0.94620300	1.24250500
C	2.04466100	0.48858000	0.20555900
H	1.96441400	1.17367800	-0.64892300
H	2.24354100	1.12118400	1.08033600
C	3.23291400	-0.43406100	-0.01447200
O	3.09158500	-1.65996700	-0.08318700
C	5.64718500	-0.67740400	-0.23403400
H	6.19297100	-0.66957900	0.71741300
H	5.35857000	-1.69851600	-0.47259300
H	6.30529500	-0.28972200	-1.01647900
C	4.69623000	1.56865200	0.07834900
H	3.84504300	2.17013700	-0.23514500
H	4.91185600	1.77535800	1.13403700
H	5.56126600	1.87074200	-0.51607500
N	4.45467400	0.15080600	-0.14635700
K	-3.04692800	0.22199000	-1.98003600

4-Bromostyrene/DMA monoadduct K benzylate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-3767.817250 [B3LYP/6-31+G(d,p)]

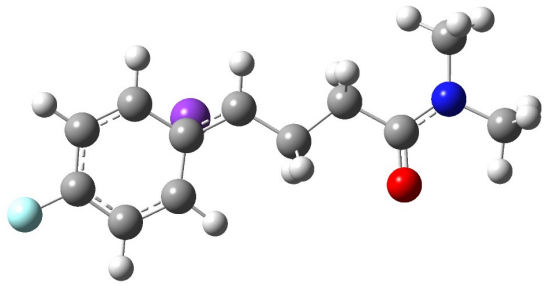
C	-3.34206900	-0.33052300	0.21106600
C	-2.89834400	0.53931100	1.22410100
C	-1.54433200	0.73456500	1.43555900
C	-0.52015900	0.07646600	0.64357900
C	-1.04222800	-0.82066800	-0.37251900
C	-2.40572200	-1.00877500	-0.57659600
H	-3.61915800	1.05984400	1.84944700
H	-1.23156900	1.41057700	2.22995200
H	-0.34839900	-1.37125800	-1.00162500
H	-2.73881400	-1.69281500	-1.35309400
C	0.84107800	0.32630400	0.81833600
H	1.14653600	0.95486300	1.65503900
C	1.92198300	-0.40817200	0.06096800
H	1.83382100	-0.26909300	-1.03006600
H	1.85836800	-1.50276700	0.19982200
C	3.31886500	0.04926100	0.49174600
H	3.40574800	1.13426700	0.34398800
H	3.43697500	-0.11332000	1.57122800
C	4.46505500	-0.64408500	-0.24079800
O	4.24827000	-1.49602600	-1.12096600
C	6.87618100	-0.96711900	-0.51779900
H	7.35144400	-1.65125700	0.19743000
H	6.53289300	-1.53513600	-1.37989300
H	7.61999000	-0.22948000	-0.83624300
C	6.08585900	0.61650400	1.19230900
H	5.25014600	1.25780000	1.46145500
H	6.40014100	0.05369500	2.08134900
H	6.91779600	1.25589800	0.88087700
N	5.74028100	-0.28458900	0.09604700
K	-0.29422800	2.49272800	-1.17632800
Br	-5.22659200	-0.60405000	-0.06982100

-3767.591937 [M06-2X/6-31++G(d,p)]

C	3.12450500	-0.25792400	-0.35691900
C	2.70346900	0.82805800	-1.14841000
C	1.36213800	1.09180500	-1.32540600
C	0.31515300	0.28837700	-0.71282700
C	0.81133300	-0.85396200	0.04006500
C	2.16355600	-1.10585900	0.20351600
H	3.44510000	1.46822600	-1.61910700
H	1.06996200	1.94406600	-1.93492400

H	0.10082200	-1.53582600	0.49727900
H	2.48106000	-1.97026100	0.78113800
C	-1.02630400	0.59075600	-0.81161800
H	-1.33282700	1.45149500	-1.40386500
C	-2.09327600	-0.26573800	-0.18593900
H	-1.93669100	-0.38624900	0.89856000
H	-2.08452900	-1.29494600	-0.58318100
C	-4.59772200	-0.51557200	0.19777600
O	-4.35521200	-1.55115100	0.82694800
C	-6.98950600	-0.88088100	0.47492100
H	-7.46515500	-1.38515200	-0.37500500
H	-6.63042800	-1.62793900	1.17898200
H	-7.73191600	-0.24373800	0.96270800
C	-6.21847600	1.05237800	-0.83723700
H	-5.44616300	1.81907200	-0.82366800
H	-6.37951700	0.72412900	-1.87151900
H	-7.14424000	1.49939300	-0.46883100
N	-5.87053400	-0.06621600	0.02715200
K	1.66259700	1.59719100	1.71761200
Br	4.97594200	-0.61304200	-0.11375300
C	-3.48192700	0.32069500	-0.40892500
H	-3.66992300	0.43433200	-1.48447200
H	-3.52508900	1.33316200	0.01300800

4-Fluorostyrene/DMA monoadduct K benzylate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-1295.922848 [B3LYP/6-31+G(d,p)]

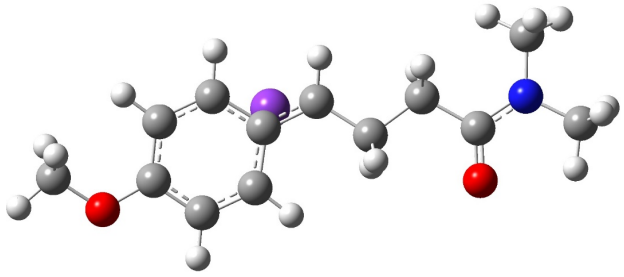
C	-4.40183100	-0.74982500	0.07567000
C	-4.05206900	0.00043000	1.20238500
C	-2.71365900	0.26658100	1.45809700
C	-1.63954200	-0.19620200	0.60114100
C	-2.08164200	-0.98208600	-0.53432400
C	-3.43220100	-1.24448300	-0.78531200
H	-4.82713600	0.36615600	1.87142200
H	-2.45651900	0.84957600	2.34087200
H	-1.34327100	-1.39321500	-1.21672600
H	-3.72582900	-1.83852200	-1.64759300
C	-0.29392100	0.13396600	0.83340600
H	-0.04422200	0.60262400	1.78615300
C	0.83930400	-0.47888900	0.04415800
H	0.74745900	-0.27826900	-1.03662700
H	0.85449200	-1.58472600	0.10927400
C	2.20157800	0.04340900	0.51070200
H	2.20913100	1.14055000	0.44611200
H	2.33607000	-0.19021000	1.57491100
C	3.39249900	-0.50350300	-0.27260300
O	3.23444500	-1.25310200	-1.25306000
C	5.82438600	-0.68625800	-0.51150000

H	6.35903700	-1.35403900	0.17614200
H	5.51967500	-1.24832200	-1.39171800
H	6.50398700	0.11963800	-0.80883100
C	4.91070200	0.67699800	1.32653700
H	4.06975500	1.32230000	1.57157700
H	5.13665100	0.04266600	2.19407300
H	5.77876900	1.31389700	1.13345100
N	4.64133400	-0.12597900	0.13600300
K	-1.31956400	2.34131300	-1.06072700
F	-5.74809500	-1.01435700	-0.17403800

-1295.588944 [M06-2X/6-31++G(d,p)]

C	-4.33439700	-0.71455700	0.14318200
C	-3.99647000	0.14176000	1.19269300
C	-2.66617800	0.42059500	1.44879700
C	-1.58283900	-0.13750800	0.66855800
C	-2.00845900	-1.02477500	-0.39089500
C	-3.35444700	-1.29694200	-0.64073900
H	-4.78270500	0.58228100	1.80047200
H	-2.41798300	1.09049100	2.26969400
H	-1.25961700	-1.50592900	-1.01361300
H	-3.64040900	-1.96800900	-1.44695300
C	-0.24861900	0.21690200	0.86883200
H	0.00877600	0.82628700	1.73389000
C	0.86876600	-0.41497300	0.08409900
H	0.75929800	-0.25636900	-1.00399200
H	0.89477600	-1.51526300	0.19146800
C	2.22470500	0.13790600	0.50743100
H	2.23433800	1.22791500	0.37391600
H	2.37491600	-0.03439700	1.58113300
C	3.39544100	-0.46157900	-0.25545800
O	3.22018000	-1.27431500	-1.16998500
C	5.81271000	-0.67597600	-0.49127700
H	6.30452600	-1.34043300	0.22935100
H	5.50730600	-1.25309700	-1.36095900
H	6.52439600	0.09693400	-0.79518700
C	4.90679900	0.79206600	1.26189000
H	4.11947200	1.53065000	1.40226500
H	5.01019900	0.19924800	2.17926600
H	5.84350100	1.32670700	1.08955900
N	4.64191000	-0.05422200	0.10735900
K	-1.51950500	2.02734400	-1.26666100
F	-5.66300700	-0.98333300	-0.10422900

4-Vinylanisole/DMA monoadduct K benzylate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1311.168384 [B3LYP/6-31+G(d,p)]

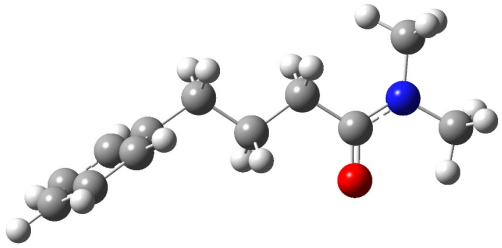
C	-4.03407500	-0.67047200	-0.05684100
C	-3.66572300	0.07459800	1.07728500
C	-2.32368900	0.33416500	1.35349600
C	-1.23873500	-0.12095400	0.52044200
C	-1.67159400	-0.89838800	-0.61900600
C	-3.01711100	-1.15186100	-0.88933400
H	-4.41883600	0.45697800	1.75965000
H	-2.08425400	0.91388400	2.24432900
H	-0.92695700	-1.30924200	-1.29574600
H	-3.29072700	-1.74303000	-1.76148000
C	0.11361000	0.21145900	0.76751300
H	0.35022800	0.61167200	1.75580000
C	1.24592900	-0.45784600	0.02101900
H	1.17787300	-0.28973400	-1.06632100
H	1.23730100	-1.56286100	0.12174700
C	2.61230600	0.04746900	0.49435600
H	2.64707300	1.14133000	0.39089300
H	2.72055600	-0.14983200	1.56900300
C	3.80577400	-0.55430500	-0.24316800
O	3.65192000	-1.33353300	-1.20110100
C	6.23781800	-0.80007900	-0.42372100
H	6.74011600	-1.45933400	0.29594300
H	5.93937500	-1.38125000	-1.29360400
H	6.94397100	-0.02034600	-0.72891200
C	5.32008800	0.64648200	1.34580100
H	4.48472100	1.30995400	1.55881700
H	5.52628800	0.03767000	2.23631000
H	6.19935900	1.26535400	1.14412400
N	5.05506900	-0.19138600	0.17878500
K	-0.89713300	2.45666800	-1.04807700
O	-5.34715300	-0.97954400	-0.42259900
C	-6.38590800	-0.54780000	0.44311200
H	-7.32016600	-0.89570900	-0.00158700
H	-6.28153300	-0.97974100	1.44782300
H	-6.41462200	0.54706900	0.52903900

-1310.815434 [M06-2X/6-31++G(d,p)]

C	-3.96061800	-0.65039400	0.01965900
C	-3.60840100	0.21815100	1.06321700
C	-2.27409200	0.48426200	1.34770200
C	-1.17825000	-0.08826600	0.61058300
C	-1.59401400	-0.99019000	-0.43675100
C	-2.93395700	-1.24613000	-0.71347400
H	-4.37195500	0.69801800	1.66824800
H	-2.04526100	1.16827500	2.16343100
H	-0.83834000	-1.49195100	-1.03543200
H	-3.19993400	-1.93082500	-1.51655200
C	0.16088600	0.26660000	0.82092800
H	0.41183900	0.85341800	1.70404800
C	1.28225300	-0.41075300	0.07965100
H	1.18841200	-0.29334900	-1.01447500
H	1.29959000	-1.50734200	0.23058300
C	2.63834000	0.14524800	0.49854300
H	2.65908600	1.22950100	0.32423700
H	2.77341900	0.01284500	1.58003000
C	3.81437500	-0.49101400	-0.22555000
O	3.64606500	-1.33162100	-1.11591500
C	6.23257800	-0.73659300	-0.41790100
H	6.70111400	-1.38990500	0.32814600
H	5.93539200	-1.33081700	-1.27884900

H	6.96109800	0.01840000	-0.72688000
C	5.31724800	0.79775500	1.27172500
H	4.53145700	1.54298800	1.38165400
H	5.40963800	0.23362800	2.20819200
H	6.25768700	1.32348300	1.09195600
N	5.05985700	-0.08326800	0.14192600
K	-1.16133000	2.07445900	-1.28979800
O	-5.26183000	-0.97279100	-0.34326200
C	-6.29222100	-0.41557400	0.44178500
H	-7.23125900	-0.79007500	0.03343100
H	-6.20615500	-0.72246900	1.49233300
H	-6.28821400	0.68102200	0.39129200

Styrene/DMA monoadduct (**6**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

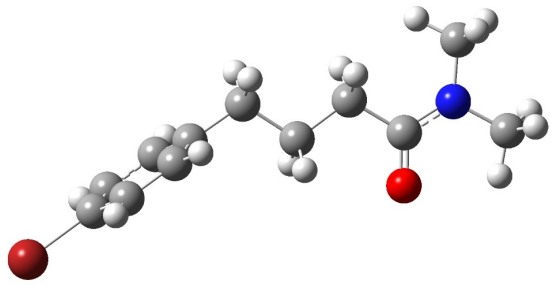
-597.342570 [B3LYP/6-31+G(d,p)]

C	-4.96826900	0.60012500	-0.05703800
C	-4.31221800	0.24501200	-1.24040200
C	-3.02915000	-0.30934000	-1.19290900
C	-2.37579900	-0.51847300	0.03245100
C	-3.04736800	-0.15921200	1.21212900
C	-4.33064200	0.39513600	1.17108500
H	-5.96654400	1.02694000	-0.09129300
H	-4.80018200	0.39444000	-2.19968800
H	-2.52993900	-0.58796000	-2.11818900
H	-2.56203300	-0.31956300	2.17216700
H	-4.83293700	0.66220400	2.09683900
C	-0.97255500	-1.08639900	0.07957700
H	-0.84420300	-1.66441900	1.00341800
H	-0.83380700	-1.78684000	-0.75368900
C	0.11736100	0.00289500	0.01131700
H	-0.01680800	0.70586900	0.84064400
H	-0.00321200	0.58284400	-0.91039200
C	1.52518400	-0.59548800	0.06501500
H	1.63850100	-1.18738100	0.98267100
H	1.66165800	-1.29910900	-0.76624200
C	2.63334200	0.45686500	0.01372000
O	2.35952500	1.66848500	-0.04178500
C	5.02455100	0.96830200	-0.08583200
H	5.53484400	0.83784400	-1.04846100
H	4.63309800	1.98130600	-0.02183700
H	5.75179800	0.80465700	0.71645100
C	4.32067200	-1.39003300	0.01015000
H	3.52751000	-2.03855200	0.37485900
H	4.59413700	-1.70102200	-1.00666300
H	5.19260600	-1.52700300	0.65655600
N	3.92409300	0.01593300	0.04165100

-597.053691 [M06-2X/6-31++G(d,p)]

C	-4.90504700	-0.63646000	0.04386500
C	-4.23698900	-0.36404200	1.23834200
C	-2.97165000	0.22180800	1.21398900
C	-2.35299500	0.54487900	0.00110400
C	-3.03299500	0.26678800	-1.18985800
C	-4.29858300	-0.31905300	-1.17178700
H	-5.89153900	-1.08946400	0.06101600
H	-4.70295500	-0.60421700	2.18944400
H	-2.45573500	0.43459300	2.14778200
H	-2.56478900	0.51451200	-2.14001900
H	-4.81209300	-0.52439300	-2.10638100
C	-0.96102100	1.12753500	-0.02361300
H	-0.84394900	1.76426200	-0.90900600
H	-0.81235900	1.76670300	0.85530300
C	0.11236100	0.03190500	-0.04025900
H	-0.03901200	-0.61601200	-0.91070700
H	-0.00016300	-0.60316300	0.84572300
C	1.51711800	0.62001400	-0.07540000
H	1.63800400	1.24408500	-0.97013600
H	1.67021900	1.28432900	0.78455100
C	2.59710400	-0.45296800	-0.07181900
O	2.29943600	-1.65187700	-0.09358500
C	4.96699300	-0.99932600	0.07189600
H	5.43759100	-0.91790200	1.05857200
H	4.56476300	-2.00170100	-0.05479600
H	5.72480900	-0.80830200	-0.69332300
C	4.27998000	1.36243500	0.09826700
H	3.56713500	2.03076900	-0.38149800
H	4.37507600	1.63775600	1.15582100
H	5.25001700	1.50229300	-0.38362200
N	3.88769100	-0.03146100	-0.05262800

4-Bromostyrene/DMA monoadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-3168.483164 [B3LYP/6-31+G(d,p)]

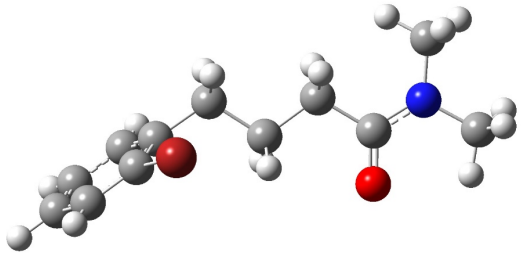
C	-3.30505600	-0.08333600	-0.00263500
C	-2.64717100	-0.30119200	-1.21202400
C	-1.31214000	-0.71273000	-1.18851500
C	-0.62879400	-0.90816800	0.02111300
C	-1.32440900	-0.68336400	1.21860200
C	-2.65953800	-0.27157500	1.21835000
H	-3.16114700	-0.15633000	-2.15601500
H	-0.79899000	-0.88872200	-2.13044000
H	-0.82093400	-0.83628800	2.16972600
H	-3.18320700	-0.10376500	2.15316700
C	0.82544500	-1.32459900	0.03364700
H	1.01998800	-1.93789900	0.92216300
H	1.02943400	-1.95832100	-0.83824300

C	1.79995500	-0.12922000	0.02511800
H	1.60636800	0.50839800	0.89445000
H	1.61653300	0.48744000	-0.86152600
C	3.25766600	-0.59679200	0.03900600
H	3.43590500	-1.21835200	0.92601000
H	3.44698900	-1.24374500	-0.82704400
C	4.26308600	0.55516400	0.02876500
O	3.87682200	1.73698300	0.02728900
C	6.59445300	1.29393100	-0.04893900
H	7.10329500	1.26711000	-1.02081200
H	6.11128800	2.26052600	0.07605300
H	7.34334200	1.15363900	0.73769200
C	6.11941000	-1.12150600	-0.06310300
H	5.37826000	-1.86250600	0.22640800
H	6.45843400	-1.34042200	-1.08403500
H	6.97616100	-1.21848400	0.61082600
N	5.58956800	0.23670400	0.03131500
Br	-5.13144900	0.49243600	-0.01863400

-3168.273180 [M06-2X/6-31++G(d,p)]

C	-3.27284600	-0.08176400	-0.00577300
C	-2.61375700	-0.29871600	-1.21088000
C	-1.28945800	-0.73099800	-1.18446700
C	-0.62089000	-0.94723500	0.02462700
C	-1.31383800	-0.72163100	1.21807300
C	-2.63839500	-0.28935300	1.21398700
H	-3.12445600	-0.13534500	-2.15341000
H	-0.77007200	-0.90502900	-2.12360600
H	-0.81356100	-0.88771000	2.16892700
H	-3.16823900	-0.11855000	2.14454700
C	0.82724700	-1.36351600	0.04109000
H	1.02420500	-1.97251200	0.93144100
H	1.03906900	-1.99259200	-0.83169100
C	1.77745100	-0.15911200	0.03574500
H	1.57044000	0.47758500	0.90268200
H	1.59240000	0.45216300	-0.85453700
C	3.23223800	-0.61047900	0.06093800
H	3.41616500	-1.22178900	0.95351400
H	3.44093500	-1.25507400	-0.80193900
C	4.20754000	0.55868200	0.05440500
O	3.79898300	1.72439500	0.07271800
C	6.51674800	1.32563500	-0.07170500
H	6.99052800	1.30385900	-1.06019900
H	6.02614900	2.28539800	0.07182000
H	7.29085500	1.19153900	0.68921900
C	6.06137700	-1.08760000	-0.10741400
H	5.37564600	-1.83015500	0.29489600
H	6.26457400	-1.31963800	-1.15989000
H	6.99906100	-1.15613500	0.44925000
N	5.53217500	0.26041900	0.03945800
Br	-5.07175100	0.51149800	-0.02544900

2-Bromostyrene/DMA monoadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-3168.481725 [B3LYP/6-31+G(d,p)]

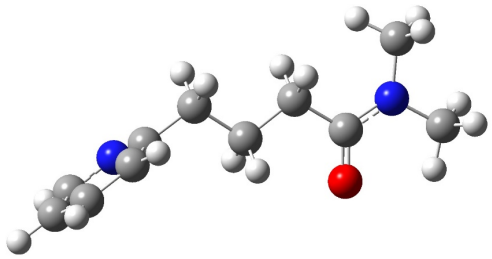
C	-4.27454900	1.44964600	-0.59916600
C	-3.78891800	0.14095600	-0.57231400
C	-2.53339700	-0.11600400	-0.01875200
C	-1.72381700	0.89782100	0.51439700
C	-2.24497800	2.20326800	0.47177900
C	-3.49846200	2.48526300	-0.07251400
H	-5.25218500	1.65072900	-1.02624600
H	-4.38319300	-0.67223600	-0.97440400
H	-1.64460300	3.01111400	0.88220900
H	-3.86640100	3.50667600	-0.08347500
C	-0.34282300	0.65866900	1.08175300
H	-0.11555700	1.46101700	1.79306300
H	-0.32665100	-0.27940000	1.64768400
C	0.75225900	0.62295600	-0.00399700
H	0.75421300	1.57340100	-0.54800000
H	0.52164900	-0.15629500	-0.73708400
C	2.13550500	0.36907000	0.59925000
H	2.36041000	1.14199400	1.34559400
H	2.13371200	-0.58480100	1.14194200
C	3.25142900	0.34736900	-0.44602300
O	3.00077900	0.54465700	-1.64780400
C	5.61873600	0.01483200	-0.96910900
H	5.99868800	-1.01367000	-1.01063100
H	5.26185600	0.30595100	-1.95473800
H	6.43855900	0.67476600	-0.66602100
C	4.88103400	-0.21327800	1.36874000
H	4.11089600	0.10020400	2.06947200
H	5.04766200	-1.29205400	1.48495600
H	5.80796200	0.30674200	1.62938400
N	4.52231600	0.11486700	-0.00900900
Br	-1.94004500	-1.94453900	0.00364400

-3168.273487 [M06-2X/6-31++G(d,p)]

C	-4.26166400	1.36680000	-0.63574500
C	-3.74138900	0.07587400	-0.60227500
C	-2.49553500	-0.14285400	-0.02007700
C	-1.73270000	0.89117300	0.53058900
C	-2.28611900	2.17727700	0.48210800
C	-3.53401200	2.42007800	-0.08451000
H	-5.23500400	1.54128300	-1.08235300
H	-4.29761200	-0.75734700	-1.01748400
H	-1.71701600	2.99991000	0.90774000
H	-3.93316500	3.42920700	-0.10311400
C	-0.35871400	0.68308900	1.11103200

H	-0.14043500	1.50549100	1.80109100
H	-0.33150200	-0.24275700	1.69649800
C	0.71961400	0.63913500	0.02099500
H	0.71641700	1.58585600	-0.52947800
H	0.48675400	-0.14695400	-0.70519100
C	2.09900600	0.39290900	0.61775200
H	2.32851300	1.16850900	1.35936100
H	2.11063800	-0.56268100	1.15723400
C	3.19279200	0.38089600	-0.44123600
O	2.92393300	0.58561400	-1.62960500
C	5.53728600	0.02168400	-0.99280400
H	5.86925600	-1.02104400	-1.05887600
H	5.18079300	0.34953400	-1.96652000
H	6.38595100	0.63918400	-0.68515300
C	4.81366900	-0.22011000	1.34280300
H	4.11360100	0.19939300	2.06224800
H	4.84206100	-1.30986900	1.46297900
H	5.80621800	0.17866200	1.56537100
N	4.46250300	0.14937600	-0.02059500
Br	-1.84365300	-1.92578900	0.00985300

2-Vinylpyridine/DMA monoadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-613.394025 [B3LYP/6-31+G(d,p)]

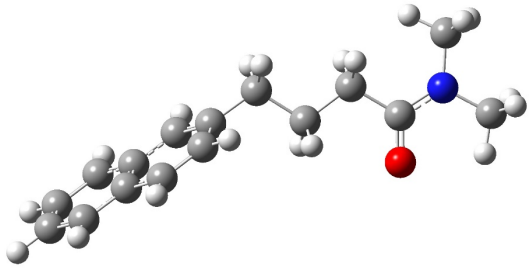
C	-4.90638100	-0.61898700	0.05609700
C	-4.40992300	0.09506800	1.14827100
C	-3.13655300	0.65739900	1.06032800
C	-2.38963100	0.49328200	-0.11632200
C	-4.09687600	-0.73258400	-1.07555500
H	-5.89176600	-1.07287800	0.07416000
H	-5.00338100	0.21439700	2.05000000
H	-2.72117700	1.22125600	1.89005900
H	-4.44903100	-1.27706500	-1.94932900
C	-0.99352400	1.05745300	-0.24787300
H	-0.87347800	1.45804800	-1.26150100
H	-0.86945800	1.89231000	0.45172000
C	0.09688100	-0.00072500	0.01595100
H	-0.04396600	-0.84414600	-0.66772400
H	-0.01506900	-0.39738900	1.03094700
C	1.50224500	0.57976800	-0.15909100
H	1.61114500	0.97805800	-1.17595700
H	1.63786900	1.43380400	0.51683300
C	2.61282200	-0.43926700	0.10046900
O	2.34031100	-1.60908200	0.42154300
C	5.00442000	-0.93122800	0.25776700
H	5.51553300	-0.62761200	1.18023200
H	4.61541800	-1.93992100	0.37950200
H	5.73033700	-0.91391400	-0.56176300
C	4.30601800	1.35739800	-0.31705400

H	3.48405100	1.94273800	-0.72155800
H	4.67268900	1.84685300	0.59454700
H	5.11553200	1.35378900	-1.05377200
N	3.90298500	-0.01948300	-0.04167100
N	-2.87080400	-0.19496500	-1.17071000

-613.105023 [M06-2X/6-31++G(d,p)]

C	-4.84740700	-0.63853400	0.10803400
C	-4.34347800	0.10162400	1.17464700
C	-3.08630900	0.68384400	1.05020100
C	-2.36673600	0.51038100	-0.13744000
C	-4.06112600	-0.75816900	-1.03543700
H	-5.82257200	-1.11008900	0.15388400
H	-4.92016900	0.22500700	2.08602500
H	-2.65926500	1.26945300	1.85838100
H	-4.42100600	-1.32506100	-1.89074700
C	-0.98115600	1.07916700	-0.30101200
H	-0.87013900	1.44606700	-1.32742500
H	-0.84874300	1.93088800	0.37532200
C	0.09272100	0.02159900	-0.01516900
H	-0.05983700	-0.83856900	-0.67492600
H	-0.01612500	-0.34445000	1.01171400
C	1.49471600	0.58294400	-0.21425200
H	1.60726500	0.94752100	-1.24303800
H	1.65044900	1.45129400	0.43798200
C	2.57957400	-0.44842300	0.06600200
O	2.28730000	-1.60900200	0.37186600
C	4.95126200	-0.93820700	0.31679900
H	5.39242600	-0.64029300	1.27524600
H	4.56257100	-1.95050100	0.39916600
H	5.72857100	-0.90445700	-0.45129600
C	4.25728900	1.34954600	-0.26477800
H	3.52915800	1.87432400	-0.88028600
H	4.37643900	1.88409700	0.68544200
H	5.21418100	1.36178000	-0.79086200
N	3.86866300	-0.03663900	-0.04706400
N	-2.85119200	-0.20330700	-1.16509100

2-Vinylnaphthalene/DMA monoadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-750.951206 [B3LYP/6-31+G(d,p)]

C	0.40499500	-0.04718100	-1.25429200
H	0.48189700	-1.05614200	-1.67687700
H	0.66819500	0.65346600	-2.05804400
C	1.42356900	0.10196300	-0.10538400
H	1.17561200	-0.60508900	0.69367500
H	1.34448200	1.10381000	0.33038900
C	2.85739300	-0.13930100	-0.58382700

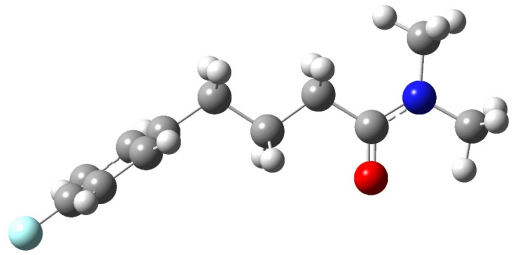
H	2.93422700	-1.14131500	-1.02527400
H	3.10263900	0.56540900	-1.38875700
C	3.89739500	-0.00326500	0.52920500
O	3.55251000	0.26916700	1.69237800
C	6.24945900	-0.01644100	1.20607400
H	6.86250200	0.86138400	0.96633400
H	5.78833400	0.12287700	2.18141300
H	6.90045200	-0.89692500	1.23022900
C	5.69997300	-0.43785800	-1.15440500
H	4.90402800	-0.76070800	-1.82077700
H	6.16062600	0.46880900	-1.56749700
H	6.45948800	-1.22567700	-1.12596200
N	5.20664800	-0.19905800	0.19964500
C	-1.02153600	0.20576800	-0.81591100
C	-1.89723500	-0.83530300	-0.56905800
C	-1.48245600	1.54174000	-0.62552300
C	-3.23206300	-0.60636800	-0.13055100
H	-1.56906200	-1.86272500	-0.71325000
C	-2.76731300	1.80297100	-0.20295900
H	-0.80369700	2.36747700	-0.82475700
C	-4.14026200	-1.67267200	0.12453200
C	-3.68030700	0.74260800	0.05841600
H	-3.10120700	2.82883300	-0.06846000
C	-5.42886000	-1.41802400	0.54730100
H	-3.80139100	-2.69562400	-0.01891600
C	-5.01524100	0.97260100	0.49394300
C	-5.87138900	-0.08262900	0.73390700
H	-6.11101900	-2.24129700	0.73890300
H	-5.35140100	1.99672400	0.63549700
H	-6.88804800	0.10512700	1.06678600

-750.600295 [M06-2X/6-31++G(d,p)]

C	0.41276700	-0.16891500	-1.27379500
H	0.48227900	-1.20125600	-1.63545700
H	0.68627200	0.48528200	-2.11170900
C	1.41053600	0.03819600	-0.12665600
H	1.15585400	-0.63066400	0.70228000
H	1.32463000	1.06050000	0.25839600
C	2.84221300	-0.21906000	-0.57840000
H	2.93310300	-1.24088600	-0.96863000
H	3.10036400	0.44982800	-1.40888900
C	3.85252000	-0.03050200	0.54515400
O	3.48264000	0.23423000	1.69394000
C	6.19074700	0.09454700	1.22054800
H	6.74060600	1.00585300	0.95846600
H	5.72251400	0.22302700	2.19356200
H	6.89661400	-0.74011800	1.26013100
C	5.64749300	-0.36587800	-1.13408900
H	4.94764100	-0.95111100	-1.72804500
H	5.82482500	0.59586900	-1.63052500
H	6.59207000	-0.91244200	-1.09182700
N	5.16387300	-0.17804100	0.22640700
C	-1.00392200	0.12430900	-0.84783800
C	-1.89622800	-0.88261200	-0.56034300
C	-1.42418400	1.47722100	-0.69586600
C	-3.21858300	-0.60156500	-0.11731400
H	-1.59525200	-1.92282500	-0.67182900
C	-2.69163700	1.78424100	-0.27097200
H	-0.72182500	2.27485200	-0.92730800
C	-4.14875100	-1.63516600	0.18061100

C	-3.62554300	0.75439500	0.03161700
H	-3.00123000	2.82071900	-0.16354200
C	-5.41979400	-1.33370800	0.60734800
H	-3.83571800	-2.66971200	0.06530000
C	-4.94653300	1.03672700	0.47325200
C	-5.82407200	0.01765300	0.75586000
H	-6.12169300	-2.13094200	0.83170800
H	-5.25036300	2.07455300	0.58386200
H	-6.83110300	0.24261500	1.09299100

4-Fluorostyrene/DMA monoadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-696.593788 [B3LYP/6-31+G(d,p)]

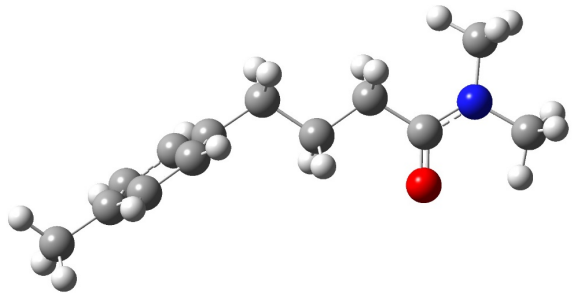
C	4.50338400	0.34324200	0.02528000
C	3.87357200	0.06553300	1.23094700
C	2.57202700	-0.44417700	1.19227300
C	1.90989800	-0.67185700	-0.02475900
C	2.59248300	-0.37792800	-1.21591600
C	3.89431700	0.13240800	-1.20433100
H	4.38891100	0.23893700	2.16968100
H	2.06807000	-0.67123200	2.12811800
H	2.10440300	-0.55257700	-2.17119600
H	4.42550900	0.35696700	-2.12317300
C	0.48633100	-1.18791900	-0.05147100
H	0.33565300	-1.79449300	-0.95310000
H	0.32301700	-1.85196400	0.80643100
C	-0.56226200	-0.05703100	-0.02261400
H	-0.40531800	0.60836900	-0.87856200
H	-0.41736600	0.55262300	0.87608900
C	-1.99068400	-0.60617700	-0.04975100
H	-2.13115400	-1.22297500	-0.94695800
H	-2.14682100	-1.27680800	0.80497300
C	-3.05960100	0.48682000	-0.02609900
O	-2.74114600	1.68857200	-0.00826000
C	-5.42998100	1.08838200	0.06347400
H	-5.94065000	1.00768900	1.03133700
H	-5.00209400	2.08375600	-0.03435900
H	-6.16608000	0.92588100	-0.73092800
C	-4.81322000	-1.29609600	0.03937500
H	-4.04489600	-1.98466800	-0.30462200
H	-5.09630700	-1.56416300	1.06571500
H	-5.69053600	-1.42176500	-0.60204400
N	-4.36557600	0.09277400	-0.03678400
F	5.78069700	0.83969300	0.04974600

-696.274841 [M06-2X/6-31++G(d,p)]

C	4.45089300	0.36501900	0.02697400
C	3.82026300	0.10510800	1.23315000

C	2.53492400	-0.43393900	1.20001700
C	1.89245600	-0.70861200	-0.01239800
C	2.57126300	-0.43204600	-1.20431800
C	3.85702400	0.10700900	-1.19793800
H	4.32729200	0.31856100	2.16790300
H	2.02418500	-0.64552700	2.13608600
H	2.08866900	-0.64130700	-2.15570500
H	4.39177200	0.32276300	-2.11655200
C	0.47768700	-1.23358900	-0.03503700
H	0.32990300	-1.85471900	-0.92665700
H	0.30841900	-1.87706200	0.83667000
C	-0.55113500	-0.09564200	-0.03327300
H	-0.37891100	0.55522600	-0.89756000
H	-0.40941100	0.52485000	0.85881300
C	-1.97734500	-0.62959500	-0.06748700
H	-2.12363300	-1.24421300	-0.96485800
H	-2.15332100	-1.29104700	0.79015000
C	-3.01550200	0.48434700	-0.05666400
O	-2.67057500	1.67061200	-0.06406600
C	-5.36216800	1.12554200	0.07212400
H	-5.83785200	1.06429200	1.05794800
H	-4.92090500	2.11120800	-0.05526500
H	-6.12538200	0.96282300	-0.69424600
C	-4.77789100	-1.26045200	0.08546900
H	-4.05986200	-1.96102600	-0.33559000
H	-4.95611000	-1.51712100	1.13686300
H	-5.71757500	-1.37042800	-0.46100000
N	-4.32232300	0.11529400	-0.04924000
F	5.70119600	0.89020900	0.04627800

4-Methylstyrene/DMA monoadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

34

-636.639013 [B3LYP/6-31+G(d,p)]

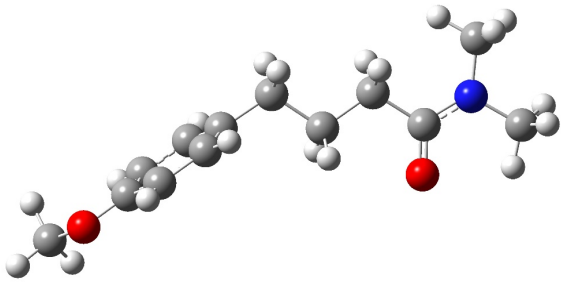
C	4.53857000	0.33130000	0.01618500
C	3.84659500	0.07264800	1.21017700
C	2.54318000	-0.42991100	1.19589000
C	1.87716000	-0.69015700	-0.01240000
C	2.56834800	-0.43103300	-1.20495400
C	3.87322300	0.07205400	-1.19096800
H	4.33448600	0.26324900	2.16354500
H	2.03589300	-0.62387300	2.13850000
H	2.08202200	-0.62524800	-2.15847400
H	4.38180100	0.26206300	-2.13338500
C	0.45040800	-1.19780300	-0.02671500
H	0.29503400	-1.82590600	-0.91311000
H	0.28183100	-1.83896900	0.84790500
C	-0.59321100	-0.06174300	-0.02592600

H	-0.43336400	0.58107200	-0.89852000
H	-0.44476000	0.56970400	0.85703200
C	-2.02460200	-0.60391500	-0.03825700
H	-2.17013600	-1.23931800	-0.92155600
H	-2.18149900	-1.25544500	0.83109400
C	-3.08934000	0.49333800	-0.03444200
O	-2.76676900	1.69411600	-0.03400900
C	-5.45622700	1.10810700	0.04062200
H	-5.94582900	1.07221100	1.02220200
H	-5.02819700	2.09689700	-0.10970800
H	-6.20992300	0.91343800	-0.72939500
C	-4.85205000	-1.27945600	0.06517500
H	-4.08229500	-1.97991700	-0.25013900
H	-5.14880100	-1.51885500	1.09476700
H	-5.72204000	-1.41900000	-0.58343600
N	-4.39732500	0.10500700	-0.04163200
C	5.96113300	0.84344100	0.03531000
H	6.10709500	1.58865200	0.82416300
H	6.67212800	0.02930400	0.22447300
H	6.23286400	1.30074600	-0.92064900

-636.327338 [M06-2X/6-31++G(d,p)]

C	4.48727700	0.33919700	0.02195400
C	3.79570200	0.08515800	1.21316000
C	2.50499300	-0.43696100	1.19681800
C	1.85852700	-0.72501100	-0.01134500
C	2.54850600	-0.47346800	-1.19977700
C	3.84217600	0.05018200	-1.18335000
H	4.27813000	0.29549300	2.16521000
H	1.99003500	-0.62853100	2.13596100
H	2.06946000	-0.69210800	-2.15188300
H	4.35809900	0.23280100	-2.12292900
C	0.43987500	-1.23920300	-0.02890600
H	0.28665600	-1.86898300	-0.91387200
H	0.26471400	-1.87172800	0.85006900
C	-0.58310600	-0.09591400	-0.03959900
H	-0.40974100	0.54242300	-0.91296300
H	-0.43602000	0.53571100	0.84383700
C	-2.01201400	-0.62332000	-0.06299100
H	-2.16306600	-1.25005900	-0.95123700
H	-2.18856500	-1.27228400	0.80407000
C	-3.04669700	0.49371100	-0.06518800
O	-2.69898500	1.67890900	-0.09232000
C	-5.39174900	1.14218700	0.06496900
H	-5.86779900	1.09156100	1.05123200
H	-4.94783600	2.12543500	-0.07159500
H	-6.15537100	0.97440700	-0.69997900
C	-4.81204600	-1.24459900	0.11109400
H	-4.10036000	-1.95221100	-0.30906600
H	-4.97931000	-1.48768800	1.16752600
H	-5.75800200	-1.35897900	-0.42345500
N	-4.35453600	0.12812500	-0.04612900
C	5.88387400	0.90839400	0.05135700
H	5.88790800	1.91266300	0.48713200
H	6.54857500	0.28695000	0.65901700
H	6.30422000	0.97485900	-0.95479200

4-Vinylanisole/DMA monoadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

35

-711.843782 [B3LYP/6-31+G(d,p)]

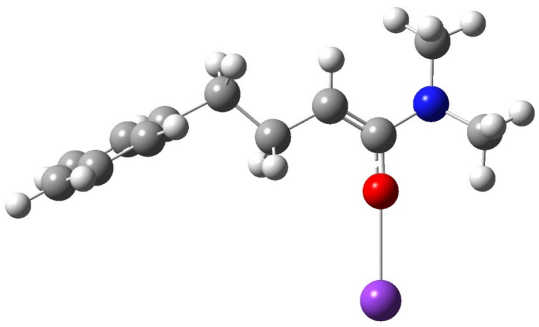
C	4.09836300	0.05317200	0.25666400
C	3.38945400	-0.55929700	1.30185300
C	2.07623300	-0.97853200	1.10298900
C	1.42762700	-0.80404800	-0.13253900
C	2.15423500	-0.19492700	-1.16228500
C	3.47594700	0.23505900	-0.98471300
H	3.88235000	-0.70300900	2.25871700
H	1.54530700	-1.45506400	1.92381200
H	1.68672500	-0.05033400	-2.13358600
H	3.99918400	0.69776500	-1.81307700
C	-0.01306300	-1.22805800	-0.32918100
H	-0.16134900	-1.54709300	-1.36884300
H	-0.22530800	-2.10173400	0.30039600
C	-1.02312200	-0.11034400	0.00199800
H	-0.81686200	0.76411600	-0.62474500
H	-0.88404300	0.21216300	1.03991200
C	-2.46907500	-0.56616300	-0.20852600
H	-2.60140300	-0.90224300	-1.24523300
H	-2.67811800	-1.44094100	0.42072300
C	-3.49937300	0.52178700	0.09628400
O	-3.14138100	1.65260200	0.46920000
C	-5.84793500	1.18101800	0.28485900
H	-6.36898700	0.87751700	1.20195500
H	-5.38649800	2.15371700	0.44127800
H	-6.58241000	1.24882200	-0.52422800
C	-5.31609300	-1.12739200	-0.39057300
H	-4.55802100	-1.72936300	-0.88626800
H	-5.65155200	-1.65347100	0.51283800
H	-6.16924500	-1.03283400	-1.06882800
N	-4.81714700	0.20728900	-0.06695100
O	5.38439200	0.43074400	0.54396800
C	6.15434100	1.05849700	-0.48328000
H	7.12665600	1.27046000	-0.03819000
H	6.28420000	0.39316200	-1.34445900
H	5.69007300	1.99592100	-0.81016500

-711.508661 [M06-2X/6-31++G(d,p)]

C	4.05855000	0.14165100	0.25323600
C	3.30202000	-0.11065500	1.40457800
C	1.99989100	-0.57814400	1.29098700
C	1.41360100	-0.80872000	0.03771300
C	2.18295300	-0.55054900	-1.09538400
C	3.49667300	-0.07946700	-1.00528700
H	3.75552700	0.06015000	2.37603600

H	1.42595000	-0.77547400	2.19381900
H	1.75480500	-0.72091600	-2.08064000
H	4.05849900	0.10393600	-1.91339700
C	-0.01719200	-1.27507000	-0.07558300
H	-0.15635000	-1.80077700	-1.02798100
H	-0.23485800	-1.99645100	0.72204900
C	-1.01616000	-0.11416800	0.00981400
H	-0.80093200	0.61291400	-0.78103700
H	-0.88831200	0.41214000	0.96230800
C	-2.45258600	-0.60518200	-0.11841800
H	-2.58243900	-1.12904200	-1.07379200
H	-2.67009900	-1.34029500	0.66684600
C	-3.46857500	0.52546300	-0.03283800
O	-3.10256700	1.69726300	0.10516500
C	-5.80249700	1.21058400	0.05176900
H	-6.27001800	1.11661400	1.03919900
H	-5.34691200	2.19394300	-0.03847800
H	-6.57452300	1.09147900	-0.71313500
C	-5.27014100	-1.18105800	-0.13916000
H	-4.54417600	-1.85887600	-0.58321700
H	-5.50719000	-1.52479300	0.87521300
H	-6.18170500	-1.22076300	-0.73983700
N	-4.78131700	0.19002000	-0.12835800
O	5.32744600	0.59540500	0.45975600
C	6.13468400	0.82908700	-0.68338100
H	7.09705600	1.17337100	-0.30783300
H	6.27332700	-0.09181200	-1.26030400
H	5.69520800	1.60052600	-1.32497400

Monoadduct K enolate (**7**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-1196.693213 [B3LYP/6-31+G(d,p)]

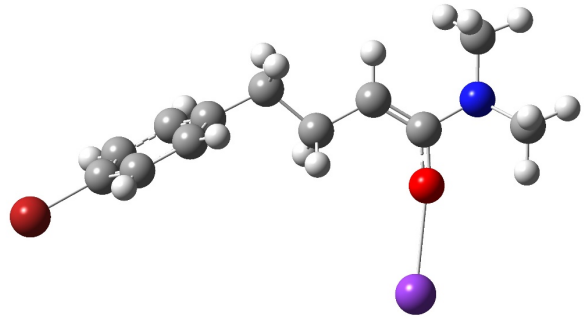
C	-2.23505300	-0.53507600	-0.10718900
N	-3.47283700	-1.25712300	-0.26951000
C	-4.59722700	-0.73307500	0.50172200
H	-5.53770000	-1.12583100	0.10003700
H	-4.54053300	-1.01698700	1.57086700
H	-4.60820800	0.35418800	0.43510100
C	-3.43390200	-2.71075700	-0.25666100
H	-3.15008700	-3.13162700	0.72657200
H	-4.42674200	-3.09613200	-0.51090500
H	-2.72467200	-3.08104100	-1.00139600
O	-2.34783900	0.75973800	-0.11081900
K	-2.44160400	3.27608500	0.01105000
C	-1.03325300	-1.20656500	-0.00167700
H	-1.00139700	-2.28896800	0.05505100

C	0.28739000	-0.47416100	0.03940000
H	0.34611500	0.28024000	-0.76134400
H	0.42114500	0.09816400	0.97468600
C	1.49484800	-1.42827300	-0.10238500
H	1.40775200	-1.96850500	-1.05386300
H	1.44446600	-2.18239400	0.69383300
C	2.83120600	-0.72157300	-0.04153100
C	3.42258900	-0.19379000	-1.20155600
C	3.50127200	-0.54233000	1.18007300
C	4.63907700	0.49384300	-1.14517000
H	2.92523100	-0.32711800	-2.15973000
C	4.71831700	0.14437400	1.24391100
H	3.06636500	-0.94959300	2.09013500
C	5.29222700	0.66692800	0.08008400
H	5.07825300	0.88976800	-2.05695000
H	5.21926500	0.26708500	2.20047300
H	6.23884300	1.19781700	0.12646600

-1196.388010 [M06-2X/6-31++G(d,p)]

C	-2.09989500	-0.61145400	0.05181000
N	-3.43074000	-1.00233600	-0.31625700
C	-4.47054500	-0.13496000	0.21811100
H	-5.41830000	-0.34602900	-0.28599500
H	-4.61758600	-0.28842400	1.30328000
H	-4.20151600	0.90652400	0.04907800
C	-3.78090400	-2.40151700	-0.17440000
H	-3.75526600	-2.74334900	0.87593700
H	-4.79367600	-2.55337600	-0.55807900
H	-3.09926200	-3.02690600	-0.75517200
O	-1.86679100	0.65809200	-0.00900500
K	-1.77245600	3.13027600	-0.02861800
C	-1.16298100	-1.55352800	0.41736600
H	-1.40856900	-2.60701900	0.46218800
C	0.26169100	-1.14322500	0.65952400
H	0.29198700	-0.16536000	1.15899600
H	0.76369100	-1.85642000	1.32794900
C	1.10606200	-1.02567700	-0.63267500
H	0.58671900	-0.33829100	-1.31046100
H	1.14393300	-2.00594700	-1.12252600
C	2.50314800	-0.52894900	-0.36521100
C	2.75866700	0.84295900	-0.24189700
C	3.56442600	-1.41969200	-0.16642900
C	4.03500900	1.31248000	0.06588100
H	1.94407400	1.54883400	-0.39348500
C	4.84428500	-0.95693200	0.14207700
H	3.38367800	-2.48861000	-0.25803300
C	5.08439100	0.41233200	0.25912800
H	4.21247200	2.38064500	0.15188900
H	5.65385500	-1.66612400	0.28809500
H	6.07980500	0.77519600	0.49621900

4-Bromostyrene/DMA monoadduct K enolate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-3767.835464 [B3LYP/6-31+G(d,p)]

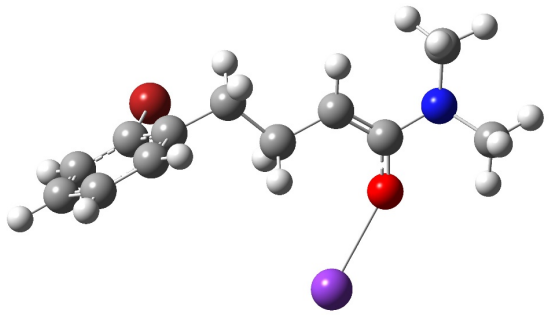
C	-3.87533800	-0.34578700	-0.14258900
N	-5.21302500	-0.87722100	-0.22845100
C	-6.20838600	-0.16125400	0.56630600
H	-7.21504800	-0.42799600	0.22680100
H	-6.13784700	-0.40591300	1.64419400
H	-6.06530200	0.91205900	0.44798400
C	-5.38805100	-2.31880100	-0.14635500
H	-5.11991600	-2.73417400	0.84350200
H	-6.43804500	-2.56209200	-0.33867900
H	-4.77939700	-2.82234300	-0.90179700
O	-3.78987300	0.94997800	-0.19033300
K	-3.21741300	3.40554100	-0.10897900
C	-2.78223600	-1.18499100	-0.05365000
H	-2.90168600	-2.26022600	0.01625300
C	-1.37210500	-0.64350500	-0.07700900
H	-1.15966400	-0.09358400	-1.01035200
H	-1.20811400	0.09470600	0.72563900
C	-0.31435500	-1.75835000	0.07161600
H	-0.44764800	-2.48425200	-0.74067400
H	-0.49996600	-2.29805500	1.00912200
C	1.10776200	-1.24714200	0.05933800
C	1.82394800	-1.13022700	-1.14192900
C	1.74006500	-0.84297000	1.24541300
C	3.12638200	-0.62438500	-1.16936200
H	1.36099800	-1.44307000	-2.07441900
C	3.04135600	-0.33381200	1.24215500
H	1.21106800	-0.92971600	2.19112000
C	3.71887600	-0.22860100	0.02851000
H	3.66548600	-0.54316500	-2.10697800
H	3.51499800	-0.02787500	2.16872600
Br	5.49867300	0.47943100	0.00563700

-3767.609992 [M06-2X/6-31++G(d,p)]

C	-3.97373900	-0.09427700	-0.16285900
N	-5.33720700	-0.51386200	-0.29181800
C	-6.28603500	0.32619500	0.42488200
H	-7.30255800	0.09174100	0.09532200
H	-6.23393400	0.16494400	1.51755600
H	-6.07361100	1.37341300	0.21776800
C	-5.61882900	-1.92273300	-0.10189300
H	-5.39741100	-2.26614200	0.92477300
H	-6.67882700	-2.10322600	-0.30093800
H	-5.03236700	-2.52604100	-0.79855800

O	-3.77158000	1.18020400	-0.24067800
K	-1.96975900	2.93832500	-0.03982700
C	-2.95964900	-1.01178600	-0.00262300
H	-3.14920400	-2.07360200	0.09727000
C	-1.52862600	-0.54726600	0.01008100
H	-1.28937200	0.04272700	-0.89166200
H	-1.31744100	0.12162800	0.86338100
C	-0.54018500	-1.72024900	0.08535600
H	-0.72508100	-2.39397500	-0.76003200
H	-0.73696200	-2.29160300	1.00072700
C	0.89527300	-1.26654500	0.06692700
C	1.57752600	-1.10261800	-1.14335300
C	1.56315500	-0.94528700	1.25333100
C	2.88806000	-0.63081300	-1.17870500
H	1.07741100	-1.35015600	-2.07653800
C	2.87350800	-0.47095900	1.24090100
H	1.05339200	-1.06926500	2.20564600
C	3.52028000	-0.31785500	0.01961100
H	3.40883300	-0.51063600	-2.12243200
H	3.38465400	-0.22737700	2.16578900
Br	5.30018700	0.33057000	-0.01380400

2-Bromostyrene/DMA monoadduct K enolate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-3767.834386 [B3LYP/6-31+G(d,p)]

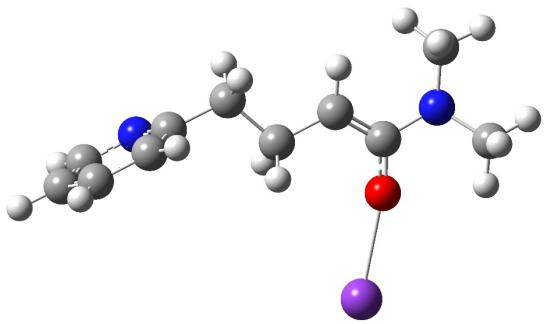
C	-3.02252000	-0.23825900	0.13086800
N	-4.26513500	-0.96487600	0.16629100
C	-5.45783200	-0.14234700	0.35225300
H	-6.34815800	-0.70937300	0.05937500
H	-5.58882900	0.17385700	1.40555900
H	-5.38322500	0.75033600	-0.26735700
C	-4.32225500	-2.19496800	0.93964100
H	-4.20848300	-2.03062000	2.02790000
H	-5.29087600	-2.67724600	0.77292000
H	-3.53924500	-2.88623600	0.61741100
O	-3.04609800	0.87692900	-0.53581800
K	-1.83377200	3.00589900	-1.24949200
C	-1.88822000	-0.73910400	0.74043200
H	-1.91592800	-1.64607900	1.33343200
C	-0.55918400	-0.03567400	0.60079900
H	-0.30358500	0.13154300	-0.45784900
H	-0.57464300	0.97168000	1.05314000
C	0.59264600	-0.82289300	1.26399100
H	0.64299700	-1.82451400	0.82254000
H	0.36146100	-0.95727100	2.32738300
C	1.93169300	-0.13438900	1.14575300
C	2.38621500	0.69612300	2.18659500

C	2.76253500	-0.22881500	0.01946400
C	3.59459000	1.39004600	2.11304700
H	1.76875800	0.78864900	3.07649800
C	3.97601200	0.45471500	-0.07914300
C	4.39473100	1.27053200	0.97367000
H	3.90978200	2.01773800	2.94116900
H	4.58929500	0.34923700	-0.96742100
H	5.33872600	1.80165500	0.89951600
Br	2.26508200	-1.35075800	-1.46016000

-3767.607420 [M06-2X/6-31++G(d,p)]

C	-2.96120600	-0.14628200	0.14198000
N	-4.20120700	-0.86271900	0.14449900
C	-5.37440600	-0.01900000	0.32029000
H	-6.27391700	-0.58308200	0.05640600
H	-5.48003000	0.32506900	1.36583700
H	-5.29512200	0.85352100	-0.32562600
C	-4.27468600	-2.05962100	0.95770700
H	-4.15762800	-1.85004300	2.03629000
H	-5.24885400	-2.53273600	0.80581300
H	-3.49922000	-2.76938200	0.66023800
O	-2.95674000	0.95962100	-0.52686100
K	-1.57169500	2.89947600	-1.32251600
C	-1.85184700	-0.64293900	0.78810200
H	-1.88255300	-1.55379800	1.37368900
C	-0.53641200	0.07674300	0.66661300
H	-0.23635500	0.18644100	-0.38920900
H	-0.58985900	1.10612000	1.06185500
C	0.59011100	-0.64709300	1.42097400
H	0.59842800	-1.70318700	1.12893800
H	0.38331700	-0.61245800	2.49630600
C	1.93662800	-0.03147800	1.15536500
C	2.48869300	0.89015700	2.05476600
C	2.67400900	-0.29436100	-0.00414600
C	3.71057900	1.51278200	1.81354100
H	1.93916700	1.11267200	2.96586900
C	3.89544000	0.31744900	-0.27135500
C	4.41516600	1.22919000	0.64476800
H	4.10912500	2.22052900	2.53360700
H	4.43458400	0.07727900	-1.18109500
H	5.36945800	1.70595300	0.44635500
Br	2.01376000	-1.53783300	-1.28102000

2-Vinylpyridine/DMA monoadduct K enolate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1212.745410 [B3LYP/6-31+G(d,p)]

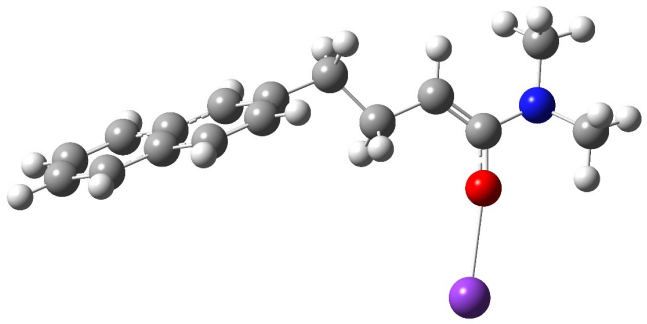
C	-2.29481500	-0.47326900	-0.11605300
N	-3.55036400	-1.16251500	-0.27892500
C	-4.66647900	-0.59749000	0.47521000
H	-5.61360200	-0.97148800	0.07136000
H	-4.62583000	-0.86667500	1.54881900
H	-4.64819900	0.48848500	0.39238500
C	-3.55069300	-2.61640100	-0.24723500
H	-3.28287100	-3.03165000	0.74282300
H	-4.55218500	-2.97836800	-0.50172000
H	-2.84805100	-3.01523700	-0.98339100
O	-2.36962200	0.82390200	-0.12990200
K	-1.98499900	3.31421500	0.03270200
C	-1.11182800	-1.17611800	0.00089900
H	-1.10667900	-2.25831100	0.06626600
C	0.22480800	-0.47348000	0.04389800
H	0.30879100	0.26870000	-0.76532600
H	0.36422100	0.10487800	0.97484100
C	1.40762100	-1.46058100	-0.07883700
H	1.32281500	-2.00575200	-1.02612200
H	1.34231000	-2.19799400	0.73083800
C	2.75416500	-0.78075100	-0.02989000
C	3.45588600	-0.63746400	1.17881400
C	4.42066900	0.34876900	-1.16797700
C	4.68074900	0.02835600	1.18904200
H	3.04157100	-1.04914400	2.09429800
C	5.17987600	0.53687300	-0.01225300
H	4.77708900	0.72474600	-2.12501100
H	5.23673700	0.14524000	2.11481900
H	6.12961300	1.05981300	-0.05741100
N	3.23986100	-0.29023000	-1.18869000

-1212.438915 [M06-2X/6-31++G(d,p)]

C	-2.43716100	-0.24445900	-0.10868000
N	-3.75889100	-0.76936200	-0.28629300
C	-4.76603700	-0.12807100	0.54685200
H	-5.76396400	-0.39613300	0.18713300
H	-4.68618900	-0.44445700	1.60343600
H	-4.64464500	0.95258800	0.49756900
C	-3.90707100	-2.21064200	-0.28974600
H	-3.64252500	-2.66878500	0.68043100
H	-4.94867200	-2.45974100	-0.51139900
H	-3.27644100	-2.65650600	-1.06233500
O	-2.35501800	1.04393800	-0.04101600
K	-0.89965400	3.08154100	0.00959800
C	-1.34173200	-1.07552700	-0.05284000
H	-1.43354400	-2.15490600	-0.06886700
C	0.04045100	-0.48336700	0.01569500
H	0.19860600	0.25037200	-0.79183500
H	0.20536800	0.07556000	0.95392300
C	1.13782600	-1.55264400	-0.09634100
H	1.02463400	-2.08676800	-1.04635600
H	1.01653800	-2.28173700	0.71329700
C	2.51545800	-0.95034100	-0.03660900
C	3.22015000	-0.86862700	1.17110500
C	4.21385800	0.13315400	-1.14885400
C	4.46840700	-0.25651000	1.19286500
H	2.78654200	-1.28463000	2.07551100
C	4.98237300	0.25972200	0.00537800
H	4.58261900	0.51917000	-2.09641900
H	5.03157400	-0.18600400	2.11851900

H	5.95174400	0.74425900	-0.03196600
N	3.01214600	-0.45338000	-1.18054000

2-Vinylnapthalene/DMA monoadduct K enolate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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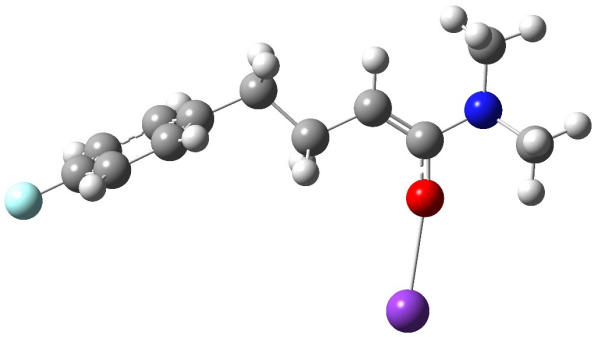
-1350.302699 [B3LYP/6-31+G(d,p)]

C	-3.49469700	-0.41368900	-0.17670300
N	-4.77748500	-1.03186000	-0.40782600
C	-5.89801300	-0.39897800	0.28388900
H	-6.84233900	-0.72159500	-0.16790300
H	-5.92918100	-0.66232800	1.35926400
H	-5.81403100	0.68371200	0.19759700
C	-4.86133500	-2.48318800	-0.36249700
H	-4.66664300	-2.89942900	0.64402500
H	-5.86757600	-2.79182300	-0.66395500
H	-4.14634100	-2.92993800	-1.05813500
O	-3.49255300	0.88563600	-0.20886000
K	-3.15489600	3.38362200	-0.18973000
C	-2.36490200	-1.18200100	0.02222500
H	-2.42628300	-2.26281100	0.08211300
C	-0.99174000	-0.56230900	0.13812100
H	-0.76299600	0.07956200	-0.72939700
H	-0.91438300	0.10877800	1.01074400
C	0.12180800	-1.62706000	0.25239500
H	0.09106000	-2.27249400	-0.63408900
H	-0.09617000	-2.26918500	1.11699500
C	1.50800400	-1.04167800	0.40070800
C	2.38601100	-0.97434100	-0.66607200
C	1.93126000	-0.51805500	1.65856200
C	3.68238800	-0.39974900	-0.54022900
H	2.08872400	-1.37275400	-1.63421400
C	3.17818700	0.04513400	1.82032800
H	1.25238000	-0.57376500	2.50615800
C	4.59145400	-0.32972400	-1.63386900
C	4.09109700	0.12370600	0.73093400
H	3.48219900	0.43333200	2.78939400
C	5.84279800	0.23120500	-1.47935400
H	4.28316100	-0.72660600	-2.59792400
C	5.38819600	0.69457200	0.85882100
C	6.24617300	0.74831100	-0.22075300
H	6.52563600	0.27822700	-2.32283600
H	5.69447500	1.08898100	1.82457500
H	7.23401200	1.18630900	-0.11092600

-1349.934185 [M06-2X/6-31++G(d,p)]

C	-3.60986200	-0.19147700	-0.20444900
N	-4.93589400	-0.68762100	-0.43053700
C	-5.97105100	0.05192100	0.27764700
H	-6.95255800	-0.21464100	-0.12589200
H	-5.97137200	-0.17732700	1.35939900
H	-5.80822000	1.12043800	0.14885900
C	-5.13729300	-2.11861100	-0.32358800
H	-4.95205800	-2.49974800	0.69699100
H	-6.17147700	-2.35237600	-0.59174300
H	-4.47639300	-2.64961400	-1.01247100
O	-3.48423000	1.09478200	-0.23821100
K	-1.95209800	3.07603800	-0.20996600
C	-2.55421500	-1.05018100	-0.00092800
H	-2.68816100	-2.12363000	0.05928800
C	-1.15573900	-0.50609200	0.12089600
H	-0.88303100	0.10487900	-0.75659200
H	-1.05294400	0.17122700	0.98676500
C	-0.11041800	-1.62292800	0.26118700
H	-0.16569900	-2.27789800	-0.61639300
H	-0.36488900	-2.23586300	1.13577600
C	1.29172400	-1.09104900	0.40838400
C	2.17052200	-1.06599500	-0.65053700
C	1.71711600	-0.55900900	1.66049200
C	3.48029500	-0.52602200	-0.52178500
H	1.86607000	-1.46868500	-1.61520300
C	2.97412700	-0.03336200	1.82185900
H	1.02646000	-0.58149100	2.50055300
C	4.39400800	-0.49779600	-1.61107300
C	3.89243400	-0.00046700	0.73572300
H	3.28735000	0.36191900	2.78494600
C	5.65482000	0.02686800	-1.45680200
H	4.07649000	-0.89887900	-2.57022200
C	5.20278600	0.53476800	0.86677200
C	6.06512400	0.54881500	-0.20318400
H	6.34344600	0.04321300	-2.29587700
H	5.51198800	0.93261600	1.83006200
H	7.06370000	0.95993900	-0.09312600

4-Fluorostyrene/DMA monoadduct K enolate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1295.945564 [B3LYP/6-31+G(d,p)]

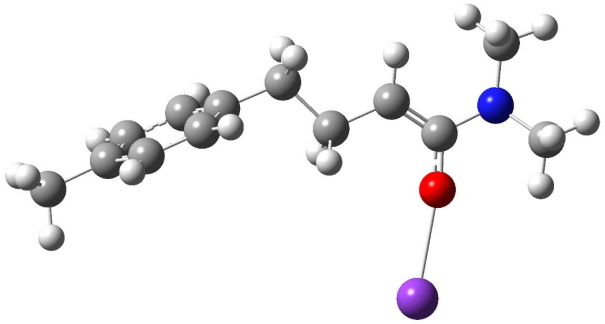
C	-2.71049800	-0.44416500	-0.11155300
N	-3.99463900	-1.08478900	-0.25099300
C	-5.07928500	-0.45935500	0.50144500
H	-6.04502600	-0.80013600	0.11260900
H	-5.04000500	-0.71020000	1.57952600

H	-5.01566800	0.62316100	0.39809700
C	-4.05363500	-2.53643700	-0.18696700
H	-3.79505900	-2.94020300	0.81028000
H	-5.07094200	-2.86296600	-0.42630300
H	-3.37365300	-2.97959400	-0.91895600
O	-2.73285400	0.85438900	-0.15471100
K	-2.36910700	3.34837300	-0.04626100
C	-1.55611500	-1.19130700	0.01489700
H	-1.59391500	-2.27142300	0.10210300
C	-0.19223400	-0.54292400	0.03542700
H	-0.08055400	0.17157000	-0.79641600
H	-0.02851900	0.05978100	0.94654900
C	0.95195300	-1.57710100	-0.05453800
H	0.83442000	-2.15700000	-0.97853600
H	0.85216300	-2.28759500	0.77655700
C	2.33142000	-0.95651100	-0.02128100
C	2.99884800	-0.61284700	-1.20810400
C	2.96923700	-0.67573900	1.19858300
C	4.25933500	-0.00648800	-1.19073000
H	2.53035900	-0.82507300	-2.16563700
C	4.22882400	-0.06947400	1.24372900
H	2.47853400	-0.93872000	2.13213300
C	4.84408600	0.25193600	0.04139600
H	4.77731000	0.25507100	-2.10750000
H	4.72385900	0.14392900	2.18534500
F	6.08149000	0.84235700	0.07221400

-1295.609862 [M06-2X/6-31++G(d,p)]

C	-2.85281800	-0.19855500	-0.13503700
N	-4.19759800	-0.68360500	-0.24555300
C	-5.14120500	0.00560400	0.62369100
H	-6.16387500	-0.24626600	0.32769900
H	-5.00925400	-0.28456000	1.68267100
H	-4.99724800	1.08118000	0.53817600
C	-4.38902600	-2.11946100	-0.20536600
H	-4.09555400	-2.56167200	0.76389700
H	-5.44639700	-2.34125200	-0.37523100
H	-3.80661000	-2.60314900	-0.99289700
O	-2.72528000	1.08785100	-0.11233000
K	-1.18572400	3.06393200	-0.09108300
C	-1.78454000	-1.06423800	-0.08826300
H	-1.91322100	-2.13989000	-0.07378400
C	-0.38229100	-0.51812200	-0.07077600
H	-0.18205700	0.11396900	-0.95363100
H	-0.21352600	0.14051900	0.79891500
C	0.67704200	-1.62928400	-0.03265300
H	0.55197200	-2.27265600	-0.91241200
H	0.50264900	-2.25705900	0.84983600
C	2.08226400	-1.08320700	0.00198000
C	2.76122500	-0.77849200	-1.18370500
C	2.71905300	-0.81393400	1.21897200
C	4.03855400	-0.21966400	-1.16692400
H	2.28421600	-0.98232100	-2.13924600
C	3.99627400	-0.25553700	1.26345100
H	2.20912600	-1.04667900	2.15052300
C	4.62584900	0.03049800	0.06295300
H	4.57260100	0.01683900	-2.08090000
H	4.49761700	-0.04781400	2.20266300
F	5.86905000	0.57387600	0.09243000

4-Methylstyrene/DMA monoadduct K enolate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1235.990465 [B3LYP/6-31+G(d,p)]

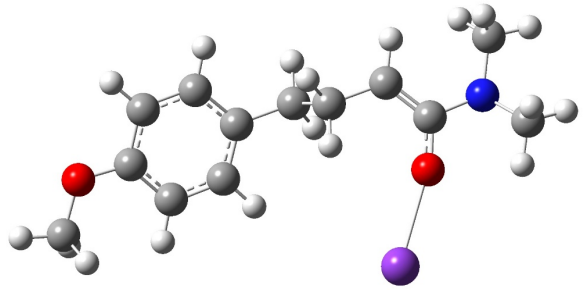
C	-2.73978300	-0.43296700	-0.11206600
N	-4.02951800	-1.06493900	-0.24485800
C	-5.10397400	-0.43345300	0.51722400
H	-6.07516900	-0.76657700	0.13534900
H	-5.05797500	-0.68692500	1.59448200
H	-5.03347800	0.64883500	0.41574300
C	-4.09775500	-2.51618500	-0.18062400
H	-3.83637500	-2.92180000	0.81518300
H	-5.11854400	-2.83598500	-0.41429800
H	-3.42473200	-2.96371900	-0.91637000
O	-2.75413900	0.86580700	-0.15816000
K	-2.37626400	3.35728100	-0.05170400
C	-1.59033500	-1.18774100	0.01172400
H	-1.63626600	-2.26736900	0.10202200
C	-0.22083800	-0.55054500	0.02884900
H	-0.10707800	0.16557600	-0.80128400
H	-0.04964600	0.04837000	0.94109900
C	0.91609500	-1.59240400	-0.06796800
H	0.79257900	-2.16547800	-0.99584400
H	0.80873600	-2.30751300	0.75874300
C	2.30113900	-0.98461600	-0.03026200
C	2.98276400	-0.64850100	-1.20946400
C	2.94306500	-0.70987400	1.18875600
C	4.25082000	-0.05863500	-1.17348500
H	2.51969900	-0.85817200	-2.17137400
C	4.20927400	-0.12017100	1.22605500
H	2.44854800	-0.96978000	2.12237700
C	4.88745700	0.22048600	0.04466800
H	4.75417500	0.18172200	-2.10734600
H	4.68053700	0.07165300	2.18767900
C	6.24763200	0.87985700	0.08827100
H	6.78056700	0.75701800	-0.85934600
H	6.15999600	1.95711800	0.27859700
H	6.86982100	0.46128900	0.88617500

-1235.661823 [M06-2X/6-31++G(d,p)]

C	-2.88445300	-0.18639500	-0.13509800
N	-4.23142200	-0.66792900	-0.23954600
C	-5.16908700	0.02678500	0.63177600
H	-6.19388900	-0.22311700	0.34147900
H	-5.03297800	-0.26033500	1.69111400
H	-5.02255400	1.10168700	0.54223800
C	-4.42687300	-2.10305200	-0.19240600

H	-4.13066700	-2.54194300	0.77757100
H	-5.48562600	-2.32244800	-0.35677800
H	-3.84920000	-2.59198400	-0.98018300
O	-2.75339700	1.09994500	-0.11937100
K	-1.19121000	3.05990100	-0.10319600
C	-1.81915800	-1.05540700	-0.08624800
H	-1.95273500	-2.13042000	-0.06594900
C	-0.41364900	-0.51691400	-0.07322700
H	-0.21283600	0.11368500	-0.95698700
H	-0.23863500	0.14076100	0.79599900
C	0.63975500	-1.63408600	-0.03821600
H	0.50808400	-2.27479100	-0.91927400
H	0.45978900	-2.26218700	0.84338300
C	2.04955900	-1.10015700	-0.00288400
C	2.74589100	-0.82072600	-1.18267400
C	2.68634300	-0.82133500	1.21248800
C	4.03236100	-0.28138000	-1.15023300
H	2.27658100	-1.03348500	-2.14110800
C	3.97110600	-0.28326500	1.24580000
H	2.16883600	-1.03644400	2.14521200
C	4.66624800	-0.00081400	0.06381000
H	4.55342300	-0.08016000	-2.08340100
H	4.44551700	-0.08455400	2.20440000
C	6.04922000	0.60019100	0.10622500
H	6.55403200	0.49541200	-0.85718500
H	6.00414100	1.66795300	0.34585700
H	6.66526500	0.11952700	0.87146100

4-Vinylanisole/DMA monoadduct K enolate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

35

-1311.195235 [B3LYP/6-31+G(d,p)]

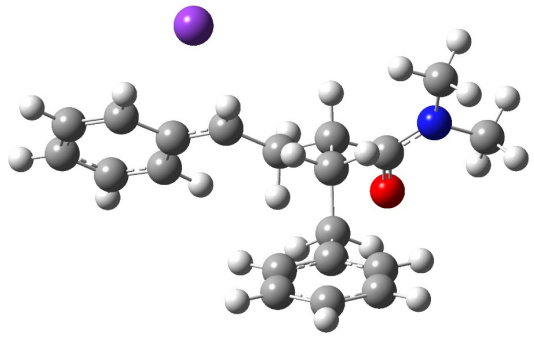
C	3.12135800	-0.34490700	-0.02005700
N	4.47122700	-0.72731100	0.31376300
C	5.51028700	0.15032700	-0.21930800
H	6.45016800	-0.02011900	0.31693100
H	5.69774200	-0.02861300	-1.29615800
H	5.21000000	1.18944200	-0.09102700
C	4.84349400	-2.13004500	0.21828100
H	4.83600000	-2.51374700	-0.81943300
H	5.85621200	-2.25703300	0.61460400
H	4.16732100	-2.74876100	0.81362200
O	2.88045500	0.92942600	0.05533600
K	1.86218900	3.23060600	-0.16811300
C	2.18575900	-1.30496600	-0.36520400
H	2.46856100	-2.35016000	-0.42828600
C	0.73050400	-0.97974600	-0.57410500
H	0.61778200	0.08508900	-0.81350200

H	0.32806700	-1.53550500	-1.43543300
C	-0.18700200	-1.29553900	0.64624900
H	0.18574800	-0.73610000	1.51285100
H	-0.08386100	-2.36096400	0.88981200
C	-1.64518500	-0.96543600	0.41479300
C	-2.18551500	0.27001500	0.79237600
C	-2.50512100	-1.87175200	-0.23379600
C	-3.52352900	0.60681000	0.54346600
H	-1.55382300	0.99478900	1.30126500
C	-3.83771600	-1.55892700	-0.49217500
H	-2.12517500	-2.84484700	-0.53692400
C	-4.35625000	-0.31357900	-0.10423400
H	-3.89531300	1.57397000	0.86085800
H	-4.49215700	-2.26983100	-0.98807700
O	-5.67944400	-0.09545200	-0.39569200
C	-6.26221800	1.15035400	-0.00985800
H	-7.30349600	1.10367300	-0.32948500
H	-6.21962900	1.28884500	1.07660600
H	-5.76560700	1.99210000	-0.50614800

-1310.840476 [M06-2X/6-31++G(d,p)]

C	3.13530600	-0.29836300	-0.05266100
N	4.49962400	-0.61430800	0.26224300
C	5.46779200	0.29663700	-0.33171700
H	6.44291200	0.15783600	0.14479100
H	5.58851400	0.11644400	-1.41622800
H	5.13923600	1.32401600	-0.18529300
C	4.91816000	-1.99495300	0.12691300
H	4.86910700	-2.35572400	-0.91641700
H	5.95258700	-2.08628300	0.47019000
H	4.29484200	-2.64572800	0.74411000
O	2.83606300	0.95679500	0.01566200
K	1.45593800	3.02629000	-0.03383700
C	2.24188400	-1.29462700	-0.38174500
H	2.55410100	-2.33029700	-0.43499700
C	0.78238900	-0.99552700	-0.57706700
H	0.65132800	-0.00346800	-1.03220200
H	0.33552600	-1.71891200	-1.27372400
C	-0.05101400	-1.02549000	0.72693000
H	0.34064900	-0.25911500	1.40623900
H	0.10309000	-1.99715800	1.21231800
C	-1.52380400	-0.80656500	0.48839500
C	-2.11399200	0.45108800	0.60957800
C	-2.34388900	-1.86741600	0.07257900
C	-3.46908200	0.66580100	0.33346600
H	-1.51016700	1.29433700	0.93673900
C	-3.69065900	-1.67978300	-0.20544000
H	-1.91474700	-2.86186700	-0.03044300
C	-4.26150300	-0.40699400	-0.07686300
H	-3.88414400	1.66034200	0.44728100
H	-4.32071600	-2.50601500	-0.52040500
O	-5.59148900	-0.31537900	-0.36732700
C	-6.19901700	0.96209400	-0.26533300
H	-7.24391200	0.82215800	-0.53890500
H	-6.13786300	1.34737900	0.75840800
H	-5.73256100	1.67596000	-0.95314400

Bisadduct K benzylate (**9**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1506.242335 [B3LYP/6-31+G(d,p)]

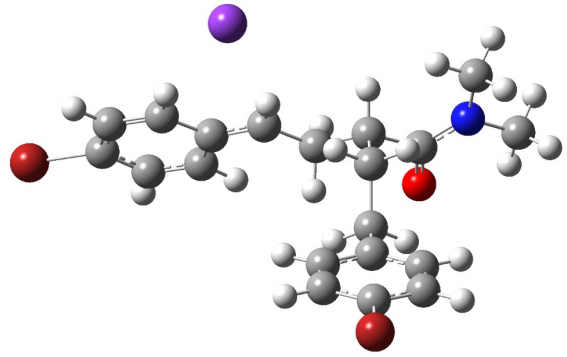
C	5.16259100	-2.34495300	0.83900500
C	4.60496200	-2.53476100	-0.44687000
C	3.46266100	-1.86449800	-0.85467100
C	2.75729200	-0.92412100	0.00001900
C	3.36010500	-0.75271500	1.31093400
C	4.50797000	-1.44297100	1.69609400
H	6.05787400	-2.87478400	1.15012400
H	5.08056300	-3.22774700	-1.14042600
H	3.06602000	-2.04735100	-1.85338300
H	2.89601000	-0.07102500	2.01940800
H	4.90584200	-1.27145000	2.69625800
C	1.63590600	-0.21032800	-0.43116300
H	1.22831900	-0.43977100	-1.41518100
C	0.86857500	0.73975000	0.45779200
H	1.48776100	1.60105100	0.77141900
H	0.57398000	0.27104200	1.41169600
C	-0.39241100	1.31545300	-0.22272100
H	-0.06407300	1.71040100	-1.19052800
C	-0.98742300	2.46376900	0.60367700
O	-0.86395600	2.48036100	1.84232600
C	-2.28367900	4.53383700	0.73843600
H	-3.37537200	4.42125300	0.75639700
H	-1.90491800	4.50609000	1.75765900
H	-2.04444300	5.50038100	0.28275300
C	-1.96796100	3.52290400	-1.46896400
H	-1.46287800	2.73822800	-2.02456400
H	-3.04817500	3.42451900	-1.63359200
H	-1.64848300	4.49114800	-1.87053500
N	-1.66736800	3.46151500	-0.04072000
K	4.23906900	1.36105800	-1.25139400
C	-1.48004100	0.24781700	-0.53116300
H	-2.28696300	0.70677300	-1.11540600
H	-1.02849800	-0.51482500	-1.17446600
C	-2.10195000	-0.44714300	0.69878100
H	-1.31094900	-0.92608300	1.28557700
H	-2.56897300	0.30221400	1.34734900
C	-3.13187900	-1.48435400	0.30117000
C	-2.75564500	-2.81252500	0.04231500
C	-4.48388000	-1.13715500	0.14715700
C	-3.69795500	-3.76390100	-0.36106100
H	-1.71471400	-3.10471200	0.16125200
C	-5.43097700	-2.08395400	-0.25626800
H	-4.79865700	-0.11578300	0.34917100

C	-5.04079900	-3.40243000	-0.51344600
H	-3.38412300	-4.78646200	-0.55254500
H	-6.47215900	-1.79277500	-0.36547300
H	-5.77486900	-4.14027700	-0.82435200

-1505.799531 [M06-2X/6-31++G(d,p)]

C	5.21572500	-1.78499400	0.86180300
C	4.60696500	-2.22801000	-0.33532800
C	3.38562600	-1.74324400	-0.75869000
C	2.64356900	-0.73768400	-0.01551900
C	3.26891400	-0.35243200	1.23913000
C	4.49774200	-0.86134300	1.63838000
H	6.17450000	-2.17372300	1.18561000
H	5.11615100	-2.96816700	-0.95048900
H	2.96108400	-2.10605000	-1.69348700
H	2.76570000	0.36858500	1.87720100
H	4.91808000	-0.51809400	2.58266200
C	1.47036700	-0.16613900	-0.47563000
H	1.06648500	-0.49244100	-1.43217200
C	0.73675500	0.88614700	0.30973600
H	1.37144900	1.77230500	0.49287700
H	0.46870200	0.53819200	1.32050600
C	-0.53824600	1.37348300	-0.38630000
H	-0.23950800	1.77346100	-1.36210000
C	-1.20452900	2.48476000	0.42534000
O	-0.99226300	2.59439700	1.63896700
C	-2.79585500	4.32664300	0.54801900
H	-3.86687800	4.09317200	0.54430200
H	-2.43103000	4.33924400	1.57200700
H	-2.65391900	5.31250800	0.09431600
C	-2.43727700	3.26981600	-1.61866300
H	-1.79427000	2.60195500	-2.18503100
H	-3.47525600	2.93160500	-1.72283300
H	-2.35740700	4.27205500	-2.05106600
N	-2.06309800	3.32661800	-0.21407800
K	5.03735300	0.83584600	-0.95798100
C	-1.56433400	0.24641600	-0.63622500
H	-2.47845200	0.66475000	-1.07596600
H	-1.15401300	-0.45167700	-1.37390200
C	-1.94379700	-0.53729100	0.62827500
H	-1.05310800	-1.04370700	1.01703200
H	-2.29172800	0.15690500	1.40269000
C	-3.01567000	-1.55698100	0.33369900
C	-2.67626200	-2.82553100	-0.15052300
C	-4.37024900	-1.24213800	0.48669400
C	-3.66281900	-3.75714800	-0.47210600
H	-1.62599300	-3.08324600	-0.27263100
C	-5.36167100	-2.17008500	0.16747900
H	-4.64914500	-0.26007500	0.86289000
C	-5.01053500	-3.43188000	-0.31315100
H	-3.37941900	-4.73803800	-0.84221500
H	-6.40786300	-1.90935000	0.29783000
H	-5.78058900	-4.15694400	-0.55810900

4-Bromostyrene/DMA bisadduct K benzylate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-6648.528803 [B3LYP/6-31+G(d,p)]

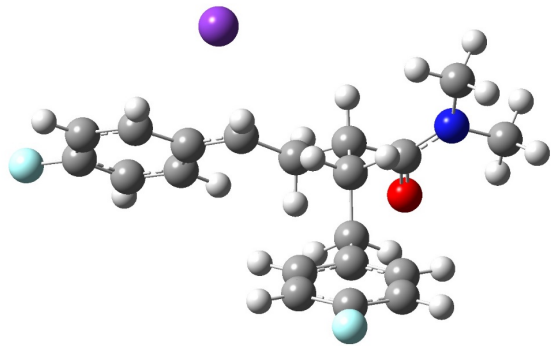
C	-4.97367100	-1.67839500	-0.19183500
C	-4.28386900	-1.82313400	1.02622000
C	-3.17180700	-1.04517500	1.29785900
C	-2.65753200	-0.05324700	0.36896400
C	-3.40905900	0.04232600	-0.87126300
C	-4.52513900	-0.74622600	-1.13347700
H	-4.62131200	-2.55040700	1.76014600
H	-2.65662600	-1.18273900	2.24734800
H	-3.09391300	0.75345100	-1.62962300
H	-5.04757900	-0.63192000	-2.07995100
C	-1.57278200	0.76869600	0.67121500
H	-1.05007100	0.60705500	1.61280800
C	-1.01565100	1.78337900	-0.29746800
H	-1.74932400	2.57878800	-0.52751600
H	-0.79854700	1.33831500	-1.28196300
C	0.25781100	2.48296500	0.22277900
H	0.00948300	2.87582100	1.21464400
C	0.65361300	3.65151600	-0.68983000
O	0.37843000	3.62439800	-1.90358500
C	1.77478100	5.80315700	-1.01524700
H	2.86984000	5.86488100	-1.02175100
H	1.41586400	5.63157600	-2.02738700
H	1.37849000	6.75432300	-0.64156800
C	1.75658200	4.85496900	1.23929800
H	1.36836600	4.06002900	1.86932100
H	2.85142800	4.84793100	1.30642900
H	1.39715200	5.81298200	1.63208600
N	1.33624200	4.70822800	-0.15204300
K	-4.21649800	2.13028000	1.75851500
C	1.46439000	1.52235900	0.42101300
H	2.29884100	2.07389700	0.87099200
H	1.17134300	0.75722100	1.14754800
C	1.96811900	0.82604900	-0.86077000
H	1.14642000	0.26199600	-1.31410900
H	2.27758600	1.58027000	-1.59232000
C	3.12247000	-0.11259900	-0.58609300
C	2.89322000	-1.45125700	-0.23335000
C	4.45048100	0.33368200	-0.65918000
C	3.94948500	-2.32291000	0.04285700
H	1.87390000	-1.82472400	-0.17781200

C	5.52226200	-0.52112600	-0.38829100
H	4.65692100	1.36361000	-0.93880000
C	5.25587700	-1.84338600	-0.03749700
H	3.75398600	-3.35496800	0.31269000
H	6.54288400	-0.15990100	-0.45157900
Br	-6.51476900	-2.76943200	-0.56500600
Br	6.71419000	-3.02243800	0.35461000

-6648.244903 [M06-2X/6-31++G(d,p)]

C	-4.74858800	-1.47385500	-0.22364500
C	-4.03885500	-1.72471000	0.96656500
C	-2.93281100	-0.97115100	1.29821800
C	-2.43696300	0.11016700	0.46078500
C	-3.19047500	0.29711200	-0.76948400
C	-4.29571300	-0.47454100	-1.09031400
H	-4.36928100	-2.51815500	1.63206200
H	-2.40933800	-1.18642200	2.22731800
H	-2.88511100	1.07266100	-1.46515800
H	-4.82318200	-0.29116200	-2.02304000
C	-1.36481800	0.90660300	0.80808400
H	-0.86833300	0.73305900	1.76084500
C	-0.88247200	2.02234300	-0.07626400
H	-1.63556100	2.82529500	-0.17623500
H	-0.71970400	1.67868800	-1.10848200
C	0.41379800	2.66958600	0.42344600
H	0.21009800	3.08357900	1.41752200
C	0.84260500	3.79904900	-0.51262100
O	0.47761400	3.81030300	-1.69446200
C	2.17211800	5.79272200	-0.92683100
H	3.21429700	5.58169300	-1.19534600
H	1.56644100	5.81596900	-1.82953100
H	2.13110300	6.76592400	-0.42983400
C	2.24469400	4.81214900	1.30756800
H	1.77656500	4.09780100	1.97905100
H	3.31879000	4.59583700	1.25853300
H	2.11404100	5.81445600	1.72617900
N	1.66049800	4.77139800	-0.02439300
K	-5.18848500	1.21061400	1.44455600
C	1.57468800	1.66089600	0.56577700
H	2.48546600	2.17730500	0.89427600
H	1.32037600	0.94216400	1.35201400
C	1.88411700	0.89092300	-0.72544500
H	0.98546300	0.35413900	-1.04858800
H	2.15113000	1.59383000	-1.52314300
C	3.00059700	-0.09870900	-0.51580000
C	2.72672700	-1.37291900	-0.00743300
C	4.32990200	0.23928200	-0.78523100
C	3.74602000	-2.29369900	0.22343400
H	1.69747500	-1.65252700	0.20676000
C	5.36496800	-0.66779400	-0.56305200
H	4.56294900	1.22436800	-1.18213200
C	5.05716800	-1.92708300	-0.06176000
H	3.52480600	-3.28133300	0.61314500
H	6.39303100	-0.40047900	-0.78105600
Br	-6.26619500	-2.52139100	-0.67713700
Br	6.45462500	-3.16686000	0.25424300

4-Fluorostyrene/DMA bisadduct K benzylate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1704.743447 [B3LYP/6-31+G(d,p)]

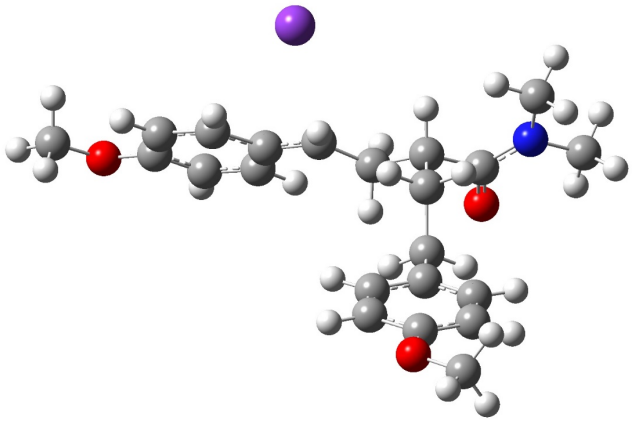
C	5.13747000	-2.18906300	0.61802800
C	4.48547400	-2.49776500	-0.57954700
C	3.32370000	-1.81844500	-0.92076300
C	2.73996300	-0.78397200	-0.08753600
C	3.46982300	-0.52815800	1.14020100
C	4.63922400	-1.21760600	1.47523900
H	4.88864400	-3.26763800	-1.23293700
H	2.82478600	-2.07356000	-1.85430200
H	3.09705300	0.21788200	1.83602000
H	5.15774500	-0.99995500	2.40608400
C	1.59590100	-0.06682200	-0.46851100
H	1.05961000	-0.39958700	-1.35566100
C	0.93321400	0.94148000	0.43917600
H	1.62566200	1.76144500	0.70588400
H	0.65506400	0.51192800	1.41803400
C	-0.31593200	1.59790500	-0.18674900
H	-0.00275500	1.97615100	-1.16613800
C	-0.80530600	2.77735900	0.66531100
O	-0.61508000	2.79092500	1.89550900
C	-1.99617100	4.90926300	0.85126700
H	-3.08930500	4.95118400	0.77204700
H	-1.71384900	4.76936500	1.89214900
H	-1.58793400	5.85847500	0.48521700
C	-1.79470100	3.90517300	-1.36905400
H	-1.35308300	3.09838200	-1.94641100
H	-2.88169700	3.88139000	-1.51418600
H	-1.41934000	4.85709000	-1.76218200
N	-1.47485400	3.80183300	0.05245500
K	3.93888600	1.54020400	-1.66026800
C	-1.48317900	0.60624000	-0.45531900
H	-2.29388800	1.13090100	-0.97551700
H	-1.12257400	-0.16255400	-1.14660000
C	-2.07060200	-0.08534200	0.79322400
H	-1.27399300	-0.61849600	1.32273600
H	-2.46070500	0.66978200	1.48439700
C	-3.17379000	-1.05946800	0.43398000
C	-2.87553600	-2.38436900	0.07594900
C	-4.51812100	-0.65550200	0.41485700
C	-3.87924500	-3.28432200	-0.29480500
H	-1.84310700	-2.72377600	0.08925100
C	-5.54067200	-1.53664300	0.04797400
H	-4.77605000	0.36263800	0.69429500

C	-5.19274800	-2.83420100	-0.30095800
H	-3.65116700	-4.30920900	-0.56812300
H	-6.58046500	-1.22729000	0.03624300
F	-6.18570300	-3.70795600	-0.66018200
F	6.30509600	-2.87461100	0.95371100

-1704.241306 [M06-2X/6-31++G(d,p)]

C	-4.98979200	-2.08586300	-0.61422800
C	-4.35953500	-2.39347600	0.59347900
C	-3.21612400	-1.70976000	0.96253400
C	-2.62401800	-0.67036200	0.14781900
C	-3.33065300	-0.40641400	-1.08616900
C	-4.48408200	-1.10529700	-1.44833400
H	-4.77380700	-3.16774500	1.23411200
H	-2.73503300	-1.95940300	1.90627800
H	-2.95268800	0.35338200	-1.76460100
H	-4.99065000	-0.88416700	-2.38460400
C	-1.51528700	0.06629200	0.56323800
H	-1.03470500	-0.20079000	1.50163800
C	-0.90241700	1.13758300	-0.29425100
H	-1.59157700	1.98769300	-0.47202100
H	-0.67230700	0.77807100	-1.31104100
C	0.37775000	1.71848100	0.31710700
H	0.10675200	2.13176400	1.29549600
C	0.93856900	2.83857800	-0.55859400
O	0.66619100	2.89396400	-1.76373700
C	2.40603700	4.76780500	-0.81094900
H	3.48224100	4.57328300	-0.88873300
H	1.96389700	4.75636700	-1.80415700
H	2.26338500	5.75239500	-0.35531400
C	2.22520100	3.75054500	1.39692500
H	1.65422900	3.06105400	2.01250600
H	3.28500700	3.47324400	1.44839200
H	2.11258000	4.75650200	1.81265400
N	1.76990200	3.75247900	0.01507100
K	-4.10952400	1.52246500	1.34777900
C	1.47647800	0.65695400	0.54676700
H	2.39395200	1.13937300	0.90703100
H	1.15117100	-0.02460400	1.33999600
C	1.81437100	-0.16755800	-0.70279500
H	0.91570300	-0.69901000	-1.03485600
H	2.12166100	0.49966600	-1.51692200
C	2.90764900	-1.16613400	-0.41349600
C	2.59466700	-2.43070100	0.09787200
C	4.25477200	-0.83550300	-0.59488800
C	3.59183400	-3.34995900	0.42071300
H	1.55199100	-2.70320800	0.24459500
C	5.27090300	-1.73731600	-0.27994000
H	4.51692600	0.14238900	-0.99143600
C	4.91166900	-2.97748500	0.22235700
H	3.35861400	-4.33387100	0.81334700
H	6.31792700	-1.49231400	-0.42207200
F	5.89196200	-3.86401200	0.52863500
F	-6.13319500	-2.76803800	-0.96915700

4-Vinylanisole/DMA bisadduct K benzylate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1735.238417 [B3LYP/6-31+G(d,p)]

C	5.24609300	-1.84211600	0.60599600
C	4.53853300	-2.17491700	-0.56256400
C	3.35573800	-1.51405900	-0.89222400
C	2.78072100	-0.46266300	-0.08749700
C	3.54163900	-0.16972800	1.10840000
C	4.72469800	-0.83666800	1.42890000
H	4.89807500	-2.95486900	-1.22698300
H	2.83865600	-1.80856700	-1.80499000
H	3.18288800	0.59423000	1.79317600
H	5.25855500	-0.57918900	2.34208400
C	1.62040600	0.24487900	-0.46613400
H	1.03500600	-0.16466900	-1.28872200
C	0.95104400	1.23883800	0.45467800
H	1.63691100	2.06314900	0.71987200
H	0.67917000	0.80363800	1.43474200
C	-0.30758100	1.88609500	-0.16299100
H	-0.00427400	2.25029200	-1.15104400
C	-0.79065700	3.07777600	0.67447800
O	-0.58015100	3.11957700	1.90090800
C	-1.99867900	5.20317100	0.83694100
H	-3.09107800	5.24898200	0.75075600
H	-1.72274900	5.07245100	1.88072800
H	-1.58446500	6.14750100	0.46440900
C	-1.81539600	4.16149000	-1.36695300
H	-1.36122100	3.35676500	-1.93740900
H	-2.90296700	4.11268600	-1.50173500
H	-1.46417200	5.11574700	-1.77649100
N	-1.47896200	4.08513400	0.05234600
K	3.95118300	1.70505000	-1.84221200
C	-1.47648500	0.88916000	-0.40569900
H	-2.28746900	1.40104900	-0.93825400
H	-1.11660500	0.10420400	-1.07909000
C	-2.06613400	0.22758800	0.85809700
H	-1.26694300	-0.28210300	1.40727800
H	-2.46421900	1.00013700	1.52570500
C	-3.16082200	-0.76568400	0.52609300
C	-2.85599000	-2.09760900	0.19082800
C	-4.50863800	-0.38949400	0.50744300
C	-3.85146600	-3.00936300	-0.15075900

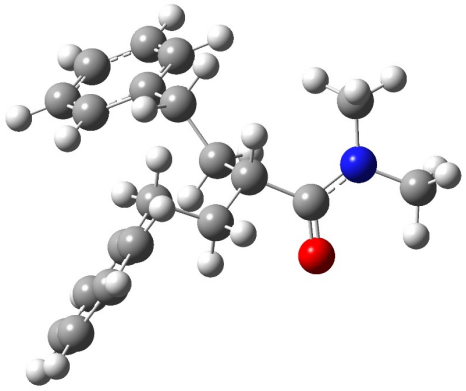
H	-1.82003600	-2.42855800	0.20158500
C	-5.52733600	-1.29014900	0.16640200
H	-4.78245000	0.63036100	0.76798400
C	-5.19697100	-2.60916100	-0.16684600
H	-3.60502900	-4.03641800	-0.40322600
H	-6.55699500	-0.95277200	0.17008200
O	-6.10620000	-3.57552600	-0.51277300
O	6.44019800	-2.44125400	1.01990700
C	6.95322500	-3.49434600	0.21868600
H	7.86664900	-3.83624400	0.70907100
H	6.24568600	-4.33193200	0.14891400
H	7.19687700	-3.15116500	-0.79619700
C	-7.49126800	-3.22592600	-0.54346900
H	-7.68494900	-2.43518900	-1.27733700
H	-8.02010300	-4.13246900	-0.83847600
H	-7.84131400	-2.90400300	0.44399700

-1735.702091 [M06-2X/6-31++G(d,p)]

C	-5.02871600	-1.82352700	-0.58658300
C	-4.36770100	-2.11100300	0.61785100
C	-3.22401400	-1.41393400	0.98472600
C	-2.63888700	-0.37158100	0.18156000
C	-3.35766800	-0.11244700	-1.04383000
C	-4.50335700	-0.82032800	-1.40005900
H	-4.73841500	-2.88312100	1.28546100
H	-2.74214500	-1.66773100	1.92768300
H	-2.99363000	0.65532200	-1.72205800
H	-5.01014900	-0.59393800	-2.33627700
C	-1.53150300	0.37987000	0.59171800
H	-1.02717800	0.10176500	1.51445400
C	-0.93092800	1.44912600	-0.27719200
H	-1.62134700	2.30040200	-0.44723100
H	-0.71375600	1.08988700	-1.29746800
C	0.35789400	2.03240000	0.31401200
H	0.10122400	2.44161100	1.29823400
C	0.90027800	3.15821300	-0.56568200
O	0.60366000	3.22277600	-1.76470600
C	2.36507000	5.08858000	-0.83444600
H	3.44281300	4.90495800	-0.91680900
H	1.91816700	5.07012700	-1.82537700
H	2.21483300	6.07316500	-0.38086500
C	2.21970700	4.06359600	1.37171300
H	1.65665800	3.37408900	1.99451700
H	3.27979100	3.78489300	1.40764000
H	2.11447300	5.06927800	1.79030400
N	1.74427800	4.06822900	-0.00321300
K	-4.13211600	1.77697100	1.41275100
C	1.46426500	0.97435400	0.52330600
H	2.38148600	1.45685700	0.88433200
H	1.14630600	0.28226200	1.31031500
C	1.80208300	0.16582300	-0.73661500
H	0.89952400	-0.35068700	-1.08245000
H	2.11865900	0.84374400	-1.53865900
C	2.88390800	-0.84918700	-0.46161200
C	2.56164600	-2.11524200	0.04851600
C	4.23217300	-0.55049100	-0.65120000
C	3.54684600	-3.04393300	0.35456800
H	1.51663400	-2.37525100	0.20592100
C	5.24194200	-1.47029500	-0.35015700

H	4.51249900	0.42358700	-1.04644600
C	4.89568600	-2.72443200	0.15572400
H	3.29383100	-4.02497600	0.74482000
H	6.27721300	-1.19788200	-0.51788300
O	5.79445800	-3.69730600	0.48080000
O	-6.17706800	-2.46354600	-1.03658100
C	-6.66805200	-3.51371200	-0.23392600
H	-7.54292300	-3.91441000	-0.74700700
H	-5.92131700	-4.30938800	-0.11480900
H	-6.96573000	-3.15533800	0.76015600
C	7.17117800	-3.40637100	0.29992200
H	7.47629100	-2.55118200	0.91261400
H	7.71227100	-4.29570800	0.61968200
H	7.39467600	-3.20064900	-0.75255200

Bisadduct (**10**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-906.908136 [B3LYP/6-31+G(d,p)]

C	5.83115600	-1.75743800	-0.21294900
C	5.54110700	-0.93315100	0.87934600
C	4.22066600	-0.55485300	1.14283700
C	3.16631300	-0.99027800	0.32428700
C	3.47185500	-1.82023500	-0.76646000
C	4.79022500	-2.20069100	-1.03572100
H	6.85560800	-2.05466700	-0.41797000
H	6.34094600	-0.58752000	1.52854200
H	4.00510500	0.08317100	1.99691100
H	2.66892800	-2.17475400	-1.40881500
H	5.00309600	-2.84576300	-1.88378600
C	1.74046300	-0.55039000	0.58904600
H	1.06065000	-1.35673800	0.29474600
H	1.60163300	-0.38858600	1.66515300
C	1.38144700	0.73983900	-0.17574600
H	1.46359000	0.55926600	-1.25243200
H	2.12923600	1.50494500	0.06848300
C	-0.01998300	1.31407800	0.13040000
H	-0.07188000	1.49800400	1.20784400
C	-0.17886700	2.64216700	-0.62366100
O	0.24939200	2.75195100	-1.78758800
C	-0.93408400	4.96789100	-0.66649900
H	-0.52468400	5.75348000	-0.02186000
H	-0.38036000	4.94105600	-1.60249100
H	-1.98516400	5.20025700	-0.87394300
C	-1.38282600	3.60719000	1.35067900

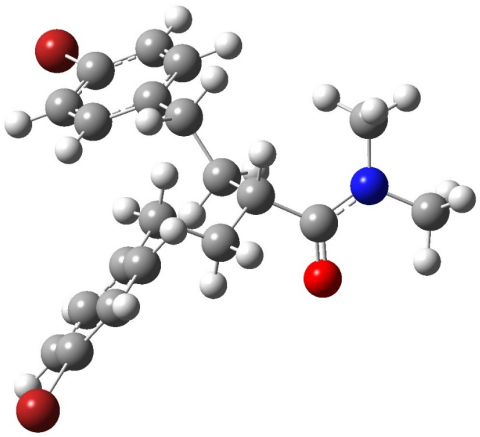
H	-1.83881100	2.63860500	1.55295100
H	-0.62893000	3.81916400	2.11864100
H	-2.16962700	4.36059600	1.42720700
N	-0.81852700	3.67087700	-0.00021900
C	-1.19665900	0.36996200	-0.26736900
H	-0.88340000	-0.25629300	-1.11188000
H	-2.04219000	0.96582200	-0.63211900
C	-1.71631900	-0.52550800	0.88088900
H	-0.90083600	-1.13619000	1.27983200
H	-2.05821400	0.11557700	1.70273000
C	-2.85139000	-1.42790400	0.44204900
C	-4.18205300	-0.98038200	0.47427200
C	-2.59807900	-2.72388000	-0.03525600
C	-5.22869100	-1.80021800	0.04087800
H	-4.40120900	0.01735400	0.84765900
C	-3.64080300	-3.54826900	-0.47005100
H	-1.57538700	-3.09269700	-0.06238000
C	-4.96131000	-3.08846800	-0.43432100
H	-6.25131200	-1.43504000	0.07903600
H	-3.42209900	-4.54928900	-0.83158100
H	-5.77313600	-3.72827400	-0.76813400

-906.482026 [M06-2X/6-31++G(d,p)]

C	-5.85653400	-1.49614900	0.23824600
C	-5.53007300	-0.76734700	-0.90596900
C	-4.19834000	-0.45484300	-1.18027000
C	-3.17370700	-0.86495700	-0.32072100
C	-3.51347400	-1.59574200	0.82347400
C	-4.84308000	-1.90995100	1.10346200
H	-6.89206200	-1.74181600	0.45253300
H	-6.31183400	-0.44350500	-1.58666400
H	-3.94827600	0.11297800	-2.07371200
H	-2.72588800	-1.92287500	1.49904100
H	-5.08779100	-2.48066300	1.99428500
C	-1.73743400	-0.48323400	-0.58699500
H	-1.08368200	-1.28421300	-0.22309400
H	-1.57228000	-0.39054600	-1.66775000
C	-1.38103500	0.83770300	0.10756000
H	-1.49097400	0.71708100	1.19099700
H	-2.10685700	1.60197500	-0.19654700
C	0.03186800	1.35021200	-0.19340600
H	0.10877400	1.52575500	-1.27435600
C	0.24457400	2.67976900	0.53435200
O	-0.40031800	2.95205600	1.55322000
C	1.38942000	4.82877700	0.64603400
H	1.24429200	5.61196900	-0.10509600
H	0.67365300	4.96289200	1.45344600
H	2.40684300	4.90774600	1.04240900
C	1.95817000	3.26834700	-1.17185700
H	2.22023300	2.21545600	-1.26737600
H	1.41991900	3.58971900	-2.07104300
H	2.88969500	3.83368200	-1.10460400
N	1.18497600	3.52230500	0.03696600
C	1.14180900	0.35220200	0.22576500
H	0.77087600	-0.26701400	1.05348000
H	2.01278800	0.89202900	0.61958400
C	1.62509300	-0.55554500	-0.91755400
H	0.78287800	-1.11342500	-1.33795600
H	2.02365800	0.06697700	-1.72802300
C	2.68940400	-1.51650300	-0.44795600

C	4.03743900	-1.14108500	-0.44259400
C	2.34540700	-2.78263400	0.03760200
C	5.01966300	-2.00995000	0.03229700
H	4.31931700	-0.15973200	-0.81899700
C	3.32361600	-3.65571200	0.51354200
H	1.30108600	-3.08787300	0.03777300
C	4.66484000	-3.27132300	0.51193100
H	6.06153200	-1.70386400	0.02449200
H	3.03843300	-4.63665000	0.88181800
H	5.42759900	-3.95086400	0.87920400

4-Bromostyrene/DMA bisadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-6049.190323 [B3LYP/6-31+G(d,p)]

C	5.54251200	-1.34669800	0.05892400
C	5.37886800	-0.34378200	1.01326800
C	4.10385300	0.18458600	1.22774400
C	2.99399300	-0.27429800	0.50325000
C	3.19381800	-1.28628700	-0.44713500
C	4.46130500	-1.82724300	-0.67769200
H	6.22654900	0.01967300	1.58375400
H	3.97440100	0.96189200	1.97639500
H	2.34837300	-1.66488100	-1.01568200
H	4.59803300	-2.61070300	-1.41500200
C	1.61947900	0.31836400	0.73014000
H	0.86649800	-0.44692200	0.51644500
H	1.51260600	0.59002400	1.78755100
C	1.36893300	1.56217000	-0.14758700
H	1.41284800	1.27946300	-1.20437500
H	2.18822700	2.27308500	0.01792800
C	0.03316900	2.28796500	0.12494100
H	0.02366100	2.56411200	1.18358700
C	-0.01532900	3.55722700	-0.73776100
O	0.38256300	3.51978900	-1.91692200
C	-0.51068400	5.93991400	-0.96829000
H	-0.03839400	6.73562700	-0.38214600
H	0.04853900	5.78561900	-1.88852200
H	-1.53374200	6.24837700	-1.21385000
C	-1.06189800	4.81836000	1.16227000
H	-1.55125900	3.90067200	1.48404000
H	-0.28462100	5.08722400	1.88809000
H	-1.81712800	5.60783700	1.16081200

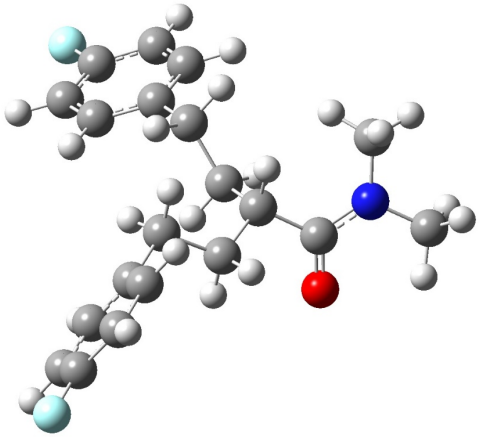
N	-0.51997800	4.69931700	-0.19346500
C	-1.23341200	1.42805800	-0.17643700
H	-0.99172600	0.69280200	-0.95365200
H	-2.02137700	2.06334300	-0.59873900
C	-1.81971800	0.71076200	1.06022500
H	-1.06685600	0.05419300	1.50605200
H	-2.06858200	1.46125100	1.82003500
C	-3.05853800	-0.09393300	0.73328300
C	-4.33219200	0.49084900	0.79255600
C	-2.96304000	-1.43754400	0.34138300
C	-5.48140900	-0.23473800	0.46931100
H	-4.43411100	1.52805300	1.10125300
C	-4.09932100	-2.18111500	0.01273300
H	-1.98891100	-1.91732500	0.29506300
C	-5.34861900	-1.56644300	0.07972300
H	-6.45887200	0.23201900	0.52287100
H	-4.00862000	-3.21934500	-0.28723400
Br	7.28537900	-2.07466800	-0.24975200
Br	-6.91357300	-2.56866600	-0.38236600

-6048.920196 [M06-2X/6-31++G(d,p)]

C	5.48004600	-1.28348700	0.04569200
C	5.29401700	-0.36018600	1.06908100
C	4.01815300	0.15416800	1.28967800
C	2.93299100	-0.24208800	0.50167300
C	3.15440400	-1.16837300	-0.52173700
C	4.42266400	-1.69443900	-0.75814300
H	6.13032600	-0.05340800	1.68764600
H	3.86664200	0.87343500	2.09066800
H	2.32215700	-1.48984100	-1.14317500
H	4.58365500	-2.41719700	-1.55041700
C	1.56153700	0.34623500	0.72271400
H	0.80891700	-0.39314700	0.42644600
H	1.41708900	0.55285400	1.79036800
C	1.37180700	1.63586900	-0.08700700
H	1.44881400	1.40717300	-1.15569000
H	2.19371100	2.32404200	0.14527100
C	0.04135200	2.34857600	0.17622500
H	0.01092500	2.63209700	1.23620600
C	-0.01935600	3.61933600	-0.67466500
O	0.61182000	3.69927100	-1.73463600
C	-0.88176900	5.87911200	-0.97347800
H	-0.62617500	6.71147100	-0.31032400
H	-0.17706400	5.84479300	-1.80107600
H	-1.89303300	6.03758600	-1.36201200
C	-1.57216400	4.58237200	1.01033600
H	-2.03542600	3.60785600	1.16509800
H	-0.94647900	4.82714400	1.87593800
H	-2.37381700	5.31965000	0.94353000
N	-0.81457200	4.62580900	-0.23508900
C	-1.19461400	1.46610700	-0.13483800
H	-0.92263900	0.72583500	-0.89890900
H	-1.99597900	2.07369700	-0.57480100
C	-1.76333800	0.75086500	1.10097400
H	-0.99412200	0.12618600	1.56453800
H	-2.04854400	1.49938500	1.84982400
C	-2.96292600	-0.09330900	0.75608400
C	-4.25069500	0.44818000	0.79921200
C	-2.81112900	-1.42542300	0.36145100

C	-5.36599000	-0.31337700	0.45672800
H	-4.38837700	1.48158900	1.10866500
C	-3.91314800	-2.20466700	0.01516500
H	-1.81774000	-1.86669300	0.32520000
C	-5.18076900	-1.63554500	0.06825200
H	-6.36208500	0.11347300	0.49594800
H	-3.78800400	-3.23878900	-0.28624500
Br	7.20721300	-1.99544500	-0.25705600
Br	-6.68640500	-2.67694300	-0.41266800

4-Fluorostyrene/DMA bisadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1105.410284 [B3LYP/6-31+G(d,p)]

C	-5.65713500	-1.78376300	0.12240400
C	-5.45477400	-0.90255600	-0.93109700
C	-4.15313900	-0.45330200	-1.17447200
C	-3.07298800	-0.87437100	-0.38273300
C	-3.33003400	-1.76897700	0.66827700
C	-4.62271100	-2.23206000	0.93252700
H	-6.29050100	-0.58193200	-1.54406200
H	-3.97913700	0.23383400	-1.99839100
H	-2.50956400	-2.11521100	1.29133100
H	-4.82339000	-2.92586000	1.74204800
C	-1.67292100	-0.35174400	-0.63426900
H	-0.95132500	-1.12966700	-0.36449900
H	-1.54591400	-0.15308100	-1.70548700
C	-1.38041500	0.93369200	0.16609300
H	-1.44729800	0.71959400	1.23770600
H	-2.16863400	1.66461700	-0.05444400
C	-0.01232700	1.58779700	-0.13115500
H	0.02033300	1.80154100	-1.20367200
C	0.08091500	2.90118100	0.65884100
O	-0.32714400	2.94704400	1.83425800
C	0.67257700	5.27084500	0.76198500
H	0.24440600	6.05287300	0.12572200
H	0.09555300	5.19316700	1.68098700
H	1.70531600	5.54697900	1.00584700
C	1.19437900	4.01107800	-1.29716300
H	1.63960600	3.05458000	-1.56503600
H	0.43744500	4.27925900	-2.04445000
H	1.98804600	4.76135000	-1.32897500
N	0.63566400	3.99000000	0.05667000
C	1.21278600	0.69333000	0.23448100

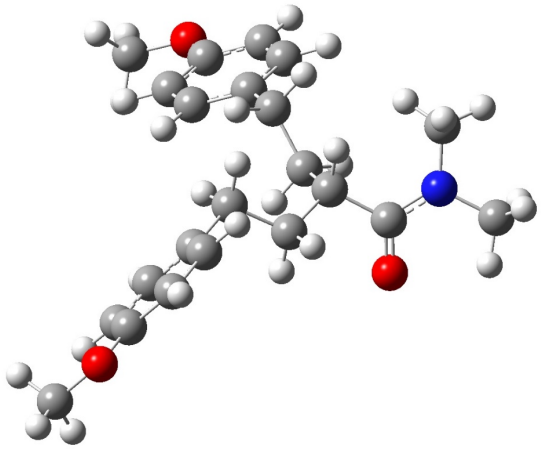
H	0.92984400	0.01066100	1.04510700
H	2.02107800	1.31672100	0.63564100
C	1.78741200	-0.11412400	-0.95184700
H	1.00888000	-0.74727700	-1.38790200
H	2.09772200	0.58408100	-1.73859700
C	2.96846100	-0.97435600	-0.55197400
C	4.27367500	-0.45707600	-0.56432300
C	2.78474700	-2.30142600	-0.13220000
C	5.36896300	-1.23150900	-0.16995000
H	4.44308900	0.56515700	-0.89221600
C	3.86378600	-3.09610400	0.26711900
H	1.78511800	-2.72742200	-0.11984300
C	5.13431400	-2.53743200	0.23875200
H	6.37904500	-0.83594000	-0.18348500
H	3.72506300	-4.12326000	0.58746500
F	6.19983000	-3.30734500	0.62367600
F	-6.92768500	-2.23330500	0.36884500

-1104.924297 [M06-2X/6-31++G(d,p)]

C	-5.66560100	-1.60042000	0.13419700
C	-5.42027600	-0.81902000	-0.98326100
C	-4.10817700	-0.41600500	-1.22855200
C	-3.06280800	-0.78815500	-0.37677900
C	-3.35989100	-1.57757700	0.73973800
C	-4.66369000	-1.99226100	1.00742800
H	-6.23721600	-0.54037500	-1.64000100
H	-3.89450200	0.19601400	-2.10122400
H	-2.55893800	-1.87744100	1.41108400
H	-4.90412200	-2.60714200	1.86792800
C	-1.65343300	-0.30619600	-0.62413200
H	-0.95101100	-1.07527900	-0.28407700
H	-1.49383200	-0.17056300	-1.70095100
C	-1.37951900	1.01122500	0.11225800
H	-1.46726100	0.84693200	1.19188700
H	-2.15832400	1.73490800	-0.15814200
C	-0.00759700	1.62593400	-0.18782400
H	0.03960500	1.84468000	-1.26239200
C	0.13198500	2.93854100	0.58667400
O	-0.49429500	3.12210400	1.63675300
C	1.11602500	5.16143500	0.75089200
H	0.96938100	5.95856400	0.01558400
H	0.36368900	5.24441300	1.53192300
H	2.11246600	5.27022700	1.19192900
C	1.76314300	3.70910700	-1.12963000
H	2.07868500	2.67674000	-1.27432800
H	1.20099100	4.04174800	-2.00980000
H	2.66534200	4.31810800	-1.04328200
N	0.98796000	3.86826400	0.09403700
C	1.17180100	0.68910200	0.17998800
H	0.85675900	0.02284400	0.99418800
H	2.01324600	1.27236300	0.57619000
C	1.69199700	-0.15008200	-0.99908400
H	0.88269900	-0.75284900	-1.42205900
H	2.03162900	0.52031100	-1.79794600
C	2.82832800	-1.04961900	-0.57859400
C	4.14925800	-0.58896900	-0.60138000
C	2.57882200	-2.34270400	-0.10685200
C	5.20337400	-1.39227000	-0.16841700
H	4.36022900	0.41311500	-0.96726600

C	3.61572200	-3.16540000	0.33136400
H	1.55838500	-2.71728800	-0.08366100
C	4.90762900	-2.66597900	0.28972700
H	6.23133600	-1.04693500	-0.18645200
H	3.43432900	-4.17103200	0.69500100
F	5.92443700	-3.45829900	0.71037500
F	-6.93749000	-2.00179700	0.38040400

4-Vinylanisole/DMA bisadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

55

-1135.911642 [B3LYP/6-31+G(d,p)]

C	-5.62311500	-1.59572900	-0.11890900
C	-5.42070000	-0.51701000	-0.99460200
C	-4.13840900	-0.01421000	-1.19773100
C	-3.02100500	-0.56204600	-0.54163900
C	-3.24484500	-1.63772500	0.32457200
C	-4.52692100	-2.16001900	0.54428300
H	-6.27587100	-0.09020600	-1.51010500
H	-4.00206300	0.81823900	-1.88422300
H	-2.40316000	-2.09015200	0.84381700
H	-4.64996300	-2.99696300	1.22123900
C	-1.63317800	0.01019400	-0.74896800
H	-0.89464300	-0.77070600	-0.53971500
H	-1.50866600	0.29248500	-1.80253900
C	-1.36218200	1.23968400	0.14241300
H	-1.42393300	0.94787100	1.19604000
H	-2.16396700	1.97043000	-0.02395600
C	-0.00695700	1.93833300	-0.10766300
H	0.02500900	2.21509200	-1.16572900
C	0.05596800	3.20403800	0.75794500
O	-0.34582900	3.16914200	1.93618900
C	0.58005800	5.58021400	0.99794800
H	0.12044400	6.38391500	0.41254100
H	0.01513500	5.43020500	1.91540800
H	1.60587100	5.87513500	1.24888400
C	1.12639300	4.45881800	-1.13355500
H	1.60749600	3.53666600	-1.45507900
H	0.35553800	4.73748900	-1.86258700
H	1.88967700	5.24053100	-1.12663000
N	0.57679500	4.34210800	0.21925600
C	1.23560600	1.04938500	0.21105900
H	0.96132800	0.31123600	0.97478400

H	2.02656500	1.66374400	0.65848400
C	1.83835900	0.32969100	-1.01656900
H	1.07738400	-0.29636400	-1.49275300
H	2.13024400	1.08258200	-1.75926100
C	3.04222200	-0.51937400	-0.66439400
C	4.33790800	0.02745000	-0.64677000
C	2.90615600	-1.86837500	-0.31672100
C	5.44698000	-0.73859900	-0.29692700
H	4.48301100	1.07063400	-0.91786400
C	4.00781300	-2.65746800	0.03956800
H	1.92004500	-2.32676200	-0.32535400
C	5.28779000	-2.08936400	0.05037100
H	6.44380200	-0.30793600	-0.29257100
H	3.85327600	-3.69852500	0.29705000
O	6.43467500	-2.76470800	0.37659700
O	-6.91804900	-2.02448700	0.01559900
C	-7.18303200	-3.12199500	0.89168800
H	-8.25994100	-3.28509900	0.84622700
H	-6.66214400	-4.02790500	0.56123100
H	-6.89222600	-2.88632100	1.92171800
C	6.33346600	-4.14592700	0.72985000
H	5.92831300	-4.73815200	-0.09852400
H	7.35076700	-4.47229000	0.94652700
H	5.70849200	-4.28300700	1.61957500

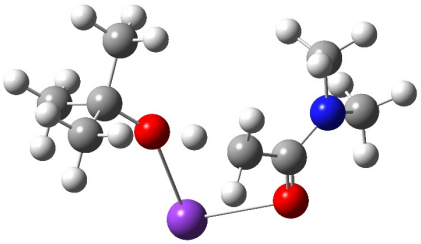
-1135.389936 [M06-2X/6-31++G(d,p)]

C	-5.62050300	-1.46536200	-0.13338100
C	-5.35160000	-0.54014100	-1.14985300
C	-4.05547100	-0.08490100	-1.34965500
C	-2.99382000	-0.53486200	-0.55178300
C	-3.28227700	-1.45574200	0.45418200
C	-4.58011200	-1.92691900	0.67472400
H	-6.17138300	-0.19546400	-1.77257200
H	-3.86115400	0.63273800	-2.14371900
H	-2.47747800	-1.82322400	1.08715400
H	-4.75770100	-2.64594900	1.46543000
C	-1.59500200	0.00057900	-0.74226600
H	-0.87616700	-0.76645300	-0.43187800
H	-1.41747300	0.20096800	-1.80666800
C	-1.37064300	1.28226500	0.07043700
H	-1.47238200	1.05455700	1.13737300
H	-2.16648700	1.99739200	-0.17255300
C	-0.01431100	1.95502700	-0.16712500
H	0.04329100	2.24334200	-1.22487900
C	0.07197900	3.21825800	0.69211800
O	-0.56776500	3.31061900	1.74622100
C	0.98689900	5.45439400	1.01235800
H	0.77266600	6.29557800	0.34568100
H	0.26133700	5.43927200	1.82249300
H	1.99251600	5.58179700	1.42624500
C	1.67695800	4.14607600	-0.96380000
H	2.10823200	3.15693900	-1.11866100
H	1.07588700	4.41963700	-1.83818900
H	2.50257300	4.85432700	-0.87658600
N	0.89915500	4.20595500	0.26817400
C	1.19034800	1.03536400	0.16071300
H	0.88556200	0.30700900	0.92399800
H	2.00384200	1.62008200	0.60994700
C	1.75853600	0.29477900	-1.06072300

H	0.97997200	-0.31758100	-1.52591500
H	2.06675500	1.03045100	-1.81413800
C	2.93718600	-0.57229900	-0.69250800
C	4.23733800	-0.04790500	-0.67522200
C	2.76723700	-1.90269900	-0.31265200
C	5.32411900	-0.82542800	-0.29925600
H	4.40054500	0.98747700	-0.96730400
C	3.84703200	-2.70431500	0.07023300
H	1.76918600	-2.33593800	-0.31692300
C	5.13340800	-2.16122700	0.07530900
H	6.33093400	-0.41960100	-0.29279100
H	3.66980600	-3.73534200	0.35246900
O	6.25640600	-2.84985200	0.42301100
O	-6.92018200	-1.85829300	-0.01250100
C	-7.23081600	-2.79959100	1.00260200
H	-8.30332000	-2.97515200	0.93264900
H	-6.69428200	-3.74130700	0.84352000
H	-6.98860400	-2.40246900	1.99442900
C	6.10272200	-4.20802100	0.80476600
H	5.67575100	-4.79991900	-0.01208500
H	7.10306000	-4.57202400	1.03436200
H	5.46753400	-4.29659200	1.69274600

10.1.2. XYZ Co-ordinates of transition states

Deprotonation of *N*,*N*-dimethylacetamide by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

30

-1120.709445 [B3LYP/6-31+G(d,p)]

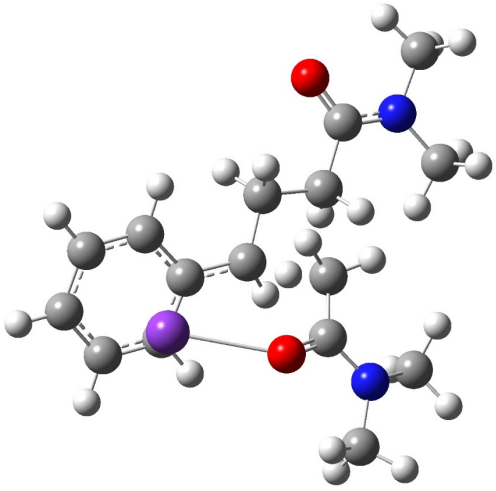
C	0.12575200	-0.10898500	-0.45078500
O	0.04732100	0.39712300	-1.61482000
C	-1.81869500	1.25955800	0.17606600
H	-2.75587800	0.69857600	0.03712800
H	-1.97733100	1.99713200	0.96927100
H	-1.58037200	1.77432100	-0.75272200
N	-0.71221600	0.38005900	0.53831600
K	-0.44188500	-1.50703700	-3.47864600
H	0.32954900	-2.34880000	-0.75762400
O	-0.26149600	-3.19973100	-1.43131400
C	-0.03706300	-4.53847400	-1.02811600
C	-0.59863500	-4.77209400	0.39222300
H	-1.67178100	-4.54943000	0.41473100
H	-0.45680500	-5.80952800	0.72010300
H	-0.09981700	-4.11585800	1.11400500
C	-0.76098200	-5.46743200	-2.02075900
H	-0.37200100	-5.31750000	-3.03467300
H	-0.62938800	-6.52423000	-1.75613300
H	-1.83496700	-5.24814300	-2.03153600
C	1.47506400	-4.85786400	-1.04042700

H	1.88706700	-4.69445900	-2.04301500
H	2.01142500	-4.20620500	-0.34194800
H	1.67135200	-5.89867500	-0.75409700
C	0.99672000	-1.23951500	-0.18336000
H	1.90563100	-1.18416800	-0.78811700
H	1.22307100	-1.46252300	0.85882400
C	-0.81274600	-0.24508200	1.85238900
H	-1.36670300	-1.19474000	1.82472000
H	0.17597400	-0.43322900	2.27476900
H	-1.33985400	0.43604400	2.52506200

-1120.422464 [M06-2X/6-31++G(d,p)]

C	0.18079900	-0.10907300	-0.40110600
O	0.22169600	0.52400100	-1.49131200
C	-1.76995300	1.22519800	0.22198600
H	-2.00338800	1.80863600	1.11622600
H	-1.39444000	1.88946800	-0.55377600
H	-2.69415300	0.75100300	-0.13560100
N	-0.75214200	0.23726100	0.54012200
K	0.20845900	-1.37921100	-3.38498700
H	0.36848400	-2.28873700	-0.80204700
O	-0.24180300	-3.13452600	-1.53270800
C	-0.06074400	-4.43928300	-1.05049500
C	-0.62863300	-4.56171300	0.37297000
H	-1.69176800	-4.29576000	0.37203500
H	-0.52433100	-5.57921300	0.76741600
H	-0.10431400	-3.87446700	1.04668400
C	-0.79497600	-5.41618300	-1.97502200
H	-0.39866500	-5.33503600	-2.99326100
H	-0.68096200	-6.45372600	-1.63931600
H	-1.86340800	-5.17524700	-2.00156800
C	1.43689200	-4.79001100	-1.02780700
H	1.85481600	-4.70042100	-2.03697300
H	1.97515500	-4.09663100	-0.37175900
H	1.61030300	-5.81126300	-0.66861200
C	1.02783200	-1.27186300	-0.16687400
H	1.97653200	-1.16451200	-0.69824400
H	1.18482800	-1.55510600	0.87344400
C	-0.97901800	-0.58976400	1.71654700
H	-1.24438800	-1.61821100	1.44419000
H	-0.09602700	-0.61716800	2.36143200
H	-1.80237100	-0.15933200	2.28793000

Deprotonation of *N*,*N*-dimethylacetamide by DMA monoadduct K benzylate (5) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1484.410012 [B3LYP/6-31+G(d,p)]

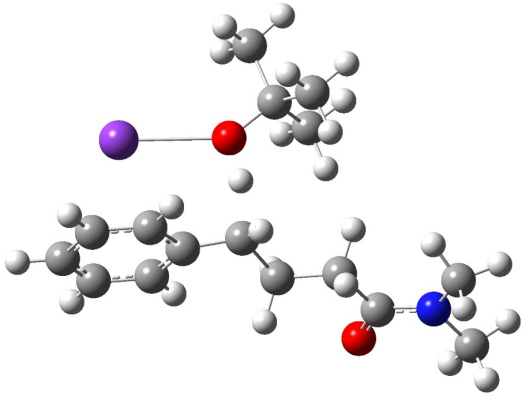
C	-0.47246300	-0.15111400	-1.03473000
O	-1.61148600	0.40884600	-1.11710100
C	-0.24679300	0.84378900	1.20234900
H	-1.07778500	1.45810700	0.86076200
H	-0.61565600	0.15578800	1.97888800
H	0.51856700	1.48513800	1.65097500
N	0.32078600	0.12372100	0.06779000
K	-3.95915900	-0.54260800	-1.76747600
H	-0.54963200	-2.36736300	-1.67902400
C	-0.03867100	-1.12695200	-2.01706600
H	-0.49948400	-0.93985900	-2.98901300
H	1.03282600	-1.30032700	-2.10743100
C	1.55728400	-0.60203300	0.33756500
H	2.11382300	-0.06869500	1.11203600
H	1.37552000	-1.62665700	0.69235800
H	2.18867900	-0.65015200	-0.55194800
C	-5.33072700	-3.50153500	-1.38626300
C	-4.55774500	-3.42377300	-0.21109600
C	-3.17071700	-3.52828100	-0.25741200
C	-2.45903900	-3.72619600	-1.48211900
C	-3.26914800	-3.79870500	-2.65768200
C	-4.66188400	-3.69252500	-2.60418100
H	-6.41340800	-3.42919600	-1.34787900
H	-5.04882800	-3.28508600	0.74978700
H	-2.60261400	-3.47251500	0.66950500
H	-2.79352100	-3.95182900	-3.62218100
H	-5.23318700	-3.76286900	-3.52761300
C	-1.01544300	-3.76822700	-1.51777900
H	-0.57715300	-4.03204300	-0.54812400
C	-0.33360500	-4.45512100	-2.69704200
H	-0.40377500	-3.83157500	-3.60109000
H	-0.82067600	-5.40677500	-2.96389200
C	1.14686600	-4.72404000	-2.41009200
H	1.64589400	-3.78649400	-2.13578900
H	1.23268400	-5.37553600	-1.53007600
C	1.90394300	-5.36401300	-3.57280800

O	1.32998100	-5.64189800	-4.64100800
C	4.02905300	-6.16699600	-4.49114000
H	3.37345200	-6.41428100	-5.32333900
H	4.77273700	-5.43121800	-4.82258100
H	4.55821300	-7.06782800	-4.16137600
C	3.99837700	-5.25837800	-2.20458000
H	4.57073500	-4.33667800	-2.37358400
H	3.35364200	-5.11736700	-1.34025100
H	4.70448700	-6.06168300	-1.97285700
N	3.23255000	-5.62720800	-3.39253800

-1483.963392 [M06-2X/6-31++G(d,p)]

C	-0.51234300	-0.30452900	-1.04853300
O	-1.54172000	0.42602600	-1.03393200
C	0.14212100	0.62400100	1.12479700
H	-0.81939300	1.12141600	1.01847500
H	0.19070700	0.13162600	2.10089400
H	0.94316800	1.37401100	1.07621700
N	0.28760700	-0.35921800	0.06615300
K	-3.70885900	-0.69179900	-1.97884700
H	-0.66652300	-2.43325400	-1.71852700
C	-0.21463000	-1.20060700	-2.15176400
H	-0.76319000	-0.91943100	-3.05129900
H	0.84099100	-1.37140000	-2.36214600
C	1.50886100	-1.14614300	0.08892800
H	1.83341600	-1.25223000	1.12626100
H	1.32990900	-2.14519300	-0.31349900
H	2.32078000	-0.67152500	-0.47997600
C	-5.36508500	-3.37050700	-1.44469500
C	-4.63096300	-3.23053700	-0.25473500
C	-3.25293700	-3.39531200	-0.24181300
C	-2.51698800	-3.72593500	-1.41743900
C	-3.28425200	-3.85714200	-2.60931700
C	-4.66996100	-3.68872200	-2.61425200
H	-6.44248800	-3.24458200	-1.45196400
H	-5.14626500	-2.98791700	0.67129100
H	-2.70895400	-3.27942000	0.69390300
H	-2.78298700	-4.11326100	-3.53826300
H	-5.21290800	-3.80728800	-3.54889900
C	-1.08124700	-3.80919500	-1.40927200
H	-0.65618400	-4.02217600	-0.42283400
C	-0.38696000	-4.51157000	-2.55921600
H	-0.49478400	-3.92198100	-3.48448300
H	-0.81851100	-5.49886800	-2.78808600
C	1.10159400	-4.66853900	-2.27387000
H	1.54238600	-3.68496900	-2.06753400
H	1.24540700	-5.26247300	-1.36134300
C	1.87401200	-5.31983600	-3.41054800
O	1.29969800	-5.73499100	-4.42291900
C	4.03653500	-5.93227000	-4.35052300
H	3.39468800	-6.41895000	-5.08149100
H	4.57600600	-5.10957300	-4.83521300
H	4.76601500	-6.65052200	-3.96676100
C	3.95251300	-4.82220400	-2.15379500
H	4.21393400	-3.77983200	-2.37530900
H	3.37890400	-4.85595700	-1.22874800
H	4.87587100	-5.38432400	-1.99874100
N	3.22051000	-5.43313900	-3.25447700

Deprotonation of HO*t*Bu by DMA monoadduct K benzylate (5) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

46

-1430.265690 [B3LYP/6-31+G(d,p)]

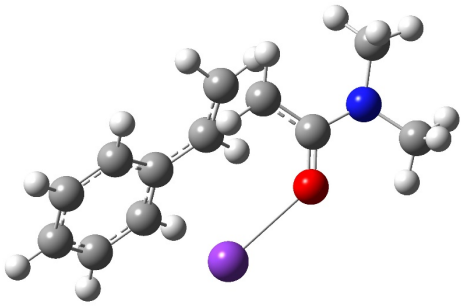
K	-4.06631200	-1.59142100	-1.50155300
H	-1.26613100	-3.01778700	-1.31168200
C	-5.66285500	-4.45752100	-0.39627900
C	-4.79756400	-4.12544200	0.66242900
C	-3.41536700	-4.17814000	0.50107800
C	-2.80330800	-4.56183700	-0.73187900
C	-3.70668600	-4.92078200	-1.77760400
C	-5.09365700	-4.86422600	-1.61103300
H	-6.74049000	-4.41660800	-0.26975200
H	-5.21028700	-3.82438800	1.62304400
H	-2.77187700	-3.91218500	1.33793300
H	-3.30832800	-5.23696600	-2.73765400
H	-5.73830300	-5.14184500	-2.44255000
C	-1.36729800	-4.47497400	-0.92200100
H	-0.82728000	-4.54699000	0.03114400
C	-0.73850600	-5.33939800	-2.01573800
H	-0.92033800	-4.91394100	-3.01302900
H	-1.17884800	-6.35102300	-2.05127200
C	0.77315700	-5.48364700	-1.81678000
H	1.23147300	-4.48874200	-1.74754900
H	0.96836600	-5.96456300	-0.84927200
C	1.48424700	-6.27502500	-2.91280700
O	0.86636800	-6.71429300	-3.89912200
C	3.55088900	-7.29623300	-3.74099700
H	2.91170500	-7.48475700	-4.60097600
H	4.45884900	-6.77739100	-4.06574800
H	3.84169300	-8.25464300	-3.29150100
C	3.60152900	-6.08638600	-1.59503600
H	4.60393800	-5.78410900	-1.91176100
H	3.14557200	-5.24571400	-1.07664300
H	3.70167200	-6.92475000	-0.89273300
N	2.83001900	-6.47171600	-2.77456300
O	-1.44036100	-1.89436600	-1.59881900
C	-0.27981700	-1.13040400	-1.89467700
C	0.35382000	-1.61408500	-3.21587700
H	-0.36740700	-1.52021900	-4.03578100
H	1.24593200	-1.03073200	-3.47533800
H	0.64560800	-2.66673600	-3.14083100
C	0.74510200	-1.24352500	-0.74638600

H	1.63516700	-0.63310500	-0.94110000
H	0.29587400	-0.90567100	0.19447500
H	1.06633200	-2.28206700	-0.61468800
C	-0.71647500	0.33772700	-2.04680600
H	-1.17865500	0.69554900	-1.11957200
H	0.13581300	0.98843800	-2.27800100
H	-1.45000600	0.43532900	-2.85563300

-1429.842295 [M06-2X/6-31++G(d,p)]

K	-3.92538900	-1.60797700	-1.57767100
H	-1.26358900	-3.17369600	-1.15094200
C	-5.70897700	-4.16847100	-0.57028800
C	-4.89384100	-3.89133000	0.53759800
C	-3.51773000	-4.07022300	0.47065600
C	-2.87214700	-4.53761600	-0.70615200
C	-3.72144800	-4.83164500	-1.80390800
C	-5.10377100	-4.64931200	-1.73367900
H	-6.78347200	-4.02720200	-0.51895600
H	-5.34027600	-3.52777400	1.45970800
H	-2.90476000	-3.83590300	1.33895800
H	-3.28675100	-5.20254500	-2.72811000
H	-5.71412900	-4.88441500	-2.60215300
C	-1.42339400	-4.56214400	-0.80596700
H	-0.94692400	-4.72131700	0.16938500
C	-0.81282900	-5.40991200	-1.91082900
H	-0.95802000	-4.93299500	-2.89207100
H	-1.28286800	-6.40375700	-1.99856500
C	0.68233500	-5.59699200	-1.68199100
H	1.15256700	-4.62284300	-1.49968200
H	0.84678800	-6.18059900	-0.76613500
C	1.40119600	-6.28162200	-2.83381900
O	0.78212100	-6.72963400	-3.80541000
C	3.52227500	-6.91468600	-3.85426300
H	4.25909200	-7.63329800	-3.48519900
H	2.84750200	-7.40901700	-4.54954500
H	4.05042800	-6.10729900	-4.37545300
C	3.53054400	-5.74758300	-1.68351200
H	3.74531000	-4.69758700	-1.91918200
H	3.01507200	-5.79926600	-0.72540000
H	4.47875800	-6.27980000	-1.58488400
N	2.75420100	-6.38500900	-2.73814700
O	-1.38601700	-2.01444900	-1.46406900
C	-0.17741100	-1.39303100	-1.82388900
C	0.37468700	-2.01493100	-3.11514300
H	-0.35483300	-1.89965300	-3.92441600
H	1.31458700	-1.54243700	-3.42289700
H	0.55651800	-3.08582800	-2.97216400
C	0.85406200	-1.54639700	-0.69548300
H	1.80527900	-1.06552900	-0.95056800
H	0.46987800	-1.09276500	0.22474700
H	1.04470700	-2.60679300	-0.49701800
C	-0.45738700	0.09470700	-2.05821000
H	-0.85510900	0.54824900	-1.14378800
H	0.45081300	0.63576600	-2.34792500
H	-1.20068200	0.21524900	-2.85448900

Reaction of *N*,*N*-dimethylacetamide K enolate (2) with styrene (3) T.S. (T.S. 4), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-1196.655285 [B3LYP/6-31+G(d,p)]

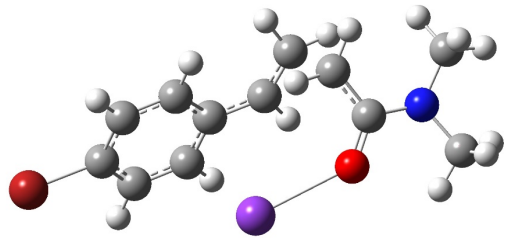
C	-4.41850500	-1.05642300	0.77690400
C	-4.08205300	0.25253300	1.15679400
C	-2.79935200	0.75147300	0.94020000
C	-1.77373300	-0.03341300	0.33510800
C	-2.14820100	-1.35236100	-0.05743100
C	-3.43323400	-1.84647400	0.16743000
H	-5.41822900	-1.44526000	0.94547500
H	-4.82806800	0.88916000	1.62711400
H	-2.56265000	1.76761600	1.25051900
H	-1.41788500	-1.99190700	-0.54439000
H	-3.67195800	-2.86059500	-0.14553000
C	-0.45262400	0.51272100	0.13625700
H	-0.34002800	1.57632000	0.34415100
C	0.63888200	-0.17340700	-0.39350400
H	0.66901200	-1.25857100	-0.34161900
H	1.61486100	0.29631200	-0.31996300
C	0.75300400	-0.33635000	-2.57614600
H	1.64994700	-0.93897500	-2.66643600
H	-0.17816400	-0.87463000	-2.71886600
C	0.73317800	1.01382400	-3.02338600
O	-0.36205200	1.64146000	-3.21361000
C	1.91795100	3.00516100	-3.83836500
H	0.95295400	3.49078100	-3.70603900
H	2.70650900	3.65736800	-3.44978200
H	2.09282400	2.86373200	-4.91840200
C	3.21533900	1.05394400	-3.10945800
H	3.28820200	0.36595300	-2.26569800
H	3.39771200	0.48786100	-4.03786100
H	4.01088700	1.79633900	-3.00354700
N	1.92902200	1.73965800	-3.11383000
K	-2.81531900	1.29853000	-2.40502500

-1196.344662 [M06-2X/6-31++G(d,p)]

C	-4.22667800	-0.63266300	0.57862100
C	-3.74362400	0.61851000	0.98512500
C	-2.39463400	0.93157800	0.86849400
C	-1.45421100	0.01249800	0.33368800
C	-1.96498600	-1.25097400	-0.06251800
C	-3.31725900	-1.56216700	0.06453600
H	-5.28063600	-0.87493000	0.66371500
H	-4.42989300	1.35741800	1.39000600

H	-2.04341100	1.91301300	1.17927200
H	-1.29444000	-1.98904100	-0.49240000
H	-3.66853900	-2.53857200	-0.25853000
C	-0.07314100	0.39044300	0.16286300
H	0.16651300	1.43582200	0.34713600
C	0.88947100	-0.42613300	-0.39978400
H	0.78535800	-1.50677900	-0.36138900
H	1.91789600	-0.07621800	-0.41112500
C	0.75864300	-0.58702100	-2.59636100
H	1.70368200	-1.06587900	-2.81999400
H	-0.12442600	-1.21617200	-2.64078000
C	0.52891100	0.77905100	-2.86793800
O	-0.63633700	1.28090600	-2.86196800
C	1.37892400	2.94419300	-3.60161300
H	2.13502100	3.65807100	-3.26360200
H	1.43588700	2.87548900	-4.70009200
H	0.39177900	3.30803200	-3.32497100
C	2.94726600	1.12313700	-3.17888900
H	3.19810600	0.39447000	-2.40597900
H	3.05824200	0.64199100	-4.16358400
H	3.66717600	1.94231400	-3.11460000
N	1.61387300	1.65711500	-2.96838200
K	-3.05630300	0.75487900	-2.24789100

Reaction of *N*,*N*-dimethylacetamide K enolate (2) with 4-bromostyrene (11) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-3767.797355 [B3LYP/6-31+G(d,p)]

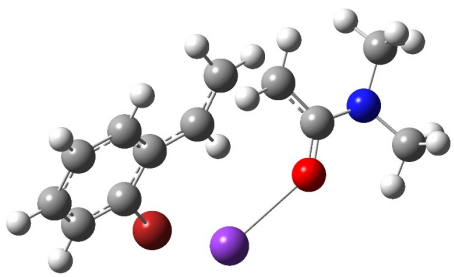
C	-3.01670500	-0.28671400	0.12684700
C	-2.47590000	0.00471300	1.38310300
C	-1.15543600	-0.33836600	1.65668200
C	-0.32399600	-0.99205800	0.70166900
C	-0.91548900	-1.25167900	-0.56868900
C	-2.23746200	-0.91201700	-0.84919500
H	-3.07875200	0.49373000	2.14159300
H	-0.74748900	-0.10976000	2.63864400
H	-0.33004700	-1.72855900	-1.34832900
H	-2.65532600	-1.13089000	-1.82682300
C	1.03170800	-1.34616800	1.03602900
H	1.39681800	-0.97525500	1.99277600
C	1.92638800	-2.01664900	0.20920600
H	1.55955200	-2.62540400	-0.61218300
H	2.85273500	-2.37408700	0.64635000
C	3.01275600	-0.78339000	-1.29550400
H	3.62629800	-1.55666100	-1.74367800
H	2.14280100	-0.48830900	-1.87248000
C	3.58631900	0.24697100	-0.50359700
O	2.94154100	1.31075600	-0.21440500

C	5.52873600	1.20532200	0.65744200
H	4.80136500	1.93045700	1.01734900
H	6.16852200	0.89140400	1.48850700
H	6.16661100	1.69474400	-0.09802700
C	5.70125800	-1.04175500	-0.31078800
H	5.16274500	-1.99076200	-0.32319500
H	6.13573900	-0.87436300	-1.31024600
H	6.52300600	-1.13464300	0.40443900
N	4.83005100	0.04714800	0.11250400
K	0.44082400	2.03208300	-0.26155700
Br	-4.84045700	0.16067000	-0.25018900

-3767.564837 [M06-2X/6-31++G(d,p)]

C	-2.59002400	0.07901600	0.18714200
C	-2.00744400	0.22951400	1.44746900
C	-0.76209300	-0.33018500	1.69577700
C	-0.04992600	-1.05891600	0.70970000
C	-0.68178600	-1.19148700	-0.55336700
C	-1.93287300	-0.63841400	-0.81021400
H	-2.52458700	0.78285000	2.22462200
H	-0.31269500	-0.19924300	2.67695400
H	-0.17527800	-1.71837000	-1.35599900
H	-2.38893000	-0.75407600	-1.78833000
C	1.25792100	-1.58973100	0.99584800
H	1.71314900	-1.26893700	1.93052200
C	2.01081000	-2.32020300	0.10095600
H	1.53517900	-2.86373200	-0.70978000
H	2.95053000	-2.74354400	0.44225900
C	3.01523200	-1.07949900	-1.47916000
H	3.78613200	-1.76818200	-1.80080800
H	2.16569100	-0.95623700	-2.14175100
C	3.29150300	0.02447500	-0.64768700
O	2.45616600	0.96381600	-0.47192700
C	4.87209400	1.28160400	0.72392700
H	4.00206000	1.87168900	1.00354200
H	5.47730500	1.08744800	1.61360700
H	5.48061400	1.86420100	0.01352400
C	5.51109200	-0.91300700	-0.13733200
H	5.13715200	-1.93827400	-0.16509600
H	6.00918200	-0.69628100	-1.09562400
H	6.25671200	-0.84792400	0.65842400
N	4.43644000	0.01781700	0.15434700
K	0.11624100	1.90905100	-0.45109000
Br	-4.29685600	0.82526900	-0.14619900

Reaction of *N*,*N*-dimethylacetamide K enolate (2) with 2-bromostyrene (12) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-3767.798293 [B3LYP/6-31+G(d,p)]

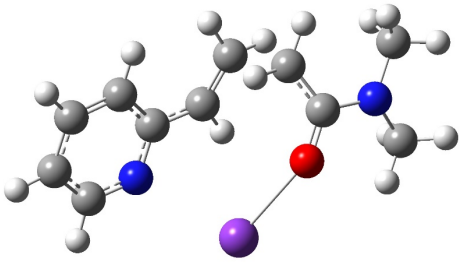
C	-4.38502200	-1.04927200	0.74491000
C	-4.07156100	0.24629600	1.16712000
C	-2.79051700	0.75725000	0.97321000
C	-1.73649500	0.02007700	0.36485100
C	-2.10915600	-1.29212800	-0.05960800
C	-3.38390100	-1.81273400	0.12752800
H	-5.38437400	-1.44492800	0.89444100
H	-4.82567200	0.85881700	1.65063100
H	-1.36171800	-1.90190100	-0.55619100
H	-3.60232500	-2.82027700	-0.21652900
C	-0.40563500	0.53947600	0.17285200
H	-0.26510800	1.59907900	0.35904900
C	0.66772600	-0.18153700	-0.33098000
H	0.67816000	-1.26604100	-0.28798000
H	1.65001800	0.27688400	-0.29708100
C	0.76301500	-0.38884000	-2.58749400
H	1.66688400	-0.98179400	-2.66198700
H	-0.16899900	-0.93400300	-2.68719100
C	0.72322000	0.96137600	-3.01705400
O	-0.37967200	1.58233500	-3.19302900
C	1.88004200	2.95442000	-3.86745800
H	0.91454700	3.43662000	-3.72627700
H	2.67095900	3.61783800	-3.50340200
H	2.03708000	2.79688000	-4.94826200
C	3.20291000	1.02471000	-3.13193100
H	3.29494900	0.34792200	-2.28069100
H	3.37391400	0.44736100	-4.05578200
H	3.99496800	1.77381500	-3.04924300
N	1.91207600	1.70114500	-3.12221900
K	-2.85060400	1.55519400	-2.41957700
Br	-2.45497000	2.53454000	1.64089400

-3767.567151 [M06-2X/6-31++G(d,p)]

C	-4.23327400	-0.60378400	0.43443100
C	-3.79600800	0.67511500	0.77969800
C	-2.44801700	1.00188000	0.67847100
C	-1.45445500	0.08743900	0.25155400
C	-1.94776000	-1.19862100	-0.09961700
C	-3.29020500	-1.53816400	-0.00662600
H	-5.28459600	-0.85896000	0.50745500
H	-4.50231700	1.42349600	1.12396800
H	-1.24462200	-1.93817600	-0.46778100
H	-3.60711200	-2.53709600	-0.29147500
C	-0.06009100	0.43086300	0.13110100
H	0.20376600	1.47432900	0.25624500
C	0.90996900	-0.44352400	-0.30178100
H	0.77742100	-1.51856200	-0.23838000
H	1.94325200	-0.11115500	-0.29801500
C	0.90480800	-0.69868500	-2.57612000
H	1.89966600	-1.09591000	-2.72956500
H	0.08052200	-1.40021900	-2.64253100
C	0.57981700	0.64778700	-2.82306400
O	-0.62006200	1.06231600	-2.85481000
C	1.28165500	2.89231300	-3.47228100
H	0.26653600	3.17996700	-3.20670100
H	1.97931000	3.64870700	-3.10277000
H	1.36238300	2.85604300	-4.57098000
C	2.97253200	1.18552900	-3.03809000

H	3.25725000	0.47028900	-2.26385700
H	3.15034600	0.72408200	-4.02248000
H	3.62421800	2.05745000	-2.94581200
N	1.59617500	1.61089400	-2.86293600
K	-3.09637900	0.70958000	-2.43323400
Br	-1.94998900	2.76335600	1.18150200

Reaction of *N*,*N*-dimethylacetamide K enolate (2) with 2-vinylpyridine (13) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

30

-1212.712075 [B3LYP/6-31+G(d,p)]

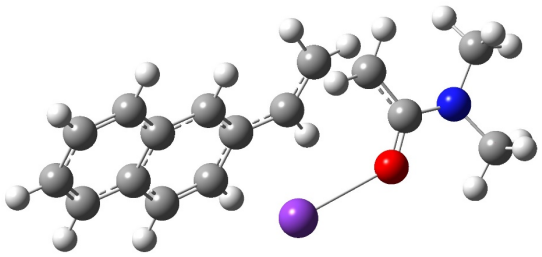
C	-4.34530600	-1.02841000	0.71583100
C	-4.02587300	0.32791800	0.68405100
C	-1.76999800	-0.06296100	0.20896700
C	-2.02897900	-1.46548600	0.20236200
C	-3.30506100	-1.93834800	0.45741800
H	-5.35802300	-1.35735900	0.92279500
H	-4.80093000	1.07322100	0.86049200
H	-1.22116000	-2.16339100	0.00960600
H	-3.49743600	-3.00824700	0.45806000
C	-0.46827300	0.50669900	-0.01610700
H	-0.42052300	1.59188600	0.05073300
C	0.65982800	-0.18034100	-0.43514800
H	0.72918000	-1.25841500	-0.33741900
H	1.61574900	0.33009800	-0.42346500
C	0.76931100	-0.50752900	-2.70513500
H	1.69852300	-1.06203000	-2.75981500
H	-0.13934700	-1.09743800	-2.75166700
C	0.66346400	0.82684600	-3.17154800
O	-0.46200300	1.42728100	-3.24820300
C	1.75470800	3.01458300	-3.49987700
H	0.74477200	3.32971100	-3.75707700
H	2.01783700	3.44863100	-2.52077800
H	2.45594100	3.40996700	-4.24275600
C	3.14796500	1.00276300	-3.28808000
H	3.43679200	0.95112900	-2.22628900
H	3.21891300	-0.00117900	-3.71308600
H	3.87645200	1.63453500	-3.80417300
N	1.81798400	1.55893700	-3.48984400
K	-2.53299200	2.40735500	-2.03332900
N	-2.80064000	0.81433900	0.43402600

-1212.399859 [M06-2X/6-31++G(d,p)]

C	-4.14369100	-0.90549500	0.76269700
C	-3.82294700	0.44654000	0.73005100
C	-1.60554600	0.05436400	0.15011700
C	-1.86428400	-1.34160300	0.12914400

C	-3.12589400	-1.81250200	0.44083900
H	-5.14604100	-1.23207100	1.01392100
H	-4.58501000	1.19301000	0.94820600
H	-1.07192300	-2.03579000	-0.12873400
H	-3.32446100	-2.88062400	0.43087600
C	-0.31014600	0.61667900	-0.13698600
H	-0.25345300	1.70280100	-0.13743300
C	0.79454300	-0.11370800	-0.51454800
H	0.86499300	-1.17706300	-0.31090800
H	1.75113300	0.39232300	-0.59412000
C	0.78266300	-0.69729400	-2.71526400
H	1.76027000	-1.15446300	-2.79204200
H	-0.06957400	-1.36517400	-2.65344700
C	0.51783700	0.60683400	-3.16949900
O	-0.65198600	1.09964700	-3.17087400
C	1.40135500	2.88033400	-3.31584700
H	2.07715800	3.43697400	-3.97132800
H	0.37468400	3.16055400	-3.54522600
H	1.62096200	3.16590600	-2.27383200
C	2.94677900	0.99630600	-3.40346600
H	3.26061200	0.88019900	-2.35390100
H	3.08278600	0.03991200	-3.91257600
H	3.60832400	1.72633200	-3.87656400
N	1.57751600	1.45454600	-3.53802200
K	-2.40476400	2.45998700	-1.94244800
N	-2.61101900	0.92730100	0.43175600

Reaction of *N*,*N*-dimethylacetamide K enolate (2) with 2-vinylnaphthalene (14) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

37

-1350.265337 [B3LYP/6-31+G(d,p)]

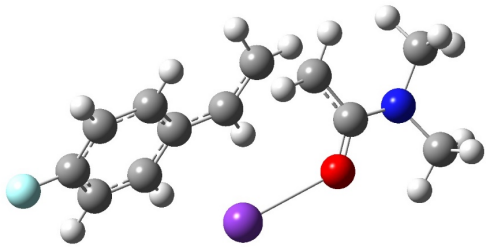
C	1.05648300	-1.31654800	1.10602900
H	1.40639700	-0.87533800	2.03818600
C	1.96085900	-2.04351400	0.34236500
H	1.60220100	-2.71384600	-0.43337100
H	2.89199400	-2.35217800	0.80567800
C	3.04011200	-0.91370000	-1.26597600
H	3.65119900	-1.71804800	-1.65843100
H	2.16200900	-0.66714800	-1.85289300
C	3.61223000	0.16935600	-0.54817800
O	2.96176600	1.24526000	-0.32355100
C	5.55353400	1.21612600	0.53448100
H	4.82308200	1.94284500	0.88486000
H	6.22536100	0.95362700	1.35787600
H	6.15653300	1.68372300	-0.26242600
C	5.74392500	-1.08134800	-0.30570700
H	5.21919800	-2.03670500	-0.25126400
H	6.15854500	-0.96879000	-1.32113800

H	6.57914300	-1.12008700	0.39872300
N	4.86396600	0.01914300	0.06714500
K	0.44854100	1.91184000	-0.50467400
C	-0.29847800	-0.99810600	0.72804800
C	-0.87044400	-1.30525300	-0.52012100
C	-1.14596900	-0.31053500	1.67150600
C	-2.21924800	-1.00066000	-0.83422200
H	-0.27339500	-1.80430100	-1.27886400
C	-2.45147000	0.00775300	1.39033100
H	-0.72782400	-0.04753200	2.64088800
C	-2.80366100	-1.33288600	-2.09400600
C	-3.04256700	-0.32726400	0.13391500
H	-3.05702800	0.52307700	2.13273900
C	-4.11909400	-1.02029100	-2.37590500
H	-2.19224600	-1.84260900	-2.83506400
C	-4.38911900	-0.01920500	-0.18607200
C	-4.92574300	-0.35696900	-1.41623000
H	-4.54225700	-1.28506300	-3.34129700
H	-4.99937700	0.49013500	0.55662200
H	-5.95897400	-0.11663000	-1.64900600

-1349.892514 [M06-2X/6-31++G(d,p)]

C	1.22881000	-1.50920300	1.13407800
H	1.64485700	-1.05225400	2.02947700
C	2.03800600	-2.29670800	0.34376200
H	1.60164200	-2.96420800	-0.39396900
H	2.99883000	-2.61603100	0.73607000
C	2.97446700	-1.20444600	-1.38266900
H	3.72182200	-1.93054700	-1.67599800
H	2.08805900	-1.13746700	-2.00394600
C	3.29866900	-0.03405700	-0.66881900
O	2.47974800	0.92723600	-0.53870600
C	4.96549200	1.33487100	0.46914600
H	4.12173700	1.96209600	0.74850900
H	5.63725000	1.23145500	1.32547800
H	5.51890600	1.83024600	-0.34510900
C	5.53652800	-0.94323700	-0.19049300
H	5.15550500	-1.96264800	-0.10724200
H	5.98365100	-0.81648600	-1.18925200
H	6.32384400	-0.81685500	0.55617100
N	4.48428400	0.02100900	0.07453300
K	0.07848700	1.71286400	-0.61598300
C	-0.10918200	-1.11222900	0.77057200
C	-0.69604600	-1.39170200	-0.46659500
C	-0.89356800	-0.34845000	1.70464900
C	-2.01167200	-0.97097600	-0.78988500
H	-0.13491300	-1.93465100	-1.22302700
C	-2.16122900	0.07834500	1.41497800
H	-0.45180200	-0.10866400	2.66926300
C	-2.60787200	-1.25379600	-2.05401100
C	-2.76943100	-0.21855200	0.15797500
H	-2.72442200	0.65463000	2.14528800
C	-3.88016700	-0.82417800	-2.34802100
H	-2.03651700	-1.82169700	-2.78417100
C	-4.07908000	0.21195100	-0.17350400
C	-4.63020000	-0.08403100	-1.39950300
H	-4.31770200	-1.05178200	-3.31566200
H	-4.64245600	0.78111900	0.56225000
H	-5.63415200	0.24736300	-1.64463700

Reaction of *N*,*N*-dimethylacetamide K enolate (2) with 4-fluorostyrene (15) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

31

-1295.904512 [B3LYP/6-31+G(d,p)]

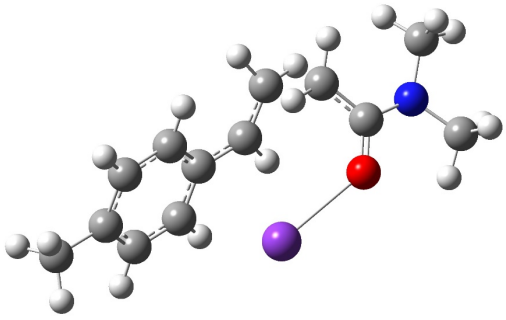
C	-4.06516400	-0.14797800	-0.12361900
C	-3.61500400	0.21885600	1.14065700
C	-2.31289400	-0.11488600	1.51069400
C	-1.42916300	-0.82304300	0.64442600
C	-1.94653100	-1.15113700	-0.64298900
C	-3.25093000	-0.82601600	-1.02194800
H	-4.27185300	0.75366300	1.81986500
H	-1.96238800	0.16507700	2.50136900
H	-1.31745700	-1.67088500	-1.35849700
H	-3.62758200	-1.08720800	-2.00637300
C	-0.09350900	-1.16243500	1.07715200
H	0.22764200	-0.72141000	2.01988300
C	0.83187600	-1.90751400	0.34779700
H	0.48372800	-2.59179500	-0.42177500
H	1.72278100	-2.24884700	0.86581900
C	1.98854800	-0.85728300	-1.17933600
H	2.55303600	-1.68838500	-1.58782500
H	1.15467000	-0.52845200	-1.79110600
C	2.64048700	0.17976000	-0.45422500
O	2.07168200	1.30022600	-0.22939300
C	4.63264200	1.06231900	0.68097100
H	3.94848200	1.83960400	1.01606300
H	5.25263300	0.73828700	1.52297800
H	5.29770700	1.48997900	-0.08823400
C	4.67017900	-1.22998800	-0.19691800
H	4.07447100	-2.14367700	-0.16709500
H	5.11423100	-1.13553700	-1.20156300
H	5.48440400	-1.34000500	0.52427900
N	3.86798200	-0.07042600	0.17276300
K	-0.41732600	2.06264000	-0.38067400
F	-5.35087500	0.18074000	-0.49835100

-1295.564468 [M06-2X/6-31++G(d,p)]

C	-3.69269800	0.16445500	-0.05358300
C	-3.20214500	0.39277200	1.22642300
C	-1.96340800	-0.13696300	1.57201400
C	-1.18487600	-0.90004300	0.66387200
C	-1.73369700	-1.08990900	-0.63057600
C	-2.97743700	-0.56952600	-0.98700000
H	-3.78467500	0.97583700	1.93260900
H	-1.57467300	0.04131900	2.57150900
H	-1.16937000	-1.63934700	-1.37732300
H	-3.38533100	-0.71843500	-1.98188200

C	0.11085500	-1.40712900	1.04933800
H	0.52249300	-1.02452100	1.98103600
C	0.90424700	-2.19894900	0.23833700
H	0.44954200	-2.81193900	-0.53580800
H	1.81120100	-2.61841400	0.66449700
C	1.98280200	-1.13668000	-1.34237700
H	2.69666600	-1.89463700	-1.64078000
H	1.15227700	-0.96647100	-2.01954000
C	2.36902000	-0.00737600	-0.58613100
O	1.62056600	1.00934000	-0.46646500
C	4.06242800	1.18549500	0.70513700
H	3.24868300	1.86417000	0.95199600
H	4.65452900	0.99072100	1.60340700
H	4.71411300	1.67072100	-0.03912500
C	4.50733800	-1.09836800	-0.03783800
H	4.04940500	-2.08876500	-0.01064900
H	5.01284500	-0.97218200	-1.00810000
H	5.26217400	-1.05450700	0.75058400
N	3.51596300	-0.06687100	0.20930300
K	-0.71822300	1.96982700	-0.50786100
F	-4.90410900	0.68062100	-0.40023100

Reaction of *N*,*N*-dimethylacetamide K enolate (2) with 4-methylstyrene (16) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

34

-1235.950037 [B3LYP/6-31+G(d,p)]

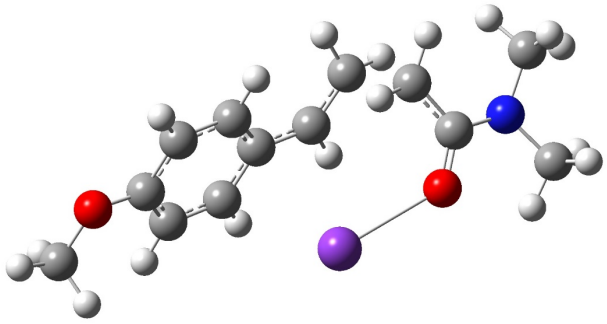
C	-4.43880700	-1.06775200	0.76738000
C	-4.07891600	0.23468400	1.16202200
C	-2.79687800	0.73745600	0.95177900
C	-1.77150600	-0.03270700	0.32992000
C	-2.15652500	-1.33963300	-0.08511000
C	-3.44362700	-1.83284900	0.13693000
H	-4.82074100	0.86900500	1.64470300
H	-2.56412900	1.74963700	1.27845900
H	-1.43551800	-1.97399900	-0.59274400
H	-3.68340900	-2.84013200	-0.20028500
C	-0.44908400	0.51422800	0.13505900
H	-0.33416900	1.57573300	0.35286300
C	0.63898000	-0.16907400	-0.41185100
H	0.66845300	-1.25472200	-0.35620100
H	1.61659300	0.29669900	-0.32854300
C	0.74187100	-0.31779400	-2.56694500
H	1.63074100	-0.93073800	-2.67039000
H	-0.19396900	-0.84589800	-2.71892300
C	0.73680500	1.03264100	-3.01989800
O	-0.35186300	1.67196300	-3.20533700

C	1.94031400	3.01394900	-3.83110900
H	0.98222400	3.51050100	-3.68949200
H	2.73927100	3.65367500	-3.44311900
H	2.10671000	2.87743500	-4.91303800
C	3.21892600	1.04346600	-3.11909000
H	3.28716400	0.34988000	-2.27966400
H	3.39130400	0.48097700	-4.05150200
H	4.02308200	1.77629300	-3.01182600
N	1.94024100	1.74362900	-3.11499500
K	-2.80203900	1.32521000	-2.38007300
C	-5.82079900	-1.62109200	1.03168500
H	-6.05798800	-2.44320600	0.34835700
H	-5.91471500	-2.01268500	2.05397100
H	-6.59213000	-0.85186900	0.91262800

-1235.616296 [M06-2X/6-31++G(d,p)]

C	-4.25114300	-0.84666600	0.53433700
C	-3.73511500	0.34760400	1.06431200
C	-2.38705000	0.66832300	0.96155100
C	-1.45809300	-0.18426100	0.31165700
C	-1.98975200	-1.38682200	-0.21865500
C	-3.34342400	-1.70144400	-0.10271800
H	-4.40955800	1.04184500	1.56212900
H	-2.02946200	1.60955200	1.37380300
H	-1.33745100	-2.07163500	-0.75280300
H	-3.70704000	-2.63219000	-0.53437200
C	-0.07589100	0.20273500	0.16413800
H	0.17147600	1.22562300	0.44197600
C	0.87550600	-0.56349600	-0.48786800
H	0.76386800	-1.64364200	-0.53739000
H	1.90757300	-0.22441400	-0.46441000
C	0.75059600	-0.52332000	-2.66329100
H	1.69718400	-0.97944700	-2.92580500
H	-0.13116500	-1.14411100	-2.78661800
C	0.52179500	0.86220700	-2.82670100
O	-0.64453700	1.35899100	-2.80057500
C	1.37668800	3.09531500	-3.31419200
H	0.38591800	3.42564400	-3.00967300
H	2.12766800	3.76562500	-2.88739200
H	1.44684500	3.15378200	-4.41223900
C	2.94396100	1.23719500	-3.07073600
H	3.18762500	0.43781200	-2.36878300
H	3.07092500	0.85450400	-4.09563100
H	3.65899200	2.04849900	-2.91698400
N	1.60525900	1.74448700	-2.82938500
K	-3.05496200	0.85063700	-2.13929300
C	-5.70866300	-1.20493300	0.68015200
H	-6.34245200	-0.31463300	0.63389400
H	-6.02734100	-1.89212900	-0.10840800
H	-5.90291200	-1.69432400	1.64159500

Reaction of *N*,*N*-dimethylacetamide K enolate (2) with 4-vinylanisole (17) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

35

-1311.153211 [B3LYP/6-31+G(d,p)]

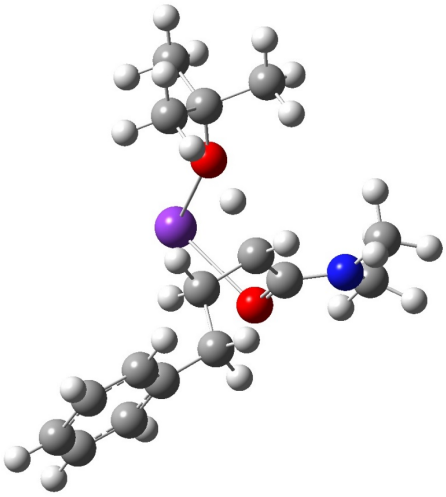
C	-4.42931000	-1.02397000	0.81422600
C	-4.10988900	0.28759300	1.19073800
C	-2.82649400	0.79073000	0.95382100
C	-1.79827100	0.02628900	0.33956400
C	-2.17089700	-1.29607300	-0.04560300
C	-3.44393200	-1.80581900	0.19248200
H	-4.84361800	0.92683700	1.66936100
H	-2.60536600	1.80964400	1.26626100
H	-1.44525800	-1.93406000	-0.54130100
H	-3.69412600	-2.81905300	-0.11144000
C	-0.47941700	0.57990000	0.12562300
H	-0.37141500	1.64643400	0.32180600
C	0.60967400	-0.10562800	-0.42384200
H	0.64969800	-1.18943400	-0.33471200
H	1.58477500	0.36709200	-0.34329700
C	0.70127600	-0.28954900	-2.54348200
H	1.56713600	-0.93511600	-2.64831200
H	-0.25058400	-0.78844800	-2.69719600
C	0.74325600	1.05122200	-3.02973600
O	-0.32306500	1.72311400	-3.22635500
C	2.01041900	2.98145200	-3.86459300
H	1.07349100	3.51512100	-3.71631600
H	2.83740300	3.59257400	-3.48971700
H	2.15944000	2.83114000	-4.94715000
C	3.22391700	0.97381500	-3.13769000
H	3.27054500	0.28736400	-2.29106300
H	3.37406600	0.39602400	-4.06444600
H	4.05293900	1.67971900	-3.04002800
N	1.96975200	1.71741700	-3.13853300
K	-2.77092800	1.43500800	-2.36399300
O	-5.66063300	-1.62231800	0.99903000
C	-6.68760900	-0.85755400	1.62443200
H	-6.93383000	0.03669200	1.03848700
H	-7.56097700	-1.50908600	1.67325600
H	-6.40116800	-0.55723400	2.63993500

-1310.796761 [M06-2X/6-31++G(d,p)]

C	-4.25204600	-0.84110400	0.67492700
C	-3.84606900	0.43774300	1.07167300
C	-2.51225200	0.82078100	0.92514800
C	-1.52470200	-0.03070100	0.37969100

C	-1.97515800	-1.31867900	-0.01484700
C	-3.29986300	-1.71213400	0.13313500
H	-4.55259400	1.14518300	1.49142200
H	-2.22420000	1.82341600	1.23316600
H	-1.27550800	-2.01972000	-0.46033700
H	-3.61992200	-2.70140200	-0.18181900
C	-0.16490400	0.42108400	0.19255900
H	0.01863800	1.48040100	0.36086700
C	0.83493700	-0.35022200	-0.38190300
H	0.79515200	-1.43417600	-0.30239500
H	1.84487900	0.05212400	-0.38287700
C	0.72140200	-0.54235100	-2.51211100
H	1.65442200	-1.04673500	-2.73377300
H	-0.17271700	-1.15563000	-2.57324900
C	0.52265100	0.81949400	-2.84564500
O	-0.63212900	1.34087800	-2.87432100
C	1.42699100	2.95083300	-3.61372500
H	1.50892000	2.86363300	-4.70907200
H	0.43956800	3.33452300	-3.36644600
H	2.18651700	3.65757900	-3.26858000
C	2.95243400	1.10676800	-3.13133700
H	3.17685900	0.38995300	-2.33970000
H	3.07098700	0.60432800	-4.10420200
H	3.68587800	1.91411100	-3.07079100
N	1.62554700	1.66975100	-2.95629300
K	-3.02023400	0.72697300	-2.21575000
O	-5.53287400	-1.31923700	0.76993500
C	-6.51116800	-0.44971600	1.31125000
H	-6.61431400	0.45696400	0.70374200
H	-7.44944600	-1.00302300	1.29995300
H	-6.26468000	-0.16985200	2.34192100

Deprotonation of monoadduct by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1430.281340 [B3LYP/6-31+G(d,p)]

C	-0.06145900	-0.07974600	-0.64953500
O	-0.10618200	0.37342000	-1.83732500
C	-2.28346300	0.91600500	-0.28344600
H	-3.09396200	0.18029700	-0.40530800
H	-2.62926200	1.68978000	0.41023300

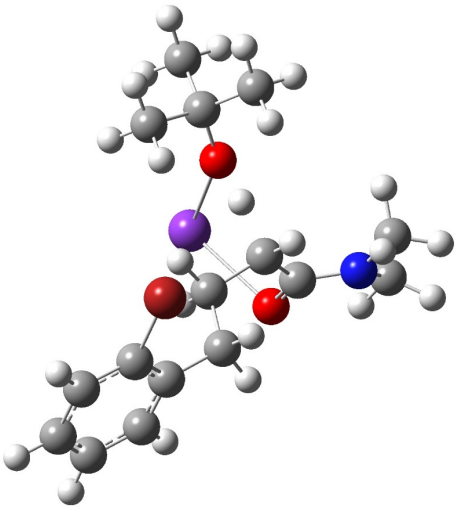
H	-2.07331000	1.36788200	-1.25085600
N	-1.06781800	0.29571200	0.23253500
K	-0.49778700	-1.65209200	-3.59445700
H	0.39640500	-2.24535900	-0.79752700
O	-0.06838200	-3.17147300	-1.46254100
C	0.03474100	-4.45540400	-0.87279400
C	-0.76463700	-4.50557900	0.44854600
H	-1.81725100	-4.26231200	0.26302300
H	-0.71923800	-5.49880800	0.91261800
H	-0.36835300	-3.77713800	1.16427700
C	-0.54953400	-5.48269600	-1.86036700
H	0.00379500	-5.45719100	-2.80637600
H	-0.49857100	-6.50325800	-1.46044100
H	-1.59945000	-5.25003700	-2.07284600
C	1.51306300	-4.80357700	-0.58994400
H	2.09282400	-4.77492000	-1.51963600
H	1.95157100	-4.08025400	0.10619800
H	1.61604400	-5.80410000	-0.15182300
C	0.94201700	-1.04744400	-0.24244700
H	1.01142200	-1.21204500	0.83414600
C	-1.17835100	-0.25453000	1.57878000
H	-1.53504000	-1.29477900	1.58171100
H	-0.22032000	-0.21569900	2.10094400
H	-1.89175600	0.35028600	2.14450400
C	2.31943000	-0.91050800	-0.88399900
H	2.89241700	-1.83169500	-0.71060200
H	2.22060500	-0.81160200	-1.97188900
C	3.15857300	0.28689600	-0.36216400
H	2.59687400	1.21108900	-0.54494100
H	3.26830700	0.18848500	0.72529900
C	4.52549600	0.38847100	-1.00197900
C	5.63957100	-0.25674300	-0.43910500
C	4.71107700	1.09742500	-2.20105800
C	6.89568000	-0.19851400	-1.05167800
H	5.52206400	-0.80614700	0.49237700
C	5.96422100	1.16014600	-2.81851700
H	3.86446700	1.61069100	-2.65179400
C	7.06339300	0.51081800	-2.24574400
H	7.74299800	-0.70237500	-0.59423800
H	6.08316800	1.71927500	-3.74278800
H	8.03875600	0.56088000	-2.72134700

-1429.853536 [M06-2X/6-31++G(d,p)]

C	-0.12767300	0.00451700	-0.63440500
O	0.02111700	0.44348400	-1.80787000
C	-2.30503300	1.10838000	-0.58425400
H	-3.06676900	0.41629100	-0.97053400
H	-2.78373400	1.79455900	0.11879600
H	-1.89355600	1.67457900	-1.41706400
N	-1.22976700	0.39789400	0.08927100
K	-0.14412800	-1.64737600	-3.47948200
H	0.20689900	-2.12582200	-0.60985500
O	-0.30259400	-3.07409800	-1.27922500
C	0.22089500	-4.33813900	-0.96576200
C	0.63318600	-4.40162200	0.51441600
H	-0.22287500	-4.14953300	1.15105700
H	0.98772200	-5.40203200	0.78698500
H	1.43429300	-3.68355500	0.72197200
C	-0.85310600	-5.39995200	-1.23293100

H	-1.16498700	-5.35907400	-2.28260200
H	-0.48690000	-6.41107600	-1.01879600
H	-1.73088800	-5.20718200	-0.60635400
C	1.44804100	-4.62527000	-1.84520700
H	1.15902000	-4.61350500	-2.90304100
H	2.20599200	-3.84933900	-1.68734700
H	1.89659000	-5.60102200	-1.62392900
C	0.76679400	-0.99657800	-0.07283900
H	0.73322000	-1.08309300	1.01424500
C	-1.56899100	-0.24014400	1.35207000
H	-1.73992000	-1.31819700	1.23444800
H	-0.78300700	-0.09254700	2.09680500
H	-2.48407800	0.21470700	1.73415200
C	2.18675200	-0.97047800	-0.60874500
H	2.72492600	-1.86167800	-0.25624300
H	2.18152100	-1.03520700	-1.70533000
C	2.99536200	0.27826100	-0.20639300
H	2.44982200	1.16751300	-0.54376600
H	3.05301400	0.32365400	0.88798100
C	4.38320800	0.27243300	-0.79448900
C	5.45606900	-0.30578600	-0.10583600
C	4.61700000	0.78678200	-2.07571300
C	6.72713200	-0.36702400	-0.67760300
H	5.29184700	-0.70977800	0.89088600
C	5.88537400	0.72968900	-2.65268600
H	3.79272800	1.24043800	-2.62259200
C	6.94619400	0.15054500	-1.95464800
H	7.54689300	-0.81767500	-0.12566100
H	6.04620100	1.13935100	-3.64565200
H	7.93504500	0.10524000	-2.40054900

Deprotonation of 2-bromostyrene monoadduct by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-4001.423426 [B3LYP/6-31+G(d,p)]

C	-1.90010900	-1.71255400	-0.61606200
O	-1.93025500	-2.39688700	0.45581500
C	-3.79891500	-3.05601400	-1.42167900
H	-4.76521600	-2.54687300	-1.28096200
H	-3.89449700	-3.73645700	-2.27455500
H	-3.57233000	-3.63034100	-0.52573400

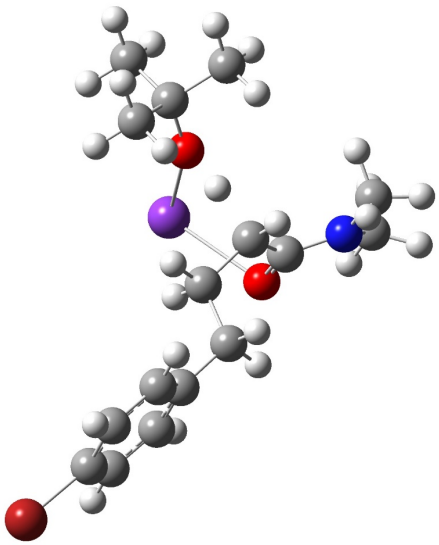
N	-2.72170900	-2.10265600	-1.66620000
K	-2.83409600	-0.84981400	2.50125800
H	-1.95247600	0.43539300	-0.03585200
O	-2.67237500	1.10701300	0.70581000
C	-2.65821600	2.50751800	0.48981200
C	-2.93256500	2.82976500	-0.99597700
H	-3.90043200	2.41576200	-1.30146800
H	-2.95018700	3.91165300	-1.17656000
H	-2.15830800	2.39142000	-1.63485500
C	-3.76567000	3.13374200	1.35856900
H	-3.58688800	2.91432000	2.41773500
H	-3.80883000	4.22338200	1.23692000
H	-4.74228900	2.71856600	1.08400000
C	-1.29306400	3.10450500	0.89940200
H	-1.08627100	2.88572900	1.95356600
H	-0.48612200	2.67079900	0.29906200
H	-1.26996600	4.19322800	0.76500000
C	-1.11765700	-0.49257200	-0.71807600
H	-1.00406800	-0.10053000	-1.73005300
C	-2.85431000	-1.32417900	-2.89249700
H	-3.44089200	-0.40510500	-2.74734900
H	-1.87735400	-1.05160500	-3.29623100
H	-3.36470200	-1.93712900	-3.63983500
C	0.19552100	-0.45450200	0.05450100
H	0.50600000	0.58860200	0.19172700
H	0.05140900	-0.86805200	1.05957800
C	1.36358500	-1.22129200	-0.62186900
H	1.10094800	-2.28313600	-0.68420100
H	1.47654300	-0.85766500	-1.64903000
C	2.66814300	-1.08299300	0.12612100
C	3.52814800	0.01817400	-0.00258900
C	3.05173200	-2.06538000	1.05776700
C	4.69749800	0.15271000	0.74792300
C	4.21784000	-1.95821800	1.81654700
H	2.41070600	-2.93482800	1.18028900
C	5.04538200	-0.84246500	1.66358000
H	5.33276800	1.02177300	0.61553600
H	4.47882000	-2.74174600	2.52160600
H	5.95583900	-0.74199500	2.24640300
Br	3.13098800	1.41232600	-1.26917400

-4001.075497 [M06-2X/6-31+G(d,p)]

C	1.12429500	2.08994700	-0.02964700
O	0.78620600	2.47504600	1.12293600
C	2.57620400	4.04669500	-0.16406100
H	3.56136800	3.79509500	0.25358500
H	2.70695900	4.83245400	-0.91210200
H	1.93977000	4.41341500	0.63832700
N	1.94753300	2.89104500	-0.78377800
K	1.75122000	0.51185100	2.71311800
H	1.70319400	-0.05460700	-0.00135900
O	2.48243500	-0.82951000	0.64038200
C	2.82844200	-1.95561500	-0.12237500
C	3.57013400	-1.52515500	-1.39872200
H	4.46432000	-0.94890800	-1.13480800
H	3.87693100	-2.38865100	-2.00049200
H	2.92162000	-0.88988000	-2.01263200
C	3.74261000	-2.85596800	0.71566100
H	3.22060700	-3.17714900	1.62386800
H	4.05179400	-3.74808200	0.15837200

H	4.64050900	-2.30272400	1.01225600
C	1.56685700	-2.74118600	-0.51863100
H	1.00440100	-3.01962800	0.38016000
H	0.91868100	-2.12491500	-1.15190200
H	1.81736200	-3.65436000	-1.07140300
C	0.75350400	0.77280900	-0.53400100
H	0.83591900	0.66100100	-1.61780900
C	2.56166100	2.40315200	-2.00967100
H	3.16938600	3.20420900	-2.43309400
H	3.20760600	1.53565000	-1.82413800
H	1.80748400	2.12489500	-2.75008800
C	-0.56460200	0.22474500	-0.01726100
H	-0.57633200	-0.86498600	-0.13902900
H	-0.66556900	0.41416600	1.05874400
C	-1.80388500	0.81452400	-0.72118000
H	-1.94538000	1.85196900	-0.39893100
H	-1.62211400	0.83141300	-1.80144100
C	-3.04530500	0.01957500	-0.42363000
C	-3.30792700	-1.21407100	-1.02977500
C	-3.96670600	0.45669800	0.53633100
C	-4.41789300	-1.98822900	-0.70495500
C	-5.09076900	-0.29381100	0.87246400
H	-3.79012400	1.41313500	1.02174400
C	-5.31454500	-1.52305100	0.25457500
H	-4.58095100	-2.93849000	-1.20148200
H	-5.78605400	0.07748100	1.61873100
H	-6.18598000	-2.11758500	0.50835100
Br	-2.12463600	-1.88309900	-2.36142700

Deprotonation of 4-bromostyrene monoadduct by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-4001.423128 [B3LYP/6-31+G(d,p)]

C	-0.05813100	-0.08234300	-0.64396900
O	-0.10403700	0.37339400	-1.83059900
C	-2.27208500	0.92656800	-0.26528700
H	-3.09039400	0.19818800	-0.37769000
H	-2.60476700	1.70617500	0.42832300
H	-2.06529300	1.37294300	-1.23596400
N	-1.05837500	0.29606900	0.24271600

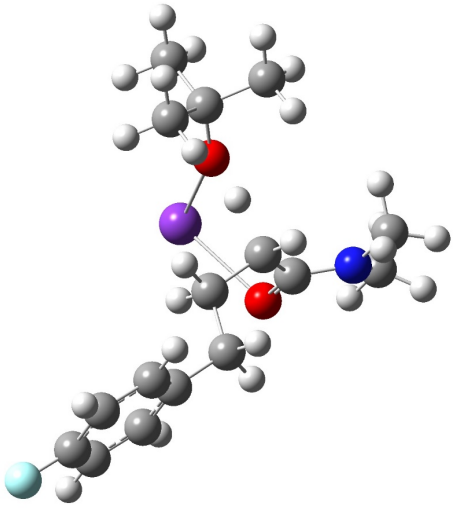
K	-0.49553100	-1.64493200	-3.59703700
H	0.39590900	-2.25001000	-0.80253900
O	-0.06849700	-3.17401600	-1.47148000
C	0.03309700	-4.45868700	-0.88309800
C	-0.77164600	-4.51098000	0.43490800
H	-1.82371900	-4.26853800	0.24525900
H	-0.72720800	-5.50457500	0.89827900
H	-0.37903500	-3.78277700	1.15291900
C	-0.54630400	-5.48521400	-1.87427900
H	0.01106600	-5.45830000	-2.81786400
H	-0.49644700	-6.50617800	-1.47525000
H	-1.59543700	-5.25294300	-2.09099600
C	1.51052800	-4.80618800	-0.59459700
H	2.09412800	-4.77573700	-1.52182500
H	1.94564300	-4.08370300	0.10453400
H	1.61237600	-5.80730700	-0.15757800
C	0.94255700	-1.05608600	-0.24313300
H	1.01451300	-1.22437100	0.83267200
C	-1.16244300	-0.25073000	1.59089600
H	-1.52340400	-1.28942900	1.59842800
H	-0.20097900	-0.21457500	2.10691900
H	-1.86987500	0.35820700	2.15965000
C	2.31896900	-0.91825400	-0.88614700
H	2.89699200	-1.83430700	-0.70341100
H	2.22110600	-0.82936000	-1.97497700
C	3.14792600	0.28980400	-0.37330500
H	2.58222400	1.20830400	-0.57016800
H	3.25197100	0.20486100	0.71550900
C	4.51665500	0.39301200	-1.00438800
C	5.63430700	-0.22053400	-0.41706900
C	4.70111800	1.07012600	-2.22052000
C	6.89599400	-0.16707800	-1.01571800
H	5.52296400	-0.74583000	0.52815600
C	5.95285400	1.13559700	-2.83744300
H	3.85488300	1.56096300	-2.69466700
C	7.03820800	0.51060800	-2.22519800
H	7.74845900	-0.64507300	-0.54535600
H	6.07639200	1.66471900	-3.77610700
Br	8.75779300	0.57704900	-3.06781600

-4001.074590 [M06-2X/6-31++G(d,p)]

C	-0.13392200	0.02656300	-0.59725700
O	-0.00146300	0.47266400	-1.76979200
C	-2.29817100	1.15189800	-0.49726800
H	-3.07583400	0.47273300	-0.87447300
H	-2.75418900	1.83789500	0.22081400
H	-1.89541000	1.71991400	-1.33320700
N	-1.21922900	0.42180900	0.14875600
K	-0.18489900	-1.60223100	-3.46074400
H	0.19741200	-2.10755900	-0.59627200
O	-0.31488600	-3.05250600	-1.27192600
C	0.22400200	-4.31549700	-0.98124700
C	0.65414600	-4.39493000	0.49308800
H	-0.19595500	-4.15658300	1.14286400
H	1.01823300	-5.39638300	0.74871900
H	1.45323200	-3.67463300	0.70055900
C	-0.84305900	-5.38388500	-1.25008400
H	-1.16742300	-5.33215200	-2.29548200
H	-0.46483100	-6.39418200	-1.05362500

H	-1.71531500	-5.20776500	-0.61099000
C	1.44354800	-4.58018000	-1.87843200
H	1.14137700	-4.56264700	-2.93249700
H	2.19494000	-3.79732000	-1.72368900
H	1.90612200	-5.55263200	-1.67190100
C	0.76430800	-0.98450600	-0.05938700
H	0.75244000	-1.07637900	1.02768100
C	-1.53899400	-0.22263000	1.41351000
H	-1.70932500	-1.30034800	1.29305100
H	-0.74273800	-0.07711100	2.14788400
H	-2.44964400	0.22823300	1.81047300
C	2.17361300	-0.96133600	-0.62251300
H	2.72282700	-1.84115700	-0.25904100
H	2.15149000	-1.05114300	-1.71730900
C	2.97964900	0.30138800	-0.26239600
H	2.43917000	1.17733900	-0.63929700
H	3.02814600	0.38889200	0.82967100
C	4.37121800	0.26547300	-0.83459600
C	5.42955200	-0.29667000	-0.11291000
C	4.62214200	0.72016400	-2.13364800
C	6.70331700	-0.41113400	-0.66611900
H	5.25699100	-0.65388800	0.89945100
C	5.88852900	0.61549900	-2.70638200
H	3.81343000	1.16408400	-2.70961800
C	6.91444800	0.04155300	-1.96354100
H	7.51722700	-0.85035400	-0.09969800
H	6.07295700	0.97058500	-3.71447800
Br	8.63584400	-0.14041100	-2.73300600

Deprotonation of 4-fluorostyrene monoadduct by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1529.532389 [B3LYP/6-31+G(d,p)]

C	-0.06012100	-0.08009700	-0.64977800
O	-0.10302600	0.37258200	-1.83775700
C	-2.28141600	0.91800300	-0.28598100
H	-3.09340500	0.18386100	-0.40701000
H	-2.62566300	1.69341600	0.40664900
H	-2.07006400	1.36818800	-1.25392100
N	-1.06722100	0.29564800	0.23095400
K	-0.50513300	-1.65402400	-3.59282400

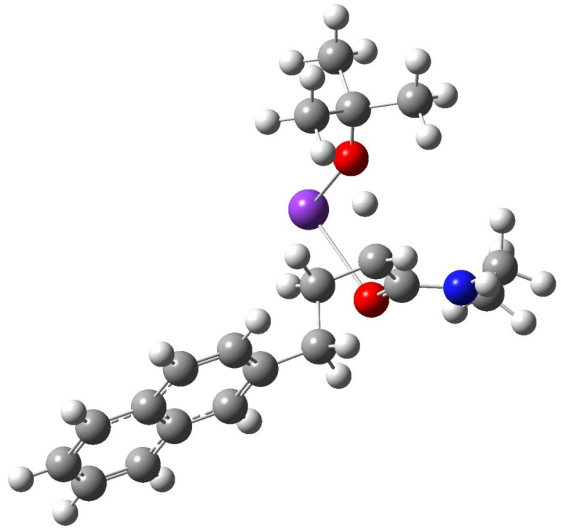
H	0.39729700	-2.24542600	-0.79602700
O	-0.06793800	-3.17172300	-1.46144400
C	0.03507600	-4.45581200	-0.87209200
C	-0.76537700	-4.50665900	0.44858200
H	-1.81794200	-4.26381500	0.26223500
H	-0.71992700	-5.49995100	0.91251600
H	-0.37001500	-3.77817100	1.16478600
C	-0.54806100	-5.48298600	-1.86047500
H	0.00612400	-5.45707800	-2.80597100
H	-0.49724500	-6.50365400	-1.46080100
H	-1.59783300	-5.25049200	-2.07384000
C	1.51326500	-4.80367800	-0.58811400
H	2.09381100	-4.77451900	-1.51730100
H	1.95098600	-4.08052200	0.10870700
H	1.61616400	-5.80433200	-0.15027600
C	0.94264000	-1.04822400	-0.24123900
H	1.01143700	-1.21215000	0.83548800
C	-1.17923400	-0.25400700	1.57735300
H	-1.53549800	-1.29437000	1.58024200
H	-0.22189500	-0.21452200	2.10076300
H	-1.89360800	0.35079100	2.14183800
C	2.32021000	-0.91205300	-0.88228400
H	2.89320500	-1.83311600	-0.70816400
H	2.22161500	-0.81376900	-1.97025400
C	3.15876400	0.28548700	-0.36080200
H	2.59748900	1.20986000	-0.54270500
H	3.26978200	0.18796900	0.72640600
C	4.52551900	0.38848400	-1.00120100
C	5.63948200	-0.25918900	-0.44162500
C	4.71047400	1.10041100	-2.19827600
C	6.89888900	-0.20591000	-1.04795800
H	5.52654800	-0.81199500	0.48744500
C	5.95907100	1.16963000	-2.82422900
H	3.86677100	1.61627800	-2.64951000
C	7.02675500	0.51008200	-2.23030300
H	7.76048400	-0.70207500	-0.61349200
H	6.10323400	1.72399200	-3.74572700
F	8.25716000	0.57332300	-2.83236000

-1529.075644 [M06-2X/6-31++G(d,p)]

C	-0.12273100	0.00136000	-0.63216700
O	0.02903200	0.44125500	-1.80487000
C	-2.29762000	1.11023100	-0.58335100
H	-3.06138500	0.42089700	-0.97046500
H	-2.77438500	1.79751000	0.11994000
H	-1.88377200	1.67565400	-1.41551000
N	-1.22508600	0.39561500	0.09018100
K	-0.14388000	-1.64614500	-3.48061900
H	0.20821000	-2.12873300	-0.60969700
O	-0.30337600	-3.07461100	-1.28187900
C	0.21679400	-4.34040200	-0.97011900
C	0.62623400	-4.40778800	0.51068500
H	-0.23034300	-4.15470300	1.14622700
H	0.97771600	-5.40961300	0.78199800
H	1.42880500	-3.69216400	0.72105600
C	-0.85892200	-5.39938800	-1.24148400
H	-1.16886700	-5.35561200	-2.29161900
H	-0.49527700	-6.41175600	-1.02889000
H	-1.73743100	-5.20610100	-0.61608200

C	1.44500700	-4.62825800	-1.84784300
H	1.15794800	-4.61396300	-2.90617900
H	2.20409800	-3.85401200	-1.68715100
H	1.89132400	-5.60525600	-1.62754900
C	0.76936600	-1.00202200	-0.07040700
H	0.73455200	-1.08946900	1.01655500
C	-1.56674300	-0.24247400	1.35232800
H	-1.73859900	-1.32027700	1.23407000
H	-0.78165300	-0.09587700	2.09822200
H	-2.48191000	0.21318400	1.73322400
C	2.18981400	-0.97626300	-0.60493700
H	2.72846300	-1.86647600	-0.25063200
H	2.18561000	-1.04253200	-1.70147100
C	2.99576200	0.27401100	-0.20356200
H	2.44807800	1.16205600	-0.54023500
H	3.05471000	0.32106000	0.89046400
C	4.38367600	0.27426400	-0.79216700
C	5.46360500	-0.28136200	-0.09674100
C	4.61020900	0.77246100	-2.08093800
C	6.73843200	-0.33955000	-0.65995600
H	5.30838100	-0.67429200	0.90498800
C	5.87457400	0.72666000	-2.66654200
H	3.78274400	1.20843800	-2.63596000
C	6.91206500	0.16778100	-1.93725700
H	7.58142100	-0.76512000	-0.12608800
H	6.05869600	1.11588100	-3.66216100
F	8.14828500	0.11958700	-2.49518800

Deprotonation of 2-vinylnapthalene monoadduct by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1583.891578 [B3LYP/6-31+G(d,p)]

C	-2.02594300	-1.73642500	-0.18642200
O	-1.60820900	-2.02810200	0.97931000
C	-3.68007200	-3.54550900	0.04953500
H	-4.67938000	-3.17944600	0.33254200
H	-3.80612900	-4.48208300	-0.50443200
H	-3.10746900	-3.73645700	0.95483800
N	-2.96765900	-2.57342700	-0.77267300
K	-2.27205800	-0.08185400	2.74836400
H	-2.46540000	0.43366300	-0.19098500

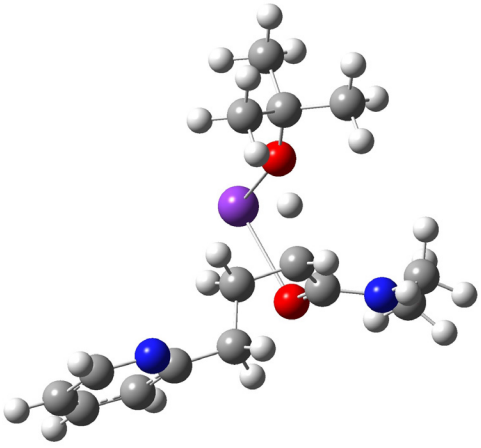
O	-3.10317400	1.16822500	0.56297600
C	-3.65853400	2.32769000	-0.03187800
C	-4.62470400	1.93848100	-1.17283100
H	-5.42367500	1.29391700	-0.78868600
H	-5.08717100	2.82222800	-1.63008800
H	-4.09211600	1.38950700	-1.95701500
C	-4.43599700	3.09504200	1.05377400
H	-3.76578300	3.37232900	1.87572700
H	-4.88849500	4.01221500	0.65615600
H	-5.23652100	2.46785300	1.46300300
C	-2.54066100	3.23380200	-0.59404300
H	-1.84995900	3.52331500	0.20647800
H	-1.96753300	2.70365400	-1.36250700
H	-2.94794000	4.14865600	-1.04228100
C	-1.62377100	-0.51005300	-0.85338900
H	-1.87993000	-0.45613500	-1.91279700
C	-3.59084100	-2.28168100	-2.05848800
H	-4.34045200	-1.47962100	-1.99215800
H	-2.84532200	-1.99830200	-2.80379700
H	-4.09234500	-3.18533600	-2.41489300
C	-0.20195700	-0.02579800	-0.58711400
H	-0.11397000	1.02614300	-0.89137300
H	0.00808200	-0.05239100	0.48898500
C	0.90397200	-0.83751500	-1.31371600
H	0.82998600	-1.88694600	-1.00571000
H	0.70490200	-0.80567000	-2.39321200
C	2.30114000	-0.32737600	-1.04217600
C	3.12400700	-0.92814400	-0.10586900
C	2.78784700	0.82434600	-1.72938100
C	4.42543500	-0.42995300	0.18377100
H	2.77756500	-1.81084900	0.42828700
C	4.04204400	1.33588000	-1.47739600
H	2.15216900	1.30061900	-2.47208900
C	5.27813200	-1.04583300	1.14372900
C	4.89867200	0.72923800	-0.51577700
H	4.39512300	2.21142500	-2.01682100
C	6.53593200	-0.53998300	1.40097300
H	4.92087800	-1.92507400	1.67407300
C	6.20075900	1.22630300	-0.22887600
C	7.00276700	0.60743100	0.70833700
H	7.17510000	-1.01995700	2.13652300
H	6.55549900	2.10491300	-0.76207900
H	7.99471700	0.99639800	0.91925100

-1583.400236 [M06-2X/6-31++G(d,p)]

C	1.01765500	1.93435500	-0.15667300
O	0.66013200	2.13610500	1.03606100
C	2.55767500	3.81275400	0.07885900
H	1.91149600	4.08382900	0.91109000
H	3.50751200	3.43138000	0.48017200
H	2.76736600	4.70162800	-0.52101800
N	1.88930000	2.82026600	-0.74750600
K	1.63562800	0.13560900	2.51687700
H	1.56201000	-0.14745100	-0.39764500
O	2.37932200	-0.89900100	0.21392300
C	2.37273900	-2.23052900	-0.23092000
C	2.07893100	-2.29588500	-1.73877300
H	2.81364400	-1.69640200	-2.28863000
H	2.12278800	-3.32614600	-2.10953000

H	1.08245000	-1.89478500	-1.95428700
C	3.74898600	-2.85060300	0.03915000
H	3.97893400	-2.79576200	1.10907100
H	3.78794700	-3.90171900	-0.27071800
H	4.52163500	-2.29824800	-0.50673200
C	1.30143300	-3.03013700	0.52802400
H	1.52296600	-3.02489500	1.60197600
H	0.31767700	-2.57102400	0.37689900
H	1.25319600	-4.07345700	0.19447700
C	0.62789900	0.73294200	-0.87894300
H	0.74588000	0.79308700	-1.96192700
C	2.50554900	2.52948800	-2.03327200
H	3.11248100	1.61509100	-2.00195900
H	1.75304000	2.41961200	-2.81780000
H	3.15282100	3.36529300	-2.30272200
C	-0.71292300	0.14172000	-0.48094900
H	-0.83056800	-0.83786000	-0.96518300
H	-0.74452300	-0.04960100	0.60046100
C	-1.92562900	1.01885000	-0.84890600
H	-1.84403100	1.97525300	-0.32041600
H	-1.88430500	1.23361100	-1.92466800
C	-3.23611400	0.35350800	-0.51767800
C	-3.95913900	0.68000200	0.60756500
C	-3.72194000	-0.68644900	-1.36298400
C	-5.17010300	0.00933700	0.93677800
H	-3.60655800	1.47114600	1.26726400
C	-4.88492300	-1.35452700	-1.07620600
H	-3.15392200	-0.94475800	-2.25393400
C	-5.92714400	0.34300500	2.09385200
C	-5.64299400	-1.02645500	0.08228600
H	-5.24532200	-2.14177900	-1.73363800
C	-7.09402700	-0.32222000	2.38596800
H	-5.56621300	1.13489600	2.74527700
C	-6.85265200	-1.69690900	0.40833800
C	-7.56287500	-1.35487600	1.53414300
H	-7.66299500	-0.05864900	3.27214900
H	-7.20676500	-2.48639800	-0.24962400
H	-8.48543700	-1.87332000	1.77566400

Deprotonation of 2-vinylpyridine monoadduct by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1446.334677 [B3LYP/6-31+G(d,p)]

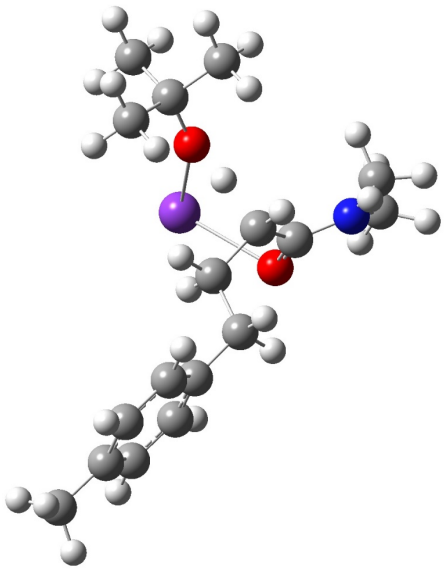
C	0.94059100	1.75126900	-0.09871700
O	0.68690900	1.97338600	1.12778700
C	2.56663900	3.59900200	-0.01016100
H	3.60637600	3.25415800	0.10165000
H	2.58323600	4.56593700	-0.52468700
H	2.13048300	3.72494700	0.97883600
N	1.76618600	2.64455000	-0.76959700
K	1.66712500	-0.00764300	2.69420200
H	1.41633500	-0.40682500	-0.26773200
O	2.15174800	-1.16995100	0.36028600
C	2.67604800	-2.26000200	-0.37647800
C	3.47966400	-3.14748600	0.59228500
H	2.83032000	-3.51726200	1.39432300
H	3.91948800	-4.01235200	0.07985100
H	4.29185100	-2.57015000	1.04904500
C	1.53318700	-3.09107100	-1.00040500
H	0.93995900	-2.47599000	-1.68590300
H	1.91878500	-3.95151200	-1.56129000
H	0.86561400	-3.46500000	-0.21552400
C	3.61069500	-1.75006200	-1.49627600
H	3.05953800	-1.10964300	-2.19357100
H	4.42767000	-1.15983900	-1.06512200
H	4.04990400	-2.57755600	-2.06745300
C	0.47763600	0.54562800	-0.76404900
H	0.58402200	0.54929700	-1.85001700
C	2.19201600	2.44161200	-2.14964500
H	2.95930600	1.65954200	-2.24485400
H	1.34674400	2.17714700	-2.78788200
H	2.61421200	3.37757000	-2.52475500
C	-0.88251100	0.00818400	-0.33092200
H	-0.99898400	-1.02062200	-0.69617800
H	-0.93548600	-0.04362300	0.76343200
C	-2.09316800	0.83871400	-0.83815000
H	-2.00779100	1.86008800	-0.44999600
H	-2.05114400	0.89294700	-1.93195700
C	-3.42189800	0.25081700	-0.43224600
C	-4.06903900	0.65340400	0.74852300
C	-5.10265300	-1.27731700	-0.86906500
C	-5.27459800	0.05516800	1.11106200
H	-3.62804800	1.42990000	1.36655800
C	-5.80925300	-0.93644200	0.28492000
H	-5.48726800	-2.04188400	-1.54129700
H	-5.78938400	0.35851600	2.01820000
H	-6.74610500	-1.42995400	0.52204200
N	-3.94110000	-0.70720900	-1.22814500

-1445.907348 [M06-2X/6-31++G(d,p)]

C	0.75656300	1.78930900	-0.60807100
O	0.50900000	2.24858100	0.54020500
C	2.19019300	3.72743300	-0.98016400
H	3.19868600	3.48310700	-0.61644400
H	2.28046400	4.46213300	-1.78391200
H	1.61896400	4.15822800	-0.16046900
N	1.50252700	2.54770000	-1.48047100
K	1.78034200	0.67991200	2.30118200
H	1.43419400	-0.24258800	-0.43423800
O	2.36195300	-0.77441700	0.25598500
C	2.78334800	-1.99466200	-0.29238000

C	3.85909300	-2.59703300	0.61781600
H	3.45031600	-2.75768400	1.62164400
H	4.22550000	-3.55628500	0.23359300
H	4.70742900	-1.90845900	0.69844300
C	1.59735800	-2.96833700	-0.39110100
H	0.83222800	-2.55994300	-1.06073300
H	1.90607500	-3.94758900	-0.77533200
H	1.14774800	-3.10711100	0.59854300
C	3.36807100	-1.77451100	-1.69722700
H	2.60697300	-1.33992400	-2.35514000
H	4.21437100	-1.08011700	-1.64676900
H	3.71594100	-2.71370700	-2.14346100
C	0.37610900	0.43459000	-0.98332600
H	0.36593300	0.24246000	-2.05738800
C	2.01626600	1.98365700	-2.71992000
H	2.70558100	1.14926700	-2.53597000
H	1.20483000	1.63026100	-3.36036800
H	2.55286500	2.76627800	-3.25836000
C	-0.86820000	-0.09365300	-0.29053400
H	-0.98146600	-1.16389100	-0.50551500
H	-0.76169200	-0.00723100	0.79914500
C	-2.16717800	0.62564500	-0.70492000
H	-2.07354000	1.68994700	-0.46260000
H	-2.29488900	0.53214500	-1.78906500
C	-3.37369100	0.04606400	-0.01912300
C	-3.85779700	0.59004300	1.17761500
C	-4.97082900	-1.61026600	0.03947900
C	-4.94387900	-0.00632300	1.80804600
H	-3.38293600	1.47195100	1.59728800
C	-5.51890200	-1.13484400	1.22798300
H	-5.39296500	-2.48796100	-0.44495800
H	-5.33712300	0.40223700	2.73395800
H	-6.36865300	-1.63475500	1.67927000
N	-3.92640000	-1.04376600	-0.57576500

Deprotonation of 4-methylstyrene monoadduct by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

49

-1469.578435 [B3LYP/6-31+G(d,p)]

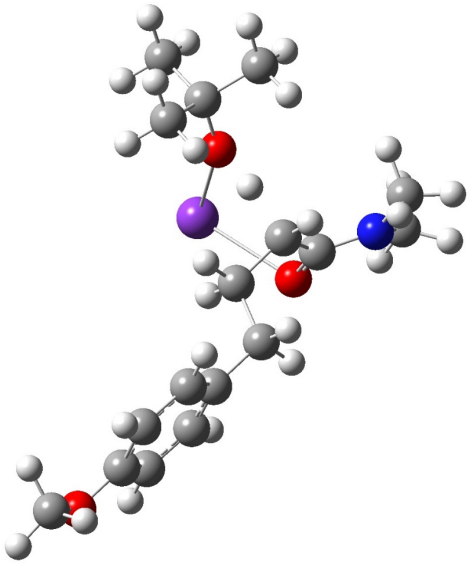
C	0.94828700	1.74608800	-0.12554400
O	0.66709700	1.97721700	1.09356200
C	2.58167100	3.58511400	-0.00511800
H	3.61367900	3.23030500	0.14296400
H	2.62524300	4.54681000	-0.52775800
H	2.11626300	3.72472100	0.96845000
N	1.79480300	2.63265500	-0.78109200
K	1.58914600	-0.01186200	2.68623100
H	1.43412700	-0.40631800	-0.27940800
O	2.17624400	-1.14845200	0.36356700
C	2.68409200	-2.27201800	-0.33322000
C	3.48599000	-1.82029700	-1.57401400
H	4.30779400	-1.16025400	-1.27337700
H	3.91253000	-2.67549600	-2.11316000
H	2.84247900	-1.26796000	-2.26739500
C	3.61507700	-3.04310800	0.62123500
H	3.06288900	-3.36467200	1.51195200
H	4.04018300	-3.93368800	0.14140200
H	4.44218600	-2.40118000	0.94597900
C	1.53024200	-3.19810500	-0.77748900
H	0.95488500	-3.52970200	0.09468800
H	0.84965300	-2.66656300	-1.45160300
H	1.90275300	-4.08778700	-1.30045200
C	0.49589700	0.53898900	-0.79459800
H	0.62289800	0.53749900	-1.87845400
C	2.26816400	2.41000300	-2.14236400
H	3.03791100	1.62639500	-2.19893500
H	1.44634700	2.13671200	-2.80681700
H	2.70399600	3.34051500	-2.51568600
C	-0.87087600	0.00246300	-0.38087200
H	-0.97563700	-1.03362300	-0.73150300
H	-0.94238800	-0.03623600	0.71293700
C	-2.07876200	0.81674400	-0.91644100
H	-1.98368900	1.85155200	-0.56462700
H	-2.02293400	0.84591900	-2.01204800
C	-3.41803800	0.25605100	-0.49120700
C	-4.12104100	-0.65278600	-1.29529700
C	-3.98511400	0.59514500	0.74960700
C	-5.33814600	-1.20343800	-0.87687200
H	-3.71623800	-0.93169400	-2.26593700
C	-5.19935400	0.04695900	1.16754300
H	-3.46976700	1.30387000	1.39454500
C	-5.90009700	-0.86667500	0.36226000
H	-5.85923200	-1.90174200	-1.52799900
H	-5.61219600	0.33609500	2.13181100
C	-7.21116800	-1.46279400	0.82351800
H	-7.92973700	-0.68289400	1.10034400
H	-7.66561200	-2.07722600	0.04097800
H	-7.07074100	-2.09739100	1.70693700

-1469.128214 [M06-2X/6-31++G(d,p)]

C	0.76863900	1.77085300	-0.65503900
O	0.30505100	2.27886200	0.40227200
C	2.23327700	3.71370300	-0.84666200
H	3.17880500	3.50185600	-0.32692400
H	2.43189600	4.43002400	-1.64790600
H	1.53380300	4.14995500	-0.13708200
N	1.65424800	2.50497800	-1.41102900
K	1.13384800	0.83381300	2.49191900

H	1.40053600	-0.23024400	-0.22115700
O	2.15219600	-0.70379400	0.69062900
C	2.73432800	-1.91991300	0.30363500
C	3.64873800	-1.70626000	-0.91338400
H	4.42281600	-0.96832900	-0.67400800
H	4.13843000	-2.63696400	-1.22341300
H	3.06276300	-1.32602700	-1.75794700
C	3.56174900	-2.46546000	1.47267000
H	2.91818300	-2.61914700	2.34634700
H	4.03835100	-3.42024800	1.22074600
H	4.34445400	-1.74833200	1.74408600
C	1.64216800	-2.93757800	-0.06439800
H	0.96594100	-3.08272200	0.78579500
H	1.05288500	-2.56652300	-0.91064000
H	2.06904500	-3.90906600	-0.34009100
C	0.47959200	0.39194800	-1.02226400
H	0.68847300	0.13683500	-2.06246300
C	2.39189800	1.90321800	-2.51104900
H	3.07715100	1.11724100	-2.16675800
H	1.71577500	1.47663900	-3.25480300
H	2.97808100	2.68340300	-2.99972800
C	-0.87310000	-0.12016200	-0.55748900
H	-0.92741400	-1.20618100	-0.71262100
H	-0.98671800	0.04026100	0.52279900
C	-2.07535500	0.53631800	-1.26381200
H	-2.01394200	1.62120800	-1.11535500
H	-1.99653900	0.34819000	-2.34172700
C	-3.39449600	0.02108200	-0.74723300
C	-4.01580700	-1.09043200	-1.32636800
C	-3.99997600	0.59571500	0.37591400
C	-5.20107900	-1.60729900	-0.80365200
H	-3.56350700	-1.55881100	-2.19815800
C	-5.18525300	0.08003200	0.89861600
H	-3.53354500	1.45836100	0.84800400
C	-5.80812000	-1.02906700	0.31594100
H	-5.66279000	-2.47270400	-1.27371100
H	-5.63496600	0.54654800	1.77224900
C	-7.11023700	-1.56381800	0.85840200
H	-7.96333700	-1.07351000	0.37691000
H	-7.20247700	-2.63782900	0.67725500
H	-7.19270500	-1.38676000	1.93390400

Deprotonation of 4-vinylanisole monoadduct by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

50

-1544.782817 [B3LYP/6-31+G(d,p)]

C	-0.16207200	-0.08023000	-0.65850400
O	-0.21303600	0.36564700	-1.84907800
C	-2.44620600	0.78145200	-0.33520500
H	-3.20723800	-0.00306100	-0.47111400
H	-2.85194700	1.53252200	0.35085100
H	-2.24650500	1.24521300	-1.29913600
N	-1.20432600	0.23796300	0.20443000
K	-0.32204600	-1.67544500	-3.62341100
H	0.43478200	-2.21707600	-0.79021000
O	0.05143800	-3.17254600	-1.46353200
C	0.20632400	-4.44465800	-0.86013000
C	-0.59588400	-4.51544900	0.45844600
H	-1.65623000	-4.31432500	0.26670400
H	-0.51389700	-5.50247600	0.93062900
H	-0.23113800	-3.76663500	1.16986800
C	-0.32950300	-5.50511400	-1.84005700
H	0.22612000	-5.46455700	-2.78418600
H	-0.23669300	-6.51889600	-1.43052500
H	-1.38744500	-5.31913300	-2.05855000
C	1.69716600	-4.72605600	-0.56902600
H	2.27767800	-4.68487500	-1.49776700
H	2.10243100	-3.97527300	0.11815700
H	1.84198900	-5.71544500	-0.11753800
C	0.89123900	-0.98344100	-0.22949600
H	0.95154700	-1.14047500	0.84884000
C	-1.30605600	-0.31320500	1.55092100
H	-1.60520800	-1.37143900	1.55249700
H	-0.36025300	-0.22012300	2.08818200
H	-2.06063900	0.25321700	2.10288200
C	2.26877200	-0.76423100	-0.84829100
H	2.89378800	-1.64894200	-0.66410400
H	2.18215300	-0.67416200	-1.93809600
C	3.02830600	0.48126200	-0.31914500
H	2.40453800	1.36738300	-0.49047700
H	3.14668600	0.38195600	0.76755000

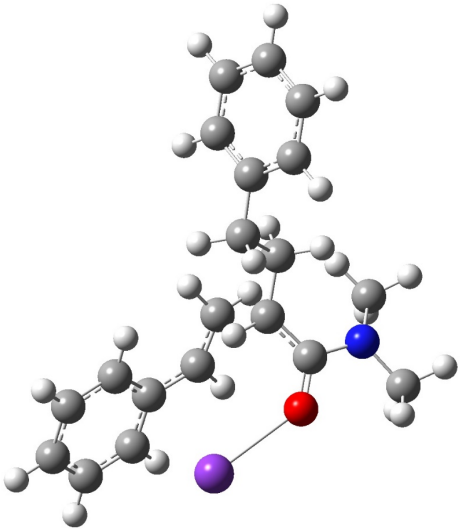
C	4.38321100	0.68500000	-0.96155600
C	5.54604000	0.12615200	-0.41707100
C	4.51793900	1.41241900	-2.15876700
C	6.79987800	0.27425200	-1.02658200
H	5.48317300	-0.43788100	0.51090500
C	5.75330300	1.57369600	-2.78140200
H	3.63823500	1.86689200	-2.60897100
C	6.90502600	1.00304100	-2.21738300
H	7.67142300	-0.17343400	-0.56374900
H	5.84477300	2.14326400	-3.70159300
O	8.07709100	1.21820800	-2.89765700
C	9.28236600	0.66771300	-2.36379100
H	9.23067700	-0.42592200	-2.31202000
H	10.07447700	0.96151900	-3.05286800
H	9.49621400	1.07226800	-1.36781200

-1544.309979 [M06-2X/6-31++G(d,p)]

C	-0.30747700	-0.05805200	-0.91870100
O	-0.10580400	0.36870200	-2.08847700
C	-2.58451900	0.80951300	-1.08007400
H	-2.16835900	1.38429200	-1.90453500
H	-3.24085600	0.02837500	-1.48971400
H	-3.18387700	1.46696800	-0.44527700
N	-1.49972200	0.23863000	-0.29782800
K	0.08898600	-1.75510400	-3.71059700
H	0.26010600	-2.14142600	-0.81421800
O	-0.06961600	-3.16006600	-1.49962700
C	0.57766400	-4.34080400	-1.10300600
C	1.92976200	-4.46385500	-1.82384800
H	2.55406700	-3.59355000	-1.59188800
H	2.47304300	-5.36967600	-1.52970800
H	1.77359200	-4.49531500	-2.90876300
C	0.81318300	-4.34463600	0.41674000
H	-0.14064000	-4.21691700	0.94192900
H	1.26953200	-5.28453200	0.74746700
H	1.47395900	-3.51995000	0.70613500
C	-0.30323700	-5.53932600	-1.47665700
H	-1.26664600	-5.46969100	-0.95977100
H	-0.49179600	-5.54042300	-2.55604800
H	0.16918400	-6.49100600	-1.20551400
C	0.63479800	-0.94934500	-0.25856800
H	0.51314800	-1.02436800	0.82290000
C	-1.88030700	-0.40202900	0.95158700
H	-1.98108300	-1.49022600	0.84258900
H	-1.15228800	-0.19784700	1.73988800
H	-2.84208000	0.00390600	1.26909500
C	2.08652000	-0.77349900	-0.66723300
H	2.68322100	-1.59446400	-0.24504500
H	2.18632900	-0.85635300	-1.75821500
C	2.71795500	0.56074100	-0.22713900
H	2.12138300	1.38123300	-0.64402100
H	2.65603700	0.63587400	0.86553000
C	4.15308300	0.69266900	-0.67008900
C	5.20729700	0.27899500	0.14382900
C	4.47050300	1.17436400	-1.94882900
C	6.53872500	0.33631400	-0.28148500
H	4.99319200	-0.09915800	1.14122100
C	5.78450400	1.24149900	-2.39241800
H	3.66928900	1.50473700	-2.60684700

C	6.82767600	0.82006100	-1.55841900
H	7.32537000	0.00667800	0.38690900
H	6.02625900	1.61861100	-3.38149500
O	8.08538900	0.92163700	-2.07697600
C	9.16530800	0.47997400	-1.27016800
H	9.06246100	-0.58231600	-1.02295100
H	10.06666000	0.63093900	-1.86265200
H	9.23258300	1.06575400	-0.34695600

Reaction of monoadduct K enolate (**7**) **with styrene** (**3**) **T.S.** (**T.S. 8**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1506.223261 [B3LYP/6-31+G(d,p)]

C	-4.34296200	-0.73864800	0.91081600
C	-4.04431900	0.62693400	1.04683700
C	-2.76518300	1.10866600	0.77860400
C	-1.70354200	0.25088600	0.36244000
C	-2.03755300	-1.12931000	0.22208700
C	-3.32069200	-1.60436900	0.49572800
H	-5.34066000	-1.11376400	1.11770100
H	-4.81860700	1.32178200	1.36415200
H	-2.56002100	2.17129500	0.89394300
H	-1.27764600	-1.83209100	-0.10689700
H	-3.52787800	-2.66552800	0.37596100
C	-0.39326400	0.78763400	0.08914700
H	-0.31332600	1.87416000	0.10676900
C	0.72432400	0.05383900	-0.30243100
H	0.78215100	-1.00783200	-0.07419700
H	1.68956200	0.54988800	-0.29314500
C	0.91073400	-0.50833000	-2.42340100
H	-0.02460800	-1.06317000	-2.40130000
C	0.73796300	0.72598700	-3.11942400
O	-0.42672300	1.16103900	-3.40311800
C	1.55121100	2.73577400	-4.25198400
H	0.78446500	2.54132300	-5.00162700
H	1.20275600	3.56249000	-3.61201500
H	2.47000600	3.05767000	-4.75321000
C	3.02064900	1.66027600	-2.64895800
H	3.19601300	0.76751500	-2.05545400

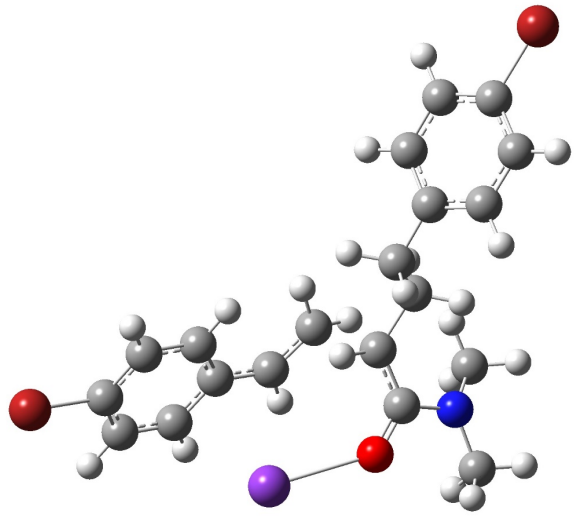
H	3.90461300	1.83504500	-3.27287700
H	2.92130900	2.51465200	-1.95948600
N	1.83561000	1.52400700	-3.49220000
K	-2.86368800	0.72361400	-2.58685700
C	2.14581200	-1.38524400	-2.48864200
H	2.81278800	-1.07579200	-3.30451900
H	2.75120500	-1.31777200	-1.56583600
C	1.78997000	-2.87830200	-2.69296500
H	1.11612500	-3.19223300	-1.88589400
H	1.23065000	-2.98137400	-3.63083400
C	3.00307300	-3.78270900	-2.72119700
C	3.68116600	-4.04096400	-3.92403700
C	3.50501400	-4.35862100	-1.54248600
C	4.82501100	-4.84488100	-3.95042600
H	3.30613400	-3.61055700	-4.84994300
C	4.64891100	-5.16332900	-1.56197900
H	2.99109300	-4.17860700	-0.60098000
C	5.31472300	-5.40899300	-2.76739600
H	5.33040700	-5.03366500	-4.89370200
H	5.01654600	-5.60101300	-0.63778100
H	6.20133300	-6.03636600	-2.78563600

-1505.771787 [M06-2X/6-31++G(d,p)]

C	-4.26102500	-0.51159500	0.60845100
C	-3.89250000	0.82380800	0.81693900
C	-2.56670700	1.22177600	0.69209800
C	-1.53882700	0.30735100	0.34718600
C	-1.93322700	-1.04183500	0.15493400
C	-3.26340300	-1.43580500	0.28535700
H	-5.29662900	-0.82196400	0.69759000
H	-4.64932500	1.56091000	1.07156700
H	-2.30383600	2.26610200	0.84531000
H	-1.19038300	-1.78547000	-0.11952400
H	-3.52549600	-2.47728800	0.11873500
C	-0.18565600	0.76858900	0.14312600
H	-0.03956400	1.84710300	0.14523900
C	0.85787100	-0.04338400	-0.24518500
H	0.83860300	-1.11255400	-0.04400400
H	1.85891100	0.37430100	-0.30022200
C	0.84535500	-0.64089000	-2.38696600
H	-0.07897800	-1.20055200	-2.25019300
C	0.60443600	0.61692000	-2.97795700
O	-0.56871600	1.08480300	-3.09359300
C	1.29897200	2.68169900	-4.04703100
H	0.50968100	2.51685200	-4.77978200
H	0.93933300	3.42089700	-3.31436300
H	2.17680400	3.09494500	-4.55210100
C	2.85201400	1.58353500	-2.57530800
H	3.15249400	0.64155200	-2.12197300
H	3.68667900	1.95057400	-3.18062300
H	2.66960200	2.31374400	-1.76953500
N	1.67715400	1.42428100	-3.42245100
K	-2.96939700	0.52232500	-2.40591900
C	2.09106700	-1.47362900	-2.53007200
H	2.69898700	-1.14521600	-3.38552900
H	2.74994500	-1.39289800	-1.64324400
C	1.76215400	-2.96719700	-2.70401200
H	1.11786400	-3.28234100	-1.87303200
H	1.18757700	-3.10210000	-3.62793200

C	3.00458200	-3.82122600	-2.73634600
C	3.68013800	-4.05858700	-3.93904800
C	3.54527800	-4.34363400	-1.55559800
C	4.86357400	-4.79653600	-3.96343100
H	3.27186300	-3.66068100	-4.86563400
C	4.72832300	-5.08262600	-1.57323400
H	3.03082700	-4.16893300	-0.61296600
C	5.39237300	-5.31124000	-2.77886600
H	5.37086700	-4.97218900	-4.90750700
H	5.12961900	-5.48185200	-0.64636500
H	6.31137900	-5.88883300	-2.79563600

Reaction of 4-bromostyrene/DMA monoadduct K enolate with 4-Bromostyrene (**11**) **T.S.**, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

47

-6648.507115 [B3LYP/6-31+G(d,p)]

C	-5.17995600	-1.66024300	0.28071700
C	-5.60432600	-0.48785200	0.91399000
C	-4.65783700	0.41325800	1.39176000
C	-3.25626500	0.18566400	1.26790400
C	-2.87517200	-1.01602200	0.60210600
C	-3.81723900	-1.92421400	0.12391600
H	-6.66257000	-0.28009500	1.03608900
H	-5.00044400	1.31919700	1.88663400
H	-1.82336600	-1.24318700	0.45999900
H	-3.48856600	-2.83186900	-0.37245700
C	-2.31377900	1.14202400	1.78958500
H	-2.74189800	2.06626200	2.17549500
C	-0.92893500	1.02785400	1.75037100
H	-0.46306400	0.05428400	1.62232700
H	-0.33862500	1.71882200	2.34241000
C	0.10468800	1.61744800	-0.14132400
H	-0.47908400	0.90032900	-0.71321000
C	-0.36439200	2.94375700	-0.36795500
O	-1.46869500	3.15778700	-0.96947900
C	-0.17443700	5.37942200	-0.26567600
H	-0.53088400	5.38070900	-1.29558800
H	-1.00935900	5.68340700	0.38638800
H	0.62552500	6.11981000	-0.16095300

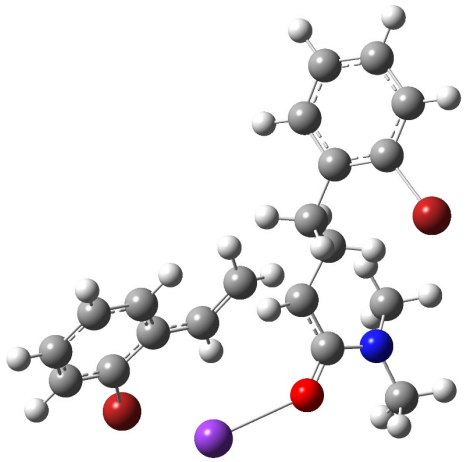
C	1.05028700	4.07185800	1.36906000
H	1.41548200	3.08295300	1.63221200
H	1.90809100	4.75252200	1.32660400
H	0.38563600	4.41778800	2.17781100
N	0.35731600	4.06707200	0.08285300
K	-3.58855000	1.78094000	-1.58863500
C	1.55250600	1.22047900	0.06091200
H	2.23201000	2.04139200	-0.20490100
H	1.77480300	0.97823100	1.11675800
C	1.93267700	-0.01943000	-0.78478200
H	1.24934900	-0.83977700	-0.53195300
H	1.76894900	0.21326400	-1.84364700
C	3.36041700	-0.47032500	-0.57819700
C	4.39361000	0.00649200	-1.39927000
C	3.69619700	-1.35231700	0.46079800
C	5.72215400	-0.37532500	-1.19532300
H	4.16052900	0.68519200	-2.21574000
C	5.01822200	-1.74530200	0.68464900
H	2.91418700	-1.74459900	1.10581400
C	6.01807300	-1.24775500	-0.14941800
H	6.50797400	0.00236100	-1.84027900
H	5.25985700	-2.42710500	1.49271400
Br	7.83787700	-1.76313400	0.15525500
Br	-6.47481200	-2.91904800	-0.35827000

-6648.213309 [M06-2X/6-31++G(d,p)]

C	-5.22003200	-1.13854500	0.06809000
C	-5.54763700	-0.00595000	0.81597100
C	-4.54073800	0.71084700	1.44789300
C	-3.17724100	0.33388200	1.36191300
C	-2.89320400	-0.83459300	0.61096500
C	-3.89627100	-1.56181700	-0.02301900
H	-6.58097900	0.31613000	0.89352700
H	-4.80427100	1.60017800	2.01463500
H	-1.86747700	-1.17369500	0.50440800
H	-3.64586300	-2.44713000	-0.59848700
C	-2.15177500	1.15233500	1.96134000
H	-2.47684500	2.10833900	2.36678800
C	-0.80526800	0.88907300	1.87163000
H	-0.43773900	-0.11631300	1.68059000
H	-0.10427600	1.52307300	2.40573900
C	0.10200300	1.36025200	-0.14406800
H	-0.48503300	0.56878100	-0.60760300
C	-0.47569300	2.62752800	-0.34749400
O	-1.64386800	2.76247800	-0.82420500
C	-0.44450900	5.05468200	-0.29549200
H	-0.82647000	5.02987300	-1.31552700
H	-1.28684600	5.26360900	0.38248500
H	0.28142500	5.86785200	-0.20392300
C	0.87251600	3.86158100	1.32386400
H	1.41247600	2.94400400	1.54797600
H	1.59000500	4.68781300	1.33148000
H	0.14010800	4.03894400	2.12898200
N	0.22411500	3.80280500	0.01990000
K	-3.64444700	1.38212500	-1.59702800
C	1.56573400	1.06536700	0.03845600
H	2.18527600	1.91853600	-0.27240100
H	1.82651500	0.87138000	1.09719400
C	1.99685300	-0.17427700	-0.76546300

H	1.37313600	-1.02476800	-0.46247900
H	1.80260300	0.00612700	-1.82888900
C	3.45063700	-0.50744600	-0.55837600
C	4.43461000	0.03889600	-1.38894700
C	3.85522600	-1.32240200	0.50423200
C	5.78773900	-0.21264400	-1.17072500
H	4.14072400	0.67216700	-2.22233800
C	5.20308900	-1.58642900	0.74010600
H	3.10616100	-1.75918100	1.16026700
C	6.15511400	-1.02402900	-0.10300700
H	6.54321600	0.21458200	-1.82086800
H	5.50806000	-2.21928600	1.56628700
Br	7.99185500	-1.36182800	0.21711200
Br	-6.58855600	-2.11992700	-0.79342000

Reaction of 2-bromostyrene/DMA monoadduct K enolate with 2-Bromostyrene (**12**) **T.S.**, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

47

-6648.507738 [B3LYP/6-31+G(d,p)]

C	-4.15547200	-1.05893700	1.00650700
C	-3.99774400	0.31584900	1.20677100
C	-2.78664300	0.93067900	0.89960600
C	-1.65875900	0.23494900	0.38352800
C	-1.87397200	-1.16423900	0.18803700
C	-3.07536000	-1.79188900	0.49404200
H	-5.09895900	-1.53944500	1.24465300
H	-4.81468300	0.90784600	1.60628400
H	-1.06235200	-1.75657100	-0.22107100
H	-3.17525100	-2.86083600	0.32498700
C	-0.40509500	0.87367900	0.06673700
H	-0.39299700	1.95831800	0.08647300
C	0.74794000	0.21667600	-0.33219400
H	0.89087200	-0.83880100	-0.12053500
H	1.66898800	0.78476400	-0.39430400
C	0.90103900	-0.40573900	-2.52354800
H	-0.05179400	-0.92366000	-2.44988400
C	0.76107300	0.83459700	-3.20371200
O	-0.39043900	1.32216700	-3.46332200
C	1.64019800	2.79467400	-4.37741300
H	0.85055900	2.62279200	-5.10857100
H	1.34105500	3.64528000	-3.74335200

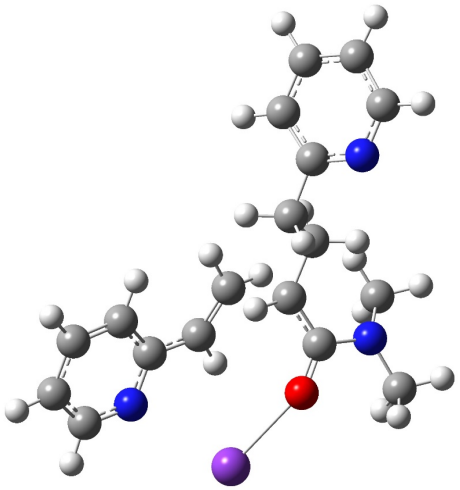
H	2.56138300	3.07023400	-4.90176900
C	3.07901200	1.69439200	-2.76732400
H	3.22509900	0.80786600	-2.15644500
H	3.96765200	1.82656100	-3.39526000
H	3.01098000	2.56515700	-2.09409400
N	1.88826100	1.58248800	-3.60632500
K	-2.84450600	1.12122900	-2.62888600
C	2.11136300	-1.31224800	-2.57400100
H	2.78779800	-1.02536800	-3.38845900
H	2.71402400	-1.25910300	-1.64833000
C	1.70885900	-2.79493200	-2.76797100
H	1.01129900	-3.07615400	-1.97083300
H	1.16712400	-2.89660900	-3.71426800
C	2.88431400	-3.74296700	-2.73057200
C	3.70659400	-4.01217700	-3.83430200
C	3.22252800	-4.38949800	-1.52773400
C	4.80924300	-4.86500400	-3.75937500
C	4.31595000	-5.25042500	-1.42772400
H	2.60107100	-4.20871000	-0.65442000
C	5.11483700	-5.49000900	-2.54881800
H	5.42003800	-5.04371700	-4.63756500
H	4.54057900	-5.73258300	-0.48112200
H	5.96930700	-6.15710900	-2.48945500
Br	-2.65772600	2.81826500	1.26201200
Br	3.33474800	-3.20319100	-5.53816900

-6648.216893 [M06-2X/6-31++G(d,p)]

C	-4.39458800	-0.16119100	0.52925400
C	-4.01209100	1.18017700	0.53864800
C	-2.67011900	1.52300300	0.41413300
C	-1.63247000	0.56897400	0.28452700
C	-2.06881100	-0.78316800	0.27559500
C	-3.40437300	-1.14052100	0.39784000
H	-5.44093300	-0.43024700	0.62117300
H	-4.75634600	1.96333700	0.63830400
H	-1.32656600	-1.56514700	0.15488400
H	-3.67765400	-2.19142600	0.38166200
C	-0.24431200	0.92628100	0.11933900
H	-0.02128700	1.97537500	-0.03783600
C	0.76874100	0.01335200	-0.03283300
H	0.66583200	-1.01887500	0.28974300
H	1.79405200	0.36434300	-0.08907400
C	0.84458300	-0.87534900	-2.15606500
H	-0.04739000	-1.46236400	-1.94488900
C	0.55645600	0.32437800	-2.82611600
O	-0.62947700	0.75100900	-2.97092700
C	1.18313100	2.31189400	-4.06661300
H	0.42947900	2.03773500	-4.80470600
H	0.75558900	3.08742100	-3.41172400
H	2.05195900	2.73327000	-4.58058200
C	2.72582900	1.45103200	-2.43896600
H	3.07988900	0.56898500	-1.90887500
H	3.55635600	1.84531300	-3.03279300
H	2.44563800	2.21563700	-1.69482000
N	1.61149300	1.13573600	-3.32564200
K	-3.11329900	0.39443400	-2.55070100
C	2.13760800	-1.63675800	-2.23437800
H	2.75154300	-1.26218200	-3.06398400
H	2.75587600	-1.52358000	-1.32352000

C	1.90355800	-3.14665300	-2.43361100
H	1.44472700	-3.56344800	-1.52999600
H	1.19405800	-3.29234800	-3.25502100
C	3.18658100	-3.87572600	-2.72440200
C	3.78270400	-3.86984900	-3.99007500
C	3.86919700	-4.56224400	-1.71185700
C	5.00160400	-4.48928100	-4.24906100
C	5.08336900	-5.20268300	-1.94829600
H	3.42629500	-4.59290400	-0.71956800
C	5.65599900	-5.16031600	-3.21817400
H	5.42592100	-4.45438300	-5.24643700
H	5.58508000	-5.72559900	-1.14019200
H	6.60310200	-5.65236100	-3.41340500
Br	-2.24567900	3.37344100	0.45030100
Br	2.92118100	-2.97798200	-5.43175200

Reaction of 2-vinylpyridine/DMA monoadduct K enolate with 2-vinylpyridine (**13**) **T.S.**, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

45

-1538.333123 [B3LYP/6-31+G(d,p)]

C	-4.32812500	-0.77914500	0.88794200
C	-4.05730000	0.56798500	0.65368100
C	-1.77555400	0.19996700	0.29982500
C	-1.98289500	-1.19607400	0.50553500
C	-3.24833100	-1.67517500	0.79910000
H	-5.33393400	-1.11300300	1.11925700
H	-4.86378300	1.29959900	0.69380300
H	-1.14473400	-1.88197900	0.44328800
H	-3.40184100	-2.73903100	0.96135700
C	-0.48899600	0.78083900	0.02068400
H	-0.48296700	1.86514400	-0.07281800
C	0.67621500	0.08542400	-0.25703800
H	0.77852600	-0.96443600	-0.00091000
H	1.61467400	0.62662200	-0.29267300
C	0.90498100	-0.59374600	-2.43860800
H	-0.02538300	-1.14747200	-2.34600100
C	0.71362200	0.63847700	-3.11640100
O	-0.45446100	1.09133900	-3.36011400
C	1.51083500	2.62150600	-4.30645700
H	0.74687600	2.40323200	-5.05273300

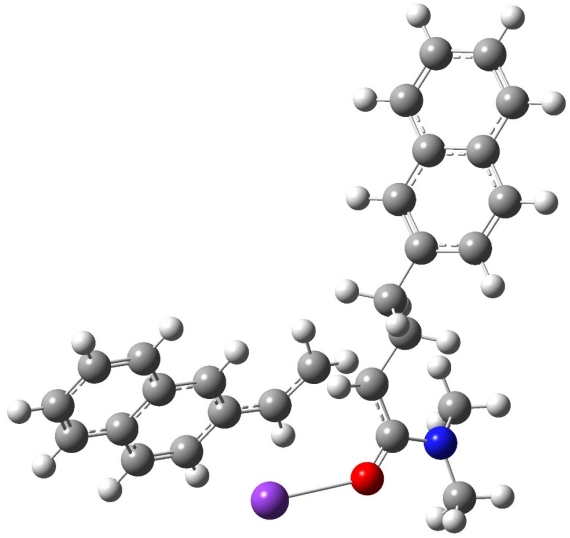
H	1.14904900	3.45376200	-3.68038300
H	2.42367000	2.95042900	-4.81419900
C	2.97401200	1.61920800	-2.65871500
H	3.18411600	0.73292900	-2.06572900
H	3.86016100	1.84119000	-3.26393000
H	2.81853700	2.46468200	-1.96749200
N	1.81625000	1.42542900	-3.52992600
K	-2.57121400	2.22116500	-2.33636800
C	2.15437000	-1.44600800	-2.47767000
H	2.82741600	-1.12868000	-3.28486400
H	2.74381300	-1.36512800	-1.54540700
C	1.82406700	-2.94499800	-2.68416600
H	1.15104700	-3.27356800	-1.88325300
H	1.29076800	-3.06537500	-3.63350300
C	3.05437600	-3.81999400	-2.70195900
C	3.52437600	-4.44418100	-1.53497700
C	4.81600100	-4.69101900	-3.91916400
C	4.68630500	-5.21317900	-1.58719200
H	2.97877300	-4.32714000	-0.60350600
C	5.35274900	-5.34250900	-2.80758100
H	5.30227500	-4.77131900	-4.88933400
H	5.06212300	-5.70478900	-0.69455500
H	6.25866300	-5.93246600	-2.90087000
N	-2.84360000	1.05919900	0.36095000
N	3.69901400	-3.94743800	-3.87957500

-1537.878239 [M06-2X/6-31++G(d,p)]

C	-4.73479000	-0.79082300	-0.61188700
C	-4.31728100	0.46212400	-0.17843900
C	-2.07177700	-0.13718500	-0.15682200
C	-2.41633900	-1.43077400	-0.62551000
C	-3.74306400	-1.75155000	-0.84529200
H	-5.78600800	-1.00114500	-0.77068600
H	-5.04821600	1.24929900	-0.00185700
H	-1.64115100	-2.16778500	-0.80560600
H	-4.01073600	-2.74321600	-1.19920500
C	-0.71136700	0.26551300	0.11329100
H	-0.57801000	1.29540100	0.43818700
C	0.39426500	-0.51150700	-0.12617300
H	0.31695800	-1.58730800	-0.25751500
H	1.36922300	-0.17197000	0.20726400
C	1.03776000	-0.52039700	-2.32897400
H	0.09295900	-1.00223700	-2.56967300
C	0.99852400	0.87036100	-2.50712900
O	-0.08625200	1.49420000	-2.72044900
C	2.02974600	3.05884400	-2.68851800
H	1.48546500	3.19452100	-3.62304000
H	1.48399100	3.59087000	-1.89265000
H	3.02254500	3.50786900	-2.78490900
C	3.03958300	1.44041900	-1.23281400
H	3.19723100	0.38317400	-1.02799100
H	4.01627400	1.89958000	-1.41368600
H	2.60560500	1.90817300	-0.33271500
N	2.19067500	1.64241300	-2.40077000
K	-1.97385800	2.81757300	-1.64719300
C	2.25667000	-1.39953000	-2.37402100
H	3.09798100	-0.89141500	-2.86534400
H	2.61362400	-1.67085400	-1.36117600
C	1.97274000	-2.71578700	-3.11995200

H	1.12154300	-3.21551700	-2.64183700
H	1.69294500	-2.49251200	-4.15467200
C	3.16583700	-3.63310800	-3.11686100
C	3.33020200	-4.59747700	-2.11486900
C	5.17104200	-4.22567600	-4.07645800
C	4.46920200	-5.39473700	-2.11592700
H	2.56710100	-4.71504100	-1.35139900
C	5.41595100	-5.20848900	-3.12065500
H	5.88538600	-4.05197500	-4.87797700
H	4.61446000	-6.15016000	-1.34990700
H	6.31912800	-5.80659600	-3.16760500
N	-3.04059000	0.79650500	0.04021400
N	4.07936400	-3.45179400	-4.08343900

Reaction of 2-vinylnaphthalene/DMA monoadduct K enolate with 2-vinylnaphthalene (14) T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

59

-1813.442609 [B3LYP/6-31+G(d,p)]

C	-2.20488500	1.01127100	1.85958000
H	-2.59953900	1.90925100	2.33300400
C	-0.82658400	0.88005000	1.74763400
H	-0.38767200	-0.09052400	1.53126500
H	-0.19507900	1.52605900	2.34781800
C	0.15184900	1.56325100	-0.15785900
H	-0.44270800	0.86384100	-0.74039100
C	-0.33032900	2.89384200	-0.32270000
O	-1.44987400	3.12363600	-0.89007100
C	-0.14637100	5.32572200	-0.14215100
H	-0.52930800	5.35935400	-1.16188700
H	-0.96487800	5.60536300	0.54087100
H	0.65412400	6.06505100	-0.03375600
C	1.11971300	3.96895800	1.41899100
H	1.49324400	2.97319200	1.64116300
H	1.97459600	4.65351400	1.37991800
H	0.47259800	4.28583000	2.25347300
N	0.39753900	4.00452100	0.14940500
K	-3.55311000	1.70271200	-1.49750700
C	1.60399900	1.16459600	0.00438800

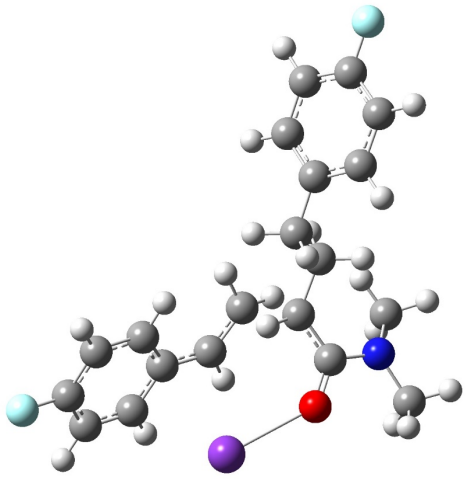
H	2.27421900	1.99914200	-0.24155700
H	1.84545400	0.88482000	1.04659100
C	1.97816400	-0.04502600	-0.88763100
H	1.30147300	-0.87681300	-0.65734100
H	1.80279200	0.22567100	-1.93670100
C	3.41067400	-0.49694400	-0.71019600
C	3.73703400	-1.56667500	0.10373900
C	4.46676000	0.20592400	-1.36180600
C	5.08590500	-1.97302500	0.30755500
H	2.94789600	-2.12269500	0.60605500
C	5.78436400	-0.15848400	-1.19088800
H	4.21993100	1.04362300	-2.00972200
C	5.42905300	-3.07295600	1.14399000
C	6.13639400	-1.25393200	-0.35276600
H	6.57422300	0.38781200	-1.70055600
C	6.74658100	-3.44291200	1.32108100
H	4.63319400	-3.61918000	1.64415000
C	7.48496500	-1.66045200	-0.15087200
C	7.78535300	-2.73024100	0.66748600
H	6.99376100	-4.28371300	1.96284000
H	8.27836700	-1.11252700	-0.65309900
H	8.81861100	-3.03109300	0.81430000
C	-3.18556400	0.10607800	1.31376500
C	-2.88297200	-1.01054400	0.51173600
C	-4.58299000	0.34224600	1.58429200
C	-3.88304600	-1.88677300	0.01921000
H	-1.84850500	-1.22734400	0.25826700
C	-5.57287400	-0.48428800	1.11412600
H	-4.84982200	1.20475200	2.19137500
C	-3.57266500	-3.02824000	-0.78108900
C	-5.26651600	-1.63132900	0.31952600
H	-6.61412100	-0.27135000	1.34634400
C	-4.56747000	-3.86315800	-1.25120300
H	-2.53087000	-3.23354600	-1.01631600
C	-6.26421300	-2.50669000	-0.17847000
C	-5.92935600	-3.60586600	-0.95028200
H	-4.30603700	-4.72657900	-1.85733500
H	-7.30578100	-2.29990200	0.05783700
H	-6.70279400	-4.26960900	-1.32541400

-1812.867090 [M06-2X/6-31++G(d,p)]

C	-2.11090000	1.05026500	2.01532000
H	-2.47962200	1.97724700	2.44950800
C	-0.75537400	0.85473500	1.90592300
H	-0.34747600	-0.13089700	1.69244000
H	-0.07483000	1.51642400	2.43275500
C	0.10105200	1.37763400	-0.13250900
H	-0.52943600	0.61634600	-0.58905800
C	-0.44628400	2.66641300	-0.26818300
O	-1.63080900	2.85024400	-0.68740900
C	-0.34038900	5.08953900	-0.14829900
H	-0.77189500	5.10829800	-1.14857500
H	-1.14257700	5.29851700	0.57684500
H	0.41208400	5.87940500	-0.06666200
C	1.01870800	3.81322000	1.36759400
H	1.51840500	2.86432300	1.55035000
H	1.77822100	4.60120800	1.35458000
H	0.33526900	4.01341500	2.20975600
N	0.30631800	3.81056900	0.09633400

K	-3.64187800	1.44323200	-1.37798900
C	1.55904200	1.02873000	-0.00835500
H	2.19595500	1.86378100	-0.33402200
H	1.85255300	0.81516600	1.03789500
C	1.91234400	-0.22174100	-0.83381000
H	1.26839600	-1.05012600	-0.51290300
H	1.68418600	-0.02510700	-1.88866600
C	3.35926900	-0.61588700	-0.68682800
C	3.75154100	-1.62855800	0.15851000
C	4.36008600	0.10658000	-1.39899400
C	5.12253000	-1.96556100	0.33271900
H	3.00240500	-2.19351100	0.71078800
C	5.69131000	-0.19245500	-1.25656500
H	4.05155900	0.90593300	-2.06908500
C	5.53658000	-3.01188200	1.20222000
C	6.11188300	-1.23657200	-0.38640800
H	6.44418600	0.36346500	-1.80968800
C	6.86853000	-3.31630300	1.34991700
H	4.77883200	-3.56731200	1.74898000
C	7.48188400	-1.57351700	-0.21468500
C	7.85338300	-2.58894300	0.63355600
H	7.17320600	-4.11735900	2.01627300
H	8.23197300	-1.01270600	-0.76651900
H	8.90233900	-2.83852300	0.75909900
C	-3.10169400	0.17810600	1.42706600
C	-2.79144500	-0.92709400	0.63109400
C	-4.49658200	0.47928800	1.60910500
C	-3.79523900	-1.73157700	0.03314000
H	-1.75306700	-1.18881300	0.44290200
C	-5.48502700	-0.27561200	1.03748900
H	-4.76094700	1.34105000	2.21747500
C	-3.47576000	-2.85480600	-0.78437000
C	-5.17169800	-1.40928200	0.22913600
H	-6.52977800	-0.01713700	1.19303200
C	-4.46650100	-3.61196200	-1.36292100
H	-2.42923700	-3.10439000	-0.94118500
C	-6.17208900	-2.20740400	-0.38121200
C	-5.83247500	-3.28935400	-1.16131600
H	-4.20339300	-4.46596600	-1.97991200
H	-7.21605300	-1.94927400	-0.21977500
H	-6.60467400	-3.89582900	-1.62369300

Reaction of 4-fluorostyrene/DMA monoadduct K enolate with 4-fluorostyrene (**15**) **T.S.**, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

47

-1704.722671 [B3LYP/6-31+G(d,p)]

C	-4.69502400	-2.71908700	-0.10357800
C	-5.28214000	-1.65413200	0.57173900
C	-4.45678700	-0.68433600	1.14010000
C	-3.03445200	-0.74576300	1.05765700
C	-2.49886900	-1.85553900	0.33925700
C	-3.31598200	-2.83421000	-0.22937000
H	-6.36295200	-1.58752400	0.65113400
H	-4.91527900	0.14445400	1.67479800
H	-1.42413900	-1.95371600	0.22603000
H	-2.88815500	-3.67287600	-0.77052200
C	-2.21888600	0.27776900	1.66776500
H	-2.75588200	1.13486200	2.07239400
C	-0.82541500	0.30597500	1.68041900
H	-0.26601400	-0.61956100	1.56293900
H	-0.33804600	1.02109800	2.33559800
C	0.20806800	1.03115700	-0.10769400
H	-0.31430200	0.32351200	-0.74765800
C	-0.31062300	2.34793900	-0.30091300
O	-1.40461600	2.53702300	-0.92780800
C	-0.22135000	4.78490800	-0.10708300
H	-0.55542000	4.80617900	-1.14416200
H	-1.07963400	5.04044400	0.53525000
H	0.55040600	5.54809700	0.03826100
C	1.01736100	3.46776000	1.51071700
H	1.39377900	2.47903400	1.75758700
H	1.86357100	4.16426000	1.50180200
H	0.33088200	3.78233200	2.31378900
N	0.34731000	3.48109000	0.21283900
K	-3.50911000	1.13625000	-1.54970800
C	1.67080900	0.69848400	0.11527100
H	2.31565200	1.55869600	-0.10989200
H	1.87961200	0.43706400	1.16921500
C	2.13534700	-0.49629100	-0.75232500
H	1.48481000	-1.35539700	-0.54628200
H	1.99497600	-0.24056700	-1.80939000
C	3.57747100	-0.88568200	-0.50952100

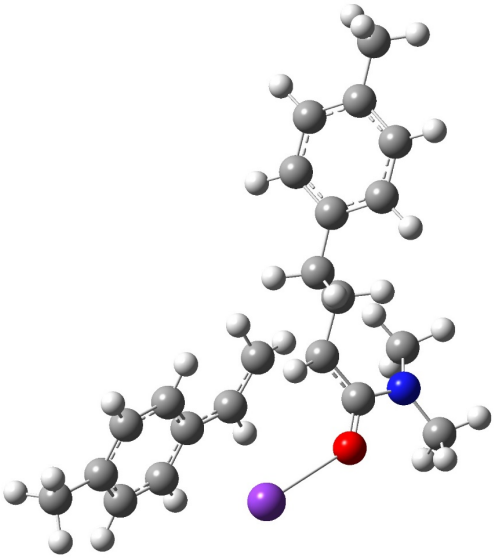
C	4.61583800	-0.31943600	-1.26654900
C	3.91897000	-1.79582800	0.50434700
C	5.95541300	-0.64148800	-1.02617800
H	4.37776200	0.38304500	-2.06096800
C	5.25069300	-2.13391400	0.76519000
H	3.13338100	-2.25420700	1.09926400
C	6.23959000	-1.54391900	-0.01021600
H	6.75854500	-0.20826000	-1.61301000
H	5.51585500	-2.83964300	1.54540600
F	-5.50421300	-3.68174700	-0.67031000
F	7.54857400	-1.87048200	0.23267000

-1704.214880 [M06-2X/6-31++G(d,p)]

C	-4.82107800	-2.30323600	-0.21685400
C	-5.31631400	-1.26827100	0.56608000
C	-4.41490600	-0.44081700	1.22719700
C	-3.01150300	-0.61599300	1.12570600
C	-2.56651700	-1.68726200	0.31035600
C	-3.46010800	-2.52734700	-0.35307800
H	-6.38789400	-1.11855900	0.65068900
H	-4.79733600	0.37339200	1.83763500
H	-1.50269900	-1.86173500	0.18183800
H	-3.10766200	-3.34161700	-0.97822900
C	-2.10614000	0.29950900	1.78430900
H	-2.55278200	1.19251600	2.21650400
C	-0.73132300	0.18985500	1.74429000
H	-0.25837600	-0.77375300	1.56164300
H	-0.13407600	0.85866400	2.35690500
C	0.23452900	0.82191200	-0.13191900
H	-0.29286900	0.05348700	-0.69554000
C	-0.35756700	2.09103700	-0.30999500
O	-1.49890600	2.22506400	-0.84453500
C	-0.38066500	4.51242800	-0.14681000
H	-0.70821800	4.52747900	-1.18587300
H	-1.26105600	4.67495200	0.49429500
H	0.32370200	5.33264000	0.01948300
C	0.88666500	3.27134000	1.47889100
H	1.41986400	2.34726000	1.69158200
H	1.59967700	4.09848800	1.54912200
H	0.11911200	3.41647700	2.25674000
N	0.29499900	3.25918200	0.14721600
K	-3.46824800	0.79824100	-1.60102700
C	1.69985100	0.56173100	0.09692600
H	2.30475600	1.44572100	-0.15043500
H	1.92128400	0.33055600	1.15724100
C	2.20632800	-0.62811400	-0.73681800
H	1.60902300	-1.51422800	-0.48684500
H	2.03855500	-0.41616500	-1.79908700
C	3.66786900	-0.91034900	-0.49446400
C	4.65255300	-0.27509900	-1.25988100
C	4.07502700	-1.76157700	0.53896300
C	6.00927400	-0.47669400	-1.00967700
H	4.35470900	0.38859400	-2.06778100
C	5.42578300	-1.98016400	0.80973500
H	3.32411100	-2.26522100	1.14275600
C	6.36277000	-1.32785900	0.02495000
H	6.77913700	0.00932100	-1.59929000
H	5.75042900	-2.64025700	1.60684700
F	-5.69675100	-3.11563700	-0.86911300

F	7.68037100	-1.53206300	0.27765300

Reaction of 4-methylstyrene/DMA monoadduct K enolate with 4-methylstyrene (**16**) **T.S.**, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

53

-1584.814137 [B3LYP/6-31+G(d,p)]

C	-4.29301900	-0.82789000	0.94747200
C	-4.04066500	0.55505200	1.03613800
C	-2.78847000	1.09241100	0.74971800
C	-1.68514700	0.28113400	0.35187800
C	-1.95909000	-1.11314700	0.25167200
C	-3.21911100	-1.63908700	0.54665900
H	-4.84525200	1.22505900	1.33529900
H	-2.64108200	2.16779700	0.83363800
H	-1.17280100	-1.79229100	-0.06524700
H	-3.37254800	-2.71310000	0.45340800
C	-0.40194400	0.87246300	0.05627300
H	-0.37313200	1.96167800	0.04085600
C	0.74402000	0.17750200	-0.33258300
H	0.85585300	-0.86988600	-0.05970000
H	1.68528800	0.71846200	-0.34329400
C	0.91155000	-0.44284600	-2.40935600
H	-0.02732400	-0.99107200	-2.37089400
C	0.74443200	0.76697300	-3.15200800
O	-0.41815700	1.20228800	-3.44247900
C	1.57512600	2.71717900	-4.37423000
H	0.79160300	2.50233300	-5.10052400
H	1.25490300	3.58120900	-3.76978900
H	2.49173400	2.99528900	-4.90502500
C	3.04397700	1.68883400	-2.73820700
H	3.20084600	0.82631200	-2.09659300
H	3.92655400	1.80558800	-3.37773700
H	2.97280900	2.58263200	-2.09707400
N	1.84694400	1.53787700	-3.56150300
K	-2.84003600	0.70796500	-2.59320700
C	2.13629800	-1.33622300	-2.47006400
H	2.79882600	-1.04908200	-3.29736900
H	2.75069900	-1.25898800	-1.55392300

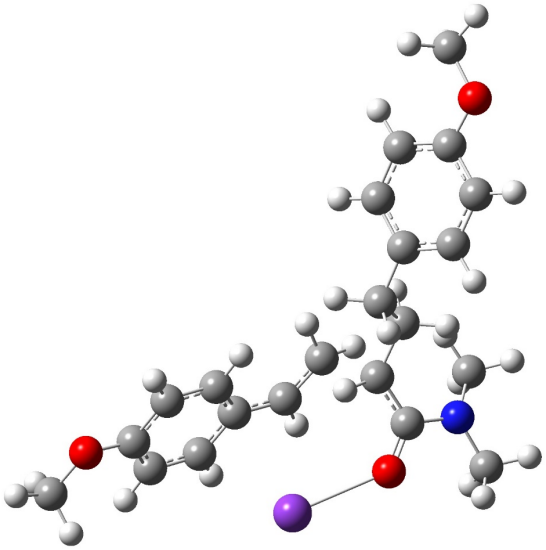
C	1.76072100	-2.82802400	-2.64489900
H	1.09378000	-3.12066300	-1.82407000
H	1.18594500	-2.93771000	-3.57291400
C	2.95935400	-3.75139900	-2.67694100
C	3.63367700	-4.02248500	-3.87832100
C	3.46112900	-4.33828100	-1.50527100
C	4.76288700	-4.84505900	-3.90664100
H	3.26994100	-3.58435900	-4.80538900
C	4.59133200	-5.16152000	-1.53276800
H	2.96078800	-4.15106900	-0.55761700
C	5.26277500	-5.43331200	-2.73410000
H	5.26136800	-5.03489700	-4.85470100
H	4.95380300	-5.60104400	-0.60612200
C	-5.64795200	-1.40612300	1.28752400
H	-5.74580300	-2.43157600	0.91678800
H	-5.81914000	-1.43407900	2.37225800
H	-6.46167600	-0.81375400	0.85277700
C	6.46287300	-6.35249500	-2.77181300
H	6.16430100	-7.38408700	-2.99810800
H	7.17665000	-6.04568700	-3.54289400
H	6.98414500	-6.36768300	-1.80981000

-1584.318936 [M06-2X/6-31++G(d,p)]

C	0.76863900	1.77085300	-0.65503900
O	0.30505100	2.27886200	0.40227200
C	2.23327700	3.71370300	-0.84666200
H	3.17880500	3.50185600	-0.32692400
H	2.43189600	4.43002400	-1.64790600
H	1.53380300	4.14995500	-0.13708200
N	1.65424800	2.50497800	-1.41102900
K	1.13384800	0.83381300	2.49191900
H	1.40053600	-0.23024400	-0.22115700
O	2.15219600	-0.70379400	0.69062900
C	2.73432800	-1.91991300	0.30363500
C	3.64873800	-1.70626000	-0.91338400
H	4.42281600	-0.96832900	-0.67400800
H	4.13843000	-2.63696400	-1.22341300
H	3.06276300	-1.32602700	-1.75794700
C	3.56174900	-2.46546000	1.47267000
H	2.91818300	-2.61914700	2.34634700
H	4.03835100	-3.42024800	1.22074600
H	4.34445400	-1.74833200	1.74408600
C	1.64216800	-2.93757800	-0.06439800
H	0.96594100	-3.08272200	0.78579500
H	1.05288500	-2.56652300	-0.91064000
H	2.06904500	-3.90906600	-0.34009100
C	0.47959200	0.39194800	-1.02226400
H	0.68847300	0.13683500	-2.06246300
C	2.39189800	1.90321800	-2.51104900
H	3.07715100	1.11724100	-2.16675800
H	1.71577500	1.47663900	-3.25480300
H	2.97808100	2.68340300	-2.99972800
C	-0.87310000	-0.12016200	-0.55748900
H	-0.92741400	-1.20618100	-0.71262100
H	-0.98671800	0.04026100	0.52279900
C	-2.07535500	0.53631800	-1.26381200
H	-2.01394200	1.62120800	-1.11535500
H	-1.99653900	0.34819000	-2.34172700
C	-3.39449600	0.02108200	-0.74723300

C	-4.01580700	-1.09043200	-1.32636800
C	-3.99997600	0.59571500	0.37591400
C	-5.20107900	-1.60729900	-0.80365200
H	-3.56350700	-1.55881100	-2.19815800
C	-5.18525300	0.08003200	0.89861600
H	-3.53354500	1.45836100	0.84800400
C	-5.80812000	-1.02906700	0.31594100
H	-5.66279000	-2.47270400	-1.27371100
H	-5.63496600	0.54654800	1.77224900
C	-7.11023700	-1.56381800	0.85840200
H	-7.96333700	-1.07351000	0.37691000
H	-7.20247700	-2.63782900	0.67725500
H	-7.19270500	-1.38676000	1.93390400

Reaction of 4-vinylanisole/DMA monoadduct K enolate with 4-vinylanisole (**17**) **T.S.**, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

55

-1735.221248 [B3LYP/6-31+G(d,p)]

C	-4.22798600	-0.87243700	0.94684700
C	-4.05368000	0.51542900	1.03276700
C	-2.81462900	1.08588000	0.72217300
C	-1.68905600	0.31794800	0.31782200
C	-1.91351000	-1.08895800	0.23141400
C	-3.14228800	-1.66396000	0.54202800
H	-4.86740400	1.16386700	1.33844100
H	-2.70805600	2.16593600	0.80540800
H	-1.10591400	-1.74185700	-0.08569200
H	-3.27814200	-2.73984000	0.46663700
C	-0.42381600	0.94702800	0.01115600
H	-0.42690300	2.03662800	-0.00961600
C	0.74255400	0.28061300	-0.37870800
H	0.88695900	-0.75676500	-0.08061400
H	1.66774500	0.84958500	-0.37858500

C	0.93235400	-0.34390200	-2.41623200
H	-0.01996300	-0.87012500	-2.40963200
C	0.81527800	0.86362500	-3.17726600
O	-0.32828300	1.32559500	-3.49821200
C	1.72686600	2.78127700	-4.39358100
H	0.95208700	2.58383800	-5.13397400
H	1.42167500	3.66010100	-3.80303300
H	2.66215800	3.02609300	-4.90786300
C	3.13603200	1.71729400	-2.72708000
H	3.25114100	0.85751400	-2.07326100
H	4.03124400	1.79366500	-3.35509500
H	3.08895800	2.62072300	-2.09762500
N	1.94561900	1.60175800	-3.56538600
K	-2.76203300	0.97995200	-2.61583600
C	2.13358200	-1.27189000	-2.45744700
H	2.80883500	-1.01531100	-3.28457500
H	2.74397200	-1.19685000	-1.53846800
C	1.71992100	-2.75539800	-2.61097400
H	1.04139500	-3.01861500	-1.78976600
H	1.14538500	-2.86409200	-3.53950300
C	2.89233700	-3.71269400	-2.62309100
C	3.58062600	-4.00405700	-3.81518200
C	3.35689000	-4.31657300	-1.44876900
C	4.68156400	-4.85672900	-3.83272700
H	3.24516200	-3.55848400	-4.74895100
C	4.46321500	-5.17740900	-1.44227000
H	2.84563700	-4.12060500	-0.50904900
C	5.13161100	-5.44898600	-2.64213300
H	5.20131600	-5.07828100	-4.76015300
H	4.78225700	-5.62428800	-0.50814000
O	-5.40459400	-1.54114600	1.22568000
C	-6.52888800	-0.76973500	1.63950300
H	-6.82901600	-0.05231300	0.86563100
H	-7.33834000	-1.48184100	1.80501500
H	-6.32321100	-0.23041200	2.57245500
O	6.21984500	-6.27573600	-2.75605300
C	6.71572500	-6.91144200	-1.57637200
H	7.56774800	-7.51098900	-1.89742800
H	7.04646600	-6.17316400	-0.83691500
H	5.95738100	-7.56425500	-1.12909400

-1734.678708 [M06-2X/6-31++G(d,p)]

C	-4.25030700	-0.58531700	0.76662400
C	-3.91908600	0.76263500	0.94121200
C	-2.60302600	1.18519600	0.75135000
C	-1.56181400	0.30624400	0.37798700
C	-1.93540500	-1.05339100	0.20971600
C	-3.24291200	-1.48489200	0.39985200
H	-4.66976200	1.49264500	1.22299500
H	-2.37266200	2.23962700	0.88614600
H	-1.19005800	-1.78390000	-0.09259200
H	-3.50448400	-2.52975300	0.25786100
C	-0.22374300	0.79636900	0.12938200
H	-0.10308600	1.87792300	0.10976400
C	0.83174600	-0.00135700	-0.27561800
H	0.84421800	-1.06203100	-0.02643900
H	1.82466300	0.43772900	-0.32652200
C	0.83185700	-0.61642900	-2.34422700
H	-0.10322400	-1.16584500	-2.23813700

C	0.61642800	0.62573100	-2.98921200
O	-0.54927900	1.09761200	-3.13981900
C	1.34825300	2.65867200	-4.09207500
H	0.55776500	2.49288600	-4.82317900
H	1.00145700	3.42031600	-3.37662900
H	2.23564200	3.04295000	-4.60312600
C	2.88903100	1.55300100	-2.60896000
H	3.15968100	0.61704000	-2.12631900
H	3.72970100	1.86864400	-3.23441800
H	2.74110000	2.31583600	-1.82738300
N	1.69950300	1.40878200	-3.43759100
K	-2.92154400	0.52351100	-2.37011400
C	2.06121400	-1.47812600	-2.47388100
H	2.66664500	-1.19110100	-3.34581300
H	2.72965700	-1.37785400	-1.59636800
C	1.70587800	-2.97028800	-2.59131300
H	1.08240300	-3.25105200	-1.73252000
H	1.09845000	-3.12276100	-3.49168000
C	2.93205700	-3.84701300	-2.63968800
C	3.59045300	-4.09807700	-3.85253600
C	3.49009300	-4.38028300	-1.47837600
C	4.75719400	-4.84884800	-3.90064000
H	3.17877400	-3.69714200	-4.77623300
C	4.66493300	-5.13922100	-1.50203900
H	3.00102900	-4.20389000	-0.52271500
C	5.30265100	-5.37249200	-2.72170500
H	5.26223000	-5.04343700	-4.84175300
H	5.06094700	-5.53573100	-0.57454700
O	-5.50655600	-1.10765800	0.92644300
C	-6.54072300	-0.20879700	1.28517300
H	-6.67254200	0.56730900	0.52251200
H	-7.44995500	-0.80453300	1.35658100
H	-6.33688000	0.26343100	2.25303400
O	6.44971800	-6.09595100	-2.86475400
C	7.04266200	-6.62577500	-1.68985600
H	7.94153200	-7.14825900	-2.01414300
H	7.31490900	-5.82605200	-0.99239200
H	6.36840100	-7.33162700	-1.19269400

10.2. REACTIONS OF *N,N*-DIMETHYLPROPIONAMIDE (DMP, 18) WITH STYRENE

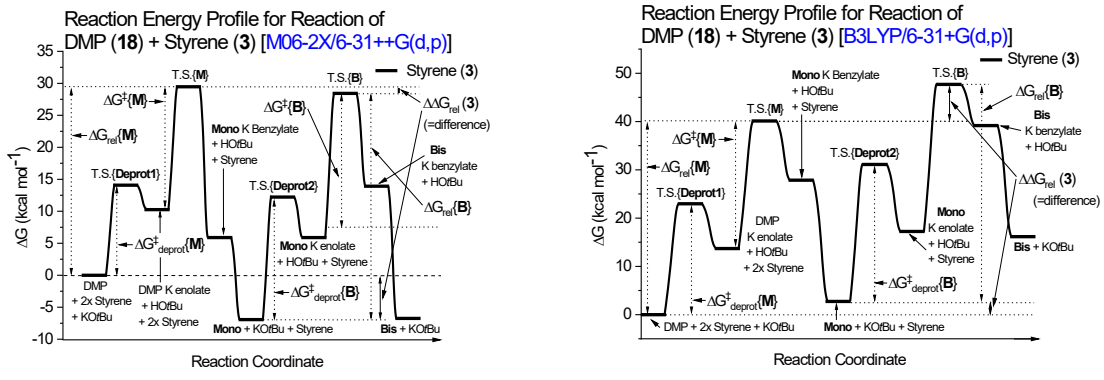
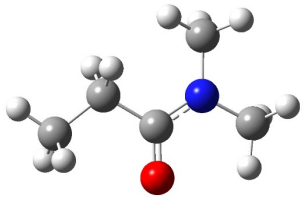


Figure S66. Left: M06-2X/6-31++G(d,p) computed reaction profile for KO*t*Bu-catalyzed reaction of DMP (**18**) with styrene (**3**, black line). The transition states for reactions of monoadduct K benzylates or bisadduct K benzylates with proton sources are not shown. Right: B3LYP/6-31+G(d,p) profile.

10.2.1. XYZ Co-ordinates of starting materials, intermediates, products

***N*,*N*-Dimethylpropionamide** (DMP, **18**), solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

18

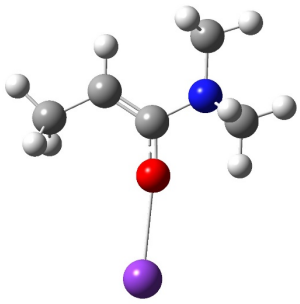
-327.057494 [B3LYP/6-31+G(d,p)]

C	0.22119900	-0.34003400	-0.02215000
O	0.49101800	-1.55355700	0.00211000
N	-1.06833700	0.10452600	-0.06133200
C	-2.17158200	-0.84970300	0.02002800
H	-2.66813600	-0.78334400	0.99661300
H	-2.90867500	-0.62854400	-0.75873000
H	-1.78687300	-1.85807100	-0.11738600
C	-1.46164000	1.50936600	0.02169300
H	-2.32157000	1.67662200	-0.63359100
H	-1.75206100	1.77884900	1.04572500
H	-0.65997500	2.16954700	-0.30119300
C	1.33396800	0.70900200	-0.02019500
H	1.18853400	1.37747300	0.83725300
H	1.23115700	1.33815000	-0.91295800
C	2.73556000	0.10030200	0.02510100
H	2.92002100	-0.54001000	-0.84198100
H	3.48507400	0.89798000	0.02738900
H	2.87768400	-0.50547400	0.92443700

-326.888459 [M06-2X/6-31++G(d,p)]

C	0.21876300	-0.34325600	-0.04268900
O	0.49379700	-1.54748800	-0.01866500
N	-1.06407900	0.10174100	-0.07888800
C	-2.16431500	-0.84242500	0.04477000
H	-2.64093600	-0.74672800	1.02742100
H	-2.91190300	-0.64005300	-0.72730900
H	-1.78239800	-1.85385900	-0.07325600
C	-1.42889300	1.50755200	0.02666500
H	-2.40076300	1.64789900	-0.45076400
H	-1.50790600	1.82399200	1.07398700
H	-0.70875700	2.14426300	-0.48493600
C	1.31783600	0.71038100	-0.04544100
H	1.14214100	1.40644300	0.78278700
H	1.23387600	1.30227400	-0.96446000
C	2.70662800	0.09484300	0.05970500
H	2.90068000	-0.57759600	-0.77889000
H	3.46528300	0.88130000	0.05741000
H	2.80875300	-0.48279100	0.98147800

***N*,*N*-Dimethylpropionamide K enolate**, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

18

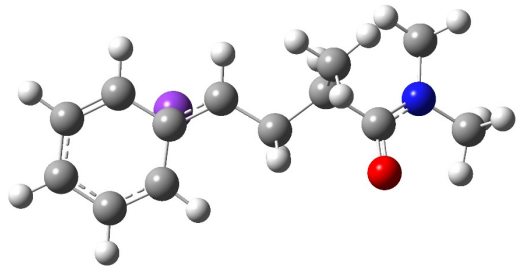
-926.408475 [B3LYP/6-31+G(d,p)]

C	0.64807300	0.28663500	-0.09152200
N	1.59943700	-0.78023000	-0.29444400
C	1.29798400	-2.01264900	0.43058800
H	1.87419700	-2.84260400	0.00723900
H	1.55147300	-1.93805300	1.50632700
H	0.23542000	-2.23627000	0.34274300
C	3.01660000	-0.45690700	-0.24238000
H	3.35380300	-0.13821800	0.76230500
H	3.59523700	-1.34262500	-0.52450800
H	3.25266200	0.34290700	-0.94898700
O	-0.60071100	-0.07331300	-0.13415400
K	-3.08197800	-0.50598200	-0.05235700
C	1.07006100	1.58814900	0.09090300
H	2.12458000	1.82698000	0.15886700
C	0.08763900	2.73257800	0.18092900
H	-0.58657600	2.78977200	-0.68883000
H	-0.57092900	2.68048400	1.06379300
H	0.61520700	3.69255800	0.23907000

-926.221304 [M06-2X/6-31++G(d,p)]

C	0.68133200	0.29928300	-0.08532200
N	1.30490500	-0.97759900	-0.30581900
C	0.72068000	-2.05740600	0.47657800
H	1.08455100	-3.01909000	0.10286400
H	0.98816200	-1.98170100	1.54717800
H	-0.36434500	-2.03037300	0.38890900
C	2.75291700	-1.02525000	-0.26834100
H	3.16312700	-0.77401000	0.72673400
H	3.08132600	-2.03627100	-0.52586400
H	3.17530000	-0.33087300	-0.99790500
O	-0.61273100	0.28130200	-0.07275100
K	-3.03953600	-0.24910900	-0.07268600
C	1.43466800	1.43869800	0.06161400
H	2.51580000	1.40016800	0.08387700
C	0.76482400	2.78373900	0.17600700
H	0.05302700	2.96540300	-0.64159900
H	0.19144800	2.90664300	1.10742700
H	1.50377500	3.59157100	0.14893300

Monoadduct K benzylate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

34

-1235.961388 [B3LYP/6-31+G(d,p)]

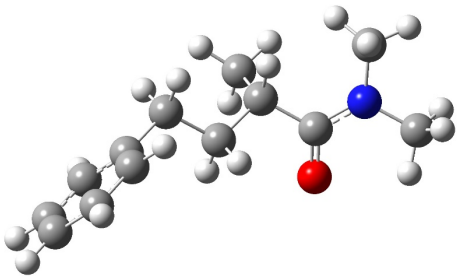
C	-4.87771500	-0.62594000	-0.55615300
C	-4.54280200	-0.42067000	0.80309000
C	-3.22660700	-0.37333700	1.23300800
C	-2.09951500	-0.52542800	0.32796900
C	-2.48142300	-0.74457400	-1.05697900
C	-3.81474600	-0.78850800	-1.46147600
H	-5.91231600	-0.66132000	-0.88384800
H	-5.33801800	-0.29868900	1.53809400
H	-3.01730500	-0.21655700	2.29110700
H	-1.70291900	-0.88578400	-1.80275700
H	-4.03178600	-0.95714800	-2.51621600
C	-0.77315400	-0.41083800	0.75152700
H	-0.58189500	-0.31196100	1.81967800
C	0.40876900	-0.63400300	-0.16310200
H	0.42190500	0.09129200	-0.99824400
H	0.37298000	-1.61764200	-0.66485100
C	1.76260300	-0.52459100	0.57298900
H	1.72472900	0.39510200	1.16480200
C	2.92117500	-0.44769300	-0.42682600
O	2.88879100	-1.11896000	-1.47559000
C	5.09120000	0.44145700	-1.10805400
H	5.93163500	-0.19463200	-0.80105800
H	4.74671000	0.12310300	-2.09004100
H	5.44177300	1.47691200	-1.15870100
C	4.23611300	1.06630900	1.10415800
H	3.47818400	0.84533500	1.85012600
H	5.20882900	0.76471600	1.50967000
H	4.25748400	2.14895000	0.93171800
N	3.99135300	0.35460700	-0.14881400
K	-1.88804600	2.42150700	-0.10295500
C	2.00377400	-1.71171200	1.53076800
H	2.05882800	-2.64911800	0.96604500
H	2.93642900	-1.60025200	2.09473500
H	1.18179500	-1.79434300	2.24679400

-1235.650195 [M06-2X/6-31++G(d,p)]

C	-4.66373800	-0.34543400	-0.74288500
C	-4.31281800	-0.98672600	0.46802600
C	-2.99814300	-1.18147200	0.83923300
C	-1.88013100	-0.73119400	0.02440700
C	-2.27734100	-0.13458000	-1.24176400
C	-3.61050200	0.04216100	-1.58775100
H	-5.70018700	-0.20011100	-1.02527500
H	-5.09991700	-1.33303900	1.13596200

H	-2.77653800	-1.67095200	1.78626200
H	-1.50524800	0.19632100	-1.93112600
H	-3.83935400	0.50998200	-2.54436600
C	-0.56348700	-0.82236900	0.43356100
H	-0.34228900	-1.28263300	1.39562800
C	0.58156400	-0.33350000	-0.41265100
H	0.48873100	0.74490400	-0.63307300
H	0.60405700	-0.81658300	-1.40474200
C	1.94045300	-0.56980400	0.25540200
H	1.87662000	-0.16916800	1.27324400
C	3.05484100	0.14347500	-0.50405100
O	2.94536100	0.37330000	-1.71482900
C	5.28305200	1.09402900	-0.57118500
H	5.97888600	0.32436200	-0.92750100
H	4.89332300	1.64174300	-1.42688800
H	5.82439900	1.77705500	0.08752100
C	4.51469600	0.10833200	1.53369400
H	3.65165200	-0.28752900	2.06169000
H	5.30171600	-0.65556600	1.52722000
H	4.88413200	0.98095300	2.08013800
N	4.18151700	0.49852800	0.17165100
K	-3.06687800	1.88447500	0.90310100
C	2.28334600	-2.06681300	0.32397600
H	2.33529700	-2.47849900	-0.69001600
H	3.24384000	-2.25145900	0.81485100
H	1.50730400	-2.60754600	0.87055800

Monoadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

34

-636.628634 [B3LYP/6-31+G(d,p)]

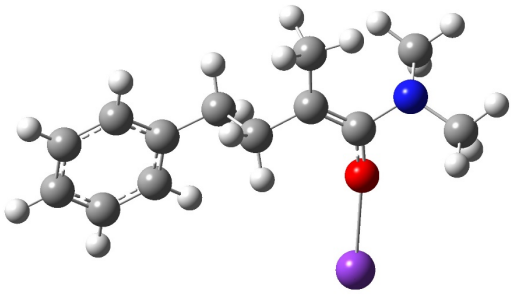
C	4.97937900	-0.71354700	0.42576500
C	4.19002100	-1.50984600	-0.41075500
C	2.93584700	-1.05733700	-0.83251700
C	2.44494700	0.19488800	-0.42900400
C	3.24933200	0.98454000	0.40834500
C	4.50426100	0.53721800	0.83381500
H	5.95532500	-1.06166800	0.75172800
H	4.55170400	-2.48057700	-0.73870000
H	2.33207200	-1.68159400	-1.48729000
H	2.89104800	1.96101300	0.72631700
H	5.11127400	1.16669900	1.47874500
C	1.07179600	0.66769300	-0.86080700
H	1.07992000	1.75989100	-0.94331900
H	0.84850300	0.27371100	-1.86036300
C	-0.03786300	0.22259900	0.11529000
H	0.16138300	0.63062100	1.11201500
H	0.00175800	-0.86933700	0.21199800

C	-1.45625200	0.63352900	-0.33470300
H	-1.57928600	0.29897400	-1.36888600
C	-2.50060200	-0.05005600	0.55726900
O	-2.30040100	-0.14916700	1.78222500
C	-4.62963000	-1.23133800	0.79238800
H	-4.81945100	-2.21896100	0.35723900
H	-4.24596600	-1.34842500	1.80358300
H	-5.57519400	-0.67788700	0.82466700
C	-3.96648100	-0.41341600	-1.44383800
H	-3.60349300	0.51840700	-1.87599800
H	-3.55860600	-1.25825100	-2.01231300
H	-5.05354400	-0.42259000	-1.55029800
N	-3.64579700	-0.51349200	-0.01755900
C	-1.67952600	2.16072900	-0.28201200
H	-1.53067700	2.53150200	0.73773200
H	-0.98074600	2.68232600	-0.94172500
H	-2.69361100	2.42998300	-0.59543300

-636.321461 [M06-2X/6-31++G(d,p)]

C	4.98642600	-0.75559900	-0.18988600
C	4.45635100	0.19905500	-1.05846000
C	3.20498200	0.75971300	-0.80197000
C	2.46364400	0.37866100	0.32199700
C	3.00575200	-0.58000600	1.18548900
C	4.25667000	-1.14380900	0.93442200
H	5.96131100	-1.19110400	-0.38548000
H	5.01831200	0.50981600	-1.93408800
H	2.79671300	1.50536700	-1.48053800
H	2.44165200	-0.88418100	2.06439200
H	4.66275800	-1.88330400	1.61803800
C	1.08755400	0.94952700	0.56648900
H	0.89767000	1.00764100	1.64538600
H	1.04840700	1.97115800	0.17432700
C	0.00108700	0.08987300	-0.09488300
H	0.10271400	-0.94252100	0.26081200
H	0.16041600	0.06436600	-1.17873800
C	-2.43719500	-0.39945800	-0.37416800
O	-2.14413100	-1.10561600	-1.34615700
C	-4.66573900	-1.33963400	-0.41419500
H	-5.23693200	-0.81095600	-1.18683300
H	-4.17166000	-2.19816000	-0.86479800
H	-5.35468000	-1.67758600	0.36271800
C	-4.19652000	0.44845900	1.19543900
H	-3.41088600	1.04874800	1.64571900
H	-4.93587300	1.12163000	0.74547700
H	-4.68725800	-0.12695700	1.98519100
N	-3.67098500	-0.46419800	0.19036500
C	-1.68687000	1.97195800	-0.40682200
H	-1.47807300	1.95369800	-1.48174300
H	-2.72658500	2.28255200	-0.26918800
H	-1.05005600	2.73038000	0.05418500
C	-1.41859400	0.58412300	0.19901900
H	-1.53329400	0.63656500	1.28704400

Monoadduct K enolate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

34

-1235.978317 [B3LYP/6-31+G(d,p)]

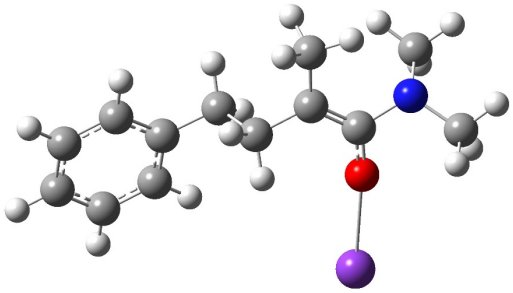
C	2.14149300	-0.40520700	-0.22171000
N	3.46883500	-0.98016500	0.02339100
C	4.57418200	-0.08604500	-0.30486000
H	4.67123000	0.77166500	0.38355600
H	5.51133400	-0.65471800	-0.27088900
H	4.44892600	0.31027300	-1.31622900
C	3.62115300	-1.52567000	1.37189300
H	4.58486400	-2.04311500	1.45707800
H	3.59157800	-0.74281000	2.15532100
H	2.82846200	-2.24741200	1.58163000
O	2.04178500	0.89148200	-0.14138200
K	1.54694500	3.35983100	-0.18741800
C	1.11304300	-1.27379800	-0.52149900
C	-0.29424600	-0.75060700	-0.67844900
H	-0.27490100	0.31726200	-0.92479800
H	-0.79555800	-1.26369400	-1.51576000
C	-1.19458600	-0.93592600	0.58212000
H	-0.73970400	-0.38272200	1.41258700
H	-1.19451700	-1.99587400	0.86421300
C	-2.61814900	-0.47080800	0.37732400
C	-2.98969100	0.86121200	0.62860100
C	-3.60126700	-1.34610600	-0.11528100
C	-4.29551300	1.30492300	0.39634100
H	-2.24783400	1.55600300	1.01638200
C	-4.90883700	-0.90903000	-0.35019800
H	-3.33918200	-2.38354000	-0.31125800
C	-5.26207000	0.42055800	-0.09512500
H	-4.55924400	2.33866800	0.60377400
H	-5.65185000	-1.60702700	-0.72682300
H	-6.27790700	0.76201000	-0.27281700
C	1.28863800	-2.76847800	-0.65487400
H	2.34248500	-3.03615500	-0.77418300
H	0.90864000	-3.34140000	0.21030700
H	0.74020300	-3.15499700	-1.52954200

-1235.650195 [M06-2X/6-31++G(d,p)]

C	2.23449500	-0.22861400	-0.26512600
N	3.59219600	-0.68326800	0.01244600
C	4.60245000	0.33817900	-0.20768900
H	4.53864400	1.17042700	0.51199100
H	5.59240400	-0.12178500	-0.11820400
H	4.50172900	0.75483300	-1.21239700
C	3.72430600	-1.24878400	1.34952600

H	4.73040700	-1.66383900	1.47735200
H	3.56717900	-0.49100800	2.13955800
H	3.00034000	-2.05321400	1.49582600
O	2.02486800	1.05016400	-0.21382500
K	0.69005400	3.16098000	-0.23220300
C	1.29172600	-1.18421600	-0.55087000
C	-0.14927200	-0.78204200	-0.69966100
H	-0.22217000	0.27533300	-0.98145800
H	-0.62889400	-1.36095400	-1.50542300
C	-0.98690600	-0.99305800	0.58558900
H	-0.53803000	-0.40033700	1.39177400
H	-0.92372100	-2.04767500	0.88105300
C	-2.42951100	-0.59999500	0.40093900
C	-2.86703300	0.69412500	0.70725700
C	-3.35397800	-1.49956200	-0.14511400
C	-4.18774800	1.08073700	0.47764600
H	-2.16331100	1.40373700	1.13750300
C	-4.67575600	-1.11983900	-0.37703100
H	-3.03137700	-2.51003600	-0.38759800
C	-5.09780800	0.17384100	-0.06656600
H	-4.50692100	2.08835700	0.72779100
H	-5.37766300	-1.83432100	-0.79712100
H	-6.12693400	0.47065800	-0.24414300
C	1.58671400	-2.65957100	-0.62809400
H	2.65742400	-2.84474300	-0.75207000
H	1.26323400	-3.22069000	0.26508300
H	1.06225800	-3.11899700	-1.47901800

Bisadduct K benzylate, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

50

-1545.518873 [B3LYP/6-31+G(d,p)]

C	-5.02909900	2.29238800	1.08221100
C	-4.53516600	2.55015900	-0.21906500
C	-3.44482000	1.87032900	-0.73554000
C	-2.72476700	0.85200400	0.01386200
C	-3.26989600	0.60392700	1.33952400
C	-4.36703100	1.30726600	1.83491700
H	-5.88530600	2.82988300	1.47849900
H	-5.02120700	3.30481700	-0.83704500
H	-3.09670900	2.10827200	-1.74076200
H	-2.80088500	-0.14593200	1.97165800
H	-4.71944300	1.07636900	2.84029800
C	-1.64988100	0.14446600	-0.52772100
H	-1.32971900	0.40804200	-1.53347100
C	-0.87568400	-0.89096500	0.25556000
H	-1.47788000	-1.79636600	0.45844700
H	-0.63649600	-0.51684000	1.26142800

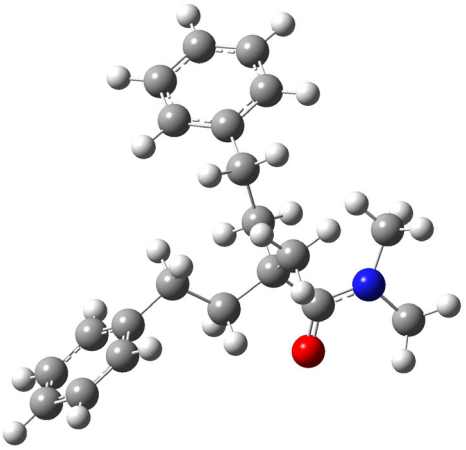
C	0.45178100	-1.39215600	-0.39876800
C	1.08778500	-2.42853600	0.58669800
O	0.57426900	-2.61167400	1.70532600
C	2.62464500	-4.18184300	1.22676100
H	3.21691100	-3.71845300	2.02605900
H	1.76775500	-4.68083600	1.67921300
H	3.24546300	-4.91932700	0.71369300
C	3.09256000	-3.03280100	-0.88297600
H	2.79366300	-2.23329900	-1.54794900
H	4.09898100	-2.80485900	-0.51146400
H	3.14146700	-3.96434200	-1.45804800
N	2.17571600	-3.18863200	0.24575800
K	-4.30320000	-1.40116000	-1.15319100
C	1.40311700	-0.18292000	-0.65136000
H	2.24265300	-0.47038400	-1.29055700
H	0.83459100	0.55995000	-1.21954500
C	1.96659200	0.49609000	0.61562600
H	1.13745500	0.83939000	1.24351500
H	2.53285900	-0.23335300	1.20699100
C	2.86280900	1.67161600	0.28407600
C	2.31702200	2.93909700	0.02092100
C	4.25635700	1.52114200	0.20498500
C	3.13592600	4.02145200	-0.31416500
H	1.24030500	3.07927800	0.08357600
C	5.08117700	2.60082400	-0.12842500
H	4.70070400	0.55021400	0.41167400
C	4.52331300	3.85610200	-0.39061400
H	2.69181900	4.99362600	-0.51009500
H	6.15765900	2.46165500	-0.17894400
H	5.16178000	4.69673100	-0.64682800
C	0.09217100	-2.08626800	-1.73677200
H	0.95411700	-2.48969700	-2.27047200
H	-0.60523300	-2.91259400	-1.55773000
H	-0.40212600	-1.37431600	-2.40285600

-1545.060781 [M06-2X/6-31+G(d,p)]

C	-5.20758900	1.77768300	0.99141200
C	-4.63634900	2.26141900	-0.20957400
C	-3.42728300	1.79569600	-0.68406200
C	-2.65872000	0.76868500	0.00319900
C	-3.24466700	0.34142900	1.26470300
C	-4.46273500	0.83322200	1.71605200
H	-6.15694500	2.15273300	1.35653700
H	-5.16595600	3.01928800	-0.78466900
H	-3.03137700	2.18992600	-1.61874500
H	-2.72207300	-0.39861700	1.86399200
H	-4.85353900	0.45911500	2.66135800
C	-1.50021800	0.22067900	-0.51563900
H	-1.14317000	0.58411500	-1.47633000
C	-0.73763800	-0.84760600	0.22297500
H	-1.37269600	-1.72967000	0.40885000
H	-0.45929300	-0.50943100	1.23452200
C	0.54336200	-1.35997400	-0.48135900
C	1.16195500	-2.44973300	0.43358000
O	0.59161800	-2.77569900	1.48083500
C	2.83777000	-4.03198100	1.08776800
H	3.22639200	-3.50675400	1.96861100
H	2.04483300	-4.70519700	1.41311600
H	3.64312300	-4.60902100	0.63321900

C	3.27002200	-2.71448400	-0.94330300
H	2.77757900	-2.27714500	-1.80446900
H	4.02082800	-2.00747400	-0.56651800
H	3.78621900	-3.61582900	-1.27950800
N	2.32171300	-3.08917700	0.09790600
K	-5.06529400	-0.78827200	-0.91235000
C	1.52060300	-0.17700100	-0.68787400
H	2.28619000	-0.40461500	-1.43473900
H	0.94080200	0.65558900	-1.09993400
C	2.21126100	0.30121400	0.59814400
H	1.45249100	0.53267800	1.35458900
H	2.83924600	-0.50128100	1.00749800
C	3.05597900	1.52481000	0.34195500
C	2.46566100	2.79362000	0.29808500
C	4.42772000	1.41814900	0.09193800
C	3.22560500	3.92711700	0.01382200
H	1.39886300	2.88991700	0.49134100
C	5.19350700	2.54930000	-0.19437600
H	4.90237500	0.43999700	0.12793000
C	4.59419900	3.80778200	-0.23434300
H	2.75101600	4.90359400	-0.01267500
H	6.25807600	2.44659900	-0.38270800
H	5.18802000	4.68921500	-0.45554700
C	0.13473500	-1.98544800	-1.82881000
H	0.95169900	-2.50200700	-2.33582600
H	-0.67234300	-2.70923300	-1.67303600
H	-0.23779200	-1.20697400	-2.49997400

Bisadduct, solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

50

-945.182730 [B3LYP/6-31+G(d,p)]

C	5.88265200	-1.51283600	-0.46881000
C	5.63082400	-0.76430800	0.68575800
C	4.31679700	-0.44741700	1.04468200
C	3.23052900	-0.86862400	0.26107200
C	3.49824800	-1.62069700	-0.89404200
C	4.81002200	-1.94085700	-1.25818100
H	6.90213400	-1.76343700	-0.74765800
H	6.45565100	-0.43091800	1.30961500
H	4.13147300	0.13072300	1.94713200
H	2.67099900	-1.96334600	-1.51151200
H	4.99311900	-2.52769100	-2.15416600

C	1.80906100	-0.50001200	0.63814100
H	1.14170300	-1.30652200	0.31716900
H	1.73802800	-0.43889300	1.72935500
C	1.37796700	0.83452600	-0.00983600
H	1.44845200	0.72780300	-1.09646800
H	2.10588500	1.60534700	0.26605900
C	-0.04865700	1.35196200	0.34331500
C	-0.26524200	2.65080800	-0.49857100
O	0.60173800	3.01755100	-1.31112800
C	-1.47638900	4.64902500	-1.12917700
H	-2.18190200	5.32605500	-0.64295400
H	-0.50063500	5.12908900	-1.19760100
H	-1.83339800	4.43929300	-2.14551900
C	-2.60778200	3.10490500	0.40146900
H	-2.54650800	2.15490600	0.91787200
H	-2.81363000	3.88734000	1.14028500
H	-3.45329800	3.05758500	-0.29556500
N	-1.38257100	3.42239000	-0.33194200
C	-1.11567600	0.27857800	-0.09297200
H	-0.66688900	-0.33289400	-0.88443200
H	-1.97616600	0.76073300	-0.56618900
C	-1.65673800	-0.66231900	1.00877200
H	-0.83019500	-1.19110000	1.49354800
H	-2.15079600	-0.07381300	1.78984700
C	-2.64097100	-1.67139300	0.45147600
C	-4.01511400	-1.38664400	0.40375300
C	-2.20053000	-2.90477100	-0.05534800
C	-4.92274600	-2.30317900	-0.13663300
H	-4.37917900	-0.44097800	0.79874000
C	-3.10349200	-3.82501100	-0.59682900
H	-1.14150800	-3.14962500	-0.02140600
C	-4.46949300	-3.52678800	-0.64028700
H	-5.98225400	-2.06338700	-0.15937700
H	-2.74083100	-4.77498000	-0.97969500
H	-5.17300000	-4.24156900	-1.05742800
C	-0.06652300	1.72071500	1.85003300
H	0.70620100	2.47095400	2.04903500
H	-1.01541400	2.12923200	2.19738600
H	0.15556300	0.84897500	2.46982300

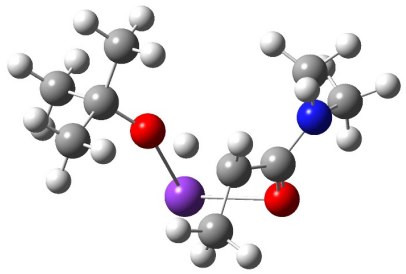
-945.743111 [M06-2X/6-31+G(d,p)]

C	5.84395700	-1.43699600	-0.53184100
C	5.61201200	-0.71393100	0.63841600
C	4.30691800	-0.40919600	1.02518800
C	3.21499000	-0.82107600	0.25346100
C	3.46022500	-1.54393900	-0.91925600
C	4.76290300	-1.85143200	-1.31111400
H	6.85871300	-1.67872800	-0.83250700
H	6.44731100	-0.39086400	1.25259700
H	4.12988700	0.15197200	1.94018800
H	2.61967700	-1.87078000	-1.52803600
H	4.93433500	-2.41670800	-2.22241600
C	1.80532500	-0.45391400	0.65199900
H	1.12927400	-1.26131400	0.34749800
H	1.75109100	-0.37716800	1.74339500
C	1.38064500	0.86841000	-0.00511300
H	1.45268700	0.75617800	-1.09279700
H	2.09960300	1.64818100	0.27206800
C	-0.04506600	1.34883300	0.34754100

C	-0.29917400	2.63980400	-0.46619500
O	0.56526900	3.08035700	-1.23169900
C	-1.62673000	4.54312900	-1.09786200
H	-2.43043600	5.13476600	-0.65700300
H	-0.70190300	5.11905300	-1.08736500
H	-1.88317900	4.31284600	-2.13845500
C	-2.67703700	2.89331600	0.37450600
H	-2.53218900	1.97102400	0.92581700
H	-2.99316300	3.66932700	1.07849100
H	-3.48048300	2.73370700	-0.35453400
N	-1.46614500	3.32375500	-0.31233400
C	-1.06701200	0.25011200	-0.09076200
H	-0.57311900	-0.39881900	-0.82489200
H	-1.91141700	0.69160100	-0.63077100
C	-1.63036400	-0.63456900	1.03268800
H	-0.81401400	-1.13548600	1.56444700
H	-2.15439100	-0.01735300	1.77270100
C	-2.58433700	-1.66275000	0.47511500
C	-3.92562300	-1.33348800	0.24757800
C	-2.14143000	-2.94315100	0.12839500
C	-4.80438000	-2.26038300	-0.31132200
H	-4.28481800	-0.34211700	0.51700400
C	-3.01681500	-3.87492400	-0.43062900
H	-1.10205200	-3.21326700	0.30253900
C	-4.35161500	-3.53560400	-0.65222300
H	-5.84276900	-1.98935300	-0.47727300
H	-2.65697300	-4.86604900	-0.69015100
H	-5.03528100	-4.25991600	-1.08390800
C	-0.07037200	1.71333600	1.84841500
H	0.72773200	2.43539400	2.04990100
H	-1.00736900	2.16120200	2.18111100
H	0.11197600	0.83400600	2.47038400

10.2.2. XYZ Co-ordinates of transition states

Deprotonation of *N*,*N*-dimethylpropionamide (DMP) by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1159.994948 [B3LYP/6-31+G(d,p)]

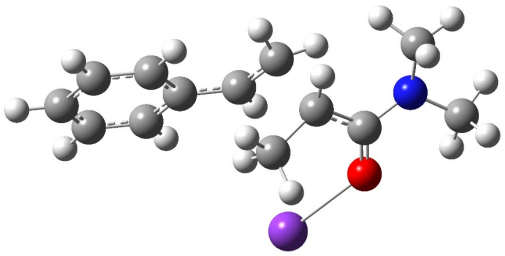
C	0.18113900	-0.10388200	-0.48991700
O	0.07938800	0.43265900	-1.64009300
C	-1.93995300	0.99367400	0.10988200
H	-2.79841100	0.31120800	0.00540700
H	-2.18909400	1.73796400	0.87372800
H	-1.77523000	1.49537500	-0.84153400
N	-0.72757200	0.27832400	0.49245600
K	-0.59551600	-1.45189100	-3.46919200

H	0.43959200	-2.28231500	-0.77923900
O	-0.17131700	-3.11420000	-1.43814600
C	-0.05495800	-4.45571600	-0.99834200
C	-0.61484700	-4.60155700	0.43384800
H	-1.66390300	-4.28510300	0.46210900
H	-0.55977000	-5.63869800	0.78754300
H	-0.05122400	-3.97327100	1.13215900
C	-0.87086900	-5.34278400	-1.95726700
H	-0.48661800	-5.24972500	-2.97975600
H	-0.82496300	-6.40047100	-1.66872900
H	-1.92233100	-5.03288500	-1.95825700
C	1.42285500	-4.90466200	-1.02108700
H	1.83259200	-4.80193200	-2.03256300
H	2.02308400	-4.28414900	-0.34676200
H	1.53302200	-5.95121200	-0.71052000
C	1.13957700	-1.15664000	-0.22433400
H	1.29422000	-1.38188800	0.83141900
C	-0.77700000	-0.35838900	1.80317300
H	-1.20883500	-1.36951800	1.76655900
H	0.21810700	-0.42350300	2.24758500
H	-1.39837200	0.25179300	2.46396100
C	2.45590600	-1.08752300	-0.99655400
H	3.08816000	-0.23064000	-0.71269900
H	3.04675600	-1.99500000	-0.82380900
H	2.28956200	-1.01215600	-2.07675500

-1159.689368 [M06-2X/6-31++G(d,p)]

C	0.21663100	-0.11935800	-0.49095200
O	0.13219600	0.45007500	-1.61414500
C	-1.85701000	1.00644900	0.12459200
H	-2.68802200	0.36250100	-0.19895100
H	-2.18707700	1.59123300	0.98661900
H	-1.60086600	1.67952200	-0.69069300
N	-0.68615200	0.22629600	0.49301700
K	-0.62461600	-1.42355000	-3.38269000
H	0.41825300	-2.23987500	-0.77483100
O	-0.24797400	-3.07868500	-1.44742400
C	-0.08684600	-4.38504100	-0.96241100
C	-0.68129600	-4.50092900	0.45011100
H	-1.74167400	-4.22481800	0.43121100
H	-0.59285900	-5.51863000	0.84820600
H	-0.16118000	-3.81674500	1.13029400
C	-0.81347400	-5.35248600	-1.90282200
H	-0.39457300	-5.27595500	-2.91240500
H	-0.72048500	-6.39159600	-1.56566100
H	-1.87794100	-5.09760400	-1.95198900
C	1.40582700	-4.75014600	-0.91056700
H	1.85054400	-4.64247000	-1.90653000
H	1.93344900	-4.07608900	-0.22637300
H	1.55969300	-5.78028100	-0.56834700
C	1.15743400	-1.19850500	-0.25426800
H	1.35639500	-1.41215100	0.79582000
C	-0.80600600	-0.55487400	1.71397500
H	-1.15837800	-1.57654500	1.51764400
H	0.14792300	-0.61167600	2.24210900
H	-1.52413800	-0.06105500	2.37100400
C	2.42051500	-1.15388200	-1.10281200
H	3.04256400	-0.26686000	-0.91712000
H	3.03778500	-2.03682900	-0.90675200
H	2.18453300	-1.15815200	-2.17258500

Reaction of *N,N*-dimethylpropionamide (DMP) K enolate with styrene T.S., solvent = *N,N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1235.941845 [B3LYP/6-31+G(d,p)]

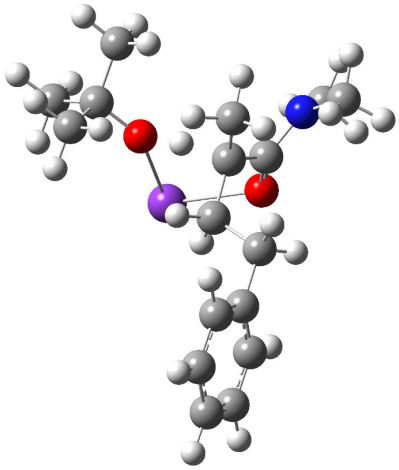
C	-4.15897100	-1.67427000	1.35292000
C	-4.24349100	-0.27336100	1.31671800
C	-3.19824700	0.49297500	0.80676800
C	-2.00184900	-0.09413500	0.29946000
C	-1.94479400	-1.51839600	0.34465100
C	-2.99280600	-2.27950200	0.85948400
H	-4.97333700	-2.27294800	1.75021900
H	-5.13453300	0.22552700	1.69236700
H	-3.29000300	1.57783000	0.79561400
H	-1.06576800	-2.03029900	-0.03666100
H	-2.90106000	-3.36377900	0.87261300
C	-0.92738200	0.74193200	-0.18270000
H	-1.12189700	1.81509000	-0.16722900
C	0.31922400	0.31067100	-0.64945300
H	0.64545000	-0.69925600	-0.41080800
H	1.13062900	1.03325700	-0.66811000
C	0.44564800	-0.07530800	-2.77328400
H	1.21560800	-0.83855800	-2.74023900
C	0.83217800	1.22453900	-3.23728100
O	-0.03107900	2.08343300	-3.61394400
C	2.56793800	2.85944700	-3.81733700
H	1.75127100	3.57787800	-3.77471100
H	3.44412600	3.27918300	-3.31383500
H	2.82849500	2.69126500	-4.87546800
C	3.23664900	0.65287000	-2.95592200
H	3.03105200	0.00781900	-2.10029200
H	3.39566600	0.01725800	-3.84193800
H	4.16697400	1.18869700	-2.75144400
N	2.16764200	1.62675100	-3.14875300
K	-2.49034800	2.60458500	-2.91253600
C	-0.93287100	-0.56307900	-3.14299400
H	-1.69411800	-0.14840300	-2.46158300
H	-1.22598000	-0.29194200	-4.16663900
H	-0.99663000	-1.65309800	-3.05334900

-1235.612633 [M06-2X/6-31++G(d,p)]

C	-4.29267900	-1.21306100	1.09256500
C	-4.07451000	0.16195700	1.18982700
C	-2.86745900	0.72091500	0.77639100
C	-1.82102300	-0.06610800	0.23634600
C	-2.06832800	-1.45967500	0.14832300
C	-3.26992000	-2.01404100	0.56990000

H	-5.23154000	-1.65150200	1.41483400
H	-4.84783800	0.80822300	1.59684000
H	-2.71246300	1.79320400	0.88815000
H	-1.30692400	-2.11225800	-0.26994900
H	-3.41625900	-3.08780600	0.48415300
C	-0.57542600	0.56045100	-0.16715800
H	-0.53370700	1.64416800	-0.05855900
C	0.54891600	-0.08755300	-0.64670500
H	0.63728200	-1.16727500	-0.54457400
H	1.49408000	0.44882500	-0.64011800
C	0.62243500	-0.31290700	-2.83979900
H	1.50650900	-0.93488000	-2.91595800
C	0.72579200	1.07514100	-3.08543400
O	-0.30308400	1.79810900	-3.25917600
C	2.10079800	3.02407000	-3.59044600
H	1.17487300	3.58194200	-3.46801800
H	2.91789700	3.57119300	-3.11272000
H	2.32289200	2.94176100	-4.66687700
C	3.18184200	0.92359600	-2.98925200
H	3.16461900	0.16238800	-2.20666300
H	3.34105200	0.42449500	-3.95848700
H	4.03240000	1.58180600	-2.79751500
N	1.96629100	1.71771100	-2.96581100
K	-2.67470900	1.81302500	-2.32049900
C	-0.70311200	-0.96899500	-3.10754200
H	-1.45987200	-0.61964600	-2.39142700
H	-1.09386500	-0.76769400	-4.11454400
H	-0.63157400	-2.05490600	-2.98579500

Deprotonation of DMP monoadduct by KO*t*Bu T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1469.557460 [B3LYP/6-31+G(d,p)]

C	-0.09934400	-0.27698200	-0.49001800
O	-0.19490600	0.04417600	-1.71299800
C	-2.37380400	0.58840000	-0.27554100
H	-3.18611900	0.55767700	0.45824300
H	-2.27496800	1.62460300	-0.63524800
H	-2.63919900	-0.04358600	-1.12380300
N	-1.15623500	0.09623700	0.36255500
K	-0.36213200	-1.79030200	-3.63956600
H	0.46612700	-2.31928200	-0.70317100

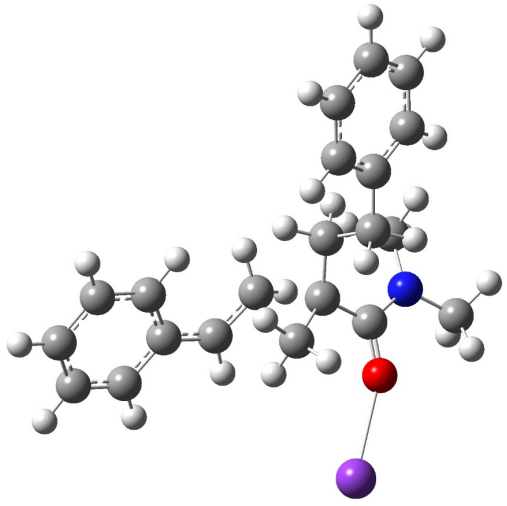
O	0.06436900	-3.22390000	-1.47373700
C	0.07634100	-4.56403800	-1.02048600
C	-0.80911700	-4.72322500	0.23540900
H	-1.83562000	-4.40765400	0.01503200
H	-0.83781000	-5.76370300	0.58255900
H	-0.43030900	-4.10250100	1.05405000
C	-0.48808000	-5.44793600	-2.15089100
H	0.12669000	-5.34745500	-3.05299300
H	-0.50892500	-6.50779200	-1.86731600
H	-1.51075000	-5.13983600	-2.39796200
C	1.51667600	-5.01890600	-0.69717700
H	2.15155100	-4.92138300	-1.58544400
H	1.94705000	-4.39899700	0.09687400
H	1.54757500	-6.06466000	-0.36647700
C	0.94992600	-1.17810200	-0.03078100
C	-0.88226900	0.78493900	1.62508500
H	-1.62238800	0.50587500	2.38418300
H	0.10794200	0.54371300	2.00032300
H	-0.93360700	1.87677700	1.48685100
C	2.30857500	-0.97528900	-0.70994800
H	2.93401600	-1.85944700	-0.52287100
H	2.17922400	-0.91217900	-1.79568100
C	3.09344400	0.28288300	-0.24647500
H	2.48268500	1.16967500	-0.45508600
H	3.23664300	0.24014100	0.83964800
C	4.43812600	0.42554100	-0.92374300
C	5.58880800	-0.17498500	-0.38521300
C	4.56670100	1.12910300	-2.13327600
C	6.82532300	-0.07818200	-1.03145700
H	5.51521600	-0.71951600	0.55360700
C	5.80040100	1.23073700	-2.78407300
H	3.69065800	1.60767100	-2.56556400
C	6.93638200	0.62568000	-2.23550100
H	7.70173300	-0.54768000	-0.59269200
H	5.87508300	1.78514900	-3.71579100
H	7.89650500	0.70557100	-2.73730700
C	1.06636900	-1.60240700	1.43160600
H	1.59285900	-0.88743700	2.08292000
H	0.08793000	-1.79434800	1.88353500
H	1.63596800	-2.53952400	1.49003300

-1469.114273 [M06-2X/6-31++G(d,p)]

C	-0.11217500	-0.29031700	-0.45417100
O	-0.20945600	-0.01819300	-1.67836400
C	-2.27772300	0.77801600	-0.20839300
H	-3.06706500	0.83488100	0.54661400
H	-2.08422100	1.79167800	-0.58811000
H	-2.61888300	0.15783900	-1.03738600
N	-1.09867300	0.18794800	0.40319000
K	-0.27424900	-1.79404900	-3.60722500
H	0.34374600	-2.29301900	-0.65590800
O	-0.15779600	-3.17052700	-1.44491400
C	0.08979900	-4.50147700	-1.08509600
C	-0.67799300	-4.85817300	0.19745300
H	-1.75267700	-4.71480900	0.03858900
H	-0.50695500	-5.89762200	0.50151500
H	-0.36197600	-4.20160200	1.01604900
C	-0.38229500	-5.41018900	-2.22751500
H	0.16190100	-5.16545300	-3.14718300

H	-0.21678800	-6.46999400	-2.00041900
H	-1.45189000	-5.25706800	-2.40923600
C	1.59311600	-4.72638600	-0.85572900
H	2.15267100	-4.45090300	-1.75707800
H	1.94783600	-4.09905000	-0.03057800
H	1.81486300	-5.77220200	-0.61305600
C	0.88738200	-1.24029600	0.01899500
C	-0.73887900	0.81768100	1.66887100
H	-1.35618800	0.44128800	2.49221900
H	0.30929000	0.64620900	1.90286100
H	-0.88965800	1.90306600	1.59331200
C	2.24671000	-1.07529000	-0.65015100
H	2.89851800	-1.90781200	-0.35010400
H	2.14777700	-1.13752500	-1.74148300
C	2.94980700	0.25320500	-0.30397300
H	2.31149900	1.07809300	-0.64505200
H	3.04330500	0.34077700	0.78540500
C	4.31157700	0.36506700	-0.93985000
C	5.46668500	-0.00701100	-0.24273900
C	4.44568100	0.78980900	-2.26779100
C	6.72134500	0.04585800	-0.85050100
H	5.37984100	-0.33922400	0.78959200
C	5.69660900	0.84475500	-2.88115100
H	3.55706900	1.08417600	-2.82270200
C	6.84074600	0.47253300	-2.17345100
H	7.60566800	-0.24273100	-0.28993400
H	5.77952900	1.18243500	-3.91013100
H	7.81619900	0.51898000	-2.64782400
C	0.97410100	-1.64891000	1.48182500
H	1.57698800	-0.98022300	2.11397300
H	-0.01714000	-1.73226100	1.94044500
H	1.44373400	-2.63866200	1.55051100

Reaction of DMP monoadduct K enolate with styrene T.S., solvent = *N*,*N*-dimethylacetamide



Charge = 0; Multiplicity = 1

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-1545.505264 [B3LYP/6-31+G(d,p)]

C	-3.57877400	-1.45272500	2.00066800
C	-3.99486500	-0.18715100	1.55491600
C	-3.15900900	0.60693500	0.77424200

C	-1.85126600	0.18623300	0.38789800
C	-1.45957200	-1.10738500	0.84544800
C	-2.29885300	-1.89493800	1.63201000
H	-4.23072700	-2.07321700	2.60853900
H	-4.98288600	0.18292900	1.82155800
H	-3.50681900	1.58587000	0.44821600
H	-0.48398500	-1.49728700	0.56923200
H	-1.95257100	-2.87429400	1.95681000
C	-1.00302300	1.05523000	-0.38721400
H	-1.46208300	1.98423600	-0.72614900
C	0.31725100	0.79629400	-0.78097100
H	0.90168400	0.06558700	-0.22345300
H	0.89776700	1.65470200	-1.10499100
C	0.58694700	-0.34066500	-2.61570400
C	0.88096400	0.70714800	-3.57955700
O	-0.03877100	1.18251700	-4.32140600
C	2.38560900	2.17344900	-4.84422200
H	1.74802100	1.90745700	-5.68633900
H	2.18661400	3.22317000	-4.57886800
H	3.43507700	2.09372000	-5.14795000
C	3.20781200	1.28056100	-2.72439800
H	2.83915400	0.97184300	-1.75097200
H	4.05247000	0.63563100	-3.00487700
H	3.58878200	2.30404700	-2.61960200
N	2.14844800	1.26691400	-3.72721300
K	-2.49436400	1.38121200	-5.07962100
C	1.63255600	-1.39521900	-2.26507800
H	2.54926900	-0.97271300	-1.84451400
H	1.21800700	-2.03194900	-1.47175700
C	2.04141500	-2.31815000	-3.44922600
H	1.14029900	-2.78596300	-3.86246700
H	2.47509600	-1.69834800	-4.24300200
C	3.02837700	-3.39045800	-3.04392600
C	4.41337700	-3.16757700	-3.12301100
C	2.58698300	-4.62331000	-2.53381500
C	5.32779200	-4.14061600	-2.70665700
H	4.77852500	-2.22361200	-3.52117100
C	3.49590900	-5.60045800	-2.11627400
H	1.51922700	-4.82064000	-2.46850600
C	4.87222200	-5.36254000	-2.20039700
H	6.39432600	-3.94602300	-2.78166200
H	3.12997700	-6.54792000	-1.72972100
H	5.58028000	-6.12124800	-1.87945300
C	-0.79892300	-0.92776400	-2.80850300
H	-1.57516400	-0.20479600	-2.52360900
H	-0.99651200	-1.24198000	-3.84394600
H	-0.93357900	-1.80222300	-2.16279100

-1545.036230 [M06-2X/6-31++G(d,p)]

C	-3.52446000	-1.41211300	1.82578300
C	-3.94975200	-0.13677900	1.43963800
C	-3.12675500	0.68468300	0.67697600
C	-1.83862600	0.27200000	0.26160700
C	-1.43500900	-1.02791000	0.65041800
C	-2.25873200	-1.84469600	1.41980300
H	-4.16488600	-2.05360300	2.42263500
H	-4.93150300	0.22082600	1.73952000
H	-3.47424900	1.67553000	0.39070100
H	-0.46921800	-1.40632200	0.32490800

H	-1.91222900	-2.83673400	1.69870700
C	-0.99253100	1.15795700	-0.51486300
H	-1.44515000	2.08979500	-0.85174700
C	0.32186600	0.89535800	-0.84905000
H	0.89849500	0.16204800	-0.28631400
H	0.90801600	1.70910300	-1.26775300
C	0.54910000	-0.44866900	-2.64378600
C	0.80349200	0.62755800	-3.55420600
O	-0.15105600	1.19243400	-4.17519800
C	2.24258900	2.17086900	-4.78405500
H	1.52452000	2.01555400	-5.58721600
H	2.09465600	3.18277100	-4.37887100
H	3.25607100	2.10771700	-5.19071700
C	3.18734000	1.01566200	-2.83907300
H	2.83622500	0.91365000	-1.81272600
H	3.84140600	0.16421600	-3.07184500
H	3.79065600	1.92623700	-2.88945200
N	2.07777300	1.14429800	-3.76914700
K	-2.64781000	1.54881100	-3.73609100
C	1.59574900	-1.47402100	-2.25943800
H	2.45353600	-1.05753000	-1.72018100
H	1.13378600	-2.17803900	-1.55304300
C	2.13667600	-2.29166600	-3.45455500
H	1.28746800	-2.75364700	-3.97291100
H	2.61467300	-1.60459900	-4.16412000
C	3.11439000	-3.35322600	-3.02022800
C	4.49362100	-3.11577700	-3.02947000
C	2.65671500	-4.58465800	-2.53369600
C	5.39207600	-4.07918200	-2.56835800
H	4.86820700	-2.16793100	-3.40976400
C	3.54888200	-5.55193500	-2.07312800
H	1.58721800	-4.78510700	-2.52108100
C	4.92226800	-5.30161200	-2.08811400
H	6.45873400	-3.87564500	-2.58747000
H	3.17321500	-6.50189400	-1.70435300
H	5.61925700	-6.05334100	-1.73082100
C	-0.84524200	-1.00962200	-2.77252800
H	-1.57372300	-0.38263500	-2.22861300
H	-1.18268800	-1.08610600	-3.81561100
H	-0.90656500	-2.00755900	-2.32455800

10.3. Reaction Profiles for *N*-Methyl-2-pyrrolidinone (NMP, 19) with Various Styrenes

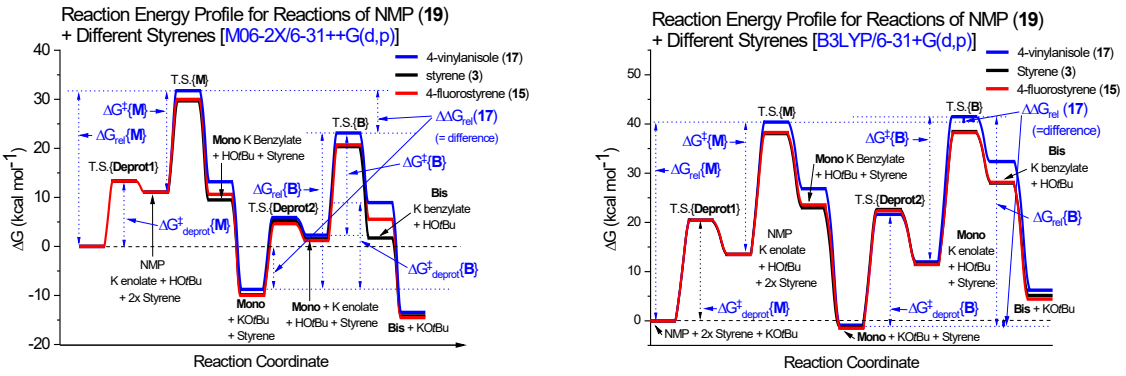
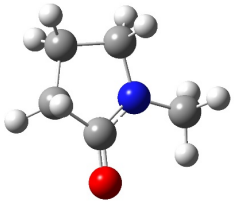


Figure S67. Computed reaction profile for KO*t*Bu-catalyzed reaction of NMP with styrene (**3**, black line), 4-fluorostyrene (**15**, red line) and 4-vinylanisole (**17**, blue line). The transition states for reactions of monoadduct K benzylates or bisadduct K benzylates with proton sources are not shown.

10.3.1. XYZ Co-ordinates of starting materials, intermediates, products

***N*-Methyl-2-pyrrolidinone** (NMP, **19**), solvent = DMSO



Charge = 0; Multiplicity = 1

16

-325.872698 [B3LYP/6-31+G(d,p)]

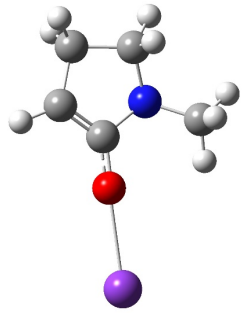
C	0.54177500	-1.38440200	0.12427500
C	1.34174300	0.90533300	0.12623400
C	1.79098000	-0.53308600	-0.18352400
H	0.54913300	-1.77789500	1.15066700
H	0.42186900	-2.22995700	-0.56019400
H	1.76434200	1.66052900	-0.54076400
H	1.58173500	1.20276200	1.15487100
H	2.04766200	-0.62585100	-1.24318900
H	2.65600500	-0.85096200	0.40212400
N	-0.56333900	-0.43698200	-0.04092700
C	-1.94663000	-0.87251000	-0.01685600
H	-2.58892900	-0.00251400	-0.15843400
H	-2.13152800	-1.59491500	-0.81861000
H	-2.18914300	-1.34581900	0.94274100
C	-0.17648000	0.86339800	-0.00201700
O	-0.93451200	1.84388800	-0.04142400

-325.715663 [M06-2X/6-31++G(d,p)]

C	0.54175600	-1.37622500	0.13374200
C	1.33666600	0.90071900	0.13676100
C	1.78033000	-0.52798400	-0.19648200

H	0.55308600	-1.74132800	1.16969400
H	0.42237900	-2.23525600	-0.53236900
H	1.76334100	1.66958200	-0.50928600
H	1.56074100	1.16922800	1.17565500
H	2.00328900	-0.60956900	-1.26364600
H	2.65901900	-0.84913300	0.36378200
N	-0.55813000	-0.43691300	-0.05232000
C	-1.93710300	-0.86839100	-0.01474100
H	-2.57512100	-0.00101300	-0.18596100
H	-2.11853000	-1.61461100	-0.79312800
H	-2.17790400	-1.30858800	0.95963300
C	-0.17607600	0.85956600	-0.00459500
O	-0.93210400	1.83162100	-0.04328000

***N*-Methyl-2-pyrrolidinone K enolate**, solvent = DMSO



Charge = 0; Multiplicity = 1

16

-925.223723 [B3LYP/6-31+G(d,p)]

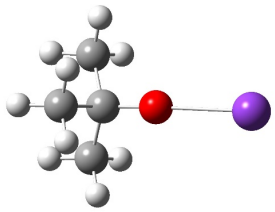
C	-1.28455300	-1.50864600	0.19366600
H	-0.93785400	-2.53617900	0.23502800
C	-0.44185400	-0.43316500	-0.02238500
O	0.84259400	-0.34109100	-0.02410200
C	-0.72939500	2.02694800	0.10300500
H	0.31859700	2.12778400	-0.18591300
H	-1.30332300	2.83208500	-0.36847400
H	-0.80142000	2.15685800	1.20088200
C	-2.61088600	0.43376300	0.06919100
H	-2.76043800	0.71565600	1.13029300
H	-3.33597500	0.99235300	-0.53407200
N	-1.23285300	0.73718100	-0.33409900
K	3.36408400	-0.12569100	-0.00263700
C	-2.71483200	-1.09694100	-0.07814900
H	-3.46283900	-1.50965000	0.61110000
H	-3.05600600	-1.35407700	-1.09920600

-925.047514 [M06-2X/6-31++G(d,p)]

C	-1.17361100	-1.50095000	0.19898100
H	-0.75796600	-2.49782000	0.28509100
C	-0.40931800	-0.37765300	-0.02399600
O	0.85940800	-0.19139500	-0.01547100
C	-0.84907100	2.03192200	0.11567200
H	0.18133200	2.21686100	-0.19127100
H	-1.49209000	2.80711300	-0.31215700
H	-0.90531000	2.10897200	1.21758500
C	-2.61677200	0.34199600	0.06172400
H	-2.76502200	0.61126400	1.12545400
H	-3.38209900	0.85309800	-0.53179100

N	-1.27120200	0.72946800	-0.35530300
K	3.34002100	-0.12720600	-0.00650300
C	-2.62375900	-1.18678700	-0.08010700
H	-3.34384900	-1.64185100	0.60900300
H	-2.93707200	-1.46699800	-1.10110000

Potassium *tert*-butoxide, solvent = DMSO



Charge = 0; Multiplicity = 1

15

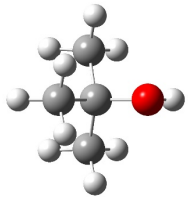
-832.973818 [B3LYP/6-31+G(d,p)]

C	-1.14292500	0.00091000	-0.00155000
C	-1.70925200	1.44751400	0.00410500
H	-2.80776400	1.47607300	0.02260600
H	-1.33905100	1.98989700	0.88322600
H	-1.36948600	1.98471200	-0.89028700
C	-1.66736300	-0.72620400	1.26730700
H	-2.76484200	-0.75508400	1.31985300
H	-1.29815300	-1.75918400	1.28364300
H	-1.29668100	-0.22099900	2.16788900
C	-1.71239100	-0.73412000	-1.24576900
H	-1.37584800	-0.23251700	-2.16173500
H	-1.34080200	-1.76625200	-1.27130700
H	-2.81087100	-0.76622500	-1.25756300
O	0.24233400	0.01303600	-0.02551800
K	2.72928500	0.00087900	-0.00193300

-832.823685 [M06-2X/6-31++G(d,p)]

C	-1.12666100	-0.00008500	-0.00001500
C	-1.68201200	-0.42697900	-1.37612700
H	-2.77927400	-0.43356100	-1.40618700
H	-1.31970900	0.26085200	-2.14945300
H	-1.32396800	-1.43391900	-1.62208700
C	-1.67151600	1.40877500	0.31910600
H	-2.76851500	1.44783500	0.32894800
H	-1.30548100	1.73079400	1.30133800
H	-1.30725400	2.12212300	-0.42990700
C	-1.67700600	-0.97797600	1.06058100
H	-1.31819100	-1.99219200	0.84830900
H	-1.31161700	-0.68838800	2.05300300
H	-2.77417300	-0.99875900	1.08881500
O	0.25111700	-0.00316800	-0.00318800
K	2.69170600	-0.00062400	-0.00045000

***tert*-Butanol**, solvent = DMSO



Charge = 0; Multiplicity = 1

15

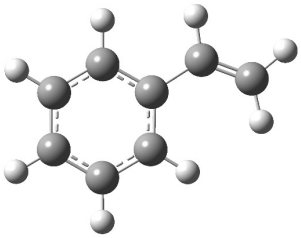
-233.601294 [B3LYP/6-31+G(d,p)]

C	-0.00662300	-0.00000400	0.00944800
C	0.67595100	-1.26502900	-0.52930900
H	0.61011000	-1.30910900	-1.62169800
H	1.73777700	-1.28149500	-0.25651200
H	0.20005900	-2.16100500	-0.11796300
C	0.67539900	1.26529900	-0.52935000
H	0.60954200	1.30931400	-1.62174100
H	0.19909500	2.16107200	-0.11803500
H	1.73721300	1.28225000	-0.25654100
C	-1.50096400	-0.00032900	-0.31884700
H	-1.98553500	-0.88879200	0.09895200
H	-1.98592800	0.88793900	0.09891400
H	-1.65557200	-0.00038600	-1.40209000
O	0.05989700	0.00004400	1.46014900
H	0.99148700	0.00022900	1.72387200

-233.474217 [M06-2X/6-31++G(d,p)]

C	-0.00603900	0.00000000	0.01463400
C	0.67070500	-1.25804500	-0.52798700
H	0.59714800	-1.29785100	-1.61909900
H	1.73284600	-1.27150300	-0.25888600
H	0.19529100	-2.15161000	-0.11263600
C	0.67065400	1.25807300	-0.52798400
H	0.59709600	1.29787700	-1.61909600
H	0.19520400	2.15161800	-0.11263200
H	1.73279500	1.27157400	-0.25888200
C	-1.49330700	-0.00002900	-0.31479100
H	-1.97374500	-0.88904800	0.10485800
H	-1.97378000	0.88897200	0.10485800
H	-1.64409300	-0.00003200	-1.39784300
O	0.06218800	-0.00000100	1.44911000
H	0.99165900	0.00001600	1.71324300

Styrene (**3**), solvent = DMSO



Charge = 0; Multiplicity = 1

16

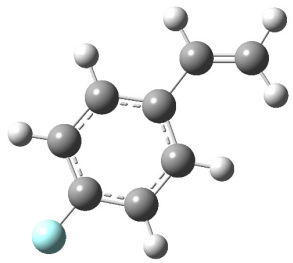
-309.575513 [B3LYP/6-31+G(d,p)]

C	-0.40636200	-1.28423700	-0.00001500
C	0.51580200	-0.22042800	-0.00002200
C	0.00937600	1.09487200	-0.00001800
C	-1.36471300	1.33203500	-0.00000100
C	-2.26931200	0.26209600	0.00001800
C	-1.78359500	-1.04834900	0.00002100
H	-0.03615600	-2.30647000	-0.00001600
H	0.69124000	1.93965000	-0.00005100
H	-1.73281000	2.35410100	-0.00002300
H	-3.33885400	0.45050900	0.00002100
H	-2.47421400	-1.88676700	0.00003000
C	1.95780200	-0.53101700	-0.00002500
H	2.18988000	-1.59570700	0.00000200
C	2.98245200	0.33674200	0.00003000
H	2.84468300	1.41438300	0.00008200
H	4.00753700	-0.01998500	0.00003900

-309.421867 [M06-2X/6-31++G(d,p)]

C	-0.40739600	-1.28262400	0.00000300
C	0.51151100	-0.22449900	-0.00000600
C	0.01545300	1.08862900	-0.00001400
C	-1.35467200	1.33032500	-0.00001100
C	-2.25998900	0.26590300	-0.00000100
C	-1.78111600	-1.04280100	0.00000600
H	-0.03809800	-2.30511400	0.00000800
H	0.70148400	1.93011900	-0.00002400
H	-1.71945500	2.35292300	-0.00001800
H	-3.32827400	0.45809400	0.00000100
H	-2.47444700	-1.87818400	0.00001300
C	1.95525100	-0.53646000	-0.00000600
H	2.19163200	-1.59989300	-0.00002900
C	2.96494500	0.34012200	0.00002400
H	2.80983000	1.41515400	0.00005100
H	3.99340000	-0.00467000	0.00002000

4-Fluorostyrene (**15**), solvent = DMSO



Charge = 0; Multiplicity = 1

16

-408.826090 [B3LYP/6-31+G(d,p)]

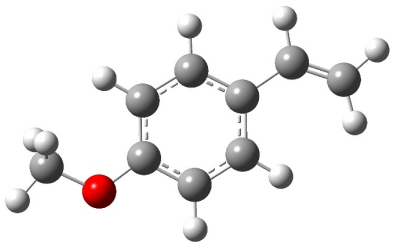
C	1.79108200	-0.09171800	-0.00000100
C	1.27127600	1.19454900	0.00000000
C	-0.11787200	1.34154300	0.00000100
C	-0.97855000	0.22772800	0.00000200
C	-0.39800100	-1.05683800	0.00000000
C	0.98533600	-1.22585000	-0.00000200
H	1.93368400	2.05335100	0.00000000
H	-0.54062900	2.34230400	0.00000200
H	-1.02768000	-1.94045000	0.00000100

H	1.43524700	-2.21282200	-0.00000300
C	-2.43533600	0.45522200	0.00000500
H	-2.72807600	1.50460100	0.00000700
C	-3.40821800	-0.46990500	0.00000100
H	-3.20979800	-1.53800600	-0.00000500
H	-4.45183000	-0.17195800	0.00000100
F	3.14786400	-0.25393300	-0.00000500

-408.643043 [M06-2X/6-31++G(d,p)]

C	1.78605300	-0.09265800	-0.00000200
C	1.26990700	1.19168600	0.00000000
C	-0.11581000	1.34038100	0.00000200
C	-0.97175700	0.23065600	0.00000200
C	-0.39988300	-1.05142700	0.00000000
C	0.97977100	-1.22295300	-0.00000200
H	1.93636900	2.04690500	0.00000000
H	-0.53999500	2.34063500	0.00000300
H	-1.03333800	-1.93247200	0.00000000
H	1.43056600	-2.20931400	-0.00000300
C	-2.43076400	0.45868100	0.00000300
H	-2.72727100	1.50678700	0.00000700
C	-3.38872400	-0.47389200	0.00000100
H	-3.17417200	-1.53863700	-0.00000300
H	-4.43478300	-0.18697600	0.00000200
F	3.12998500	-0.25664000	-0.00000300

4-Vinylanisole (**17**), solvent = DMSO



Charge = 0; Multiplicity = 1

20

-424.078033 [B3LYP/6-31+G(d,p)]

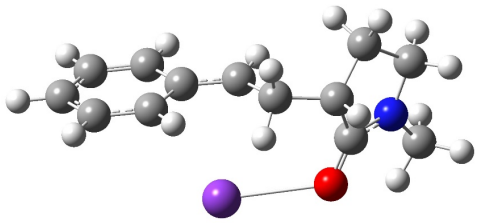
C	-1.33242200	-0.28670900	-0.00007500
C	-0.86920200	1.03446500	-0.00009100
C	0.50825300	1.27858700	0.00000200
C	1.45173100	0.23886300	0.00007900
C	0.95749200	-1.08412800	0.00017200
C	-0.40530800	-1.34535900	0.00009700
H	-1.55700600	1.87124400	-0.00024500
H	0.85446400	2.30918400	-0.00006800
H	1.64688100	-1.92276500	0.00031800
H	-0.77578800	-2.36589100	0.00011000
C	2.88628600	0.56882700	0.00024800
H	3.10208200	1.63719000	0.00083600
C	3.92685600	-0.28156200	-0.00031700
H	3.80762100	-1.36156800	-0.00101300
H	4.94566300	0.09275900	-0.00014400
O	-2.64937100	-0.64797300	0.00001500
C	-3.64132900	0.38322700	-0.00008500
H	-4.60221300	-0.13107900	0.00017900
H	-3.56033500	1.00880300	0.89568600

H	-3.56054500	1.00863500	-0.89595900

-423.877313 [M06-2X/6-31++G(d,p)]

C	-1.32847100	0.29004400	-0.00002400
C	-0.87447800	-1.02944100	0.00000100
C	0.50035700	-1.27692600	-0.00006000
C	1.44021800	-0.24346700	-0.00012700
C	0.95699200	1.07792500	-0.00018500
C	-0.40128700	1.34363500	-0.00012800
H	-1.56539400	-1.86367400	0.00006600
H	0.84550100	-2.30787200	-0.00004000
H	1.65077100	1.91311800	-0.00030900
H	-0.77263000	2.36354700	-0.00018400
C	2.87692200	-0.57436600	-0.00013400
H	3.09754900	-1.64141600	-0.00056800
C	3.90134900	0.28606900	0.00038000
H	3.76280300	1.36348300	0.00089000
H	4.92418200	-0.07477000	0.00031500
O	-2.63810500	0.65189700	0.00003600
C	-3.60928200	-0.38407200	0.00012500
H	-4.57837100	0.11243300	0.00017100
H	-3.51680000	-1.00824700	-0.89501400
H	-3.51669100	-1.00819300	0.89529100

Styrene/NMP monoadduct K benzylate, solvent = DMSO



Charge = 0; Multiplicity = 1

32

-1234.784146 [B3LYP/6-31+G(d,p)]

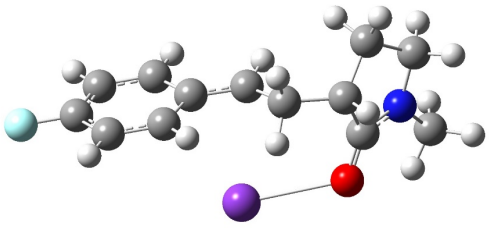
C	-4.74196400	-0.18248900	0.33577400
C	-3.95915100	-0.29526700	1.50940900
C	-2.59552700	-0.53050300	1.45752200
C	-1.87057300	-0.67558100	0.20755300
C	-2.70662900	-0.56429600	-0.97444100
C	-4.07864400	-0.32567900	-0.89390400
H	-5.81122400	0.00040300	0.38543300
H	-4.43726900	-0.19769500	2.48379900
H	-2.03353200	-0.61182500	2.38779800
H	-2.25643700	-0.68863300	-1.95643800
H	-4.64824500	-0.25605200	-1.82063800
C	-0.48608200	-0.86964500	0.16439600
H	0.03825600	-1.01690600	1.10728500
C	0.28391200	-1.06715600	-1.11729300
H	-0.00104500	-0.31440500	-1.87339300
H	0.06717500	-2.03443900	-1.61614500
C	2.30562500	0.35321300	-0.40087700
O	1.86831000	1.48198500	-0.69451900
N	3.33816100	0.11672700	0.44092800
K	-0.71756300	2.17636300	-0.25561700
C	4.15553100	1.15338100	1.04253300
H	4.24923000	0.98332600	2.12002100

H	5.15998800	1.16093400	0.60155700
H	3.68085200	2.11955100	0.86831200
C	2.48469000	-2.02465400	-0.05231600
H	2.75938700	-2.93734800	-0.58645300
H	1.80795100	-2.30028700	0.76159200
C	3.71676800	-1.29710900	0.51689600
H	3.94110200	-1.57279200	1.55221400
H	4.62011800	-1.47361700	-0.08406400
C	1.81293000	-0.98006400	-0.96733500
H	2.25846800	-1.04898200	-1.97201400

-1234.471890 [M06-2X/6-31++G(d,p)]

C	-4.62454400	-0.14175600	0.39542900
C	-3.82291700	-0.18288000	1.55694100
C	-2.47068700	-0.45258400	1.50078600
C	-1.77753100	-0.71289900	0.25563600
C	-2.62914900	-0.66855600	-0.91447800
C	-3.99081900	-0.39287300	-0.82617500
H	-5.68642300	0.07228000	0.44968800
H	-4.27830500	0.00365800	2.52844200
H	-1.88988800	-0.47171600	2.42208800
H	-2.20061200	-0.88192400	-1.89079300
H	-4.57611800	-0.37879100	-1.74476900
C	-0.40375800	-0.91594800	0.19132200
H	0.16554600	-0.94097600	1.11891400
C	0.32654300	-1.10745600	-1.10935800
H	0.00239600	-0.36407600	-1.86188800
H	0.12433800	-2.08221100	-1.59182700
C	2.24547500	0.38654700	-0.39816700
O	1.75075000	1.48187400	-0.69822700
N	3.25588300	0.20427500	0.47265700
K	-0.86177300	2.00376300	-0.43000000
C	3.99104000	1.28172700	1.09627300
H	4.06779600	1.10896400	2.17327900
H	5.00072300	1.35094600	0.67662600
H	3.45905200	2.21539800	0.91306900
C	2.54968500	-1.96961300	-0.05635800
H	2.88621900	-2.86199100	-0.58672500
H	1.86854600	-2.28058400	0.74078800
C	3.72116400	-1.17747900	0.54293700
H	3.93824800	-1.44766900	1.58021300
H	4.64377100	-1.28820100	-0.04237700
C	1.84430600	-0.96383000	-0.97791300
H	2.29837100	-1.00393200	-1.97877100

4-Fluorostyrene/NMP monoadduct K benzylate, solvent = DMSO



Charge = 0; Multiplicity = 1

32

-1334.033791 [B3LYP/6-31+G(d,p)]

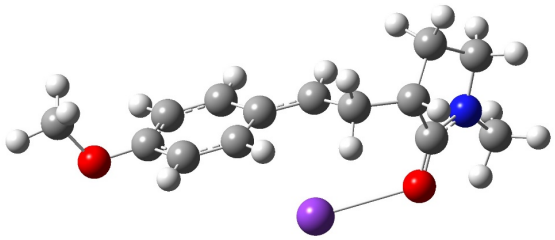
C	-4.36659300	-0.20454600	0.22563300
C	-3.66001400	-0.34164900	1.42507400
C	-2.29100300	-0.56436200	1.39005800
C	-1.53676500	-0.65889500	0.15433500
C	-2.34286100	-0.52577200	-1.04431500
C	-3.72281300	-0.29901300	-0.99942800
H	-4.18639400	-0.27614000	2.37422700
H	-1.75481700	-0.67044500	2.33162400
H	-1.87158700	-0.61751900	-2.01867600
H	-4.29392600	-0.20503800	-1.92014800
C	-0.14517700	-0.83448000	0.13938900
H	0.35081200	-1.03704000	1.08695700
C	0.63968000	-1.02795100	-1.13316300
H	0.38191800	-0.25792400	-1.88214100
H	0.40956700	-1.98288200	-1.65187900
C	2.68360200	0.34520600	-0.38593000
O	2.27509200	1.48470500	-0.67992200
N	3.70280400	0.08306700	0.46462500
K	-0.29757600	2.20930600	-0.22430400
C	4.53782400	1.09974100	1.07600200
H	4.61883600	0.92490400	2.15373500
H	5.54580700	1.08645500	0.64323600
H	4.08599700	2.07659600	0.90049900
C	2.80686300	-2.03695900	-0.04477000
H	3.06609900	-2.95416200	-0.57893500
H	2.11604100	-2.29941300	0.76154000
C	4.04937000	-1.33903400	0.53855000
H	4.25809400	-1.62359600	1.57473100
H	4.95402100	-1.53334500	-0.05494900
C	2.16800300	-0.97470700	-0.96310500
H	2.62404500	-1.04930300	-1.96273800
F	-5.74351400	0.01749500	0.26907800

-1333.691280 [M06-2X/6-31++G(d,p)]

C	-4.26483600	-0.19824500	0.27773400
C	-3.53469700	-0.24839000	1.46741100
C	-2.17396700	-0.48761600	1.42585100
C	-1.44964400	-0.69498400	0.19024600
C	-2.27071700	-0.63058400	-0.99823200
C	-3.64495500	-0.38852100	-0.94312200
H	-4.04282100	-0.09795200	2.41647700
H	-1.61777900	-0.52355700	2.36053200
H	-1.81842600	-0.80520900	-1.97035600
H	-4.23480000	-0.35478900	-1.85590800
C	-0.06815700	-0.87802100	0.15226900
H	0.48046800	-0.93526200	1.09017700
C	0.67990100	-1.04326700	-1.14046200
H	0.38633600	-0.27041500	-1.87751700
H	0.46314100	-1.99742600	-1.65846200
C	2.62003200	0.38887500	-0.36369700
O	2.15288900	1.50181000	-0.64258800
N	3.61550500	0.16324700	0.51418000
K	-0.45835500	2.04018000	-0.42463200
C	4.36595200	1.20823000	1.17379700
H	4.42044400	1.00999800	2.24780400
H	5.38386800	1.26148100	0.77213400
H	3.86022300	2.15872100	1.00324500
C	2.86783200	-1.98082400	-0.07644700
H	3.19125400	-2.86793000	-0.62357500

H	2.16871200	-2.29451400	0.70386500
C	4.04885500	-1.22997500	0.55641800
H	4.24643300	-1.53007200	1.58943200
H	4.97621400	-1.34739900	-0.02000500
C	2.19791500	-0.93745300	-0.98249100
H	2.66593500	-0.96242700	-1.97748500
F	-5.62146500	0.04008400	0.33038300

4-Vinylanisole/NMP monoadduct K benzylate, solvent = DMSO



Charge = 0; Multiplicity = 1

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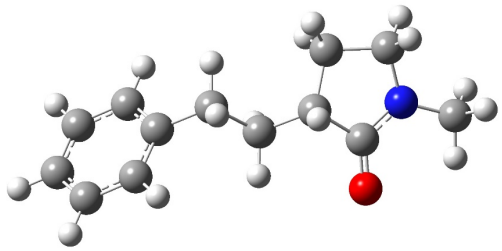
-1349.280479 [B3LYP/6-31+G(d,p)]

C	-4.00311100	0.05286000	0.15949100
C	-3.29169700	-0.16919400	1.35583200
C	-1.93957800	-0.47393600	1.33743500
C	-1.17169500	-0.58014900	0.11144100
C	-1.95076800	-0.35534800	-1.09049100
C	-3.31399400	-0.04756400	-1.05148100
H	-3.81688700	-0.09431400	2.30671500
H	-1.42286500	-0.63294200	2.28324100
H	-1.46973200	-0.43809700	-2.06164200
H	-3.85451300	0.11664100	-1.98255200
C	0.20809200	-0.83486000	0.11310700
H	0.67215400	-1.09762200	1.06228700
C	1.00736900	-1.03484300	-1.14958300
H	0.77433600	-0.25337700	-1.89364200
H	0.76801500	-1.98105800	-1.68034000
C	3.06817900	0.29914500	-0.37597800
O	2.68344600	1.44641400	-0.67189000
N	4.07631500	0.01781500	0.48189500
K	0.13079700	2.22472800	-0.18744400
C	4.92687300	1.01876200	1.09772100
H	4.99619500	0.84506700	2.17646100
H	5.93765400	0.98421600	0.67267500
H	4.49614700	2.00407500	0.91640500
C	3.14243400	-2.08409200	-0.03271300
H	3.38619300	-3.00829200	-0.56213800
H	2.44035000	-2.32924100	0.76922600
C	4.39467500	-1.41069300	0.55847100
H	4.59108600	-1.69902700	1.59602400
H	5.29906200	-1.62312000	-0.02926400
C	2.53410300	-1.01086700	-0.95897900
H	3.00193600	-1.09494000	-1.95265900
O	-5.35998800	0.41001500	0.18903600
C	-6.25999000	-0.70255700	0.21797100
H	-6.14292700	-1.32685700	-0.67768900
H	-6.09426500	-1.32217700	1.10896100
H	-7.27430300	-0.29489200	0.24547700

-1348.921456 [M06-2X/6-31++G(d,p)]

C	-3.92518000	0.05751700	0.17220800
C	-3.19447800	-0.07416400	1.36605700
C	-1.84729000	-0.37885600	1.34775600
C	-1.10804100	-0.58621400	0.12095100
C	-1.90162300	-0.43875100	-1.07844400
C	-3.26231500	-0.13306500	-1.03571700
H	-3.70572500	0.07562100	2.31572100
H	-1.31083300	-0.46540800	2.29137800
H	-1.43708500	-0.59734500	-2.04807000
H	-3.82425300	-0.03830900	-1.96382600
C	0.26358600	-0.83408200	0.10174700
H	0.79167800	-0.94351400	1.04696600
C	1.02951700	-0.98570300	-1.18243100
H	0.78251600	-0.17512900	-1.89560600
H	0.78255900	-1.91059500	-1.73826200
C	3.01438100	0.33703100	-0.32721000
O	2.59571000	1.47670200	-0.57302900
N	3.99018800	0.04226800	0.55221600
K	0.00840400	2.11641700	-0.37183400
C	4.77353600	1.03376500	1.25477700
H	4.80220500	0.80137400	2.32293500
H	5.79905700	1.05547800	0.87001600
H	4.31079900	2.00952000	1.10563600
C	3.15781500	-2.04808200	-0.11271900
H	3.44828000	-2.93290700	-0.68158600
H	2.43556600	-2.35179800	0.65036000
C	4.36304900	-1.36906200	0.55479800
H	4.53606200	-1.70957900	1.57964800
H	5.29068900	-1.50891800	-0.01617500
C	2.54718800	-0.94987500	-0.99512200
H	3.03167200	-0.96293700	-1.98259100
O	-5.27912400	0.38823600	0.20211400
C	-6.12584800	-0.74381400	0.34244200
H	-5.99445600	-1.43353200	-0.50077300
H	-5.91220900	-1.27786300	1.27672800
H	-7.15597900	-0.38133200	0.35958800

Styrene/NMP monoadduct (20a), solvent = DMSO



Charge = 0; Multiplicity = 1

32

-635.450385 [B3LYP/6-31+G(d,p)]

C	4.98736800	-0.32577600	0.60935900
C	4.41710100	-1.09630100	-0.40952500
C	3.13879500	-0.79220100	-0.88789700
C	2.40555600	0.28307200	-0.36048100
C	2.99165000	1.04979300	0.65937300
C	4.26954300	0.75005400	1.14230900

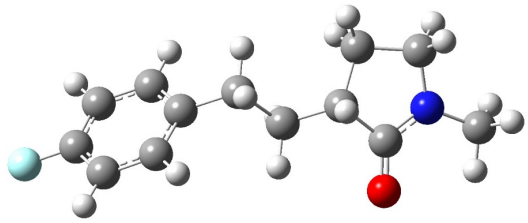
H	5.98148800	-0.55811100	0.98036900
H	4.96822800	-1.93036800	-0.83520500
H	2.70596600	-1.39336600	-1.68425000
H	2.44362200	1.89190400	1.07586300
H	4.70501300	1.35849200	1.93021100
C	1.00731900	0.58649800	-0.85708400
H	0.81787200	1.66312500	-0.77420000
H	0.93309600	0.33155900	-1.92187500
C	-0.08069000	-0.18703600	-0.08408900
H	-0.03021200	0.07924200	0.98033700
H	0.12090100	-1.26214200	-0.15117700
C	-1.49579800	0.08220100	-0.60652200
H	-1.52827100	-0.17597300	-1.67672600
C	-2.55996400	-0.79653600	0.06061000
O	-2.44273700	-2.00009900	0.33287100
N	-3.66710600	-0.04346400	0.27865200
C	-3.55427100	1.32282300	-0.23517000
H	-4.09146300	1.41201900	-1.19013900
H	-3.99871900	2.03201400	0.47005100
C	-2.03554700	1.51217600	-0.40250200
H	-1.79682200	2.18736400	-1.22685800
H	-1.61359000	1.93663200	0.51590200
C	-4.93133600	-0.57575400	0.75066300
H	-5.67716900	-0.58054100	-0.05404500
H	-4.77309100	-1.59757600	1.09728100
H	-5.31356500	0.03269700	1.57666300

-635.153240 [M06-2X/6-31++G(d,p)]

C	4.94387000	0.39681200	-0.56304600
C	4.36272700	1.05123100	0.52378700
C	3.09207400	0.68238000	0.96313500
C	2.38116700	-0.34295100	0.32869300
C	2.97398500	-0.99216500	-0.75949900
C	4.24535400	-0.62708600	-1.20375700
H	5.93408300	0.68040700	-0.90582200
H	4.89970200	1.84721100	1.03097600
H	2.64283500	1.19395500	1.81154300
H	2.43498500	-1.79290500	-1.26111100
H	4.69180000	-1.14415800	-2.04796500
C	0.98466000	-0.69434800	0.78012700
H	0.78256700	-1.75124900	0.57069500
H	0.90205100	-0.55807600	1.86561100
C	-0.07145300	0.17684200	0.08742500
H	-0.04306300	-0.00852400	-0.99517700
H	0.16985800	1.23541200	0.23784900
C	-1.47769300	-0.09015900	0.60940800
H	-1.51207900	0.15022700	1.68309600
C	-2.52614800	0.80000000	-0.05020000
O	-2.39415500	1.99531500	-0.31727000
N	-3.63453900	0.05989700	-0.27354700
C	-3.53576200	-1.30072400	0.24138600
H	-4.05104700	-1.37636900	1.20854100
H	-4.00294500	-2.00339500	-0.45402400
C	-2.02081500	-1.50613200	0.37663000
H	-1.76916400	-2.20397300	1.17691300
H	-1.61801300	-1.89974900	-0.56388600
C	-4.89132600	0.61058200	-0.72833800
H	-5.62203900	0.63196200	0.08812500
H	-4.71555700	1.62698400	-1.08156100

H	-5.29279900	0.00474000	-1.54532300

4-Fluorostyrene/NMP monoadduct (23a), solvent = DMSO



Charge = 0; Multiplicity = 1

32

-734.701194 [B3LYP/6-31+G(d,p)]

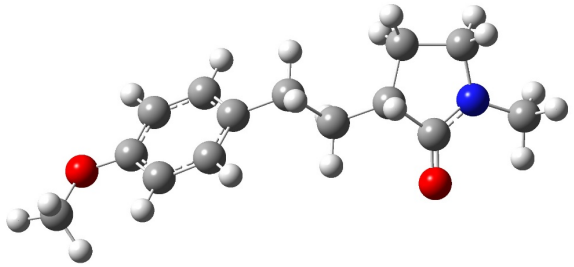
C	4.55100400	0.20172200	-0.35358500
C	4.00222200	0.93103200	0.69255000
C	2.70121200	0.62157200	1.10084000
C	1.96047500	-0.39587500	0.47833100
C	2.56217500	-1.10613800	-0.57257900
C	3.86156600	-0.81526500	-0.99981700
H	4.57837400	1.71361300	1.17481000
H	2.26027500	1.18109900	1.92157800
H	2.01203900	-1.90321000	-1.06582100
H	4.33004900	-1.36507100	-1.80925800
C	0.53931100	-0.69618500	0.90740900
H	0.33076400	-1.76051500	0.74864800
H	0.43430400	-0.50988500	1.98349600
C	-0.50431500	0.15092500	0.15077000
H	-0.42148300	-0.04601800	-0.92662400
H	-0.28339700	1.21453800	0.29573900
C	-1.94209400	-0.12009100	0.60599500
H	-2.00805600	0.07080200	1.68866700
C	-2.96409700	0.82178300	-0.04047200
O	-2.81313800	2.03688400	-0.23294000
N	-4.07759800	0.10835900	-0.34307900
C	-4.00999700	-1.28933100	0.08713400
H	-4.58185600	-1.42619700	1.01593500
H	-4.44358600	-1.94317100	-0.67592900
C	-2.50213700	-1.52220300	0.29301100
H	-2.30552800	-2.25279700	1.08036300
H	-2.05659900	-1.89686900	-0.63582900
C	-5.31326200	0.69733300	-0.82325500
H	-6.08704400	0.66824700	-0.04593300
H	-5.12183500	1.73516500	-1.09827200
H	-5.67801100	0.15092500	-1.69900200
F	5.82638900	0.49334200	-0.76061100

-734.374583 [M06-2X/6-31++G(d,p)]

C	4.50412600	0.23087300	-0.34512300
C	3.94629200	0.89688800	0.73440300
C	2.65703100	0.54346300	1.12889600
C	1.93898100	-0.45464500	0.46033300
C	2.54456000	-1.09992500	-0.62298400
C	3.83346200	-0.76438600	-1.03729500
H	4.51056500	1.66736200	1.24847000
H	2.20185500	1.05387900	1.97394500
H	2.00335300	-1.87985200	-1.15261300
H	4.31294900	-1.26126800	-1.87361700

C	0.52221500	-0.77984800	0.86634800
H	0.29678800	-1.82223500	0.61316200
H	0.41676200	-0.68225000	1.95381900
C	-0.49046900	0.14680300	0.18156900
H	-0.41483200	0.02640400	-0.90792700
H	-0.24284100	1.19079400	0.40587700
C	-1.92283300	-0.12989000	0.62116100
H	-2.00278600	0.03291600	1.70686700
C	-2.92429500	0.82658200	-0.01878200
O	-2.76008800	2.03518900	-0.19144700
N	-4.03241700	0.12667100	-0.34761800
C	-3.97984100	-1.27039900	0.06572900
H	-4.54488400	-1.40926100	0.99742300
H	-4.42196600	-1.90961600	-0.70347500
C	-2.47702100	-1.51452500	0.25995400
H	-2.27814700	-2.27283200	1.01894300
H	-2.03330200	-1.84796400	-0.68545600
C	-5.25624000	0.73331500	-0.82072900
H	-6.03515800	0.67869100	-0.05197300
H	-5.05400100	1.77838900	-1.05644100
H	-5.60984700	0.21827200	-1.71828200
F	5.75858900	0.56494800	-0.73830100

4-Methoxystyrene/NMP monoadduct (24a), solvent = DMSO



Charge = 0; Multiplicity = 1

36

-749.952153 [B3LYP/6-31+G(d,p)]

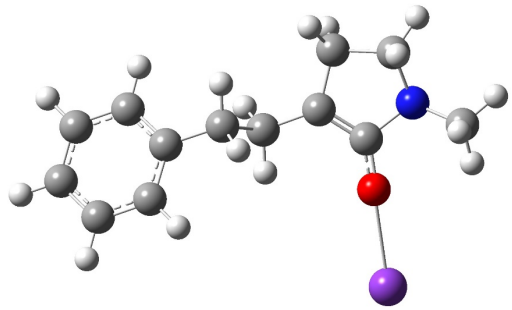
C	4.15639700	-0.07851100	-0.33722800
C	3.62800900	0.60359500	0.76569800
C	2.30858900	0.35108900	1.16498200
C	1.49383800	-0.56746700	0.49336000
C	2.04888200	-1.24202100	-0.60905400
C	3.35725600	-1.00641700	-1.02353800
H	4.22211600	1.32035700	1.31992400
H	1.91475600	0.88627900	2.02597500
H	1.44733500	-1.96818300	-1.15091200
H	3.77741900	-1.53611600	-1.87327900
C	0.05818200	-0.80428500	0.91364600
H	-0.20239300	-1.85503500	0.73777400
H	-0.04199100	-0.63096700	1.99262400
C	-0.94392000	0.10227600	0.16993600
H	-0.86119700	-0.07313200	-0.91129300
H	-0.67868900	1.15188800	0.34097000
C	-2.39606400	-0.11775100	0.60713800
H	-2.46370100	0.04881100	1.69376000
C	-3.37292700	0.88112700	-0.02309900
O	-3.17197600	2.09381000	-0.18305900

N	-4.51168200	0.22182000	-0.35375000
C	-4.50542500	-1.18807400	0.04017800
H	-5.09256700	-1.32560600	0.95933600
H	-4.95694200	-1.80371300	-0.74401600
C	-3.01055100	-1.48738400	0.25448300
H	-2.85209800	-2.24462600	1.02509500
H	-2.57113000	-1.85741300	-0.67916400
C	-5.71676600	0.87344000	-0.83027100
H	-6.50032400	0.85402400	-0.06251400
H	-5.47996000	1.90992800	-1.07333600
H	-6.09291800	0.36734900	-1.72528400
O	5.43079900	0.08506400	-0.81473200
C	6.28974700	1.01748400	-0.15507500
H	7.23467300	0.98621300	-0.69778600
H	5.87852900	2.03257800	-0.19543100
H	6.45878400	0.73102500	0.88919700

-749.606933 [M06-2X/6-31++G(d,p)]

C	4.10935500	-0.05039500	-0.35992000
C	3.61993600	0.49308000	0.82923100
C	2.31057300	0.20363600	1.22611900
C	1.47523200	-0.61524800	0.46801400
C	1.99009600	-1.15103700	-0.72162200
C	3.28626900	-0.87712500	-1.13530400
H	4.23563500	1.13150700	1.45177400
H	1.93882000	0.63036600	2.15494500
H	1.36251100	-1.79581500	-1.33301300
H	3.68333300	-1.29515600	-2.05511000
C	0.04581700	-0.87258300	0.87744400
H	-0.23423200	-1.89802800	0.60698200
H	-0.04933000	-0.79068000	1.96718800
C	-0.92587300	0.11262600	0.21549600
H	-0.84554100	0.02427700	-0.87683500
H	-0.64026100	1.13861500	0.47502700
C	-2.37239900	-0.12446700	0.63201800
H	-2.45919800	0.00695500	1.72144000
C	-3.33301100	0.88562400	0.01196400
O	-3.12670100	2.09295800	-0.12054800
N	-4.46020500	0.23507800	-0.35162400
C	-4.46034500	-1.17597200	0.01480900
H	-5.04361700	-1.32697900	0.93332100
H	-4.91257200	-1.77329000	-0.78179700
C	-2.96959100	-1.47717200	0.22095100
H	-2.80718100	-2.26461600	0.95858200
H	-2.52404200	-1.79682400	-0.72840300
C	-5.65576600	0.89814800	-0.82084800
H	-6.44660300	0.84728400	-0.06408200
H	-5.41452900	1.94230200	-1.02155600
H	-6.01492900	0.42382500	-1.73849100
O	5.36586300	0.16201200	-0.84292700
C	6.22848400	0.99816400	-0.08790400
H	7.16518600	1.04333600	-0.64143500
H	5.81153000	2.00622100	0.01087300
H	6.41050900	0.57771300	0.90708300

Styrene/NMP monoadduct K enolate, solvent = DMSO



Charge = 0; Multiplicity = 1

32

-1234.802435 [B3LYP/6-31+G(d,p)]

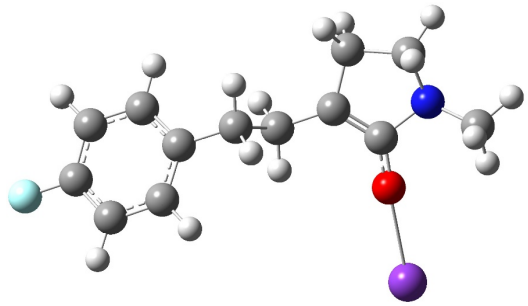
C	-0.96613000	-1.10898900	-0.13970600
C	-2.13748100	-0.37288300	-0.12245800
O	-2.33888100	0.90131100	-0.11170900
C	-4.47698600	-0.86845200	0.52456200
H	-4.73675700	0.16023200	0.26688500
H	-5.31127600	-1.52169900	0.24660200
H	-4.34848400	-0.93000700	1.62361500
C	-2.77836100	-2.60535800	0.12531800
H	-2.82556500	-2.77271500	1.21925900
H	-3.37996500	-3.38192400	-0.36118000
N	-3.27793300	-1.26337200	-0.19386800
K	-2.71175600	3.39685300	-0.26479700
C	-1.30791300	-2.57121300	-0.32499100
H	-0.69815700	-3.27423200	0.25848200
H	-1.21900500	-2.89052900	-1.38363500
C	0.39953400	-0.54616400	-0.38367600
H	0.80697600	-0.90384600	-1.34872700
H	0.33159200	0.54656700	-0.46678800
C	1.45502800	-0.88774300	0.70852500
H	1.50549600	-1.97807800	0.81924500
H	1.10358300	-0.48588000	1.66636600
C	2.83357900	-0.34730000	0.40073900
C	3.23637900	0.91668000	0.86383200
C	3.73417200	-1.07434300	-0.39647900
C	4.49375200	1.43867800	0.54300800
H	2.55811400	1.49547700	1.48697100
C	4.99224300	-0.55780100	-0.72237800
H	3.44734400	-2.05827400	-0.76082400
C	5.37779300	0.70282000	-0.25346100
H	4.78382800	2.41661400	0.91792800
H	5.67250500	-1.14090900	-1.33745700
H	6.35607300	1.10451900	-0.50185100

-1234.484525 [M06-2X/6-31++G(d,p)]

C	-0.86956400	-1.07587200	-0.13388800
C	-2.06992500	-0.40393700	-0.17893100
O	-2.33904700	0.85047100	-0.22994100
C	-4.36095400	-0.96535000	0.48358900
H	-4.69066000	0.01843100	0.14540500
H	-5.15492700	-1.69215200	0.28657800
H	-4.19592700	-0.92349100	1.57675900
C	-2.60164800	-2.63583400	0.18168300
H	-2.65348400	-2.72821700	1.28330600

H	-3.15744700	-3.46985000	-0.25956100
N	-3.15878400	-1.34851900	-0.22740700
K	-3.12933000	3.19859200	-0.22077000
C	-1.13208700	-2.55737100	-0.24967500
H	-0.49928800	-3.19473600	0.38003900
H	-1.01262900	-2.91994700	-1.28822500
C	0.47199300	-0.46114100	-0.36116600
H	0.91382800	-0.82343200	-1.30779900
H	0.36344000	0.62694300	-0.46464400
C	1.49909000	-0.74922500	0.75750000
H	1.54817600	-1.83346400	0.91783800
H	1.13961500	-0.29984900	1.69030500
C	2.87361700	-0.22767000	0.42457800
C	3.29996400	1.03194100	0.86153000
C	3.73637900	-0.97436300	-0.38811500
C	4.55235100	1.53107300	0.50112800
H	2.64350200	1.62547800	1.49413900
C	4.98809300	-0.48127800	-0.75298700
H	3.41978600	-1.95604700	-0.73430800
C	5.40124000	0.77593400	-0.30851600
H	4.86667600	2.50856500	0.85519400
H	5.64247300	-1.07875800	-1.38099800
H	6.37672400	1.16170400	-0.58839900

4-Fluorostyrene/NMP monoadduct K enolate, solvent = DMSO



Charge = 0; Multiplicity = 1

32

-1334.053087 [B3LYP/6-31+G(d,p)]

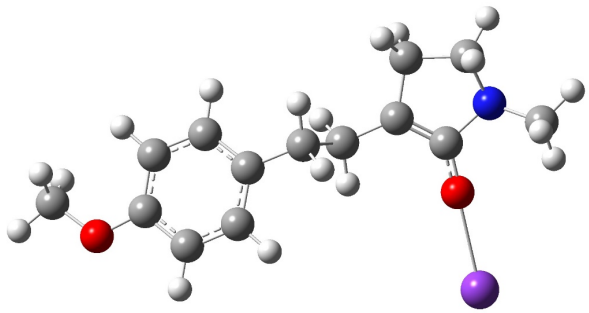
C	-1.38742500	-1.11553700	-0.12597000
C	-2.52336800	-0.32502000	-0.13006000
O	-2.66542400	0.95683300	-0.11698800
C	-4.89752800	-0.71240800	0.46223300
H	-5.10061400	0.32939200	0.20597800
H	-5.75566600	-1.32241300	0.15974500
H	-4.79849300	-0.78681000	1.56350400
C	-3.27327200	-2.52593900	0.09052800
H	-3.35016800	-2.69589600	1.18232300
H	-3.90075200	-3.27078800	-0.41250500
N	-3.70200000	-1.16048400	-0.23054500
K	-3.03802000	3.45339600	-0.26062100
C	-1.79391100	-2.55864000	-0.33014300
H	-1.23044700	-3.29409500	0.25967900
H	-1.69895700	-2.87396000	-1.38947900
C	0.00584900	-0.61404200	-0.34568300
H	0.40090300	-0.95555800	-1.32214300
H	-0.00781200	0.48291600	-0.38902700
C	1.03720100	-1.04714000	0.73589000

H	1.04279400	-2.14230100	0.79919200
H	0.69737200	-0.67442400	1.70927900
C	2.43916300	-0.55092700	0.46063900
C	2.90767700	0.64670400	1.02563800
C	3.29702000	-1.24966100	-0.40590900
C	4.18571000	1.14023800	0.74288100
H	2.26690800	1.20476300	1.70349200
C	4.57847700	-0.77703800	-0.70631600
H	2.96324900	-2.18296100	-0.85186500
C	4.99183600	0.41241100	-0.12144000
H	4.54930100	2.06253400	1.18381700
H	5.24262200	-1.31806700	-1.37227700
F	6.24833000	0.88376300	-0.40465800

-1333.706272 [M06-2X/6-31++G(d,p)]

C	-1.29548200	-1.10461500	-0.13814000
C	-2.44917500	-0.35558500	-0.18648100
O	-2.63602400	0.91453000	-0.21353800
C	-4.78513500	-0.78124000	0.42009900
H	-5.02705900	0.23789600	0.11336000
H	-5.62712700	-1.43514100	0.17332700
H	-4.64915700	-0.79363800	1.51796400
C	-3.12946500	-2.55544900	0.11707500
H	-3.20602900	-2.66472800	1.21566900
H	-3.73010500	-3.34339200	-0.34926100
N	-3.59525800	-1.22718200	-0.27446000
K	-3.41516100	3.26818300	-0.20875100
C	-1.65082900	-2.56376800	-0.28874300
H	-1.07138600	-3.25282800	0.33807900
H	-1.53645300	-2.91253800	-1.33252300
C	0.08411400	-0.56989200	-0.33581800
H	0.52281900	-0.95301600	-1.27572800
H	0.04022100	0.52279700	-0.43619500
C	1.07174900	-0.91838700	0.80038700
H	1.07541000	-2.00567600	0.94466500
H	0.70881800	-0.46987500	1.73211200
C	2.47185300	-0.44245600	0.50722600
C	2.91743200	0.80993600	0.94564900
C	3.33789800	-1.21750700	-0.27419600
C	4.18900100	1.28348200	0.62186700
H	2.26131400	1.42728900	1.55413800
C	4.61303100	-0.76729100	-0.61264700
H	3.00991000	-2.19349100	-0.62338800
C	5.00814800	0.47921600	-0.15366300
H	4.54333500	2.25023800	0.96293300
H	5.28981700	-1.36403200	-1.21468400
F	6.24887600	0.92778200	-0.47337300

4-Vinylanisole/NMP monoadduct K enolate, solvent = DMSO



Charge = 0; Multiplicity = 1

36

-1349.304166 [B3LYP/6-31+G(d,p)]

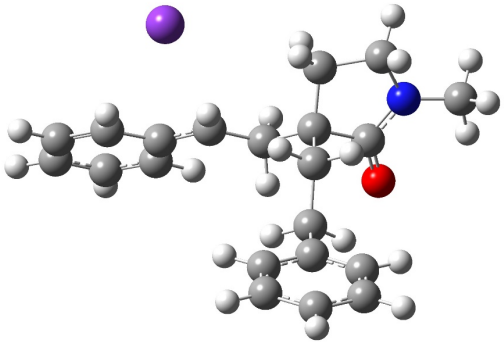
C	-1.82222400	-1.12055200	-0.14185800
C	-2.95229300	-0.32597200	-0.21356900
O	-3.08712800	0.95677400	-0.24521500
C	-5.34880200	-0.68325400	0.30305700
H	-5.53590600	0.35119100	0.00793300
H	-6.19931500	-1.29787800	-0.01142100
H	-5.29005600	-0.72403700	1.40900400
C	-3.72327800	-2.51436000	0.05175000
H	-3.84325500	-2.64626600	1.14495800
H	-4.33513700	-3.27346400	-0.44929000
N	-4.13187200	-1.15879600	-0.33192500
K	-3.34010300	3.47106500	-0.21873300
C	-2.22858800	-2.56844600	-0.30896100
H	-1.69273200	-3.28383400	0.32939600
H	-2.09323800	-2.92323300	-1.35127600
C	-0.41709900	-0.63421700	-0.31838600
H	0.02722400	-1.04130300	-1.24718800
H	-0.42558600	0.45744600	-0.43684000
C	0.55596200	-0.99101000	0.84202500
H	0.54468900	-2.07804500	0.98989600
H	0.16931300	-0.54256700	1.76561100
C	1.97693000	-0.52933800	0.60394100
C	2.39629600	0.76119600	0.97706700
C	2.91538700	-1.34687300	-0.03799900
C	3.68894000	1.21264300	0.72102900
H	1.69803900	1.42406700	1.48310200
C	4.22122000	-0.91377800	-0.30745200
H	2.63066700	-2.35345400	-0.33614300
C	4.61147900	0.37549500	0.07427800
H	4.00192800	2.20872600	1.02005000
H	4.91173200	-1.58595800	-0.80303900
O	5.86105500	0.90369800	-0.13155000
C	6.84310700	0.09213900	-0.77798000
H	6.52779000	-0.18180500	-1.79139000
H	7.74510700	0.70221300	-0.83095400
H	7.05015800	-0.81625100	-0.20053500

-1348.938793 [M06-2X/6-31++G(d,p)]

C	-1.83087700	-1.09083300	-0.14256900
C	-2.94920400	-0.29276200	-0.22381900
O	-3.07796600	0.98488300	-0.25046900
C	-5.31936000	-0.62094200	0.30752400

H	-5.50909200	0.40841400	-0.00077200
H	-6.17946500	-1.23882200	0.03213200
H	-5.21736900	-0.64388500	1.40894400
C	-3.73232300	-2.46168600	0.04642700
H	-3.84711100	-2.57076000	1.14175900
H	-4.35188900	-3.22145900	-0.44146500
N	-4.12830800	-1.11336100	-0.35292100
K	-3.13665500	3.46155300	-0.24451300
C	-2.24313800	-2.53272700	-0.31262700
H	-1.71447500	-3.24881500	0.32860500
H	-2.11073900	-2.88197300	-1.35419700
C	-0.42469000	-0.61117600	-0.28966600
H	0.02587600	-0.99048100	-1.22580800
H	-0.42342700	0.48456700	-0.36677500
C	0.51728400	-1.02269000	0.86344600
H	0.48992200	-2.11425900	0.96992500
H	0.13183300	-0.59896300	1.79839400
C	1.93719500	-0.56919400	0.63682400
C	2.38377600	0.67806100	1.09807500
C	2.83364800	-1.34187900	-0.10200600
C	3.67047600	1.12986900	0.83521600
H	1.70966100	1.30454800	1.67820000
C	4.13304900	-0.90738900	-0.38127800
H	2.51595400	-2.31401200	-0.47298900
C	4.55309700	0.33762500	0.09128900
H	4.01419000	2.09301600	1.19983200
H	4.79448500	-1.54308000	-0.95818300
O	5.79609300	0.86047200	-0.11527100
C	6.72197400	0.08102200	-0.85499600
H	6.35824200	-0.10181000	-1.87210000
H	7.64146800	0.66314000	-0.89602100
H	6.91609000	-0.87596500	-0.35839900

Styrene/NMP bisadduct K benzylate, solvent = DMSO



Charge = 0; Multiplicity = 1

48

-1544.351698 [B3LYP/6-31+G(d,p)]

C	4.97550100	-2.56310700	0.92360500
C	4.37060300	-2.78250200	-0.33637800
C	3.25044600	-2.07554600	-0.74271600
C	2.61688900	-1.06429100	0.08724500
C	3.26384800	-0.86743100	1.37347900
C	4.38994400	-1.59435000	1.75687300
H	5.85359400	-3.12162700	1.23344900
H	4.79171200	-3.52799500	-1.01039300
H	2.81620000	-2.28185500	-1.72089900

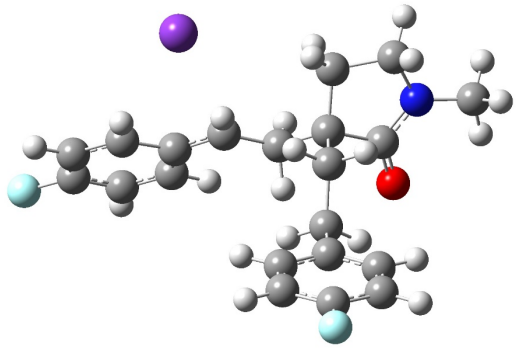
H	2.85349300	-0.13510200	2.06431700
H	4.82475200	-1.39895000	2.73706400
C	1.51998000	-0.31526000	-0.34611800
H	1.08224500	-0.55891100	-1.31232400
C	0.82344300	0.69905900	0.52725600
H	1.49988600	1.53033700	0.81205900
H	0.51477700	0.26826500	1.49580000
C	-0.42206100	1.35028000	-0.11143200
C	-1.01426700	2.42209300	0.82660500
O	-1.19751100	2.30763100	2.04813800
C	-2.05986700	4.66389100	0.62208200
H	-3.07019100	4.71447100	0.19698400
H	-2.13263900	4.56342900	1.70567900
H	-1.53328300	5.59292900	0.37863000
N	-1.33705000	3.52197500	0.09692900
K	4.26659400	1.07367500	-1.19483200
C	-1.54268900	0.32022000	-0.45261400
H	-2.40756400	0.86001600	-0.86156400
H	-1.17244800	-0.32021600	-1.26102600
C	-2.02206600	-0.57782800	0.70634200
H	-1.17507400	-1.16351600	1.07886900
H	-2.36934600	0.04849700	1.53404400
C	-3.13030800	-1.51699200	0.27641900
C	-2.84039000	-2.80019000	-0.21498200
C	-4.47608200	-1.11834600	0.33240900
C	-3.86010200	-3.65854200	-0.63910300
H	-1.80559400	-3.13198800	-0.26033500
C	-5.50017100	-1.97165600	-0.09030100
H	-4.72411700	-0.13124000	0.71614400
C	-5.19551600	-3.24663100	-0.57915400
H	-3.61185000	-4.64883000	-1.01129700
H	-6.53437100	-1.64298700	-0.03350400
H	-5.98953800	-3.91266300	-0.90459400
C	-1.05649100	3.38151100	-1.33035900
H	-0.61235200	4.30282400	-1.72174200
H	-1.98679700	3.19606700	-1.88588600
C	-0.08949800	2.18603300	-1.37557500
H	-0.18638500	1.61423700	-2.30165100
H	0.94217000	2.54762400	-1.31113600

-1543.906139 [M06-2X/6-31++G(d,p)]

C	5.02291800	-2.09075700	0.84729500
C	4.38768700	-2.42774200	-0.37048100
C	3.19912400	-1.84514400	-0.76073500
C	2.51740500	-0.84361100	0.04282100
C	3.17086400	-0.55962500	1.30991300
C	4.36664700	-1.16534100	1.67449100
H	5.95577000	-2.55575500	1.14536000
H	4.84968400	-3.16146500	-1.02899400
H	2.75113900	-2.12817900	-1.71203400
H	2.71620700	0.15764200	1.98788900
H	4.81089400	-0.89922300	2.63268500
C	1.36904200	-0.19745900	-0.37885600
H	0.95006800	-0.45780100	-1.34885500
C	0.67282300	0.83813600	0.45941400
H	1.33073700	1.70347200	0.67328600
H	0.40060100	0.45091500	1.45675200
C	-0.59770600	1.39323100	-0.19085800
C	-1.25460200	2.44664000	0.70754900

O	-1.41496900	2.36573800	1.92741600
C	-2.49436800	4.56402400	0.41617300
H	-3.49599500	4.50919100	-0.02505500
H	-2.57308800	4.48471100	1.50080200
H	-2.04632000	5.52670700	0.15246100
N	-1.66971300	3.47869100	-0.06316300
K	5.03717300	0.62253100	-0.82500200
C	-1.65336100	0.29919200	-0.47771100
H	-2.57131200	0.77602800	-0.85150700
H	-1.27923600	-0.33264100	-1.29212900
C	-2.00762400	-0.59929200	0.71431800
H	-1.10431200	-1.12571600	1.04292100
H	-2.35520100	0.01587400	1.55089900
C	-3.06486000	-1.60598700	0.33274900
C	-2.70695900	-2.83547700	-0.23235100
C	-4.42470600	-1.31326400	0.48468500
C	-3.68007500	-3.75096500	-0.63248200
H	-1.65259400	-3.07553800	-0.35576400
C	-5.40268800	-2.22462900	0.08635000
H	-4.71827700	-0.36165600	0.92285800
C	-5.03290100	-3.44772500	-0.47411800
H	-3.38201600	-4.70159600	-1.06505400
H	-6.45313000	-1.98136100	0.21627900
H	-5.79224600	-4.15955000	-0.78307000
C	-1.39595700	3.29406200	-1.48132000
H	-1.04560100	4.23153300	-1.92344700
H	-2.31044700	2.98860600	-2.00834700
C	-0.32348200	2.19747800	-1.47695700
H	-0.35657800	1.58076200	-2.37812100
H	0.66939100	2.65575000	-1.41130600

4-Fluorostyrene/NMP bisadduct K benzylate, solvent = DMSO



Charge = 0; Multiplicity = 1

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-1742.852572 [B3LYP/6-31+G(d,p)]

C	4.86096700	-2.60701700	0.94421900
C	4.31639500	-2.83370600	-0.32346900
C	3.22744200	-2.08282700	-0.74521700
C	2.61035500	-1.05589300	0.07528400
C	3.23429400	-0.87972500	1.37454900
C	4.32998000	-1.64250100	1.78985100
H	4.74563300	-3.59610900	-0.96899300
H	2.81050000	-2.27597700	-1.73228900
H	2.83699600	-0.13626300	2.05942500
H	4.76859400	-1.48372400	2.77227700
C	1.53886900	-0.27513100	-0.37733500

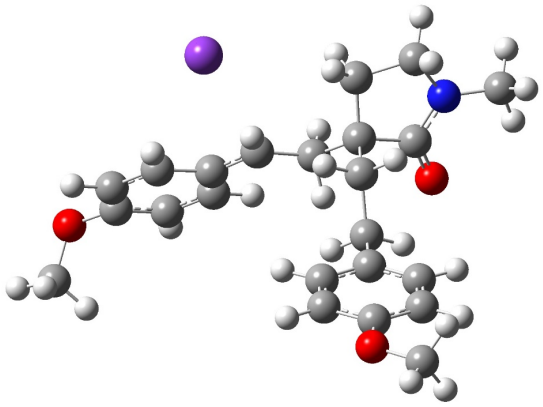
H	1.10013500	-0.51869800	-1.34277000
C	0.84139300	0.73282900	0.50164500
H	1.51095000	1.57077200	0.78610800
H	0.54241900	0.29756300	1.47194200
C	-0.41453600	1.37458600	-0.12620200
C	-1.00983500	2.43823900	0.81932300
O	-1.18264100	2.31850900	2.04184900
C	-2.07840700	4.67025700	0.62947100
H	-3.09257700	4.71250100	0.21274200
H	-2.14133200	4.56590100	1.71331800
H	-1.56257900	5.60489800	0.38447000
N	-1.34910700	3.53669800	0.09519300
K	4.22502000	1.12789800	-1.24341800
C	-1.52795800	0.33489200	-0.46102300
H	-2.40229800	0.86741900	-0.85929300
H	-1.15923600	-0.29899800	-1.27520900
C	-1.98602000	-0.57193600	0.69944100
H	-1.12989100	-1.15118900	1.06041000
H	-2.33005700	0.04679300	1.53396400
C	-3.08984200	-1.52035900	0.27863800
C	-2.79294800	-2.79755000	-0.22345200
C	-4.43870100	-1.13620700	0.35284000
C	-3.80178100	-3.67092500	-0.64267200
H	-1.75737800	-3.12161000	-0.28481300
C	-5.46579900	-1.99061600	-0.06002800
H	-4.69600600	-0.15523300	0.74383800
C	-5.11876400	-3.24209600	-0.55087900
H	-3.57414300	-4.65997700	-1.02617100
H	-6.50847600	-1.69703200	0.00098800
C	-1.07900500	3.40246200	-1.33473500
H	-0.64728100	4.32903900	-1.72754700
H	-2.01196600	3.20903300	-1.88300600
C	-0.10034100	2.21698000	-1.39057700
H	-0.19797800	1.64674900	-2.31752900
H	0.92764200	2.58963100	-1.33260000
F	-6.11687400	-4.09024200	-0.95504700
F	5.95749900	-3.36318800	1.35937200

-1742.342415 [M06-2X/6-31++G(d,p)]

C	4.77717800	-2.40876400	0.62978900
C	4.14419300	-2.63916300	-0.59358400
C	3.04547600	-1.87893500	-0.95057300
C	2.50409200	-0.83702300	-0.10534000
C	3.21120000	-0.65456100	1.14223500
C	4.31906400	-1.42904000	1.49187500
H	4.52094400	-3.41409000	-1.25612200
H	2.56239400	-2.06909400	-1.90702100
H	2.87135400	0.10440300	1.84119200
H	4.82626600	-1.26735200	2.43976200
C	1.44043500	-0.02428100	-0.49801500
H	0.94906700	-0.22414800	-1.44740300
C	0.87902200	1.03242400	0.40993200
H	1.60781800	1.84430200	0.62193600
H	0.63437100	0.63253600	1.41036000
C	-0.37884200	1.70882500	-0.14315200
C	-0.89935200	2.77228300	0.82986400
O	-1.00103200	2.65281800	2.05280800
C	-1.97763300	4.99073200	0.69016200
H	-3.00617000	5.02832300	0.31383800

H	-1.99381400	4.87684300	1.77438600
H	-1.47310800	5.92571200	0.42920500
N	-1.27096000	3.86518000	0.12319900
K	4.13804100	1.29715100	-1.21696700
C	-1.53016000	0.70687500	-0.40001700
H	-2.43603800	1.26234100	-0.68360400
H	-1.25913200	0.09187300	-1.26610200
C	-1.85715300	-0.22200000	0.77597000
H	-0.96244900	-0.80430500	1.02325500
H	-2.11936300	0.37180100	1.65753300
C	-2.98481500	-1.16167600	0.42630000
C	-2.72537900	-2.35443300	-0.25878700
C	-4.31294800	-0.84292100	0.72912100
C	-3.75588600	-3.21517100	-0.63366700
H	-1.69780700	-2.61704800	-0.50033400
C	-5.36214600	-1.68708500	0.36493300
H	-4.53358700	0.07888300	1.26142400
C	-5.05516900	-2.85672500	-0.31071900
H	-3.56356000	-4.14389500	-1.15986100
H	-6.39456900	-1.45060900	0.59907100
C	-1.09626500	3.71658200	-1.31475200
H	-0.69751100	4.64044900	-1.74413500
H	-2.06173400	3.50598800	-1.79504500
C	-0.11790200	2.53922800	-1.41503000
H	-0.25406100	1.96348400	-2.33353400
H	0.91057400	2.91679000	-1.39638800
F	-6.06734000	-3.68703600	-0.66816600
F	5.87292500	-3.16950600	0.97437000

4-Vinylanisole/NMP bisadduct K benzylate, solvent = DMSO



Charge = 0; Multiplicity = 1

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-1773.349365 [B3LYP/6-31+G(d,p)]

C	4.95583800	-2.18574200	0.36788300
C	4.29490200	-2.28975800	-0.87178200
C	3.20400900	-1.48708200	-1.17196300
C	2.67095500	-0.50429600	-0.24582500
C	3.39736700	-0.42366400	1.00807100
C	4.49138300	-1.24442000	1.29183300
H	4.65323700	-3.01062400	-1.60493200
H	2.71852400	-1.59925800	-2.14090000
H	3.08023900	0.29420000	1.75986000
H	5.00299100	-1.14665700	2.24827000

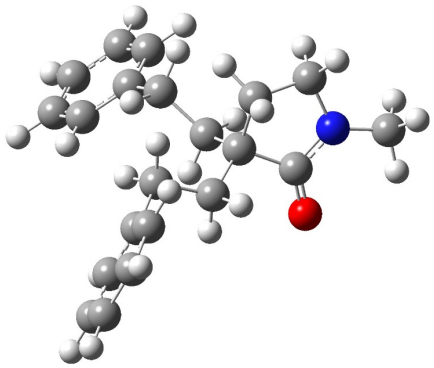
C	1.58925900	0.32583200	-0.56666900
H	1.08374100	0.16773300	-1.51724100
C	0.99777100	1.30515600	0.41554400
H	1.70879100	2.11768500	0.67512400
H	0.78130000	0.82993700	1.38833100
C	-0.29623300	1.99757900	-0.06328800
C	-0.77750700	3.02844000	0.97821800
O	-0.83534900	2.85987000	2.20583100
C	-1.81775100	5.28189500	0.98375000
H	-2.85746200	5.37232100	0.64513700
H	-1.80582100	5.11692200	2.06181500
H	-1.29487700	6.21673400	0.75431700
N	-1.16241900	4.16250900	0.33601100
K	4.23565800	1.70511400	-1.54815900
C	-1.45816500	0.99518500	-0.34142100
H	-2.34843600	1.56078900	-0.64875000
H	-1.16967800	0.38629000	-1.20546700
C	-1.84830000	0.05272200	0.81540300
H	-0.97830700	-0.55382900	1.09046700
H	-2.11651000	0.64405000	1.69645400
C	-2.99907800	-0.86029600	0.44400300
C	-2.77828600	-2.06236900	-0.25299200
C	-4.32360900	-0.52916900	0.75190800
C	-3.83197600	-2.89255900	-0.62694800
H	-1.76161200	-2.35652600	-0.50338200
C	-5.39988900	-1.34968500	0.38611100
H	-4.53197600	0.38956300	1.29549600
C	-5.15309200	-2.53918300	-0.30979400
H	-3.64924500	-3.82054800	-1.16060800
H	-6.40764100	-1.05261700	0.65134600
C	-1.02430000	4.08949400	-1.11704000
H	-0.61010800	5.02560700	-1.50625900
H	-2.00644800	3.93702600	-1.58663000
C	-0.07934000	2.89126600	-1.31289700
H	-0.27249800	2.36555200	-2.25117700
H	0.95730100	3.24377700	-1.33278300
O	-6.12367500	-3.41908600	-0.71523200
O	6.08993900	-2.96547900	0.64285200
C	-7.48644700	-3.11331400	-0.41361800
H	-7.79685400	-2.17491600	-0.88724700
H	-8.07311000	-3.93701300	-0.82084200
H	-7.64848000	-3.04951500	0.66843800
C	5.79725400	-4.24636700	1.21035800
H	6.75327600	-4.75082400	1.37598000
H	5.27056400	-4.14148500	2.16808400
H	5.18262100	-4.84954800	0.52936600

-1772.805518 [M06-2X/6-31++G(d,p)]

C	5.02594400	-2.00651500	0.33939400
C	4.28080200	-2.27178100	-0.82246300
C	3.10307500	-1.59744700	-1.08599500
C	2.56805100	-0.58484600	-0.20033700
C	3.35887200	-0.36214500	0.99011000
C	4.54211100	-1.05708300	1.23622800
H	4.64978700	-3.01730900	-1.52500200
H	2.55765700	-1.82052900	-2.00159800
H	3.02580800	0.37282900	1.71761500
H	5.11013600	-0.85359400	2.14269800
C	1.44364700	0.17776600	-0.51154400

H	0.88961900	-0.04638400	-1.42028900
C	0.92691700	1.23089900	0.42707800
H	1.68990800	2.01120500	0.63131700
H	0.69195000	0.82380100	1.42710600
C	-0.31890800	1.95944700	-0.08512200
C	-0.77773100	3.02197200	0.91945000
O	-0.85095900	2.88574200	2.14278100
C	-1.77829600	5.27971500	0.84635800
H	-2.80945400	5.36940000	0.48648100
H	-1.78416300	5.13920200	1.92758600
H	-1.23898200	6.19946100	0.60111700
N	-1.12816600	4.13996000	0.24168500
K	4.16722300	1.42073500	-1.51487800
C	-1.50956700	1.00376900	-0.33854400
H	-2.39616700	1.59473800	-0.61109800
H	-1.26793500	0.38811300	-1.21300800
C	-1.86707100	0.07670500	0.82965500
H	-0.98768700	-0.52769000	1.08065500
H	-2.11919100	0.67187800	1.71339500
C	-3.01525800	-0.83512400	0.47205100
C	-2.79308300	-1.99797900	-0.28057700
C	-4.32830900	-0.53699900	0.83151000
C	-3.83998300	-2.82872400	-0.65476500
H	-1.77692400	-2.25675400	-0.57233200
C	-5.39974600	-1.35970200	0.46604900
H	-4.53203300	0.35777000	1.41547300
C	-5.15252800	-2.51186000	-0.28152000
H	-3.66348800	-3.73159600	-1.23131200
H	-6.40420800	-1.09136200	0.77135100
C	-0.98801800	4.01468200	-1.20222200
H	-0.56457800	4.93234300	-1.62138300
H	-1.96987100	3.84924100	-1.66650200
C	-0.05541500	2.80497500	-1.34640000
H	-0.23332300	2.25238000	-2.27191500
H	0.98678800	3.14343400	-1.34432500
O	-6.11608200	-3.38644300	-0.68899400
O	6.22697000	-2.67190000	0.57735600
C	-7.45568900	-3.11118600	-0.31188200
H	-7.79402400	-2.15578900	-0.72755500
H	-8.05730800	-3.92005100	-0.72408100
H	-7.56200100	-3.09428300	0.77826900
C	6.05370600	-3.91796700	1.23859900
H	7.04397000	-4.36022700	1.36645300
H	5.58715500	-3.77430100	2.22101900
H	5.42793600	-4.59221500	0.64094800

Styrene/NMP bisadduct (20b), solvent = DMSO



Charge = 0; Multiplicity = 1

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-945.015302 [B3LYP/6-31+G(d,p)]

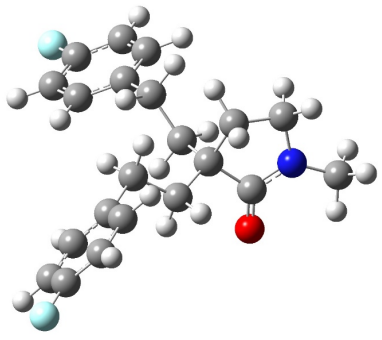
C	-5.75002700	-1.89968500	0.30592500
C	-5.52458900	-0.99820900	-0.73954400
C	-4.22411600	-0.57721900	-1.03590300
C	-3.12615800	-1.04620100	-0.29741000
C	-3.36694700	-1.95359900	0.74695800
C	-4.66497700	-2.37694600	1.04882700
H	-6.75883800	-2.23016200	0.53608400
H	-6.35921600	-0.62559300	-1.32708000
H	-4.05880200	0.12058900	-1.85364000
H	-2.52937000	-2.33547500	1.32628400
H	-4.82772800	-3.08180300	1.85957500
C	-1.72057800	-0.56465500	-0.59776300
H	-1.01988000	-1.38489100	-0.41437300
H	-1.64591400	-0.30700400	-1.66078100
C	-1.33264200	0.65455000	0.26503400
H	-1.32618700	0.35897800	1.32048000
H	-2.12109900	1.41175900	0.16172600
C	0.01859300	1.33307900	-0.05688800
C	0.19612600	2.53951900	0.89337600
O	-0.00018700	2.52807400	2.11676300
C	1.08409300	4.85137200	0.77311100
H	0.59761400	5.69799600	0.27770700
H	0.81743800	4.84918400	1.83056000
H	2.17070100	4.96683800	0.67615100
N	0.64546900	3.60183600	0.18052400
C	1.25640200	0.41083900	0.21789600
H	1.03233100	-0.18866200	1.10809100
H	2.11575500	1.03702200	0.48980300
C	1.72498600	-0.52551200	-0.92062600
H	0.89386700	-1.13290500	-1.28867600
H	2.07745700	0.07436100	-1.76616000
C	2.84894200	-1.43531600	-0.46510000
C	4.18649600	-1.01194900	-0.52500300
C	2.57917000	-2.71204100	0.05327300
C	5.22400300	-1.83603300	-0.07776600
H	4.41828200	-0.02967500	-0.93046200
C	3.61283000	-3.54107300	0.50068700
H	1.55099500	-3.06270000	0.10288800
C	4.94038400	-3.10504800	0.43794900
H	6.25202700	-1.48929500	-0.13699300
H	3.38135600	-4.52730700	0.89356400
H	5.74495100	-3.74840200	0.78234800
C	0.04095000	2.02109800	-1.44512700
H	-0.98239500	2.29078100	-1.72741800
H	0.44801400	1.40056800	-2.24440700
C	0.85916600	3.30601900	-1.23553500
H	1.93028300	3.16271000	-1.43636400
H	0.50892200	4.13769500	-1.85490500

-944.581990 [M06-2X/6-31++G(d,p)]

C	-5.71595500	-1.69816700	0.32566300
C	-5.44793200	-0.89950800	-0.78624900
C	-4.13678700	-0.52122000	-1.07624700
C	-3.07520100	-0.93531800	-0.26499200
C	-3.35619000	-1.73650100	0.84764500
C	-4.66492400	-2.11617800	1.14318300

H	-6.73542000	-1.99464500	0.55224900
H	-6.25944500	-0.57264400	-1.42960200
H	-3.93158000	0.10090900	-1.94472200
H	-2.53898900	-2.06718900	1.48535500
H	-4.86483400	-2.74034600	2.00908900
C	-1.66222800	-0.48489100	-0.54744300
H	-0.96944800	-1.29375600	-0.28936500
H	-1.54686000	-0.28279700	-1.61960500
C	-1.30967600	0.77043900	0.26112500
H	-1.34168300	0.53029700	1.33104200
H	-2.08119300	1.53212700	0.08463600
C	0.05836200	1.38054200	-0.05811800
C	0.31104500	2.58156000	0.86306500
O	0.07781200	2.62063700	2.07152300
C	1.46556800	4.75921400	0.71486600
H	1.11376300	5.64489000	0.17858600
H	1.15958300	4.82061700	1.75957300
H	2.55937000	4.72304500	0.65894100
N	0.88852800	3.56558000	0.13848300
C	1.22851500	0.39198000	0.22784100
H	0.92070100	-0.26460500	1.05187300
H	2.10106500	0.94730600	0.59776600
C	1.70830400	-0.46563200	-0.95612600
H	0.86382600	-0.95358600	-1.45280900
H	2.18859900	0.17908400	-1.70055100
C	2.69830900	-1.50647700	-0.49101300
C	4.04717100	-1.17540300	-0.31916700
C	2.28218600	-2.80372800	-0.17335900
C	4.95905300	-2.11584900	0.15887200
H	4.38502300	-0.17141000	-0.56749500
C	3.19073100	-3.74913400	0.30350600
H	1.23725600	-3.07655100	-0.30457500
C	4.53246200	-3.40694600	0.47252900
H	6.00259500	-1.84233900	0.28312700
H	2.85089000	-4.75271700	0.54135000
H	5.24096900	-4.14116000	0.84318100
C	0.13332400	2.03584900	-1.44868300
H	-0.85311000	2.43803900	-1.70538400
H	0.43718800	1.35937000	-2.24857800
C	1.11308600	3.19767300	-1.25400900
H	2.15896200	2.89249400	-1.40321200
H	0.90524400	4.04757300	-1.90977800

4-Fluorostyrene/NMP bisadduct (23b), solvent = DMSO



Charge = 0; Multiplicity = 1

48

-1143.517854 [B3LYP/6-31+G(d,p)]

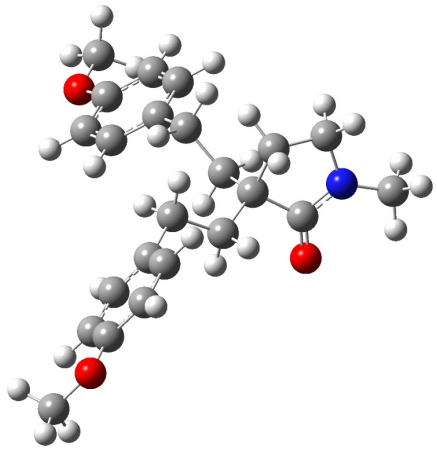
C	-5.59149300	-1.88492400	0.18677300
C	-5.46401700	-0.88313200	-0.76598500
C	-4.18302200	-0.39656000	-1.04412800
C	-3.04992000	-0.89878700	-0.38477100
C	-3.23211300	-1.91349600	0.56814300
C	-4.50277200	-2.41665900	0.86426200
H	-6.34083500	-0.50014100	-1.27731300
H	-4.06756200	0.38426200	-1.79126500
H	-2.36974900	-2.32366500	1.08704500
H	-4.64572600	-3.20365600	1.59716500
C	-1.67004500	-0.34132900	-0.67207400
H	-0.93342000	-1.13768100	-0.53163100
H	-1.61614800	-0.03448000	-1.72317400
C	-1.32796900	0.85546300	0.24062600
H	-1.29980800	0.51539200	1.28223000
H	-2.14933000	1.58117800	0.17572000
C	-0.01079700	1.60581000	-0.06033000
C	0.11597000	2.78206300	0.93545700
O	-0.07414800	2.71425500	2.15790000
C	0.89654100	5.13483700	0.90226100
H	0.37600000	5.97764300	0.43595000
H	0.62707300	5.08248500	1.95771100
H	1.97756100	5.29949600	0.81440800
N	0.51240400	3.89051300	0.26263200
C	1.26978800	0.73298700	0.17575600
H	1.08095800	0.09604800	1.04786500
H	2.10157500	1.38947600	0.46189000
C	1.77182500	-0.14364800	-0.99550600
H	0.96900600	-0.78072500	-1.37564000
H	2.08499700	0.49780200	-1.82560900
C	2.94461700	-1.00950000	-0.57917500
C	4.25919900	-0.52132300	-0.64818900
C	2.74462400	-2.30921100	-0.08745700
C	5.34802600	-1.29698100	-0.23840500
H	4.44111100	0.47889200	-1.03244700
C	3.81705800	-3.10501000	0.32726700
H	1.73752400	-2.71324700	-0.02903800
C	5.09731400	-2.57502000	0.24229500
H	6.36500000	-0.92342700	-0.29462200
H	3.66567800	-4.11145200	0.70286300
C	-0.02604200	2.34742100	-1.42084800
H	-1.06159700	2.58357600	-1.68833800
H	0.40292300	1.77750400	-2.24597000
C	0.73707500	3.65717400	-1.16341100
H	1.81310000	3.56610000	-1.36860000
H	0.35153400	4.49559200	-1.75185100
F	-6.84133400	-2.37221400	0.46524700
F	6.15615800	-3.34619400	0.64316000

-1143.024883 [M06-2X/6-31++G(d,p)]

C	-5.46526600	-1.83408500	0.19973500
C	-5.31582800	-0.92945400	-0.83898500
C	-4.03741000	-0.44140700	-1.10667200
C	-2.93166400	-0.85078000	-0.35391500
C	-3.13211400	-1.76573200	0.68541500
C	-4.40046600	-2.26749600	0.97342200
H	-6.17898000	-0.62324700	-1.42002100
H	-3.89921700	0.26951100	-1.91743500
H	-2.28283400	-2.09518800	1.27900000

H	-4.56544700	-2.98129600	1.77311600
C	-1.56003600	-0.27967800	-0.62129100
H	-0.80653600	-1.04596600	-0.40776500
H	-1.47101300	-0.02010300	-1.68358600
C	-1.29454800	0.96094200	0.24155000
H	-1.30027200	0.67356100	1.30028300
H	-2.12124200	1.67085700	0.10251900
C	0.02213400	1.68489600	-0.05618800
C	0.18028900	2.86244500	0.91472000
O	-0.04453100	2.82803000	2.12497300
C	1.12381100	5.14301300	0.85593000
H	0.65883400	6.01124600	0.38059000
H	0.84946600	5.11517700	1.91073500
H	2.21221100	5.23084600	0.76606700
N	0.66110000	3.92391800	0.23155800
C	1.26369500	0.77668400	0.18922400
H	1.00618100	0.06095800	0.98050400
H	2.09176600	1.37808800	0.58806200
C	1.80557200	0.01485300	-1.03226700
H	0.99585000	-0.49196900	-1.56605500
H	2.25413400	0.72530300	-1.73500700
C	2.84789700	-0.99402600	-0.61364400
C	4.18080700	-0.60939400	-0.43211800
C	2.49311600	-2.32078200	-0.34678500
C	5.14354100	-1.51861000	0.00394200
H	4.47466800	0.41689400	-0.63853300
C	3.43771800	-3.24914700	0.08912700
H	1.46280700	-2.63950000	-0.48441700
C	4.74501900	-2.82188900	0.25517100
H	6.17991000	-1.23120500	0.14433400
H	3.17373900	-4.28081100	0.29492900
C	0.03636200	2.40047500	-1.41929100
H	-0.98366400	2.71738300	-1.66347300
H	0.40137000	1.78862700	-2.24531200
C	0.90213500	3.64214300	-1.17783200
H	1.97075800	3.44893200	-1.34883200
H	0.60525800	4.49650400	-1.79220700
F	-6.70329700	-2.31824700	0.46793100
F	5.67354300	-3.71554100	0.67721600

4-Vinylanisole/NMP bisadduct (24b), solvent = DMSO



Charge = 0; Multiplicity = 1

56

-1174.018857 [B3LYP/6-31+G(d,p)]

C	-5.67058400	-1.57777700	-0.05175200
C	-5.48475300	-0.47354400	-0.89860700
C	-4.20335000	0.01796900	-1.13371900
C	-3.07082000	-0.56708000	-0.53913300
C	-3.27829700	-1.66767300	0.29974700
C	-4.55886200	-2.17876400	0.55102600
H	-6.35191700	-0.01785400	-1.36721000
H	-4.08033800	0.87099200	-1.79705500
H	-2.42480000	-2.14926400	0.77134700
H	-4.66902900	-3.03575900	1.20480500
C	-1.68189000	-0.00955700	-0.77925800
H	-0.95452500	-0.81968000	-0.67152600
H	-1.60957500	0.34999500	-1.81307100
C	-1.33508200	1.13641700	0.19488100
H	-1.32507400	0.74418500	1.21837500
H	-2.14642700	1.87542500	0.15629500
C	-0.00427700	1.88326700	-0.05158000
C	0.12273400	3.01080300	0.99843800
O	-0.08217000	2.89006400	2.21465500
C	0.92893600	5.35368500	1.08383300
H	0.42617000	6.22411800	0.64983200
H	0.64358700	5.25656400	2.13195500
H	2.01322000	5.50773900	1.01883000
N	0.53819200	4.14542300	0.38231800
C	1.26148900	0.98227800	0.16006000
H	1.04998700	0.30516300	0.99602700
H	2.09717100	1.61171800	0.49206400
C	1.77306100	0.15850000	-1.04471100
H	0.96698600	-0.44729700	-1.46794500
H	2.10466700	0.83757300	-1.83717900
C	2.92939500	-0.74200900	-0.65701000
C	4.25287700	-0.29019200	-0.71301500
C	2.71048400	-2.05299700	-0.19712900
C	5.33019500	-1.09818100	-0.32564900
H	4.46044100	0.71574700	-1.07062200
C	3.76635300	-2.87396000	0.19101200
H	1.69604900	-2.44125600	-0.14540800
C	5.08602100	-2.39921800	0.13102200
H	6.33795900	-0.70557500	-0.39014600
H	3.58658900	-3.88664700	0.53929300
C	0.00803000	2.68612700	-1.37677800
H	-1.02117800	2.94439800	-1.64843000
H	0.44404100	2.14990400	-2.22048300
C	0.77923500	3.97562900	-1.04992600
H	1.85711400	3.88452000	-1.24575400
H	0.40863800	4.84364500	-1.60417000
O	-6.96573600	-1.99325600	0.11729300
O	6.05902900	-3.27717400	0.53181500
C	-7.21415500	-3.11542600	0.96673200
H	-8.29416600	-3.26315100	0.95548800
H	-6.71825500	-4.01661100	0.58842000
H	-6.88303800	-2.91713900	1.99243100
C	7.42126700	-2.84635900	0.49262900
H	7.58220900	-1.98139500	1.14603500
H	8.00996100	-3.68967700	0.85402100
H	7.72915500	-2.59703500	-0.52922100

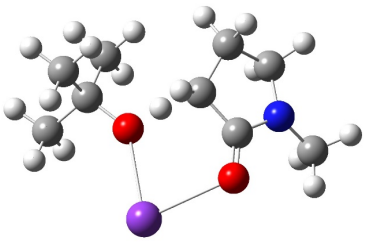
-1173.491738 [M06-2X/6-31++G(d,p)]

C	-5.51368200	-1.58197900	-0.03872000

C	-5.34346600	-0.48769200	-0.89633400
C	-4.07323300	0.02103300	-1.12868900
C	-2.94066400	-0.54024700	-0.52124500
C	-3.13074900	-1.62801000	0.32863800
C	-4.40124600	-2.15666100	0.57822500
H	-6.21828600	-0.05497400	-1.37168000
H	-3.95498200	0.86967600	-1.79922100
H	-2.26990400	-2.08452200	0.81209600
H	-4.50195700	-3.00532300	1.24425500
C	-1.56938500	0.05057200	-0.74327100
H	-0.81484900	-0.72612900	-0.57682800
H	-1.47318000	0.37917700	-1.78634800
C	-1.30864800	1.23463500	0.19717000
H	-1.32486800	0.88035500	1.23535300
H	-2.13337700	1.95351100	0.09628300
C	0.01119600	1.97372500	-0.04298600
C	0.15900800	3.09686800	0.99208700
O	-0.07833100	2.99837800	2.19660200
C	1.10965100	5.37382900	1.06825400
H	0.66164500	6.27025800	0.63041100
H	0.81492600	5.29387600	2.11494200
H	2.20038500	5.45586800	1.00360500
N	0.64820300	4.19354100	0.37267500
C	1.24988000	1.05261800	0.16676500
H	0.98121900	0.29216800	0.91147400
H	2.07184300	1.62919100	0.61236100
C	1.81258500	0.36096600	-1.08669400
H	1.01051400	-0.11894000	-1.65688400
H	2.26468400	1.11147500	-1.74442600
C	2.85590400	-0.66394600	-0.71257500
C	4.19401600	-0.30681900	-0.55439900
C	2.50012000	-1.99610800	-0.45763300
C	5.16297300	-1.23256000	-0.15584200
H	4.49895200	0.71930800	-0.74856700
C	3.44567700	-2.93248400	-0.06277400
H	1.46395100	-2.30645200	-0.57453800
C	4.78475200	-2.55357600	0.09206100
H	6.19241600	-0.91171900	-0.04920600
H	3.16922400	-3.96453900	0.12943800
C	0.04242200	2.76230400	-1.36483300
H	-0.97402300	3.09561900	-1.60273900
H	0.41542700	2.19495500	-2.21849400
C	0.90880900	3.98573800	-1.04601100
H	1.97906300	3.79618300	-1.21161500
H	0.62435300	4.87242500	-1.61907100
O	-6.79492200	-2.01580600	0.12884200
O	5.64261700	-3.53811700	0.48165600
C	-7.00411800	-3.12964100	0.98235100
H	-8.07716300	-3.31500500	0.97889500
H	-6.47812700	-4.01515400	0.60920000
H	-6.67356600	-2.91021800	2.00336400
C	7.00921800	-3.19298600	0.64559800
H	7.13128900	-2.42475900	1.41667100
H	7.51507000	-4.10555500	0.95756900
H	7.44086500	-2.83866400	-0.29667400

10.3.2. XYZ Co-ordinates of transition states

Deprotonation of NMP (19) with KO*t*Bu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

31

-1158.813939 [B3LYP/6-31+G(d,p)]

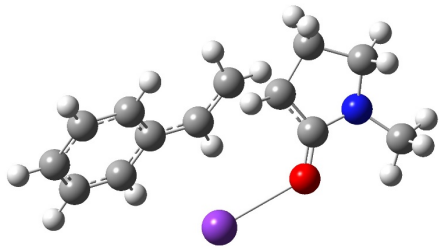
C	-0.20201300	-0.18657000	0.58453300
O	0.93528700	0.36357800	0.62170200
C	-1.14378000	1.46449200	-1.02096000
H	-0.25214800	2.04865700	-0.78747300
H	-1.04009900	1.05482000	-2.03907600
H	-2.01706000	2.12489700	-1.00592700
C	-2.40064200	-0.53527900	-0.14384700
H	-3.36551100	-0.02651600	-0.04132700
H	-2.37947800	-1.02249700	-1.13389100
N	-1.29247200	0.41568100	-0.03232900
K	2.85196600	-1.33478600	-0.27856700
C	-2.10565500	-1.54997300	0.97923000
H	-2.59001200	-1.22066200	1.91169700
H	-2.51454200	-2.53745600	0.73559300
H	0.08938400	-2.40163100	0.15232200
O	0.80852800	-3.03383600	-0.59317300
C	0.57076200	-4.43051900	-0.64896000
C	1.67648600	-5.06576000	-1.51229800
H	2.66154700	-4.86896600	-1.07330300
H	1.54980800	-6.15233900	-1.59664800
H	1.66180800	-4.63972000	-2.52213500
C	0.61443700	-5.04168400	0.76925200
H	-0.16360800	-4.60130500	1.40229600
H	0.46041900	-6.12753900	0.74534300
H	1.58603600	-4.84364000	1.23681100
C	-0.80444300	-4.71632500	-1.29011500
H	-1.60688900	-4.26977100	-0.69242900
H	-0.84811500	-4.28421400	-2.29646400
H	-0.99939600	-5.79304800	-1.37006600
C	-0.57674600	-1.50229600	1.06577600
H	-0.12604800	-1.77332200	2.02460500

-1158.518098 [M06-2X/6-31++G(d,p)]

C	-0.22881400	-0.44760200	0.54833100
O	0.78511700	-0.23931700	1.25443700
C	0.84529400	0.32186200	-1.54738800
H	1.19825700	-0.52239400	-2.15741500
H	0.60267100	1.15307300	-2.21616800
H	1.64243000	0.62649100	-0.86791200
C	-1.49336100	-0.59802400	-1.41154800
H	-1.92146400	0.12086200	-2.11736600
H	-1.21985600	-1.50466800	-1.97639400
N	-0.31055300	-0.04563900	-0.76438200

K	1.05951800	-2.29177100	2.96055200
C	-2.41882000	-0.93169600	-0.22774000
H	-3.07179000	-0.07315400	-0.02047100
H	-3.06358100	-1.78488900	-0.46319300
H	-0.97090900	-2.50683500	1.00677800
O	-0.49386800	-3.62540300	1.28681700
C	-0.07218400	-4.32712800	0.14551500
C	-1.26894600	-4.60386400	-0.77739400
H	-1.72828200	-3.65993400	-1.09247800
H	-0.97270400	-5.16000400	-1.67436100
H	-2.02483000	-5.18714100	-0.23968600
C	0.98484900	-3.51240300	-0.62050100
H	1.84688400	-3.31124800	0.02679200
H	1.34110100	-4.04401500	-1.51056000
H	0.56841000	-2.55015000	-0.93839400
C	0.54406500	-5.65761100	0.58991900
H	1.39522700	-5.47032100	1.25453300
H	-0.19759200	-6.24736700	1.13952400
H	0.89415900	-6.24764800	-0.26527100
C	-1.42835900	-1.19224800	0.90800400
H	-1.78425900	-0.96734300	1.91759200

Reaction of NMP K enolate with styrene (**3**) **T.S.**, solvent = DMSO



Charge = 0; Multiplicity = 1

32

-1234.760131 [B3LYP/6-31+G(d,p)]

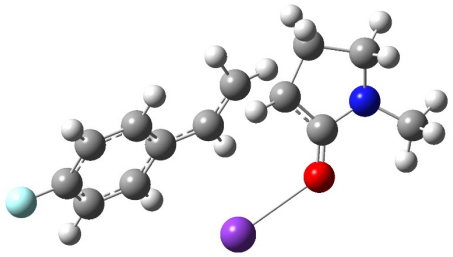
C	-2.01619300	1.40998600	0.04993400
C	-1.78652100	2.74213200	0.42484400
C	-0.54910800	3.34288300	0.19963900
C	0.53053100	2.64252100	-0.41122900
C	0.26472300	1.29718800	-0.79770900
C	-0.97354600	0.70031600	-0.56363400
H	-2.97964700	0.94099400	0.22596800
H	-2.57886600	3.31652600	0.89940100
H	-0.39268300	4.37457100	0.51039500
H	1.04247300	0.71847300	-1.28748900
H	-1.13065000	-0.33122200	-0.87107500
C	1.80390600	3.29586100	-0.62088800
H	1.83644100	4.36103900	-0.39216300
C	2.94423700	2.70244700	-1.14954900
H	3.05796400	1.62123600	-1.11752700
H	3.88414700	3.24463200	-1.08588700
C	3.19563300	2.52560200	-3.33951800
H	2.29796100	1.94113300	-3.50252700
C	3.23827600	3.89048400	-3.72978200
O	2.28532200	4.71850100	-3.83856200
C	4.92120300	5.49503100	-4.59709200
H	4.18834700	6.26869700	-4.36175400
H	5.91497200	5.84527900	-4.29972400
H	4.92662600	5.33947200	-5.69064300

C	5.40491400	3.09106900	-4.10771800
H	5.53984900	2.93291200	-5.19246900
H	6.39919000	3.21021300	-3.66345500
N	4.58287400	4.28337500	-3.87893000
K	-0.19892300	4.45742200	-3.02766200
C	4.58516000	1.93647200	-3.47498000
H	4.63031800	1.03450800	-4.09534900
H	5.01220100	1.66168700	-2.49413800

-1234.439728 [M06-2X/6-31++G(d,p)]

C	-1.95211800	1.51553300	-0.08020900
C	-1.71036900	2.82434800	0.34985100
C	-0.45798300	3.40615700	0.18394100
C	0.61633900	2.70517400	-0.41758700
C	0.34418900	1.38648200	-0.85759200
C	-0.91090600	0.80714300	-0.68447500
H	-2.92996900	1.06272400	0.04680800
H	-2.50657700	3.39658400	0.81846000
H	-0.28987900	4.42608500	0.52398600
H	1.12463200	0.81521600	-1.35242700
H	-1.07963400	-0.20707100	-1.03674300
C	1.89716900	3.35085300	-0.62302600
H	1.93914700	4.42016500	-0.42537800
C	3.00959300	2.71813700	-1.13849300
H	3.10291200	1.63527800	-1.07615500
H	3.96042100	3.24751500	-1.14143200
C	3.16870700	2.43989600	-3.31304900
H	2.28035100	1.82941500	-3.42565200
C	3.16632300	3.80995000	-3.64421300
O	2.19675100	4.61230800	-3.71608700
C	4.76562400	5.46236300	-4.50912400
H	4.04416400	6.22862600	-4.22296300
H	5.77429600	5.82158000	-4.28750800
H	4.68912100	5.29418500	-5.59683400
C	5.33625500	3.09359100	-4.06253800
H	5.41724600	2.97113100	-5.15674400
H	6.34518000	3.22335500	-3.65931000
N	4.49997400	4.25376600	-3.76096200
K	-0.20243600	3.89379200	-3.06708700
C	4.57421200	1.90455000	-3.43830300
H	4.66392900	1.00783700	-4.05832500
H	5.00446600	1.65477000	-2.45210200

Reaction of NMP K enolate with 4-fluorostyrene (**15**) **T.S.**, solvent = DMSO



Charge = 0; Multiplicity = 1

32

-1334.010353 [B3LYP/6-31+G(d,p)]

C	-1.96832500	1.40379500	0.05420000

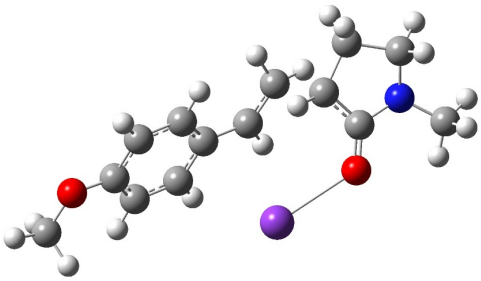
C	-1.79184200	2.72568800	0.44696700
C	-0.55896200	3.33433100	0.21156600
C	0.52228000	2.65021700	-0.41324700
C	0.26933100	1.30490700	-0.80744500
C	-0.95747400	0.68324400	-0.57062600
H	-2.60134200	3.26468900	0.92960400
H	-0.41547400	4.36483900	0.52899300
H	1.04651600	0.73696000	-1.30877700
H	-1.13127100	-0.34454600	-0.87479100
C	1.78909500	3.31711500	-0.62724500
H	1.81166500	4.38265000	-0.40050200
C	2.93291600	2.73039300	-1.15645200
H	3.05637500	1.65026300	-1.11398400
H	3.86859600	3.28027200	-1.09424900
C	3.18244500	2.53992000	-3.33774500
H	2.27903000	1.96524400	-3.50493200
C	3.24234100	3.90277400	-3.73534900
O	2.29940700	4.74135300	-3.84912300
C	4.94710100	5.48531300	-4.60119600
H	4.22224800	6.26770200	-4.36991300
H	5.94351000	5.82412800	-4.29940200
H	4.95590700	5.32866100	-5.69449400
C	5.40021000	3.07601900	-4.10539300
H	5.53727700	2.91242900	-5.18900900
H	6.39418100	3.18541800	-3.65795600
N	4.59119100	4.27841200	-3.88369200
K	-0.18905500	4.49319000	-3.04894100
C	4.56505500	1.93347700	-3.47085200
H	4.59938500	1.02951300	-4.08893200
H	4.98754200	1.65574800	-2.48884800
F	-3.18304500	0.79326200	0.28330400

-1333.660412 [M06-2X/6-31++G(d,p)]

C	-1.90698000	1.46171900	-0.00181700
C	-1.72633100	2.77090900	0.42005300
C	-0.49503300	3.37908200	0.19736900
C	0.57461400	2.70429000	-0.44003500
C	0.32252700	1.37804300	-0.86726000
C	-0.90355300	0.75441800	-0.64392400
H	-2.53614200	3.29742000	0.91480900
H	-0.34513300	4.40331500	0.53060600
H	1.09730600	0.82485900	-1.38946700
H	-1.08545300	-0.26389900	-0.97254700
C	1.84025500	3.37531500	-0.67099300
H	1.86621200	4.44496200	-0.47306800
C	2.96023100	2.75727900	-1.19026700
H	3.06778400	1.67577600	-1.11962400
H	3.90526700	3.29730700	-1.18665200
C	3.14179800	2.48641400	-3.34981800
H	2.23753000	1.90662600	-3.49364000
C	3.19276000	3.85875800	-3.67544700
O	2.25329300	4.69485100	-3.75625700
C	4.86574500	5.46505600	-4.48995100
H	4.16664400	6.25213100	-4.20496200
H	5.88188600	5.78315700	-4.24133100
H	4.80609400	5.31799800	-5.58157500
C	5.34261300	3.06948400	-4.06585800
H	5.43748200	2.95175900	-5.15938900
H	6.34855700	3.16260400	-3.64541900

N	4.54132900	4.25471900	-3.76878900
K	-0.16086600	4.02737700	-3.11216600
C	4.53027600	1.90444100	-3.46082700
H	4.59704200	1.00856300	-4.08469500
H	4.93756700	1.63492000	-2.46998900
F	-3.10850700	0.85772600	0.21447000

Reaction of NMP K enolate with 4-vinylanisole (**17**) **T.S.**, solvent = DMSO



Charge = 0; Multiplicity = 1

36

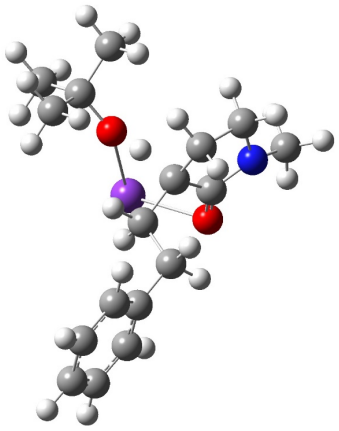
-1349.258902 [B3LYP/6-31+G(d,p)]

C	-1.63878000	0.91763000	0.27864600
C	-1.49655600	2.24583800	0.70029900
C	-0.31603900	2.94376300	0.42358000
C	0.77507000	2.36639200	-0.27708700
C	0.58276000	1.01982400	-0.70402800
C	-0.58499900	0.31614200	-0.42687700
H	-2.28832800	2.74932500	1.24386800
H	-0.22958900	3.97094700	0.77353000
H	1.36647500	0.51725900	-1.26322700
H	-0.69919900	-0.71120000	-0.76307000
C	1.98335000	3.12331100	-0.53526600
H	1.95060400	4.17926200	-0.26656900
C	3.12545700	2.63921700	-1.17285600
H	3.32740200	1.56913400	-1.16760000
H	4.02763500	3.24544400	-1.12529500
C	3.23037800	2.55807500	-3.32171000
H	2.35656400	1.93341800	-3.46998500
C	3.17781300	3.93291700	-3.69284900
O	2.17983200	4.71241200	-3.70653000
C	4.71469200	5.64406500	-4.62841800
H	3.96426400	6.37123800	-4.31375600
H	5.70915900	6.03126700	-4.38403400
H	4.65241100	5.52904800	-5.72495500
C	5.34521900	3.24992100	-4.25395000
H	5.41320300	3.12389400	-5.34890200
H	6.36040300	3.41110000	-3.87498600
N	4.48279700	4.39213900	-3.93869300
K	-0.21554600	4.13665300	-2.77517400
C	4.63054400	2.04118700	-3.59487600
H	4.66135600	1.16162100	-4.24700600
H	5.14860500	1.75678300	-2.66196300
O	-2.75499600	0.13450900	0.49657900
C	-3.84657900	0.71021700	1.20964000
H	-4.60873200	-0.06746900	1.27215400
H	-3.54963200	1.01021900	2.22213300
H	-4.25675800	1.57905500	0.68026500

-1348.891865 [M06-2X/6-31++G(d,p)]

C	-1.57824800	0.98282500	0.19783500
C	-1.42447200	2.29144700	0.66205600
C	-0.22950100	2.97399500	0.42852700
C	0.85548400	2.39875300	-0.26663600
C	0.65603100	1.07548000	-0.73679700
C	-0.52546000	0.38476400	-0.50351100
H	-2.21930000	2.79248000	1.20321200
H	-0.13128800	3.99144700	0.80166600
H	1.44121000	0.58126100	-1.30211000
H	-0.65524900	-0.62836600	-0.87357400
C	2.06678600	3.15405500	-0.52762000
H	2.03847600	4.21528600	-0.28744800
C	3.18493200	2.63500100	-1.15693600
H	3.37354900	1.56206700	-1.12801900
H	4.09262900	3.23638000	-1.17954700
C	3.20096800	2.46539200	-3.29106100
H	2.33912500	1.81430500	-3.38371600
C	3.10232600	3.84345600	-3.59017100
O	2.09180800	4.59318900	-3.55080900
C	4.53770900	5.60473100	-4.52528800
H	3.80433500	6.31948300	-4.15022200
H	5.54155200	6.00898500	-4.36969800
H	4.38097900	5.47372500	-5.60922900
C	5.25792800	3.25101500	-4.21981000
H	5.24929500	3.16376700	-5.32023700
H	6.29063500	3.42314400	-3.90122900
N	4.39444600	4.35635800	-3.81011500
K	-0.21285600	3.73427000	-2.75730800
C	4.61339600	2.00779100	-3.56906400
H	4.68569800	1.13557500	-4.22484500
H	5.14486000	1.75096000	-2.63546400
O	-2.70449500	0.22143600	0.36917500
C	-3.78024800	0.80607600	1.08107000
H	-4.56681300	0.05308500	1.11658900
H	-3.48212000	1.07041500	2.10213800
H	-4.15384600	1.70052400	0.56923100

Deprotonation of styrene/NMP monoadduct (20a) with KO*t*Bu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

47

-1468.388171 [B3LYP/6-31+G(d,p)]

C	-0.15365100	-0.19831400	0.58723000

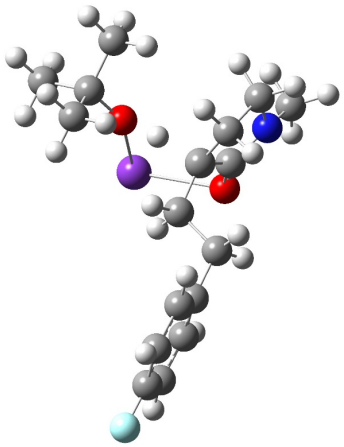
O	0.98968100	0.32223600	0.72570000
C	-0.77690400	1.26442000	-1.32392900
H	0.09823100	1.84750900	-1.03251700
H	-0.54601400	0.72489800	-2.25725600
H	-1.61086700	1.94590800	-1.52154700
C	-2.23420100	-0.57601900	-0.41797300
H	-3.18379400	-0.03711300	-0.50901500
H	-2.09226800	-1.16673100	-1.33864000
N	-1.11801300	0.35627800	-0.24723200
K	2.92378600	-1.41549000	-0.07285800
C	-2.14052700	-1.46885700	0.83365200
H	-2.75499100	-1.03799900	1.64056300
H	-2.53223900	-2.47444600	0.63741000
H	0.06753400	-2.38421100	0.33075600
O	0.85481700	-3.06699800	-0.30581000
C	0.44068900	-4.37741900	-0.65233800
C	1.65872800	-5.12064200	-1.23268700
H	2.46127600	-5.17406000	-0.48793400
H	1.40309700	-6.14388800	-1.53515300
H	2.04296900	-4.58990800	-2.11148200
C	-0.07150200	-5.13341000	0.59283900
H	-0.93814600	-4.62203200	1.02585400
H	-0.37060700	-6.15942900	0.34539800
H	0.71217200	-5.18016200	1.35755000
C	-0.67750600	-4.32154200	-1.71627100
H	-1.54945600	-3.78448500	-1.32673900
H	-0.32303100	-3.79317600	-2.60885900
H	-1.00278900	-5.32491600	-2.01835400
C	-0.64295200	-1.43943000	1.15952900
C	-0.19470200	-1.79204000	2.57237800
H	-0.51052100	-2.81723500	2.81006100
H	0.90255400	-1.79922600	2.61420800
C	-0.70817100	-0.84799800	3.69494900
H	-0.36613300	0.17062600	3.47580900
H	-1.80393500	-0.82906100	3.67955900
C	-0.23689000	-1.25674500	5.07229400
C	0.99177700	-0.80168700	5.58055200
C	-0.99355700	-2.13538000	5.86604100
C	1.45060700	-1.20975100	6.83694200
H	1.59182100	-0.11552500	4.98695000
C	-0.54028600	-2.54763100	7.12329400
H	-1.95123500	-2.49537100	5.49641100
C	0.68578700	-2.08629800	7.61437700
H	2.40195200	-0.84009500	7.21026500
H	-1.14617200	-3.22403900	7.72027900
H	1.03855800	-2.40181100	8.59215000

-1467.952775 [M06-2X/6-31++G(d,p)]

C	-0.17538100	-0.23224300	0.61535200
O	0.94103200	0.30892800	0.79343200
C	-0.78177800	1.22734100	-1.27707000
H	0.05032300	1.84630500	-0.93982400
H	-0.48294700	0.69691700	-2.19368400
H	-1.63689100	1.86744400	-1.51012100
C	-2.19652200	-0.67035900	-0.44975400
H	-3.15932000	-0.16882600	-0.58591700
H	-1.97756800	-1.25352800	-1.35966100
N	-1.13109700	0.30084500	-0.22430000
K	2.89165800	-1.47579100	0.32332700

C	-2.12316700	-1.55723500	0.80085300
H	-2.75383900	-1.12661200	1.59407000
H	-2.49642900	-2.56804600	0.59954200
H	0.10265000	-2.35479800	0.34152000
O	0.94198300	-3.03669300	-0.29972200
C	0.46365600	-4.31372300	-0.63175800
C	1.62304400	-5.13698300	-1.20326700
H	2.42129000	-5.22566600	-0.45794500
H	1.30156000	-6.14539200	-1.48900500
H	2.03339800	-4.63992900	-2.08925400
C	-0.09200100	-5.01594900	0.61741700
H	-0.93470600	-4.44726400	1.02743100
H	-0.43935400	-6.03017800	0.38891600
H	0.68478600	-5.07853200	1.38789200
C	-0.65051800	-4.20305500	-1.68394500
H	-1.48745400	-3.62091800	-1.28110400
H	-0.27256800	-3.68852900	-2.57450100
H	-1.02869800	-5.18729900	-1.98398000
C	-0.63786700	-1.50406100	1.14839300
C	-0.20674200	-1.83933300	2.56338000
H	-0.53644800	-2.85625200	2.81844200
H	0.89121300	-1.85769600	2.62159100
C	-0.72135000	-0.86556000	3.64357500
H	-0.37178200	0.14433600	3.39703500
H	-1.81687000	-0.84645400	3.62489500
C	-0.24772200	-1.25159100	5.02119600
C	0.98874200	-0.80607600	5.50460000
C	-1.00202500	-2.11595900	5.82356200
C	1.45779400	-1.20888200	6.75482000
H	1.58671200	-0.13353500	4.89296800
C	-0.53818100	-2.52314200	7.07442700
H	-1.96504200	-2.47037100	5.46230600
C	0.69536600	-2.07079000	7.54450200
H	2.41717800	-0.84814900	7.11397700
H	-1.14084900	-3.19065200	7.68330700
H	1.05770700	-2.38476000	8.51849000

Deprotonation of 4-fluorostyrene/NMP monoadduct (23a) with KO*t*Bu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

47

-1567.639323 [B3LYP/6-31+G(d,p)]

C	-0.16560700	-0.19912600	0.58863000

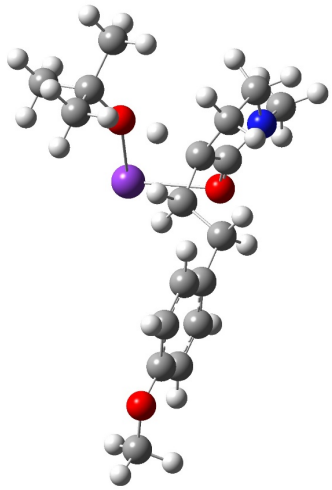
O	0.97295100	0.33045600	0.73156300
C	-0.79414200	1.25908100	-1.32429800
H	0.07498400	1.84942400	-1.02955600
H	-0.55546600	0.72208500	-2.25709400
H	-1.63320900	1.93353800	-1.52437200
C	-2.23972700	-0.59338300	-0.42365300
H	-3.19310300	-0.06171600	-0.51752000
H	-2.09041400	-1.18279400	-1.34394700
N	-1.13124500	0.34743700	-0.24929800
K	2.92356300	-1.39131400	-0.06634900
C	-2.14323200	-1.48573500	0.82815900
H	-2.76413000	-1.06006800	1.63290500
H	-2.52612900	-2.49438300	0.63030500
H	0.07351300	-2.38279700	0.33285000
O	0.86845100	-3.05880700	-0.30197800
C	0.46594700	-4.37192000	-0.65197600
C	1.69212600	-5.10517600	-1.22789100
H	2.49165400	-5.15400600	-0.47959100
H	1.44542500	-6.12974600	-1.53325900
H	2.07645700	-4.57010800	-2.10401500
C	-0.04593200	-5.13339800	0.59000300
H	-0.91857000	-4.62942400	1.01969000
H	-0.33583900	-6.16146100	0.34009700
H	0.73461600	-5.17485700	1.35821000
C	-0.64794300	-4.32328200	-1.72078800
H	-1.52568700	-3.79336400	-1.33452500
H	-0.29357000	-3.79121800	-2.61121500
H	-0.96424100	-5.32875000	-2.02544100
C	-0.64699800	-1.44438600	1.15909000
C	-0.20071700	-1.79288600	2.57343500
H	-0.50904000	-2.82047400	2.81078300
H	0.89644700	-1.79109600	2.61912400
C	-0.72600700	-0.85220300	3.69291100
H	-0.39094400	0.16893600	3.47571900
H	-1.82160100	-0.84049700	3.67312900
C	-0.25876200	-1.25627800	5.07317300
C	0.96371200	-0.79213700	5.58729000
C	-1.01245400	-2.14011700	5.86344000
C	1.42771800	-1.19060000	6.84491500
H	1.56395500	-0.10229200	4.99970900
C	-0.57065400	-2.55416300	7.12419300
H	-1.96522600	-2.50955100	5.49288100
C	0.64506100	-2.06701900	7.58441600
H	2.36910400	-0.82817500	7.24458300
H	-1.15507800	-3.23268100	7.73680000
F	1.08739900	-2.46194500	8.82107900

-1567.174993 [M06-2X/6-31++G(d,p)]

C	-0.19022500	-0.23251300	0.61341300
O	0.91981300	0.32105300	0.79301700
C	-0.80952800	1.21794600	-1.28185500
H	0.01556200	1.84591500	-0.94405000
H	-0.50402100	0.69001700	-2.19768700
H	-1.67109400	1.84877400	-1.51634400
C	-2.20502500	-0.69418000	-0.45406500
H	-3.17281000	-0.20282800	-0.59181600
H	-1.97899900	-1.27601200	-1.36300100
N	-1.15006400	0.28853300	-0.22877600
K	2.89140300	-1.43592900	0.30535100

C	-2.12379300	-1.57864500	0.79773500
H	-2.76052000	-1.15404400	1.58932500
H	-2.48557800	-2.59374700	0.59715700
H	0.11061200	-2.35227000	0.34380500
O	0.95825100	-3.02731800	-0.29546600
C	0.49114300	-4.30804300	-0.62923400
C	1.65849400	-5.12204000	-1.19782500
H	2.45558500	-5.20455400	-0.45057400
H	1.34572700	-6.13293600	-1.48446800
H	2.06713700	-4.62167200	-2.08274400
C	-0.06257200	-5.01505500	0.61814000
H	-0.91041200	-4.45273800	1.02634600
H	-0.40202100	-6.03160500	0.38808800
H	0.71265600	-5.07269300	1.39057800
C	-0.62097300	-4.20598400	-1.68451300
H	-1.46369100	-3.63075000	-1.28385000
H	-0.24474400	-3.68818600	-2.57390400
H	-0.99049700	-5.19309000	-1.98587600
C	-0.63963300	-1.50889000	1.14728400
C	-0.20677800	-1.83803100	2.56303800
H	-0.52525100	-2.85845400	2.81853100
H	0.89124100	-1.84369200	2.62251800
C	-0.73462200	-0.86915500	3.64071600
H	-0.39274400	0.14391300	3.39713000
H	-1.82998600	-0.85806400	3.61664800
C	-0.26690200	-1.25045300	5.02193500
C	0.96237900	-0.79504400	5.51377000
C	-1.01952700	-2.12013500	5.81975200
C	1.43377800	-1.18661700	6.76639000
H	1.56158300	-0.11879800	4.90880900
C	-0.57021500	-2.52750200	7.07546600
H	-1.97686000	-2.48440300	5.45541000
C	0.65191500	-2.04843500	7.51876600
H	2.38201900	-0.83295300	7.15663000
H	-1.15080500	-3.19665800	7.70128800
F	1.09801000	-2.43441100	8.74133100

Deprotonation of 4-vinylanisole/NMP monoadduct (24a) with KO*t*Bu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

51

-1582.890061 [B3LYP/6-31+G(d,p)]

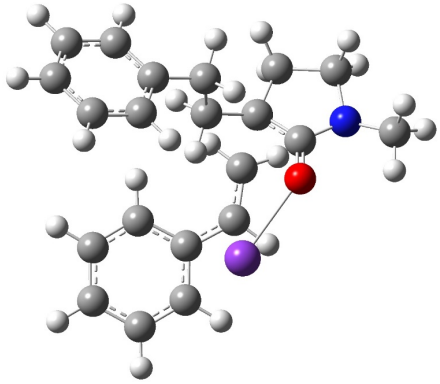
C	-0.16520400	-0.17980900	0.58033000
O	0.96043600	0.33504100	0.83648400
C	-0.56182700	1.26175500	-1.40576600
H	0.27416000	1.84983900	-1.02347900
H	-0.22446800	0.70816200	-2.29761000
H	-1.36621100	1.93992800	-1.70895900
C	-2.12388200	-0.55864800	-0.64445100
H	-3.05361800	-0.01608900	-0.84827800
H	-1.88343800	-1.16348600	-1.53498800
N	-1.02752100	0.37024800	-0.36223800
K	2.94930500	-1.45090600	0.34507300
C	-2.17669700	-1.43384300	0.62178500
H	-2.87217800	-0.98656500	1.34986900
H	-2.55348900	-2.43930900	0.39777000
H	0.06209300	-2.37144900	0.37057800
O	0.90203400	-3.06777300	-0.17673300
C	0.51786200	-4.38352500	-0.53815100
C	1.77014200	-5.11710100	-1.05458400
H	2.53654600	-5.15874400	-0.27197100
H	1.53912900	-6.14447300	-1.36279900
H	2.19141500	-4.58765300	-1.91706600
C	-0.04741500	-5.13891500	0.68408700
H	-0.94164600	-4.63581600	1.06780700
H	-0.32024600	-6.17055200	0.42955600
H	0.69689100	-5.16926100	1.48791300
C	-0.54715600	-4.34510800	-1.65597900
H	-1.44466100	-3.81925200	-1.31222600
H	-0.15671900	-3.81536300	-2.53252000
H	-0.84361900	-5.35394600	-1.96922400
C	-0.72386200	-1.41024200	1.11010200
C	-0.43319500	-1.74826700	2.56728200
H	-0.74265000	-2.78259400	2.77239300
H	0.65211200	-1.72237100	2.73414100
C	-1.09798900	-0.82130500	3.62161400
H	-0.78784800	0.21205400	3.42483100
H	-2.18699300	-0.85469100	3.49666000
C	-0.74676800	-1.19110200	5.04580200
C	0.31638900	-0.57772300	5.71960000
C	-1.45061100	-2.19683700	5.73449900
C	0.67882100	-0.93791800	7.02497600
H	0.88072400	0.20807700	5.22247500
C	-1.10765900	-2.57185700	7.03130000
H	-2.28723100	-2.69304900	5.24775200
C	-0.03675300	-1.94333300	7.68602700
H	1.50629800	-0.42899400	7.50508500
H	-1.66205700	-3.34631500	7.55322600
O	0.22622900	-2.37553900	8.96143400
C	1.30568900	-1.76881500	9.67406600
H	1.13552400	-0.69508200	9.81386000
H	1.33446700	-2.26130400	10.64627800
H	2.25968800	-1.92455300	9.15732500

-1582.407275 [M06-2X/6-31++G(d,p)]

C	-0.15500800	-0.10934200	0.49494900
O	0.95841300	0.36885000	0.81729800
C	-0.43855300	1.38888800	-1.44375600
H	0.37257600	1.96456700	-0.99620200
H	-0.05008900	0.84595000	-2.31865000
H	-1.22266800	2.07267600	-1.77992600

C	-2.05045100	-0.42951700	-0.81529000
H	-2.95797200	0.12693200	-1.06792000
H	-1.75552400	-1.02783600	-1.69366800
N	-0.96799700	0.47974900	-0.45280400
K	2.86572600	-1.47857000	0.47065000
C	-2.18292400	-1.31711800	0.42862100
H	-2.87609700	-0.84762400	1.14392100
H	-2.58645100	-2.30381200	0.17740700
H	0.02560400	-2.23804900	0.21266600
O	0.85649200	-2.93110700	-0.41421200
C	0.68740900	-4.31781700	-0.26471000
C	1.27152500	-5.02050200	-1.49550500
H	2.32982200	-4.75947200	-1.60716700
H	1.18966300	-6.11096200	-1.41666300
H	0.74105700	-4.69621900	-2.39736300
C	1.42422800	-4.80159400	0.99433900
H	1.03991500	-4.27449200	1.87538900
H	1.30173500	-5.87924600	1.15393400
H	2.49694500	-4.59137100	0.90609300
C	-0.80361500	-4.66900400	-0.14089800
H	-1.23114600	-4.21132300	0.75832100
H	-1.35096100	-4.28817400	-1.01101900
H	-0.95521200	-5.75265000	-0.08069200
C	-0.75024100	-1.35391400	0.95180600
C	-0.51082700	-1.72542000	2.40238300
H	-0.95089200	-2.71249300	2.60748400
H	0.56824600	-1.83497400	2.58570700
C	-1.06566100	-0.71301400	3.42450800
H	-0.58426400	0.25638100	3.24612500
H	-2.14000800	-0.57697000	3.25361800
C	-0.83634500	-1.14803000	4.84939200
C	0.35767600	-0.86206600	5.51221900
C	-1.79474600	-1.90648000	5.53702300
C	0.60495600	-1.30358900	6.81567200
H	1.12069900	-0.27523300	5.00496100
C	-1.57155800	-2.35542300	6.83195500
H	-2.73650100	-2.14458600	5.04731400
C	-0.36685300	-2.05543700	7.47903700
H	1.54517600	-1.05328400	7.29278000
H	-2.31951800	-2.93679300	7.36229200
O	-0.23435700	-2.53456700	8.74932800
C	0.97541200	-2.25420800	9.43536300
H	1.11750000	-1.17488700	9.55834500
H	0.88243400	-2.72233800	10.41422200
H	1.83557300	-2.67886100	8.90628200

Reaction of *N*-methyl-2-pyrrolidinone styrene monoadduct K enolate with styrene (3) T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

48

-1544.335018 [B3LYP/6-31+G(d,p)]

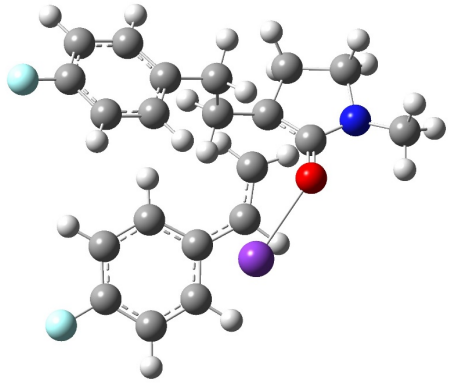
C	-2.10327300	2.05572800	0.60098100
C	-1.82277000	3.42784300	0.53945400
C	-0.57613200	3.88348800	0.11150000
C	0.46408200	2.99197500	-0.28453500
C	0.14825800	1.60326600	-0.21577600
C	-1.09594600	1.15446800	0.22012100
H	-3.07394300	1.69891600	0.93212900
H	-2.58127300	4.15085900	0.83139300
H	-0.38023500	4.95473000	0.09362600
H	0.89334500	0.87229900	-0.51473200
H	-1.28840900	0.08430500	0.25679300
C	1.74641000	3.51464000	-0.70027400
H	1.81755400	4.60232700	-0.73036700
C	2.87784800	2.78812900	-1.07063700
H	2.95551200	1.73536300	-0.80189500
H	3.83079600	3.31221600	-1.07267300
C	3.23641700	2.20430500	-3.15532000
C	3.14321200	3.50452200	-3.74228900
O	2.10086000	4.14730700	-4.05886800
C	4.67537200	5.25124900	-4.62269500
H	3.79639700	5.89775300	-4.60355900
H	5.53271600	5.80591800	-4.22683500
H	4.89445500	4.98774000	-5.67224300
C	5.43920200	3.02972000	-3.74871500
H	5.79607700	2.79057200	-4.76514500
H	6.30483700	3.36518700	-3.16663500
N	4.41892100	4.07867600	-3.81425300
K	-0.36075000	4.34043400	-3.20958100
C	4.70656000	1.82068300	-3.10962600
H	4.93044600	0.89649100	-3.65625800
H	5.05555100	1.65832400	-2.07551000
C	2.16697100	1.17019800	-3.38543200
H	2.28440800	0.34743800	-2.66577500
H	1.18314500	1.61093200	-3.18505800
C	2.14609300	0.55814900	-4.81616400
H	3.12667800	0.11559700	-5.02843000
H	1.99521300	1.36813600	-5.53880800
C	1.07045000	-0.49037200	-4.99297700
C	1.31419000	-1.83781000	-4.67767500
C	-0.21572200	-0.13826800	-5.43540800

C	0.30816200	-2.80177300	-4.79760100
H	2.30467700	-2.13499600	-4.34013700
C	-1.22610000	-1.09746200	-5.55776400
H	-0.42502800	0.89785600	-5.69212400
C	-0.96811800	-2.43487200	-5.23814900
H	0.52213300	-3.83850800	-4.55193600
H	-2.21182100	-0.80154600	-5.90672000
H	-1.75031600	-3.18232700	-5.33541000

-1543.876445 [M06-2X/6-31++G(d,p)]

C	-2.04834800	1.79846600	0.29288200
C	-1.87201100	3.18196100	0.23246600
C	-0.64044000	3.72538000	-0.12473000
C	0.47335000	2.91233300	-0.44749100
C	0.26803200	1.51209900	-0.37768400
C	-0.95958900	0.97344100	-0.01204700
H	-3.00724400	1.37201600	0.56891600
H	-2.69894600	3.84623200	0.46933700
H	-0.52164300	4.80773400	-0.14862000
H	1.08391600	0.83973900	-0.62656800
H	-1.07319000	-0.10685400	0.02859800
C	1.73489100	3.52653900	-0.82265200
H	1.72958400	4.61446700	-0.88186700
C	2.91348200	2.86544200	-1.10817600
H	3.04063400	1.82104000	-0.82110000
H	3.83776100	3.44054300	-1.13548800
C	3.32102000	2.20474500	-3.16002300
C	3.20543600	3.49907500	-3.71057900
O	2.15978200	4.12476700	-4.03022500
C	4.69200000	5.23372300	-4.61654300
H	3.83462100	5.90588700	-4.56439300
H	5.59065000	5.77863300	-4.31445700
H	4.82104800	4.90619700	-5.66221500
C	5.48545000	3.05941200	-3.72990300
H	5.76266300	2.81691100	-4.77032400
H	6.38940200	3.38557500	-3.20623000
N	4.47254100	4.11416300	-3.72876800
K	-0.29988400	4.03481600	-3.32629900
C	4.78679500	1.85626400	-3.05912100
H	5.05217700	0.91710300	-3.55814100
H	5.10897200	1.75714800	-2.00716700
C	2.24195800	1.18330200	-3.32561800
H	2.39298100	0.35512900	-2.61660000
H	1.27384100	1.63295700	-3.06248400
C	2.13477700	0.59232600	-4.74794200
H	3.08536000	0.11104200	-5.00784900
H	1.97969400	1.41605700	-5.45401800
C	1.00594000	-0.40056700	-4.85853500
C	1.20345200	-1.75288900	-4.55517800
C	-0.28392000	0.02175800	-5.20219600
C	0.14462500	-2.65990900	-4.59784900
H	2.19995400	-2.09699600	-4.28649500
C	-1.34684600	-0.88014400	-5.24693800
H	-0.45304100	1.06934900	-5.44355600
C	-1.13555300	-2.22611900	-4.94463700
H	0.31999400	-3.70595000	-4.36416800
H	-2.33863400	-0.53362400	-5.52230900
H	-1.96038300	-2.93091400	-4.98301000

Reaction of *N*-methyl-2-pyrrolidinone 4-fluorostyrene monoadduct K enolate with 4-fluorostyrene (**15**) **T.S.**, solvent = DMSO



Charge = 0; Multiplicity = 1

48

-1742.836430 [B3LYP/6-31+G(d,p)]

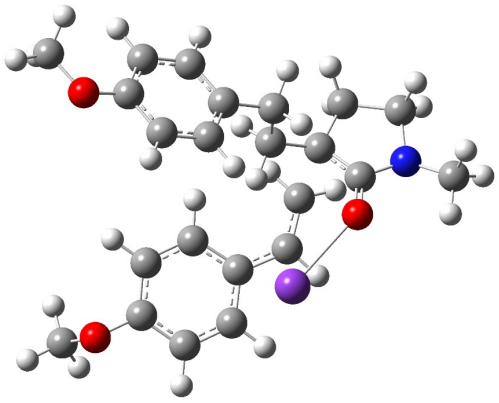
C	-2.05971600	2.06147300	0.59971000
C	-1.82437600	3.42960600	0.55911200
C	-0.57801200	3.88215300	0.12255500
C	0.45991300	2.99523300	-0.28737500
C	0.14852600	1.60538200	-0.22516900
C	-1.08917500	1.14117600	0.21688200
H	-2.59766700	4.12698400	0.86683100
H	-0.38819600	4.95360100	0.11180200
H	0.89012300	0.87616300	-0.53391400
H	-1.30438300	0.07745000	0.25620500
C	1.73983300	3.52215600	-0.70860400
H	1.80769400	4.60976000	-0.73884300
C	2.87257400	2.79694300	-1.07967900
H	2.95496800	1.74675500	-0.80094500
H	3.82370000	3.32464000	-1.08018900
C	3.23144800	2.20593800	-3.15089300
C	3.14221200	3.50278900	-3.74814600
O	2.10157300	4.14506600	-4.07026300
C	4.67983200	5.24493300	-4.62929400
H	3.80002900	5.89048700	-4.61768900
H	5.53363000	5.80107000	-4.22782900
H	4.90708500	4.97987800	-5.67659400
C	5.43807900	3.02508200	-3.74327800
H	5.80270900	2.78129000	-4.75572500
H	6.29922800	3.36374000	-3.15639500
N	4.41825500	4.07337800	-3.82122500
K	-0.35390300	4.39419700	-3.22815200
C	4.70110500	1.81912000	-3.10302700
H	4.92346500	0.89344900	-3.64768200
H	5.04800700	1.65767400	-2.06815700
C	2.16231000	1.17154800	-3.38329300
H	2.27769600	0.34988800	-2.66190800
H	1.17764600	1.61256300	-3.18752400
C	2.14684600	0.55719900	-4.81269500
H	3.12749400	0.11370300	-5.02153500
H	1.99906200	1.36515000	-5.53796800
C	1.07168600	-0.49150700	-4.99281300
C	1.31428000	-1.83874800	-4.67690900
C	-0.21324000	-0.13943400	-5.43801500

C	0.31485300	-2.80964200	-4.79595000
H	2.30181300	-2.13972100	-4.33672200
C	-1.22984100	-1.09128300	-5.56593300
H	-0.42560200	0.89497000	-5.69567500
C	-0.93842700	-2.40857200	-5.23856300
H	0.50262600	-3.85112400	-4.55670900
H	-2.22110600	-0.82104900	-5.91461800
F	-1.92574200	-3.35184500	-5.36288200
F	-3.28978500	1.60189200	1.02461300

-1742.318224 [M06-2X/6-31++G(d,p)]

C	-2.02181800	1.79736600	0.28205400
C	-1.89403400	3.17521100	0.23690900
C	-0.66326600	3.71891800	-0.12615900
C	0.45305400	2.91395400	-0.45740000
C	0.25750200	1.51235900	-0.39152100
C	-0.96112700	0.95500900	-0.02199500
H	-2.74000700	3.80770600	0.48614100
H	-0.55478900	4.80155900	-0.14406400
H	1.07422800	0.84437500	-0.64631800
H	-1.09714800	-0.12101600	0.02230000
C	1.71116000	3.53633800	-0.83535700
H	1.69762700	4.62367400	-0.89892800
C	2.89573600	2.88113500	-1.11372000
H	3.03035600	1.84164300	-0.81109900
H	3.81585000	3.46346100	-1.13522100
C	3.31685400	2.21116200	-3.14457100
C	3.20932200	3.50011700	-3.71260300
O	2.16743000	4.12399100	-4.04587500
C	4.70681800	5.22482300	-4.62046400
H	3.84856700	5.89676400	-4.58203200
H	5.60175900	5.77181700	-4.31127800
H	4.84803700	4.89086600	-5.66238100
C	5.48832800	3.05432600	-3.71036300
H	5.77495300	2.80137500	-4.74562600
H	6.38775900	3.38439300	-3.18144400
N	4.47719000	4.11045800	-3.72884400
K	-0.29492500	4.06536900	-3.35273400
C	4.78151300	1.85922800	-3.03351200
H	5.04657900	0.91504200	-3.52297100
H	5.09728200	1.76826800	-1.97897400
C	2.23879500	1.18987200	-3.31893400
H	2.37869600	0.36612000	-2.60247300
H	1.26776900	1.64342200	-3.07331000
C	2.15045800	0.58938900	-4.73804700
H	3.10268000	0.10368500	-4.98232600
H	2.00747000	1.40771700	-5.45267700
C	1.02060600	-0.40164400	-4.85817800
C	1.21254500	-1.75462700	-4.55527400
C	-0.26608000	0.02461300	-5.20829800
C	0.15802400	-2.66605700	-4.60195700
H	2.20445300	-2.10500800	-4.28074700
C	-1.33718200	-0.86637000	-5.26249700
H	-0.43434000	1.07173200	-5.44910500
C	-1.09637100	-2.19621100	-4.95595500
H	0.29965900	-3.71704100	-4.37408200
H	-2.33573700	-0.54567200	-5.53924800
F	-2.13039600	-3.07349200	-5.00899400
F	-3.22071100	1.25143300	0.62908200

Reaction of *N*-methyl-2-pyrrolidinone 4-vinylanisole monoadduct K enolate with 4-vinylanisole (17) T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

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-1773.335192 [B3LYP/6-31+G(d,p)]

C	-2.08467100	2.03675400	0.54240100
C	-1.78831900	3.40277700	0.55138500
C	-0.53274700	3.85268300	0.14063200
C	0.49159000	2.96431600	-0.29707600
C	0.14730600	1.58087400	-0.29706100
C	-1.10432200	1.13035900	0.11490100
H	-2.54627000	4.11036100	0.87779100
H	-0.32249400	4.92059700	0.17077500
H	0.87347500	0.84986300	-0.63873100
H	-1.33362000	0.06771900	0.09170300
C	1.78526000	3.48106100	-0.68842600
H	1.87636100	4.56751100	-0.67072600
C	2.90411500	2.74840300	-1.08788100
H	2.95980500	1.68487300	-0.85688100
H	3.86764600	3.25256200	-1.05665600
C	3.26089300	2.24935400	-3.17783600
C	3.21069600	3.57396200	-3.71646500
O	2.18967600	4.25866100	-4.01333900
C	4.79969900	5.31010100	-4.51384800
H	3.93946500	5.98048500	-4.47441500
H	5.66902800	5.82240500	-4.08817700
H	5.02051000	5.08457600	-5.57179700
C	5.49235300	3.03336000	-3.72553200
H	5.85369000	2.82591300	-4.74731600
H	6.36061800	3.32076200	-3.12196000
N	4.50246900	4.11236200	-3.75792900
K	-0.28295700	4.41488200	-3.18302700
C	4.71962400	1.82077800	-3.14294500
H	4.91800900	0.91483300	-3.72868800
H	5.05765600	1.60344100	-2.11529600
C	2.16972100	1.25327100	-3.47208400
H	2.26467200	0.39060600	-2.79689300
H	1.19323500	1.70207400	-3.25361100
C	2.14881100	0.72151700	-4.93315500
H	3.12361000	0.27419100	-5.16206900
H	2.02288900	1.57416500	-5.61054500
C	1.05647300	-0.29455700	-5.18610900
C	1.26716700	-1.66306800	-4.97662900
C	-0.22677600	0.10382700	-5.60372200

C	0.25259700	-2.61052800	-5.16964700
H	2.24826300	-2.01012000	-4.66008500
C	-1.25008900	-0.82011800	-5.80233100
H	-0.42690000	1.15767200	-5.78376800
C	-1.01581700	-2.18689800	-5.58510600
H	0.46656000	-3.65920300	-5.00038300
H	-2.23459600	-0.50059000	-6.13115400
O	-2.08009000	-3.02271600	-5.80974700
O	-3.35992300	1.59921600	0.89360100
C	-1.89401500	-4.42576800	-5.61436500
H	-1.62126800	-4.64924500	-4.57661600
H	-2.85383000	-4.88818000	-5.84552700
H	-1.12609100	-4.82165400	-6.28886500
C	-3.45633900	1.03798900	2.20992400
H	-4.49468800	0.72720300	2.34390000
H	-2.79931000	0.16672500	2.31838300
H	-3.19587000	1.78440700	2.97095600

-1772.782905 [M06-2X/6-31++G(d,p)]

C	-1.91601300	1.92178900	0.40745000
C	-1.71380400	3.30493100	0.37932900
C	-0.48610500	3.82849300	-0.00377600
C	0.60368400	3.00806700	-0.38906600
C	0.36293000	1.61801900	-0.34864800
C	-0.86193400	1.07879900	0.04520000
H	-2.53103800	3.95999500	0.66766100
H	-0.35314400	4.90929300	0.00388700
H	1.15034600	0.93072500	-0.64388800
H	-0.98000900	0.00082700	0.05374600
C	1.86745700	3.60778800	-0.78851800
H	1.88260100	4.69682800	-0.82144700
C	3.02532000	2.92672100	-1.12939200
H	3.14007600	1.88015700	-0.83996500
H	3.96157500	3.48441700	-1.14761100
C	3.35888400	2.30693500	-3.14957900
C	3.28559300	3.60610700	-3.70880100
O	2.25895400	4.27118100	-4.00305800
C	4.81950700	5.29085000	-4.63254600
H	3.99159200	5.99610000	-4.54984700
H	5.74586100	5.79283100	-4.33998800
H	4.91296300	4.97758000	-5.68601700
C	5.54487400	3.07343900	-3.78449000
H	5.79524700	2.82629400	-4.83031300
H	6.46920300	3.36375800	-3.27540900
N	4.57301200	4.16501000	-3.76047200
K	-0.17359200	4.26002600	-3.20080200
C	4.81293900	1.89566000	-3.10353600
H	5.01943600	0.95140100	-3.62005100
H	5.16357900	1.77095700	-2.06368400
C	2.24589700	1.32335100	-3.33681200
H	2.37946500	0.47099300	-2.65323000
H	1.29466000	1.79371300	-3.04917500
C	2.10691600	0.77791900	-4.77326000
H	3.04062300	0.27827400	-5.05886000
H	1.97103200	1.62757200	-5.45275700
C	0.94867000	-0.17834700	-4.90711100
C	1.10413900	-1.54786600	-4.69468800
C	-0.34316700	0.29378000	-5.18278100
C	0.02353700	-2.43370500	-4.75583300

H	2.09382100	-1.94476100	-4.47862800
C	-1.43100000	-0.56649600	-5.24859900
H	-0.49606700	1.35696100	-5.35656600
C	-1.25182800	-1.93882700	-5.03475300
H	0.19306400	-3.49097900	-4.58996500
H	-2.42785800	-0.19726100	-5.46947800
O	-2.37365500	-2.70945200	-5.12384700
O	-3.16064100	1.49379200	0.79240800
C	-2.22662000	-4.10633100	-4.92512000
H	-1.84725700	-4.32245300	-3.92039100
H	-3.22131200	-4.53463300	-5.03916100
H	-1.55283300	-4.54080800	-5.67160900
C	-3.37472400	0.09534600	0.85485100
H	-4.40137700	-0.04059400	1.19307900
H	-3.25081800	-0.36961800	-0.13002700
H	-2.68972200	-0.37774200	1.56787800

10.4. REACTION PROFILES FOR SARCOSINE ANHYDRIDE (21) WITH VARIOUS STYRENES

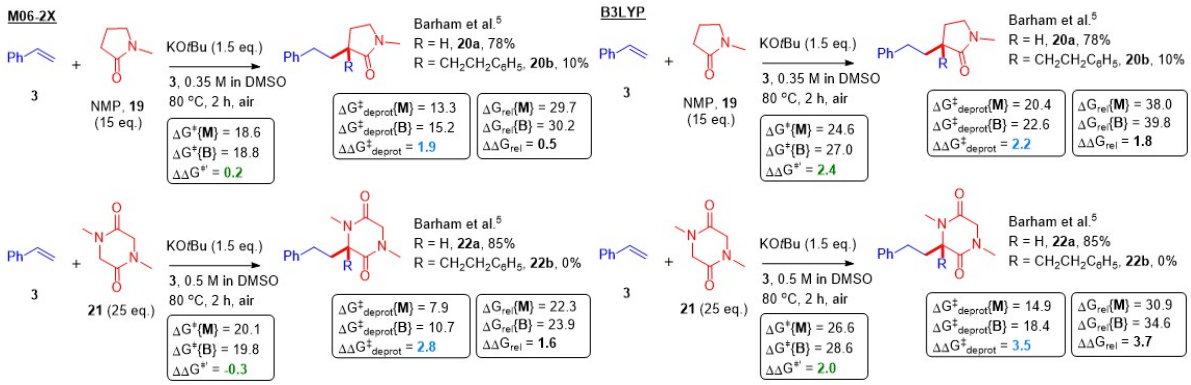
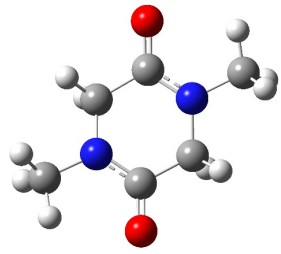


Figure S68. Application of the computational model to cyclic amide CAKES. Comparison of B3LYP/6-31+G(d,p) and M06-2X/6-31++(d,p) methods.

10.4.1. XYZ Co-ordinates of starting materials, intermediates, products

Sarcosine anhydride (**21**), solvent = DMSO



Charge = 0; Multiplicity = 1

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-494.552676 [B3LYP/6-31+G(d,p)]

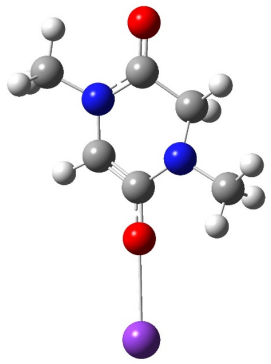
N	1.32927500	-0.46077700	0.04190800
C	2.66218800	-1.04439400	0.18221000
H	3.36453900	-0.25865300	0.45335400
H	2.64523700	-1.81022800	0.96284300
H	2.98012600	-1.50513600	-0.76022100
C	1.16659100	0.87773300	-0.03146000
O	2.09401100	1.69549000	0.05843400
C	0.24619900	-1.39796400	-0.24232200

H	0.35736200	-2.26746500	0.41064800
H	0.31661000	-1.76232200	-1.27760400
C	-1.16657200	-0.87769500	-0.03148300
O	-2.09404200	-1.69540400	0.05837200
C	-2.66220600	1.04429300	0.18223000
H	-3.36419700	0.25884100	0.45518600
H	-2.98099200	1.50343600	-0.76069400
H	-2.64489800	1.81135400	0.96164100
N	-1.32924300	0.46080700	0.04196600
C	-0.24617600	1.39795100	-0.24240300
H	-0.35737600	2.26757200	0.41039300
H	-0.31653900	1.76216200	-1.27775200

-494.333040 [M06-2X/6-31++G(d,p)]

N	-1.31270900	-0.46204400	-0.05720900
C	-2.63876300	-1.04181300	-0.21632800
H	-3.31911900	-0.26929800	-0.56863700
H	-2.59135000	-1.85346100	-0.94572800
H	-3.00121700	-1.43799500	0.73820100
C	-1.16152900	0.87277700	0.03827900
O	-2.08586500	1.68018400	-0.06127900
C	-0.24400400	-1.38577600	0.28593600
H	-0.35435700	-2.28862500	-0.31898700
H	-0.31193300	-1.68649300	1.34094700
C	1.16153300	-0.87278300	0.03791700
O	2.08586200	-1.68016100	-0.06194500
C	2.63873900	1.04186600	-0.21635300
H	3.31902900	0.26947600	-0.56905900
H	3.00134600	1.43767800	0.73827100
H	2.59123100	1.85379300	-0.94543600
N	1.31269600	0.46206300	-0.05726200
C	0.24403600	1.38569600	0.28629600
H	0.35432100	2.28872900	-0.31836200
H	0.31209200	1.68608600	1.34139200

Sarcosine anhydride K enolate, solvent = DMSO



Charge = 0; Multiplicity = 1

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-1093.918457 [B3LYP/6-31+G(d,p)]

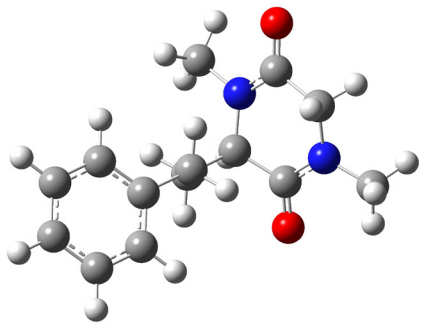
C	-0.35809000	-0.13464900	0.00981600
O	-1.63861100	-0.27284000	0.00652200
C	-0.71015300	2.29393800	-0.21051000
H	-0.96798300	2.57615700	0.82577700
H	-0.23274200	3.15431100	-0.68986200
H	-1.63342300	2.05758900	-0.73848400

K	-4.16145200	-0.54336300	0.00449600
C	0.56164400	-1.14276700	0.23209900
H	0.26495400	-2.16785700	0.40052200
N	0.19492800	1.15393800	-0.26610200
C	2.49572700	0.31605100	0.07718600
O	3.70913500	0.58442500	-0.10349400
C	1.47884000	1.40508100	0.38152200
H	1.36790500	1.48125900	1.48553800
H	1.88837900	2.35259800	0.02518400
N	1.96930200	-0.92094100	0.05314800
C	2.80348400	-2.08732800	-0.20864900
H	2.54513500	-2.53359500	-1.17609100
H	3.84947000	-1.78467100	-0.21367300
H	2.64338100	-2.83750600	0.57334600

-1093.679043 [M06-2X/6-31++G(d,p)]

C	-0.33810300	-0.27478400	-0.00475800
O	-1.60000400	-0.50429600	0.00349300
C	-0.90065500	2.09133900	-0.23327300
H	-1.23007300	2.28629500	0.80099700
H	-0.48234500	3.01446400	-0.64299300
H	-1.76992700	1.80292500	-0.82280000
K	-4.08647300	-0.47629000	0.01597300
C	0.65680700	-1.19486400	0.22866500
H	0.45154700	-2.23330000	0.44427200
N	0.10870800	1.04871800	-0.29907500
C	2.44939800	0.42496300	0.09707400
O	3.62572200	0.79897700	-0.07455600
C	1.33440000	1.40998800	0.39476200
H	1.18213100	1.44341600	1.49357500
H	1.66769400	2.39651700	0.06723200
N	2.03666400	-0.84811900	0.05618000
C	2.96589100	-1.92650600	-0.22915800
H	2.74020600	-2.37284100	-1.20336300
H	3.97988000	-1.53041700	-0.23084000
H	2.87411100	-2.70000400	0.53933500

Sarcosine anhydride/styrene monoadduct (22a), solvent = DMSO



Charge = 0; Multiplicity = 1

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-804.127765 [B3LYP/6-31+G(d,p)]

C	-1.88475000	-1.20736400	0.74092400
O	-1.70667200	-2.21449900	1.44244000
N	-2.58752300	-1.21608000	-0.41252500
C	0.27307200	0.06214000	1.14141700

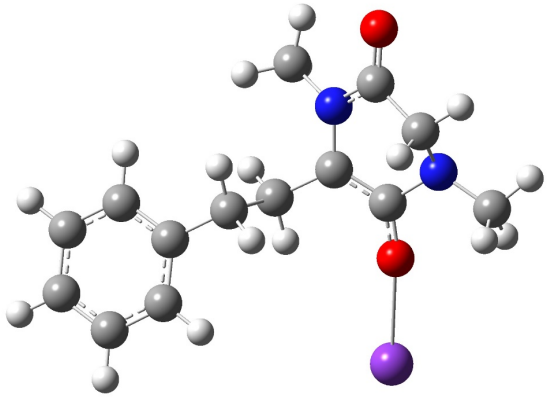
H	0.66762800	0.96012400	1.62914000
H	0.59573100	-0.79156700	1.74567900
C	0.85333100	-0.05001000	-0.28225300
H	0.50530500	0.79554000	-0.88635200
H	0.47947700	-0.96407000	-0.75909600
C	2.36853900	-0.07156800	-0.28392600
C	3.10554100	1.11756500	-0.39826800
C	3.06991300	-1.27985300	-0.14535600
C	4.50368500	1.10230800	-0.37182000
H	2.58044500	2.06279400	-0.51432100
C	4.46769400	-1.30064600	-0.11896200
H	2.51696600	-2.21269600	-0.06240100
C	5.19023600	-0.10809000	-0.23137900
H	5.05497700	2.03377000	-0.46612800
H	4.99106600	-2.24707500	-0.01506700
H	6.27618500	-0.12255900	-0.21459200
N	-1.83208500	1.30936600	0.56228700
C	-2.42591100	1.29268500	-0.64971300
O	-2.77000500	2.31830100	-1.25624600
C	-2.69023600	-0.05681300	-1.29137000
H	-3.70686700	-0.01178900	-1.69271300
H	-2.01380800	-0.16465000	-2.15083400
C	-3.15987500	-2.45827300	-0.92983600
H	-3.05283300	-3.23662200	-0.17719000
H	-4.21937900	-2.30770200	-1.15799900
H	-2.64026000	-2.76289300	-1.84518900
C	-1.58742200	2.59945400	1.21312100
H	-2.40298800	3.28079100	0.97195600
H	-1.54549800	2.44796200	2.29350000
H	-0.64596500	3.04757700	0.87767100
C	-1.27423700	0.11411800	1.21022300
H	-1.54699700	0.17572900	2.26922700

-803.771789 [M06-2X/6-31++G(d,p)]

C	-1.87832500	-1.18951400	0.76505400
O	-1.70964600	-2.19160900	1.46199200
N	-2.53835900	-1.20252500	-0.40886800
C	0.23652300	0.08061500	1.18247600
H	0.64280200	0.97821200	1.66267400
H	0.56922200	-0.77953700	1.77251900
C	0.77014200	-0.02458200	-0.25177700
H	0.42215400	0.83493600	-0.83832900
H	0.37206700	-0.93099400	-0.72707600
C	2.27879700	-0.06656200	-0.27518200
C	3.02454800	1.11369500	-0.36035600
C	2.95827200	-1.28399900	-0.16242200
C	4.41873000	1.07954300	-0.33592600
H	2.50711100	2.06644700	-0.45066900
C	4.35198500	-1.32327700	-0.13827300
H	2.38888900	-2.20863600	-0.09692300
C	5.08665700	-0.14020900	-0.22507900
H	4.98258600	2.00483500	-0.40710200
H	4.86364200	-2.27734500	-0.05407600
H	6.17168300	-0.16893200	-0.20932600
N	-1.83740800	1.30911200	0.57313000
C	-2.31833900	1.28206200	-0.68355400
O	-2.57857100	2.29834500	-1.32943100
C	-2.55243800	-0.07190100	-1.31959000
H	-3.53203300	-0.01989400	-1.80264400
H	-1.80411200	-0.20475500	-2.11361700

C	-3.03516600	-2.45983900	-0.95112300
H	-3.12732400	-3.18167200	-0.14255200
H	-4.01159100	-2.29051800	-1.41004900
H	-2.34548800	-2.84812200	-1.70852200
C	-1.55714000	2.60790200	1.17557600
H	-2.36913400	3.29427000	0.93791400
H	-1.48516600	2.48362100	2.25705200
H	-0.61855600	3.02674800	0.79566600
C	-1.29982400	0.13301200	1.25057900
H	-1.59717000	0.19966100	2.30232100

Styrene/sarcosine anhydride monoadduct K enolate, solvent = DMSO



Charge = 0; Multiplicity = 1

36

-1403.490820 [B3LYP/6-31+G(d,p)]

C	-1.02299900	-0.48206700	-0.40281700
C	-1.86936400	0.58988200	-0.16364200
O	-1.53960200	1.83635300	-0.20980800
N	-3.22886200	0.26047900	0.15219700
K	-0.48880000	4.12489900	-0.52744800
C	0.45982200	-0.32065900	-0.56295200
H	0.85044800	-0.86753400	-1.43363500
H	0.64967200	0.73886700	-0.75921300
C	1.29971300	-0.74626300	0.68167800
H	1.08855900	-1.79794100	0.91107600
H	0.95893600	-0.15827700	1.54171600
C	2.78690300	-0.55731100	0.48606200
C	3.41878900	0.63956600	0.86369000
C	3.57052600	-1.55352800	-0.12123400
C	4.78566100	0.83707800	0.64335300
H	2.83364900	1.42241200	1.34120400
C	4.93739000	-1.36141400	-0.34626300
H	3.10587300	-2.49218600	-0.41445700
C	5.55144100	-0.16360600	0.03538600
H	5.25256800	1.76922500	0.95007400
H	5.52299900	-2.14840200	-0.81389100
H	6.61387900	-0.01393700	-0.13433100
N	-1.56787100	-1.82545600	-0.41075700
C	-2.72012800	-2.12948200	0.22236500
O	-3.26539000	-3.25897900	0.21328200
C	-3.34517000	-0.95330100	0.95158500
H	-4.39838700	-1.18836400	1.11827900
H	-2.86123700	-0.84020000	1.94550000
C	-4.07819800	1.34729000	0.62078100
H	-3.81687500	1.68164100	1.64027200

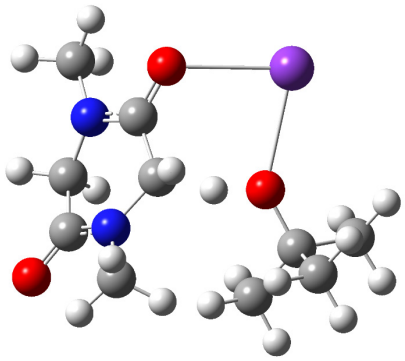
H	-3.98937800	2.20302200	-0.04798100
H	-5.11836600	1.00670500	0.62806700
C	-0.94410400	-2.82883400	-1.27299900
H	-0.88328100	-2.45314300	-2.30005000
H	0.06628900	-3.07193600	-0.93091300
H	-1.55277000	-3.73129000	-1.24802700

-1403.114783 [M06-2X/6-31++G(d,p)]

C	1.00197000	-0.46383300	0.45264700
C	1.91124000	0.55377100	0.26527500
O	1.66610400	1.81175300	0.35158600
N	3.24616900	0.14697700	-0.05744200
K	0.61588100	4.07965100	0.38418600
C	-0.46875000	-0.23030000	0.58376100
H	-0.90638100	-0.76995100	1.43737900
H	-0.61885400	0.83591000	0.78180600
C	-1.26813900	-0.61747800	-0.68428600
H	-1.03600400	-1.65708600	-0.94827600
H	-0.92437700	0.00997000	-1.51472000
C	-2.75341300	-0.45727400	-0.48862600
C	-3.39314500	0.74963700	-0.79481800
C	-3.51647600	-1.49054000	0.06884000
C	-4.75700400	0.91968700	-0.55592000
H	-2.81475300	1.56250900	-1.22906000
C	-4.88004800	-1.32642600	0.31137700
H	-3.03501800	-2.43623700	0.30969800
C	-5.50571000	-0.11882000	-0.00115700
H	-5.23603900	1.86213000	-0.80488600
H	-5.45438600	-2.14201900	0.74103300
H	-6.56764400	0.01102300	0.18333800
N	1.44980900	-1.83515200	0.39218800
C	2.56748000	-2.18471600	-0.26622600
O	3.02253100	-3.34109000	-0.32886600
C	3.26876700	-1.01587100	-0.92876000
H	4.30014000	-1.31712900	-1.12310100
H	2.77896500	-0.80668700	-1.90173800
C	4.13252200	1.20304700	-0.51628800
H	3.84234300	1.58908600	-1.50764400
H	4.11854900	2.03214900	0.18947700
H	5.14862100	0.80470900	-0.58256400
C	0.75618600	-2.82344900	1.20519700
H	0.68871500	-2.46673100	2.23746800
H	-0.25691700	-3.00226400	0.83059100
H	1.31749300	-3.75544300	1.17057900

10.4.2. XYZ Co-ordinates of transition states

Deprotonation of sarcosine anhydride (21) by KOtBu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

35

-1327.502808 [B3LYP/6-31+G(d,p)]

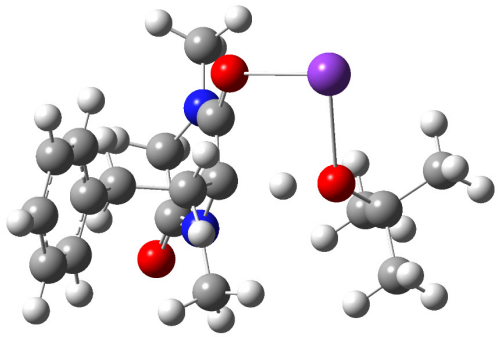
C	-1.81758800	0.93448900	0.37630700
O	-1.47440000	2.14225300	0.49031900
K	1.12176000	2.61432300	-0.20892100
H	0.10310800	-0.21427200	0.44112000
O	1.16791600	-0.04766500	-0.20235300
C	2.09838800	-1.11384300	-0.20612800
C	3.25210300	-0.74261500	-1.15786300
H	3.73246600	0.18538900	-0.82634900
H	4.01612800	-1.52929500	-1.19518000
H	2.87093800	-0.58594200	-2.17353200
C	2.66663200	-1.33602500	1.21397200
H	1.86480000	-1.59315100	1.91489700
H	3.40784700	-2.14485600	1.23460700
H	3.14913300	-0.41966100	1.57349100
C	1.42852900	-2.41361300	-0.70448000
H	0.59821500	-2.69793400	-0.04869300
H	1.02753000	-2.26760900	-1.71408200
H	2.13784500	-3.24998600	-0.73537000
C	-1.11901700	-0.12170800	1.10555900
H	-0.86359600	0.22782900	2.10791200
C	-2.69411100	-1.82502600	0.27826400
C	-2.97427000	-0.84750700	-0.85346200
H	-2.33000100	-1.11441000	-1.70916200
H	-4.00778300	-1.01136500	-1.16828500
O	-3.24325500	-2.94929800	0.26568000
N	-1.83710900	-1.39796700	1.21679400
N	-2.80781600	0.55777200	-0.49387900
C	-3.38687100	1.52188400	-1.42163400
H	-3.27150100	2.52404700	-1.01205900
H	-2.89173300	1.47979700	-2.40235000
H	-4.44985900	1.30254900	-1.55956000
C	-1.47443400	-2.25471700	2.33905900
H	-0.41204800	-2.51751900	2.29153200
H	-1.65943200	-1.72820800	3.28162400
H	-2.07277300	-3.16349800	2.30240400

-1327.144139 [M06-2X/6-31++G(d,p)]

C	-1.01907300	0.79029100	0.62007000
O	-0.49743300	1.92016400	0.74255900
K	2.15795400	1.91303100	1.21469100

H	0.65137500	-0.56604300	1.11589300
O	1.89711600	-0.67209400	0.78155000
C	2.04214000	-1.31841800	-0.45541500
C	1.46559100	-0.44318800	-1.58312000
H	2.00193900	0.51215900	-1.63111400
H	1.54671100	-0.92874400	-2.56256200
H	0.40736800	-0.22698600	-1.39421400
C	3.53271500	-1.55758300	-0.72145000
H	3.95588800	-2.19157400	0.06522800
H	3.69958600	-2.04575000	-1.68891800
H	4.06903300	-0.60206600	-0.71831100
C	1.31032300	-2.67084000	-0.44166800
H	1.71069500	-3.30080400	0.36057700
H	0.23941300	-2.52569900	-0.25513000
H	1.42296000	-3.20404000	-1.39264600
C	-2.25010700	-1.82238700	0.45705600
C	-2.36349400	-0.81676600	-0.67199800
H	-1.80630400	-1.23023800	-1.52921500
H	-3.41760500	-0.78419100	-0.96407900
O	-2.86283600	-2.89739400	0.34970400
N	-1.46089900	-1.49500700	1.48347800
N	-1.91120000	0.52956800	-0.37246100
C	-2.17011800	1.51126600	-1.41184700
H	-1.86864400	2.49353200	-1.05460300
H	-1.60669800	1.26729900	-2.32213800
H	-3.23695600	1.51490700	-1.65099000
C	-1.19249800	-2.46038900	2.53549500
H	-0.16612700	-2.83392500	2.44168200
H	-1.30338100	-1.97654200	3.50987900
H	-1.89391800	-3.28776400	2.45089100
C	-0.61132800	-0.30726600	1.49962600
H	-0.54639800	0.06924300	2.52468800

Deprotonation of sarcosine anhydride/styrene monoadduct by KOtBu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

51

-1637.072264 [B3LYP/6-31+G(d,p)]

C	-1.41055000	0.73515400	0.33874300
O	-0.98119600	1.91689400	0.24009000
K	1.64512300	2.51225400	0.21273500
H	0.50368300	-0.29752900	0.78236700
O	1.66934700	-0.15332400	0.41376600
C	2.25299400	-1.14156500	-0.42020800
C	3.23562000	-0.44026000	-1.38032100
H	3.99626600	0.10745700	-0.81147900
H	3.74910300	-1.15757200	-2.03268100
H	2.70108800	0.27441000	-2.01747800

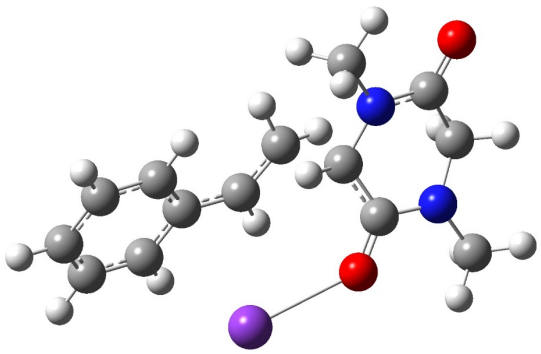
C	3.03112400	-2.16478400	0.43538600
H	2.35759200	-2.67335300	1.13352600
H	3.51834700	-2.92824300	-0.18423300
H	3.80419600	-1.65397800	1.02102200
C	1.17528400	-1.87316900	-1.24887700
H	0.46715300	-2.39406500	-0.59631500
H	0.61203600	-1.15693400	-1.85787900
H	1.62559400	-2.61348200	-1.92074700
C	-0.82059900	-0.19934100	1.29989800
C	-2.56402900	-1.89078600	0.69777600
C	-3.22463200	-0.83808200	-0.17249400
H	-3.56099300	-1.34766400	-1.08045100
H	-4.13181200	-0.48234100	0.34513400
O	-3.08893200	-3.02324400	0.77490800
N	-1.43403900	-1.54214700	1.33272800
N	-2.35932200	0.27424500	-0.54311200
C	-2.89707100	1.16912600	-1.56166200
H	-2.11789000	1.85396900	-1.89268400
H	-3.24547500	0.57416900	-2.41096000
H	-3.74271900	1.75867500	-1.17918400
C	-0.74928400	-2.56484800	2.12573200
H	-1.13497600	-2.60212100	3.15136400
H	-0.89880500	-3.54318700	1.66778200
H	0.31471800	-2.33103400	2.15724600
C	-0.66001600	0.38903500	2.70857200
H	-0.00003600	-0.25041400	3.30726300
H	-0.14651100	1.35050700	2.61489600
C	-1.98537700	0.60525200	3.48504900
H	-2.62061900	1.29036100	2.91059000
H	-2.52215200	-0.34859600	3.55095200
C	-1.77052000	1.16005200	4.87577300
C	-1.71757200	2.54603900	5.09930500
C	-1.58144500	0.30548300	5.97474200
C	-1.48286800	3.06314600	6.37714600
H	-1.86768000	3.22632600	4.26390300
C	-1.34509000	0.81655800	7.25491500
H	-1.62562700	-0.77111400	5.82632500
C	-1.29460500	2.19922200	7.46142500
H	-1.45173800	4.13906000	6.52641600
H	-1.20617600	0.13571500	8.09037400
H	-1.11559000	2.59863900	8.45558600

-1636.578405 [M06-2X/6-31++G(d,p)]

C	-0.95758400	0.73468600	0.44412200
O	-0.32475300	1.81266100	0.40597200
K	2.28151300	1.90851500	1.01623500
H	0.66131700	-0.56532100	1.09413300
O	1.90515100	-0.70862000	0.84380600
C	2.13093500	-1.36720100	-0.37717700
C	1.65270900	-0.49937900	-1.55541800
H	2.20173500	0.44972600	-1.58110400
H	1.81015100	-1.00126700	-2.51719200
H	0.58382700	-0.27674400	-1.45486900
C	3.63484600	-1.62582300	-0.52005800
H	3.98514400	-2.25286100	0.30699400
H	3.87353700	-2.12860400	-1.46468100
H	4.18113800	-0.67623800	-0.48569900
C	1.37995000	-2.70766200	-0.41622400
H	1.69616700	-3.33828200	0.42227600
H	0.29905200	-2.54080400	-0.33178400

H	1.57246400	-3.24916800	-1.34969100
C	-0.62211000	-0.28766700	1.44104300
C	-2.54083000	-1.66485900	0.65455500
C	-2.94830900	-0.50743300	-0.23492700
H	-3.29079700	-0.94519100	-1.17655200
H	-3.81544900	-0.00851400	0.22590800
O	-3.24395300	-2.68730900	0.67043500
N	-1.41966600	-1.51527000	1.36742000
N	-1.88367100	0.44008200	-0.51295600
C	-2.15927100	1.40840200	-1.56125700
H	-1.23772900	1.92713700	-1.82108000
H	-2.54344000	0.88072100	-2.43750300
H	-2.90373100	2.14735600	-1.23780500
C	-0.96255400	-2.62742500	2.18950500
H	-1.41255200	-2.59184300	3.18930800
H	-1.23939200	-3.56865900	1.71370000
H	0.12337500	-2.56096100	2.27934600
C	-0.58687400	0.26768300	2.86347300
H	-0.10009600	-0.44982300	3.53696000
H	0.03769700	1.16721600	2.86808500
C	-1.97532200	0.62594100	3.42519200
H	-2.45038100	1.35127300	2.75172800
H	-2.60549400	-0.27204900	3.43240500
C	-1.88540800	1.20334500	4.81455800
C	-1.68926100	2.57685300	5.00093200
C	-1.93117100	0.37674700	5.94303400
C	-1.54652800	3.11318600	6.28015400
H	-1.65237100	3.23046500	4.13190700
C	-1.78729700	0.90765100	7.22535700
H	-2.08378300	-0.69272000	5.81284500
C	-1.59441800	2.27865000	7.39777800
H	-1.40029200	4.18206900	6.40520200
H	-1.82798600	0.25147400	8.08969100
H	-1.48491500	2.69442700	8.39459300

Reaction of sarcosine anhydride (21) with styrene (3) T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

36

-1403.451530 [B3LYP/6-31+G(d,p)]

C	-2.01517600	1.69957200	0.10089800
C	-1.71236200	3.04246300	0.37549100
C	-0.43599700	3.54958600	0.14121800
C	0.61826500	2.74000200	-0.37811400
C	0.27835300	1.38328200	-0.66068800
C	-1.00064200	0.88268400	-0.41970600
H	-3.01010400	1.30444600	0.28263800

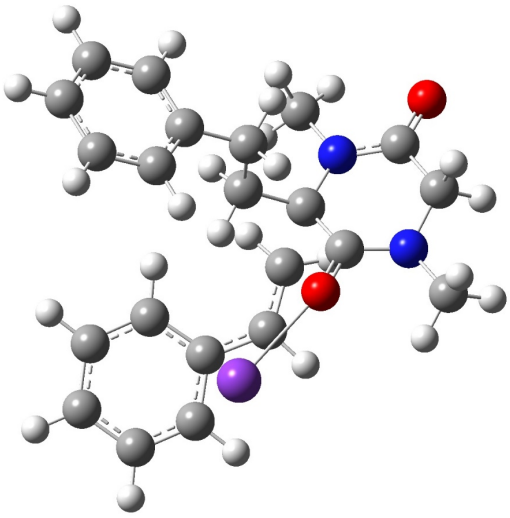
H	-2.48001400	3.69996800	0.77745800
H	-0.22620700	4.59279600	0.37128800
H	1.03128400	0.71836700	-1.07389500
H	-1.21171400	-0.15967000	-0.64879900
C	1.92837600	3.29919700	-0.60161200
H	2.01612400	4.37718500	-0.47047400
C	3.04693400	2.60110200	-1.06329300
H	3.10356900	1.52522500	-0.91471800
H	4.01307500	3.09150200	-0.98808100
C	3.24968800	2.27108400	-3.18749700
H	2.34192400	1.70114800	-3.34212000
C	3.24183000	3.58604100	-3.75056200
O	2.17225900	4.24113200	-3.91860100
C	4.56874200	5.56036000	-4.39342000
H	3.63183500	5.88497800	-4.84409200
H	4.76642100	6.18090500	-3.50595500
H	5.38691500	5.70844600	-5.10541500
K	-0.33105300	4.07856900	-3.16240600
N	4.47144200	4.14867700	-4.05249900
N	4.43490200	1.46938900	-3.35546600
C	5.65793200	2.02053200	-3.48523300
O	6.72522400	1.37393000	-3.55492000
C	4.27332800	0.01862700	-3.29980400
H	5.25298700	-0.45010000	-3.37262500
H	3.79982200	-0.27374900	-2.35750300
H	3.64061900	-0.31745200	-4.12842000
C	5.69178900	3.54212900	-3.53221300
H	6.52864300	3.82049700	-4.17843400
H	5.93259800	3.91867500	-2.52147700

-1403.068923 [M06-2X/6-31++G(d,p)]

C	-1.97332400	2.22350900	-0.33150800
C	-1.50540500	3.49629000	0.02174800
C	-0.14910200	3.79552000	-0.03175900
C	0.81439600	2.83855300	-0.44466700
C	0.31775000	1.55410000	-0.78889000
C	-1.04231700	1.25858000	-0.72773900
H	-3.03245000	1.99188300	-0.29618800
H	-2.20825100	4.26302900	0.33657500
H	0.19062000	4.79331300	0.23679600
H	1.00580800	0.78552600	-1.12847800
H	-1.38116400	0.26510400	-1.00936600
C	2.20662700	3.19518500	-0.55751900
H	2.44453600	4.25318700	-0.46606700
C	3.19400300	2.32196500	-0.97328300
H	3.07162300	1.24999800	-0.83725900
H	4.23045100	2.64869900	-0.94171200
C	3.28954200	1.93340400	-3.13125700
H	2.47973400	1.22006700	-3.22169800
C	3.03787900	3.24394300	-3.59792300
O	1.88022100	3.73370400	-3.66266500
C	3.98132900	5.45541600	-4.05134400
H	3.01166000	5.65872000	-4.50227100
H	4.03676400	5.97109800	-3.08095200
H	4.77320900	5.84445500	-4.69720800
K	-0.62163900	3.45337400	-3.15012200
N	4.14838400	4.02152400	-3.90212400
N	4.58690600	1.35893100	-3.33639300
C	5.68841500	2.11895100	-3.42877400

O	6.84592200	1.67833300	-3.52361800
C	4.67984600	-0.09189400	-3.31691000
H	4.09701000	-0.51095700	-4.14265800
H	5.72411800	-0.38015700	-3.41787800
H	4.28219500	-0.47756600	-2.37306800
C	5.44716100	3.61895200	-3.39031800
H	6.22898100	4.07971500	-3.99985300
H	5.60017100	3.96707300	-2.35270200

Reaction of sarcosine anhydride/styrene monoadduct K enolate with styrene (**3**) **T.S.**, solvent = DMSO



Charge = 0; Multiplicity = 1

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-1713.020706 [B3LYP/6-31+G(d,p)]

C	-2.15930900	2.49412700	0.55493000
C	-1.68776000	3.81544500	0.52423500
C	-0.38478100	4.10241500	0.12136500
C	0.53414200	3.08260800	-0.27909000
C	0.02019000	1.74926700	-0.24884200
C	-1.28051100	1.47070400	0.16376700
H	-3.17487700	2.26978300	0.86686200
H	-2.34249900	4.63203100	0.82144600
H	-0.04310900	5.13661500	0.12636600
H	0.65678100	0.92603500	-0.55891800
H	-1.62049000	0.43702300	0.17179000
C	1.87694900	3.42630800	-0.66308700
H	2.09434700	4.49310700	-0.71286200
C	2.91497000	2.53418800	-0.99087200
H	2.81395800	1.50732900	-0.64234900
H	3.93281100	2.91378000	-0.90498300
C	3.26978400	1.95590300	-2.95903300
C	3.14524900	3.25316600	-3.59123700
O	2.01630900	3.75751800	-3.83167500
N	4.29045400	4.01515100	-3.75079400
K	-0.42636600	4.29867600	-3.13423900
C	2.18615800	0.95133300	-3.30731300
H	2.19655400	0.11533300	-2.59902300
H	1.22461300	1.45100900	-3.17490400
C	2.26443900	0.38284700	-4.74985700
H	3.24497200	-0.08272200	-4.90317200
H	2.19196300	1.21618800	-5.45775700

C	1.17357900	-0.62655100	-5.03553100
C	1.37264400	-1.99596200	-4.79389700
C	-0.08244100	-0.21436400	-5.51115700
C	0.35071100	-2.92449500	-5.01654700
H	2.33961400	-2.33910400	-4.43323400
C	-1.10786600	-1.13799700	-5.73613800
H	-0.25617800	0.84037600	-5.71224300
C	-0.89539300	-2.49855100	-5.48822000
H	0.52949200	-3.97930700	-4.82623800
H	-2.06984400	-0.79625100	-6.10847500
H	-1.68964300	-3.21818300	-5.66485900
N	4.61295300	1.38750100	-2.89005600
C	5.72156200	1.99897700	-3.36255900
O	6.86564300	1.50383800	-3.30403800
C	5.55261500	3.34748700	-4.03103300
H	6.38024300	3.97714700	-3.69025200
H	5.69531100	3.19948900	-5.11725900
C	4.17581300	5.35293400	-4.31922000
H	3.27553800	5.83554300	-3.94224900
H	5.05192000	5.93806700	-4.02505600
H	4.12754400	5.32783700	-5.41871600
C	4.79043500	0.08743800	-2.23087100
H	4.57666000	-0.73707700	-2.91956600
H	5.82399100	0.00329300	-1.89993100
H	4.12699900	0.00918100	-1.37087500

-1712.505138 [M06-2X/6-31++G(d,p)]

C	-2.07189500	3.01791800	0.03210900
C	-1.38140400	4.21674700	0.25174400
C	0.00095900	4.27919600	0.11609500
C	0.77521400	3.14599600	-0.25417300
C	0.05259400	1.93838200	-0.45328400
C	-1.33057500	1.88054000	-0.30879200
H	-3.15121300	2.97073900	0.12891600
H	-1.93000000	5.11448400	0.52438400
H	0.51201600	5.22496600	0.28241500
H	0.58497900	1.03748400	-0.74404000
H	-1.84000900	0.93572300	-0.48031900
C	2.19825100	3.26309200	-0.43491500
H	2.60688800	4.26977200	-0.36310900
C	3.03910100	2.23554300	-0.84503300
H	2.72744300	1.20550800	-0.67055700
H	4.11432300	2.39774900	-0.76946300
C	3.24450000	1.84612000	-2.92694600
C	2.99136900	3.18583900	-3.34877000
O	1.83255300	3.66118600	-3.40929800
N	4.09478700	4.01860500	-3.50092300
K	-0.67922000	3.79103500	-2.92881200
C	2.18881700	0.82057800	-3.24817200
H	2.26297100	-0.04681000	-2.57678200
H	1.21616300	1.28047000	-3.05082700
C	2.22676500	0.32896900	-4.70993300
H	3.22096000	-0.07858600	-4.93122100
H	2.07577900	1.19141500	-5.36985700
C	1.17148900	-0.71476100	-4.97303200
C	1.43476100	-2.07161700	-4.75224300
C	-0.11486500	-0.34303500	-5.38098100
C	0.44151300	-3.03349600	-4.93712100
H	2.43061500	-2.37615800	-4.43700300

C	-1.11170800	-1.30051000	-5.56898400
H	-0.33351600	0.70839600	-5.55669800
C	-0.83601000	-2.65048800	-5.34738200
H	0.66599100	-4.08193300	-4.76454000
H	-2.10208300	-0.99294600	-5.89136500
H	-1.60922300	-3.39789400	-5.49537000
N	4.60582200	1.36116600	-3.02875900
C	5.61184400	2.05730000	-3.59010200
O	6.77175800	1.63384900	-3.70053700
C	5.26340100	3.42828200	-4.12935800
H	6.13213200	4.06720000	-3.95294400
H	5.13698200	3.34146700	-5.22386300
C	3.84662100	5.39490200	-3.89681500
H	3.01884800	5.79719700	-3.31514300
H	4.74694600	5.98273100	-3.70189600
H	3.59828700	5.47414900	-4.96578300
C	4.90209100	0.05492100	-2.45017900
H	5.97889000	-0.03162300	-2.31985400
H	4.40658000	-0.04018500	-1.48293100
H	4.55756200	-0.75313800	-3.10502200

10.5. Reaction Profiles for *N*-methyl-2-pyrrolidinone (NMP, 19) with Styrene in Presence of 18-Crown-6 or Sodium *tert*-Butoxide

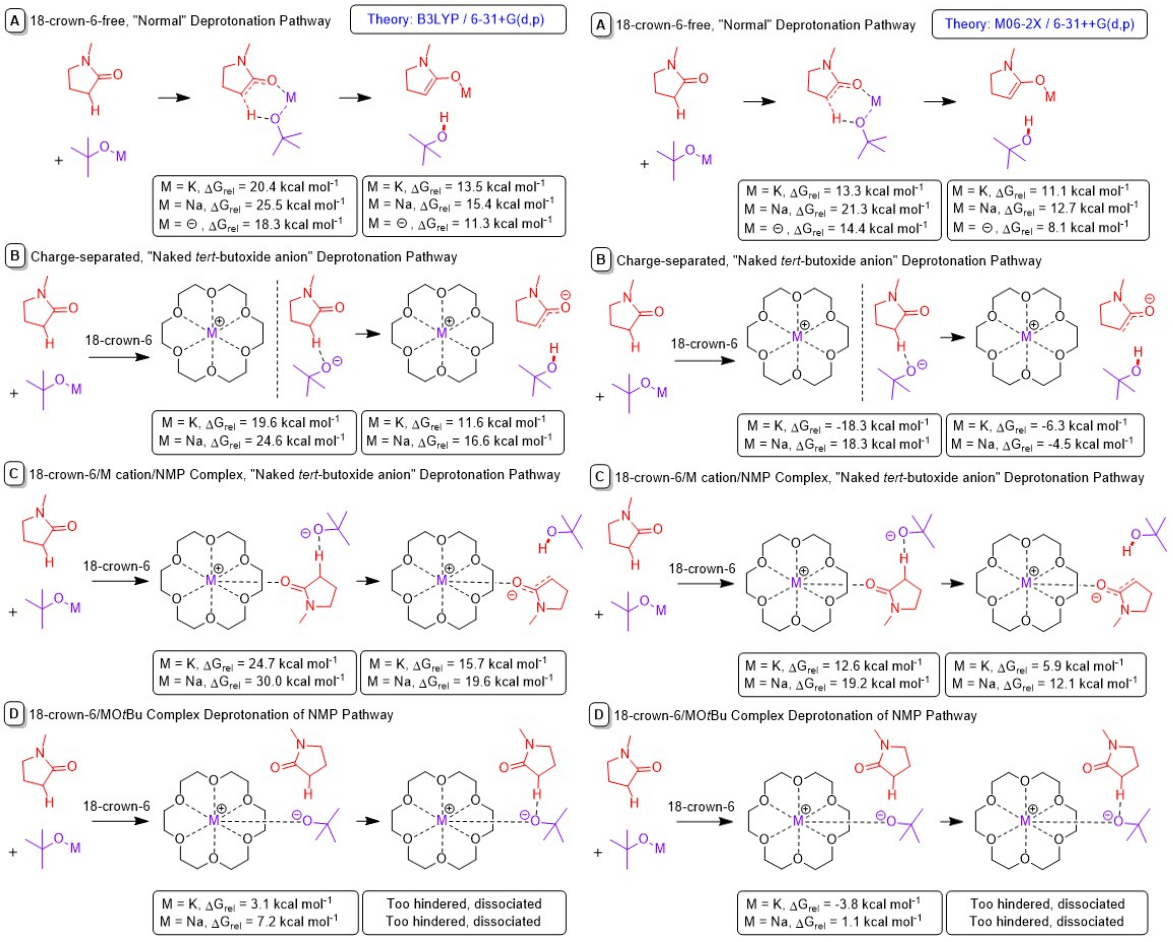


Figure S69. Computed plausible pathways for deprotonation of NMP by MO*t*Bu in the presence of 18-crown-6.

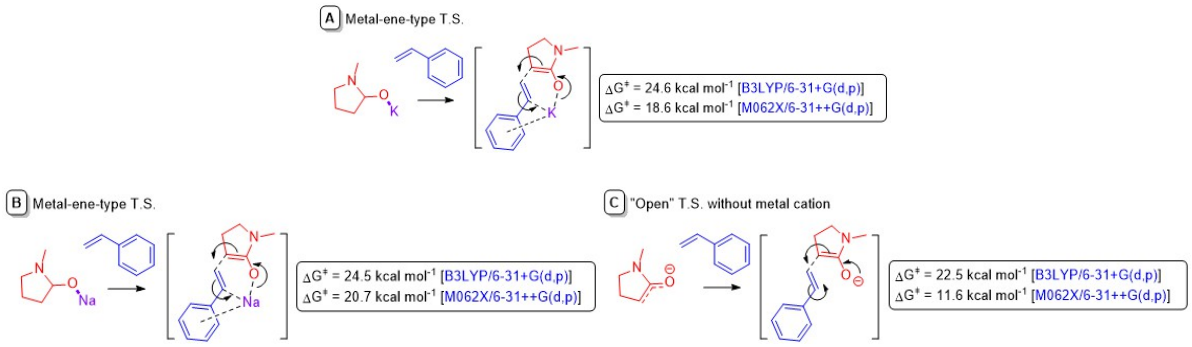
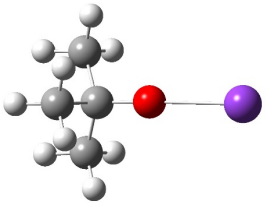


Figure S70. Metal-ene-type T.S. involving K (**A**) vs Na (**B**) vs 'open' T.S. (**C**) where K^+ is absent for the reaction of NMP with styrene following abstraction of K^+ by 18-crown-6.

10.5.1. XYZ Co-ordinates of starting materials, intermediates, products

Sodium *tert*-butoxide, solvent = DMSO



Charge = 0; Multiplicity = 1

15

-395.368774 [B3LYP/6-31+G(d,p)]

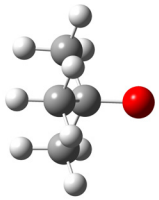
C	2.74347600	0.16102700	0.16877100
C	4.27786700	0.16471200	-0.06906600
H	2.34484100	1.17622600	0.05039800
H	2.25272600	-0.48334300	-0.57133000
H	2.47021800	-0.19877200	1.17030100
C	4.80061700	-1.28326000	0.13376200
C	4.93206500	1.07294000	1.00670200
H	5.88830200	-1.31264200	-0.00724800
H	4.57509200	-1.67919800	1.13357100
H	4.34574200	-1.95069900	-0.60891800
H	4.71515900	0.74263800	2.03192700
H	6.02095700	1.08348100	0.87410200
H	4.56861600	2.10199000	0.89494500
O	4.57682500	0.62192200	-1.34262200
Na	5.02998400	1.31278200	-3.28588600

-395.205308 [M06-2X/6-31++G(d,p)]

C	1.14587600	-1.42644500	0.29139000
C	0.63941800	0.00268300	0.00469800
H	0.83983200	-1.73042800	1.29963200
H	0.69856700	-2.12536400	-0.42609400
H	2.23795900	-1.50973900	0.22092100
C	1.10478500	0.40243300	-1.41085700
C	1.30084500	0.96110300	1.01715100
H	0.77075300	1.42258700	-1.63438600
H	2.19562800	0.36229500	-1.52499800
H	0.65594900	-0.27297200	-2.14865300
H	2.39704500	0.93932400	0.96519300
H	0.96575700	1.98736200	0.82556800

H	0.99801800	0.68862900	2.03544500
O	-0.73307600	0.06377000	0.10320600
Na	-2.82185800	0.00813600	0.01340300

***tert*-Butoxide anion**, solvent = DMSO



Charge = -1; Multiplicity = 1

14

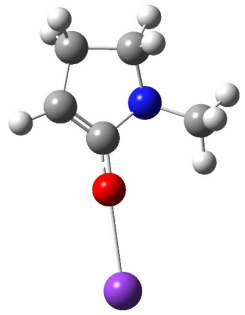
-233.101392 [B3LYP/6-31+G(d,p)]

C	-0.00001600	-0.00018400	0.12772000
C	-0.33365500	1.41319800	-0.43086900
H	-0.34222600	1.45088900	-1.52986700
H	-1.32045500	1.73200200	-0.07193700
H	0.40593300	2.13980100	-0.07119600
C	-1.05690400	-0.99365600	-0.43477100
H	-1.08447200	-1.01748400	-1.53381300
H	-0.84040500	-2.00844300	-0.07736600
H	-2.05607000	-0.71665100	-0.07484700
C	1.38933500	-0.41649800	-0.43557500
H	2.15935200	0.27802200	-0.07597100
H	1.64944500	-1.42102700	-0.07797100
H	1.42438900	-0.42573800	-1.53468900
O	0.00149300	-0.00356600	1.51107900

-272.97354 [M06-2X/6-31+G(d,p)]

C	0.00042000	-0.00004400	0.12785600
C	-0.73422100	-1.24088900	-0.43124300
H	-0.75383300	-1.26805000	-1.52897300
H	-0.24108800	-2.15258500	-0.07240800
H	-1.76905300	-1.24999800	-0.06785200
C	1.44116900	-0.01416600	-0.43392500
H	1.47283200	-0.01396600	-1.53176100
H	1.98454600	0.86752900	-0.07296700
H	1.96653800	-0.90719500	-0.07430800
C	-0.70931100	1.25556000	-0.43046500
H	-1.74327200	1.28585900	-0.06594300
H	-0.19730200	2.15679900	-0.07222200
H	-0.72957100	1.28376200	-1.52816300
O	0.00273200	-0.00061500	1.50265700

***N*-Methyl-2-pyrrolidinone Na enolate**, solvent = DMSO



Charge = 0; Multiplicity = 1

16

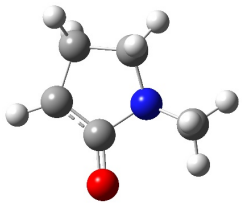
-487.615603 [B3LYP/6-31+G(d,p)]

C	-0.37890500	-1.47578900	0.17226900
H	0.23019700	-2.37340400	0.20054100
C	0.13847900	-0.21509500	-0.05671100
O	1.35256300	0.21835300	-0.09194600
C	-0.78230200	2.07873500	0.10761000
H	0.19548000	2.45234800	-0.20201400
H	-1.55873600	2.70724200	-0.34164100
H	-0.86004500	2.17712200	1.20818900
C	-2.17735600	0.04415600	0.09649300
H	-2.37118900	0.27520800	1.16247800
H	-3.03839300	0.39033800	-0.48668200
N	-0.93927800	0.70423400	-0.33490700
C	-1.87407700	-1.45937100	-0.05885000
H	-2.46627900	-2.05640600	0.64641100
H	-2.16010700	-1.79885000	-1.07245100
Na	3.47531600	-0.20780600	0.03638300

-487.426924 [M06-2X/6-31++G(d,p)]

C	-0.36765300	-1.46906700	0.12351900
H	0.24155500	-2.36473900	0.14638500
C	0.13697400	-0.21379500	-0.12630500
O	1.34040600	0.22493800	-0.21355900
C	-0.74718700	2.05835400	0.12191700
H	0.19222100	2.44987500	-0.27021900
H	-1.56870200	2.69534400	-0.21934600
H	-0.71205800	2.10516600	1.22637000
C	-2.15142100	0.05402600	0.15643100
H	-2.26167700	0.27728100	1.23510000
H	-3.04786100	0.41020200	-0.36175300
N	-0.94687300	0.70502900	-0.35384500
C	-1.87028800	-1.44454200	-0.02616300
H	-2.42434800	-2.04045500	0.70755300
H	-2.20945600	-1.77123600	-1.02457700
Na	3.42660400	-0.21872700	0.11358800

***N*-Methyl-2-pyrrolidinone 'naked' enolate**, solvent = DMSO



Charge = -1; Multiplicity = 1

15

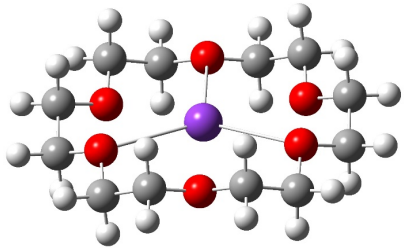
-325.354810 [B3LYP/6-31+G(d,p)]

C	1.14443400	1.05379500	0.20173600
H	1.61761800	2.03100500	0.22084400
C	-0.21520000	0.88110000	-0.02503500
O	-1.19300800	1.70946300	-0.03376700
C	-1.72655000	-1.08284800	0.10047500
H	-2.54283800	-0.41901200	-0.19112200
H	-1.88198800	-2.06072600	-0.36879600
H	-1.76950500	-1.22354500	1.19892600
C	0.73181000	-1.26038400	0.07558900
H	0.64319400	-1.55783300	1.13982100
H	0.85954000	-2.17223700	-0.52006500
N	-0.46304700	-0.51599700	-0.33388700
C	1.87606800	-0.24022200	-0.08039500
H	2.70614500	-0.47267500	0.59980200
H	2.28985800	-0.29735400	-1.10628600

-325.202110 [M06-2X/6-31++G(d,p)]

C	1.12449200	1.06408200	0.20032700
H	1.58061800	2.04574700	0.25820000
C	-0.22602700	0.87210300	-0.03171900
O	-1.21636900	1.67472500	-0.03388700
C	-1.69873000	-1.08829600	0.10925900
H	-2.52745200	-0.45180000	-0.20430500
H	-1.83506000	-2.08691400	-0.31755700
H	-1.72629500	-1.18004500	1.21161300
C	0.74185700	-1.24466000	0.07633300
H	0.64291800	-1.52149200	1.14444000
H	0.88472500	-2.16283300	-0.50407000
N	-0.45049200	-0.52081700	-0.35314100
C	1.87206800	-0.21755000	-0.07871400
H	2.69974700	-0.43912600	0.60493500
H	2.28323800	-0.26969600	-1.10308000

18-crown-6, solvent = DMSO



Charge = 0; Multiplicity = 1

42

-922.756039 [B3LYP/6-31+G(d,p)]

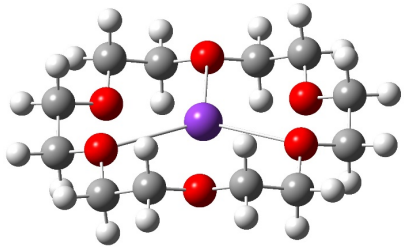
O	0.23670600	1.43658100	2.48584300
O	-0.24269300	2.87939200	0.00000000
O	0.23670600	1.43658100	-2.48584300
O	-0.23670600	-1.43658100	-2.48584300
O	0.24269300	-2.87939200	0.00000000
O	-0.23670600	-1.43658100	2.48584300
C	-0.28761700	2.75702500	2.39895700
C	0.28993000	3.45660200	-1.18709100
C	-0.29030800	0.69892100	-3.58311500
C	0.28761700	-2.75702500	-2.39895700
C	-0.28993000	-3.45660200	1.18709100
C	0.29030800	-0.69892100	3.58311500
C	0.29030800	-0.69892100	-3.58311500
C	-0.28993000	-3.45660200	-1.18709100
C	0.28761700	-2.75702500	2.39895700
C	-0.29030800	0.69892100	3.58311500
C	0.28993000	3.45660200	1.18709100
C	-0.28761700	2.75702500	-2.39895700
H	-0.02144400	3.33166600	3.29995000
H	0.03213100	4.52603500	-1.23859000
H	-0.02907400	1.19133000	-4.53287100
H	0.02144400	-3.33166600	-3.29995000
H	-0.03213100	-4.52603500	1.23859000
H	0.02907400	-1.19133000	4.53287100
H	0.02907400	-1.19133000	-4.53287100
H	-0.03213100	-4.52603500	-1.23859000
H	0.02144400	-3.33166600	3.29995000
H	-0.02907400	1.19133000	4.53287100
H	0.03213100	4.52603500	1.23859000
H	-0.02144400	3.33166600	-3.29995000
H	-1.38533400	2.72654400	2.32632200
H	1.38706300	3.36998900	-1.19299700
H	-1.38765200	0.64823600	-3.51598100
H	1.38533400	-2.72654400	-2.32632200
H	-1.38706300	-3.36998900	1.19299700
H	1.38765200	-0.64823600	3.51598100
H	1.38765200	-0.64823600	-3.51598100
H	-1.38706300	-3.36998900	-1.19299700
H	1.38533400	-2.72654400	2.32632200
H	-1.38765200	0.64823600	3.51598100
H	1.38706300	3.36998900	1.19299700
H	-1.38533400	2.72654400	-2.32632200

-922.336250 [M06-2X/6-31+G(d,p)]

O	0.22674300	1.41592600	2.45408600
O	-0.21769600	2.82565400	0.00000000
O	0.22674300	1.41592600	-2.45408600
O	-0.22674300	-1.41592600	-2.45408600
O	0.21769600	-2.82565400	0.00000000
O	-0.22674300	-1.41592600	2.45408600
C	-0.28973100	2.72894000	2.37903000
C	0.29475400	3.42274700	-1.17348800
C	-0.29186600	0.69564600	-3.55346900
C	0.28973100	-2.72894000	-2.37903000
C	-0.29475400	-3.42274700	1.17348800
C	0.29186600	-0.69564600	3.55346900
C	0.29186600	-0.69564600	-3.55346900
C	-0.29475400	-3.42274700	-1.17348800
C	0.28973100	-2.72894000	2.37903000
C	-0.29186600	0.69564600	3.55346900

C	0.29475400	3.42274700	1.17348800
C	-0.28973100	2.72894000	-2.37903000
H	-0.02466500	3.29466300	3.28491500
H	0.02687300	4.48955600	-1.20560100
H	-0.02877200	1.19878700	-4.49617500
H	0.02466500	-3.29466300	-3.28491500
H	-0.02687300	-4.48955600	1.20560100
H	0.02877200	-1.19878700	4.49617500
H	0.02877200	-1.19878700	-4.49617500
H	-0.02687300	-4.48955600	-1.20560100
H	0.02466500	-3.29466300	3.28491500
H	-0.02877200	1.19878700	4.49617500
H	0.02687300	4.48955600	1.20560100
H	-0.02466500	3.29466300	-3.28491500
H	-1.38668800	2.70203200	2.29710600
H	1.39196900	3.34165300	-1.19370400
H	-1.38869600	0.63790100	-3.48721200
H	1.38668800	-2.70203200	-2.29710600
H	-1.39196900	-3.34165300	1.19370400
H	1.38869600	-0.63790100	3.48721200
H	1.38869600	-0.63790100	-3.48721200
H	-1.39196900	-3.34165300	-1.19370400
H	1.38668800	-2.70203200	2.29710600
H	-1.38869600	0.63790100	3.48721200
H	1.39196900	3.34165300	1.19370400
H	-1.38668800	2.70203200	-2.29710600

Potassium cation/18-crown-6 complex, solvent = DMSO



Charge = 1; Multiplicity = 1

43

-1522.628029 [B3LYP/6-31+G(d,p)]

O	0.81705900	2.16469200	1.86357000
O	0.97273200	-0.43617500	3.07373600
O	0.89093000	-2.73816000	1.36140700
O	1.82692900	-2.44466000	-1.33644400
O	1.67750800	0.15220500	-2.55505200
O	1.75878500	2.44864800	-0.83487000
C	1.04931400	1.95665400	3.25688400
C	0.39111100	-1.68185000	3.45883600
C	1.52992600	-3.78632600	0.63262400
C	1.60298500	-2.24132800	-2.73180100
C	2.26884200	1.39592600	-2.93138800
C	1.12603800	3.50188000	-0.10776200
C	1.21876400	-3.63747900	-0.84071000
C	2.29986100	-0.97333600	-3.17457600
C	1.53918300	2.52899000	-2.24320400
C	1.43455000	3.35203600	1.36607700
C	0.35471200	0.68776700	3.70069300
C	1.12163200	-2.81283800	2.76821400
H	0.64928100	2.80114300	3.83682900

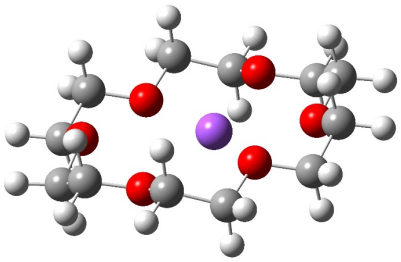
H	0.47502300	-1.81817100	4.54689900
H	1.16137600	-4.76420700	0.97549000
H	2.00766900	-3.08707500	-3.30663600
H	2.19488700	1.53597900	-4.01971700
H	1.50225600	4.47684000	-0.45056700
H	1.61295400	-4.51357300	-1.37601900
H	2.22521100	-0.89178700	-4.26880900
H	1.92159500	3.48416300	-2.63169600
H	1.04717900	4.23188600	1.90024200
H	0.43712400	0.60332100	4.79412500
H	0.74792200	-3.76907700	3.16255500
H	2.12932400	1.88548600	3.45184600
H	-0.67528600	-1.69853400	3.19034600
H	2.61687600	-3.75070500	0.79614100
H	0.52414100	-2.17203900	-2.93400900
H	3.33293900	1.40594900	-2.65372600
H	0.03907900	3.47429300	-0.27304800
H	0.13080200	-3.59846900	-0.99678200
H	3.36504400	-1.01111500	-2.90352600
H	0.46240500	2.47464400	-2.46059600
H	2.52208000	3.30449600	1.52254100
H	-0.71245300	0.72637700	3.43751000
H	2.19970300	-2.75134600	2.97693500
K	1.25745800	-0.14260300	0.24924700

-1522.193988 [M06-2X/6-31++G(d,p)]

O	0.85085200	2.11970200	1.83923200
O	0.96406800	-0.42621000	3.01732700
O	0.92414700	-2.68266800	1.33758500
O	1.80344100	-2.40459000	-1.31396800
O	1.68908900	0.14118400	-2.49206500
O	1.73007000	2.39776600	-0.81245600
C	1.06336400	1.93903700	3.22845300
C	0.38756300	-1.65810300	3.41520200
C	1.53819300	-3.74589700	0.63018900
C	1.59027800	-2.22412400	-2.70311600
C	2.26486500	1.37321400	-2.89056700
C	1.11702300	3.46125400	-0.10458400
C	1.21638800	-3.60182500	-0.83475000
C	2.29262000	-0.96500400	-3.14028500
C	1.52614900	2.49743500	-2.21105100
C	1.43907300	3.31644900	1.36022800
C	0.36037400	0.68011900	3.66515700
C	1.12666000	-2.78248600	2.73637400
H	0.65755500	2.79367200	3.78775700
H	0.46754800	-1.77913300	4.50456700
H	1.15696000	-4.71097900	0.99175800
H	1.99618800	-3.07864200	-3.26253000
H	2.18376000	1.49417000	-3.97985900
H	1.49889000	4.42614800	-0.46598700
H	1.61945600	-4.46637200	-1.38059800
H	2.20336500	-0.85978900	-4.23050900
H	1.90968300	3.45796500	-2.58221900
H	1.03709600	4.18126700	1.90644800
H	0.44885400	0.57485400	4.75543700
H	0.74251800	-3.74294800	3.10709000
H	2.14028400	1.86328500	3.43718700
H	-0.67589500	-1.68230500	3.13735700
H	2.62678100	-3.71982300	0.78292300
H	0.51323900	-2.14882200	-2.91139300

H	3.32859000	1.39771100	-2.61377900
H	0.02837400	3.43604900	-0.25701700
H	0.12718000	-3.57129500	-0.98164400
H	3.35953800	-1.01697500	-2.87969900
H	0.45227900	2.43737900	-2.43968500
H	2.52828800	3.28469900	1.50682400
H	-0.70635200	0.73238800	3.40383900
H	2.20031400	-2.72271700	2.96608500
K	1.32674300	-0.14251700	0.26255100

Sodium cation/18-crown-6 complex, solvent = DMSO



Charge = 1; Multiplicity = 1

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-1085.014904 [B3LYP/6-31+G(d,p)]

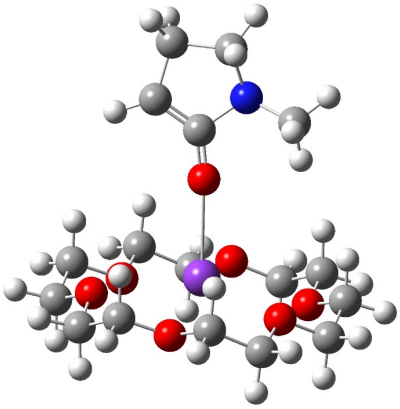
O	0.80767400	2.13461200	1.90509800
O	0.99849100	-0.41621800	3.15520500
O	0.95928700	-2.63350500	1.35600900
O	1.78954200	-2.38783900	-1.33483300
O	1.69826500	0.12910700	-2.52307200
O	1.69190500	2.34715200	-0.80282900
C	1.03072800	1.96468300	3.30143100
C	0.37982200	-1.65693100	3.46896700
C	1.55131500	-3.71525000	0.64072200
C	1.59344200	-2.24048100	-2.74130400
C	2.27022600	1.37845500	-2.90919100
C	1.10749300	3.43089400	-0.07951800
C	1.20746400	-3.58675100	-0.82316200
C	2.29353300	-0.98198000	-3.19288500
C	1.52263300	2.48879100	-2.21224600
C	1.44034700	3.29818300	1.38691700
C	0.34842200	0.69686400	3.75730800
C	1.12407500	-2.76758400	2.76750200
H	0.61788300	2.81862100	3.85960600
H	0.40830400	-1.83839300	4.55443800
H	1.16239400	-4.67481600	1.01194700
H	2.01554800	-3.10281500	-3.27630000
H	2.18537900	1.51410000	-3.99664300
H	1.50865700	4.38559800	-0.44938000
H	1.60535300	-4.45808500	-1.36234400
H	2.18240200	-0.87452700	-4.28102900
H	1.92536400	3.45537900	-2.54785300
H	1.08245300	4.19625100	1.91324900
H	0.40706200	0.62824300	4.85435700
H	0.71875900	-3.73411500	3.10101100
H	2.10984300	1.90826600	3.50858700
H	-0.67348700	-1.64761000	3.15047600
H	2.64247100	-3.70855900	0.77975800
H	0.51864500	-2.18317300	-2.96568600
H	3.33521700	1.40214300	-2.63709800
H	0.01735100	3.43475800	-0.22459300

H	0.11684300	-3.56100500	-0.95987600
H	3.36579200	-1.03224300	-2.95519200
H	0.45398100	2.45130100	-2.46944000
H	2.53007800	3.23158900	1.52458300
H	-0.71380200	0.71633800	3.47086800
H	2.19234500	-2.73371800	3.02723300
Na	1.38595500	-0.23570800	-0.05899100

-1084.561702 [M06-2X/6-31++G(d,p)]

O	0.82904200	2.10211100	1.85635000
O	0.95920700	-0.41131600	3.05038400
O	0.98950100	-2.62055500	1.34567500
O	1.74493800	-2.35331500	-1.30171300
O	1.69758600	0.13170900	-2.45064800
O	1.70931900	2.33114800	-0.78290200
C	0.99631200	1.94451900	3.25137300
C	0.39852500	-1.65108700	3.42836300
C	1.58282800	-3.69585400	0.64348200
C	1.52727300	-2.21231200	-2.69470800
C	2.28010700	1.35579100	-2.86335900
C	1.14367500	3.42404100	-0.08056900
C	1.21379900	-3.57103600	-0.80879600
C	2.24338000	-0.97181000	-3.15188000
C	1.54888200	2.47884900	-2.18156600
C	1.45712900	3.27530500	1.38263200
C	0.30530500	0.67628900	3.67195900
C	1.16867100	-2.74745400	2.74447400
H	0.55685000	2.79877400	3.78646400
H	0.46226500	-1.78534800	4.51809800
H	1.21167000	-4.65521200	1.03016600
H	1.92421400	-3.08447500	-3.23166600
H	2.19027300	1.46947600	-3.95220100
H	1.56866500	4.36780700	-0.44967300
H	1.63357900	-4.41886400	-1.36719400
H	2.10385600	-0.84126900	-4.23349600
H	1.96698800	3.43930700	-2.51360400
H	1.08302100	4.15657700	1.92379100
H	0.35440700	0.57762200	4.76608400
H	0.79348900	-3.72245600	3.08577100
H	2.06645200	1.88990100	3.49980800
H	-0.66024800	-1.69399900	3.13315300
H	2.67555100	-3.66890400	0.76380800
H	0.45022900	-2.13193600	-2.89934500
H	3.34547300	1.37212000	-2.59381900
H	0.05531800	3.44605300	-0.23525400
H	0.12098600	-3.57763300	-0.92654100
H	3.31926600	-1.05366900	-2.94201000
H	0.48122600	2.45254900	-2.44273500
H	2.54475900	3.20978800	1.53343300
H	-0.75246200	0.70394200	3.37145300
H	2.23690000	-2.67619600	2.99560400
Na	1.38725000	-0.21895500	0.01315900

NMP K enolate/18-crown-6 complex, solvent = DMSO



Charge = 0; Multiplicity = 1

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-1847.976282 [B3LYP/6-31+G(d,p)]

O	0.86431100	2.21724500	1.89513300
O	0.92277700	-0.41490300	3.04002200
O	0.76213300	-2.70512700	1.31878200
O	1.70664700	-2.37794800	-1.37163100
O	1.65885500	0.22919700	-2.57644600
O	1.82270500	2.47387900	-0.79698400
C	1.10183900	1.96509500	3.27887100
C	0.31949500	-1.64843000	3.42817700
C	1.39199100	-3.74561300	0.57370900
C	1.50927200	-2.15987100	-2.76788800
C	2.32169400	1.44806000	-2.90741500
C	1.25804900	3.55635700	-0.05870600
C	1.08351200	-3.57071500	-0.89727500
C	2.25474400	-0.91260400	-3.18968600
C	1.63807600	2.60133200	-2.20617900
C	1.55487600	3.36847700	1.41295000
C	0.35761700	0.71689700	3.69992300
C	1.01512600	-2.79031900	2.71986800
H	0.74712900	2.81225300	3.88449700
H	0.41830500	-1.79301800	4.51417000
H	1.01703500	-4.72664600	0.90138000
H	1.89592400	-3.01418100	-3.34290700
H	2.28162300	1.61858200	-3.99352600
H	1.69694000	4.50953500	-0.38866000
H	1.46867900	-4.44308400	-1.44556700
H	2.20689100	-0.82251600	-4.28506100
H	2.08028500	3.54346700	-2.56230000
H	1.22522300	4.26485800	1.95899000
H	0.44665500	0.60326400	4.79038300
H	0.63133400	-3.74168400	3.11725600
H	2.17963700	1.84010100	3.45912800
H	-0.75159800	-1.64124300	3.17804900
H	2.47948200	-3.72050400	0.73659200
H	0.43637300	-2.05532100	-2.98667700
H	3.37809200	1.39591400	-2.60561500
H	0.17175700	3.60201100	-0.22522700
H	-0.00378600	-3.51777700	-1.05435400
H	3.31199000	-0.98870000	-2.89604900
H	0.56505900	2.61186000	-2.44799100
H	2.63746400	3.25002200	1.56718000
H	-0.70965000	0.80689000	3.44943200

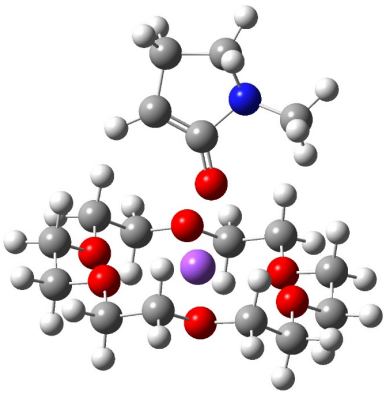
H	2.09765200	-2.74910000	2.91055000
C	-3.90811300	-1.29627600	-0.50581000
H	-3.54119500	-2.31093800	-0.38821100
C	-3.07284700	-0.19308400	-0.56890900
O	-1.81881500	-0.05554800	-0.32197200
C	-3.46590100	2.25476900	-0.53139300
H	-2.38470900	2.38697500	-0.60489200
H	-3.95764700	3.03894700	-1.11744100
H	-3.76140800	2.38726800	0.52819500
C	-5.24828600	0.59588400	-0.91879500
H	-5.61486500	0.87746100	0.08833200
H	-5.85887000	1.12428000	-1.66037700
N	-3.82949900	0.94662300	-1.04555600
K	0.74773200	-0.07423900	0.14503100
C	-5.26760600	-0.93837500	-1.06459300
H	-6.12520900	-1.37385000	-0.53541500
H	-5.38742100	-1.21255100	-2.13043000

-1847.392020 [M06-2X/6-31++G(d,p)]

O	0.32768900	2.06410100	1.39196800
O	0.10205900	-0.48665100	2.54903000
O	0.59745400	-2.73160200	0.88300700
O	2.06931300	-2.35649400	-1.47388200
O	2.10643100	0.20273200	-2.64333600
O	1.79006700	2.42479800	-0.93777800
C	-0.01989900	1.88147700	2.75040500
C	-0.52856900	-1.74588700	2.72396700
C	1.45556300	-3.73095800	0.36722100
C	2.13556400	-2.16439900	-2.87559800
C	2.71592200	1.45433500	-2.90309900
C	1.07908900	3.49309600	-0.33797100
C	1.48772600	-3.60273600	-1.13427500
C	2.86582700	-0.87648700	-3.15704700
C	1.84170100	2.54905000	-2.34778000
C	1.02699000	3.26890200	1.15199300
C	-0.77109400	0.58107200	2.87575700
C	0.42048800	-2.83078900	2.28442000
H	-0.66304100	2.70653600	3.09035700
H	-0.78459000	-1.89297500	3.78355600
H	1.08292600	-4.72953800	0.63679600
H	2.67743400	-2.99597500	-3.34786900
H	2.83500900	1.60030000	-3.98615100
H	1.57943100	4.44882700	-0.54962300
H	2.08025200	-4.42524900	-1.55940000
H	2.99673300	-0.76467500	-4.24277300
H	2.26587400	3.52373600	-2.62819400
H	0.50479300	4.11507000	1.62104600
H	-1.13517800	0.47051300	3.90781900
H	-0.00298600	-3.81195600	2.54274600
H	0.88462400	1.86234000	3.37584700
H	-1.45147800	-1.78347000	2.12605000
H	2.46729800	-3.61207400	0.78146100
H	1.12081100	-2.12421000	-3.29815800
H	3.70984600	1.49316700	-2.43419800
H	0.05671700	3.53642000	-0.74096200
H	0.46606600	-3.66307300	-1.53726500
H	3.85904100	-0.89531500	-2.68541400
H	0.82778000	2.47574300	-2.76856900
H	2.04171900	3.20860200	1.57154700

H	-1.63605600	0.57426000	2.19389200
H	1.38820700	-2.72228500	2.79595100
C	-3.55680800	-1.18259400	0.32032000
H	-3.28859500	-2.23240300	0.34797800
C	-2.80028300	-0.22208500	-0.31604700
O	-1.63450000	-0.25897200	-0.84425500
C	-2.80490400	2.23906300	-0.31724800
H	-1.99135800	2.20345000	-1.04470200
H	-3.45734600	3.08609100	-0.55186500
H	-2.36202000	2.40575600	0.68218100
C	-4.62897800	0.88373700	0.59993500
H	-4.25932800	1.21306300	1.59094600
H	-5.49238600	1.50217900	0.33202000
N	-3.55905200	1.00528400	-0.38579800
K	0.86004600	-0.16103700	-0.16959900
C	-4.92207500	-0.62328700	0.64093000
H	-5.33314000	-0.91799700	1.61330400
H	-5.68526800	-0.87519000	-0.11692900

NMP Na enolate/18-crown-6 complex, solvent = DMSO



Charge = 0; Multiplicity = 1

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-1410.364940 [B3LYP/6-31+G(d,p)]

O	1.02172800	2.20417400	1.84572900
O	0.86530300	-0.34203100	3.01406600
O	0.69740100	-2.57651100	1.32829900
O	1.62947500	-2.34971700	-1.36273300
O	1.66033800	0.21397100	-2.63334800
O	1.93519900	2.43244600	-0.84872600
C	1.20410400	2.00764800	3.24640900
C	0.20897100	-1.54088700	3.42448900
C	1.26310400	-3.66595800	0.60155100
C	1.43880500	-2.16254100	-2.76252600
C	2.36898900	1.40092000	-2.96615600
C	1.41781200	3.53347000	-0.10962200
C	0.95765500	-3.50336700	-0.86886300
C	2.22501600	-0.95412500	-3.21558200
C	1.73406900	2.57197700	-2.25273600
C	1.73222100	3.33999500	1.35515900
C	0.37876500	0.82043400	3.68376900
C	0.87240800	-2.71064900	2.73674600
H	0.87590500	2.89848900	3.80155100
H	0.29506100	-1.66712300	4.51314500
H	0.83121200	-4.61516000	0.95127500
H	1.79340800	-3.04637700	-3.31423200

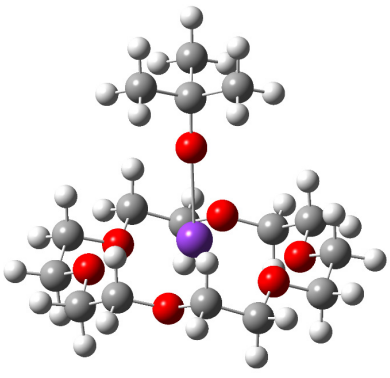
H	2.33140700	1.57923600	-4.05200400
H	1.87997900	4.47266200	-0.44963800
H	1.30120700	-4.40277400	-1.40228500
H	2.18669800	-0.89255100	-4.31420100
H	2.19917100	3.50286700	-2.61064200
H	1.42720300	4.24092200	1.90726300
H	0.47145000	0.69838100	4.77232500
H	0.41209400	-3.64476800	3.09065000
H	2.26752400	1.83390600	3.46674300
H	-0.85788000	-1.49440600	3.16266200
H	2.35055900	-3.70105400	0.76310300
H	0.36998300	-2.02527600	-2.98406700
H	3.42500700	1.30869900	-2.67055500
H	0.33053000	3.61234300	-0.25733700
H	-0.12730400	-3.40668900	-1.02306900
H	3.27857200	-1.05712100	-2.91464300
H	0.65822300	2.61590400	-2.47834400
H	2.81351500	3.19712400	1.49715100
H	-0.68165200	0.97844800	3.44012200
H	1.94416600	-2.73787200	2.98272000
C	-3.07059400	-1.30036900	-0.71955200
H	-2.53391900	-2.24154300	-0.77572900
C	-2.45072200	-0.08359500	-0.49725400
O	-1.25140800	0.21431200	-0.13886300
C	-3.27884500	2.19444800	0.01675100
H	-2.23688600	2.51737700	0.05190400
H	-3.88132800	2.99225100	-0.43111000
H	-3.63215900	2.04473400	1.05608700
C	-4.71932700	0.37906400	-0.82609900
H	-5.16326700	0.37569900	0.18904800
H	-5.39016400	0.94094600	-1.48629600
N	-3.38363800	0.98496900	-0.77961200
C	-4.45684400	-1.07033300	-1.28013300
H	-5.23478800	-1.74810200	-0.90563000
H	-4.49533000	-1.13168900	-2.38450200
Na	0.84759700	-0.04086600	0.48757000

-1409.763790 [M06-2X/6-31++G(d,p)]

O	1.11394400	2.30846000	1.62839400
O	0.59052500	-0.14720600	2.83816600
O	0.34876400	-2.41099300	1.21938100
O	1.51345800	-2.31676700	-1.30076200
O	1.79553100	0.17075500	-2.53289300
O	2.03345500	2.42435400	-0.96133500
C	1.17611900	2.13894000	3.03206100
C	-0.30635200	-1.19881000	3.13895700
C	0.94312400	-3.55458300	0.64354200
C	1.41967000	-2.16700300	-2.70291600
C	2.48536300	1.31473200	-2.99994900
C	1.61308600	3.59609000	-0.28636300
C	0.80216900	-3.45428000	-0.85162100
C	2.29231700	-1.01595500	-3.12366600
C	1.86818300	2.53068200	-2.36400000
C	1.88201400	3.40977700	1.18281700
C	0.18514100	1.07494800	3.42060000
C	0.28255700	-2.48630600	2.62718500
H	0.91637100	3.07930500	3.53815000
H	-0.45723800	-1.27213200	4.22571000
H	0.43924800	-4.46802000	0.99241900

H	1.75972800	-3.08206300	-3.20940800
H	2.40190100	1.38995500	-4.09321300
H	2.16926600	4.46819300	-0.65705000
H	1.20520900	-4.36376600	-1.32063400
H	2.27285100	-0.92864900	-4.21910500
H	2.36998300	3.43369900	-2.73807000
H	1.59346600	4.32071900	1.72540700
H	0.15120600	0.98416300	4.51597100
H	-0.34974200	-3.33147800	2.93646500
H	2.19226600	1.84718300	3.33454000
H	-1.28095200	-1.01164300	2.66124500
H	2.00477300	-3.61302800	0.92615500
H	0.37574100	-1.97554900	-2.99299800
H	3.55004500	1.24740800	-2.73303700
H	0.53958500	3.76269600	-0.45743700
H	-0.26094300	-3.36298700	-1.12033900
H	3.33043800	-1.18816700	-2.80439500
H	0.79884000	2.59314700	-2.61226800
H	2.95144300	3.22141700	1.35607200
H	-0.81741500	1.35126500	3.06045100
H	1.28821800	-2.63058300	3.04939200
C	-2.55097200	-1.05375500	-1.29985400
H	-1.86393300	-1.65638300	-1.88228400
C	-2.17938600	0.10335800	-0.65035100
O	-1.03261600	0.62651000	-0.42267200
C	-3.24065600	1.52561700	1.03821000
H	-2.36222200	2.17288900	1.00717100
H	-4.13208000	2.13966300	1.19889400
H	-3.13849700	0.83831800	1.89985500
C	-4.45282000	-0.16016200	-0.25973800
H	-4.48964600	-0.72281200	0.69329700
H	-5.41805000	0.33607400	-0.40443400
N	-3.35732600	0.80520500	-0.21186100
C	-4.05669100	-1.11332400	-1.39690900
H	-4.49785100	-2.10525100	-1.25028700
H	-4.44228000	-0.73030300	-2.35767600
Na	1.08744400	0.30079500	-0.00278400

KO*t*Bu/18-crown-6 complex, solvent = DMSO



Charge = 0; Multiplicity = 1

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-1755.724960 [B3LYP/6-31+G(d,p)]

O	0.79531400	2.17820900	1.87039600
O	0.96963100	-0.43154400	3.05320500
O	0.87619500	-2.75354600	1.36670700
O	1.80399900	-2.43146600	-1.33206800

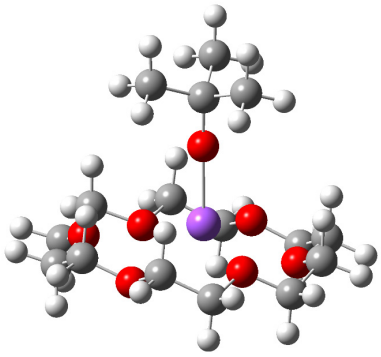
O	1.67053400	0.15472900	-2.57620000
O	1.74628300	2.42922900	-0.82597200
C	1.05207500	1.95716700	3.25549000
C	0.41951400	-1.68158300	3.46540100
C	1.53487200	-3.78232000	0.63085900
C	1.60216600	-2.23966900	-2.73118700
C	2.29652400	1.38980400	-2.91679900
C	1.12834500	3.49615700	-0.10823300
C	1.21536000	-3.63435400	-0.84067400
C	2.30744500	-0.97483200	-3.16941200
C	1.56775800	2.52866800	-2.23783200
C	1.43237000	3.35032000	1.36670100
C	0.36346800	0.68574500	3.70066900
C	1.15029600	-2.80617400	2.76512500
H	0.66660600	2.79783100	3.85152900
H	0.53575900	-1.80684500	4.55220300
H	1.19262600	-4.77081300	0.97199900
H	2.01667900	-3.08928600	-3.29379500
H	2.26245200	1.54500600	-4.00551000
H	1.52037000	4.46362500	-0.45550600
H	1.62154900	-4.50299500	-1.37980000
H	2.26165300	-0.90317000	-4.26636200
H	1.97858400	3.48071100	-2.60539100
H	1.06156600	4.24089000	1.89583500
H	0.46533200	0.59269300	4.79209600
H	0.80975800	-3.76543900	3.18275200
H	2.13535300	1.87981300	3.43000000
H	-0.65381100	-1.71950300	3.22781900
H	2.62183300	-3.72128000	0.78782700
H	0.52679200	-2.17202400	-2.95258000
H	3.35096600	1.37655600	-2.60381700
H	0.04117200	3.48510800	-0.27583500
H	0.12625600	-3.61246300	-0.99328500
H	3.36542200	-1.01085400	-2.87054700
H	0.49688900	2.49697300	-2.48742700
H	2.51926600	3.28486600	1.52250500
H	-0.70855900	0.72760700	3.45756000
H	2.23277100	-2.71943100	2.94045000
O	-1.83410300	-0.12583100	-0.37074600
K	0.67601500	-0.13959100	0.13291400
C	-3.19627900	-0.11248200	-0.61758200
C	-3.48888000	-0.28126000	-2.13505500
C	-3.91060800	-1.26872700	0.13730400
C	-3.83314500	1.22719500	-0.15197300
H	-3.00756500	0.52815800	-2.69810800
H	-3.07346300	-1.23259800	-2.49098200
H	-4.56305300	-0.26889200	-2.36819900
H	-3.73964400	-1.17143500	1.21687000
H	-4.99594300	-1.28620300	-0.03640100
H	-3.49822600	-2.23347400	-0.18401900
H	-4.91776400	1.26899900	-0.32558300
H	-3.65374400	1.36988200	0.92120000
H	-3.37014400	2.06659000	-0.68601300

-1755.166060 [M06-2X/6-31++G(d,p)]

O	0.74611700	2.12603300	1.82003800
O	0.85237400	-0.42145100	3.02283900
O	0.83268000	-2.68703700	1.33484700
O	1.69288600	-2.41669200	-1.33743600

O	1.53475600	0.13265300	-2.51825700
O	1.62607500	2.40547700	-0.83941900
C	0.90178200	1.94864100	3.21501300
C	0.26808100	-1.65658800	3.39632400
C	1.44497900	-3.74509400	0.62234700
C	1.42401100	-2.22860200	-2.71532500
C	2.07609800	1.37108600	-2.93657000
C	1.02040000	3.46302900	-0.11756700
C	1.09828100	-3.60125300	-0.83788800
C	2.11706800	-0.97347100	-3.18106400
C	1.34234600	2.47970000	-2.22513700
C	1.35387700	3.31180500	1.34474200
C	0.19084900	0.68127700	3.61629200
C	1.02719300	-2.77831300	2.73336300
H	0.46317200	2.79881900	3.75673300
H	0.31218500	-1.78165900	4.48764100
H	1.07470200	-4.71332600	0.98800800
H	1.79505500	-3.08624800	-3.29454000
H	1.95069400	1.49315500	-4.02196000
H	1.39335100	4.43125400	-0.48050400
H	1.47315100	-4.47533200	-1.38932200
H	1.99269700	-0.87354300	-4.26877900
H	1.66999300	3.44871300	-2.62761900
H	0.96997400	4.18323600	1.89418200
H	0.20437300	0.58661800	4.71139600
H	0.64938500	-3.74036900	3.10750400
H	1.96885600	1.88198100	3.47264500
H	-0.78642900	-1.68348300	3.08287100
H	2.53580700	-3.71340400	0.75891500
H	0.33916600	-2.13972800	-2.87759000
H	3.14944700	1.41499400	-2.70127800
H	-0.07102100	3.43385200	-0.25428600
H	0.00567000	-3.55240600	-0.95930900
H	3.19213200	-1.02735600	-2.95560100
H	0.25906500	2.37794700	-2.39073900
H	2.44350200	3.26214000	1.48497900
H	-0.85658800	0.71584500	3.28008800
H	2.09810100	-2.70609000	2.97327300
O	-1.41957700	-0.15317000	-0.25289600
K	1.04203700	-0.15038400	0.21412700
C	-2.76495600	-0.11564900	-0.54062000
C	-3.00206400	-0.24367600	-2.06099500
C	-3.50735800	-1.27307200	0.16214800
C	-3.38932900	1.21513700	-0.06673200
H	-2.47959000	0.56926900	-2.58006900
H	-2.58908400	-1.19496800	-2.41870500
H	-4.06496700	-0.20345900	-2.33318300
H	-3.36796500	-1.19334400	1.24730600
H	-4.58472000	-1.27972400	-0.04900500
H	-3.08370900	-2.23037800	-0.16541900
H	-4.46638200	1.27801600	-0.26987100
H	-3.23317600	1.32768200	1.01336100
H	-2.89256300	2.05335800	-0.57077500

NaO*t*Bu/18-crown-6 complex, solvent = DMSO



Charge = 0; Multiplicity = 1

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-1318.113397 [B3LYP/6-31+G(d,p)]

O	0.87288000	2.19964000	1.92676300
O	0.96937600	-0.40763800	2.96700400
O	0.89895000	-2.72378800	1.27894900
O	1.90969500	-2.51498100	-1.40839100
O	1.71352500	0.13191000	-2.52811300
O	1.71736100	2.38368000	-0.74973400
C	1.16497900	1.95040200	3.30040200
C	0.42353000	-1.66276500	3.37574000
C	1.50032300	-3.80031200	0.56474000
C	1.64822900	-2.25106300	-2.78097800
C	2.32376800	1.37713000	-2.84461300
C	1.18101100	3.50515900	-0.04870900
C	1.21170200	-3.64969900	-0.91159400
C	2.34240700	-0.96824300	-3.17904800
C	1.56900100	2.49657400	-2.16525600
C	1.51641300	3.36655500	1.41819500
C	0.45360900	0.68678500	3.72494800
C	1.15438700	-2.78606800	2.67707700
H	0.81762300	2.78842200	3.92165800
H	0.54552300	-1.78687600	4.46142800
H	1.09092800	-4.76041600	0.91430500
H	2.02564700	-3.07329500	-3.40876000
H	2.30212400	1.54854200	-3.93199100
H	1.62235700	4.43768900	-0.42902400
H	1.53845400	-4.56189200	-1.43487300
H	2.27711600	-0.84899100	-4.27137700
H	1.98114800	3.45671800	-2.50809100
H	1.16701700	4.25895400	1.95721800
H	0.62770900	0.52095500	4.79786400
H	0.79970100	-3.74362400	3.08865100
H	2.25039400	1.84124200	3.43837700
H	-0.65011000	-1.69916200	3.14168700
H	2.58716900	-3.80854900	0.73625700
H	0.56513200	-2.15954300	-2.95141600
H	3.37506000	1.37854200	-2.51901100
H	0.09166700	3.55347300	-0.19115900
H	0.12973200	-3.53134100	-1.07303700
H	3.40657600	-1.01461500	-2.90268300
H	0.50411900	2.46080100	-2.43697100
H	2.60453400	3.28251200	1.55211600
H	-0.62942700	0.78248800	3.56055500
H	2.23544600	-2.71085100	2.86890900

O	-1.36028000	0.09411400	-0.14420500
C	-2.68759200	-0.07352800	-0.49935800
C	-2.81300000	-0.50173700	-1.98752000
C	-3.36299400	-1.16762000	0.37302000
C	-3.47987600	1.24877000	-0.30900500
H	-2.37666100	0.26779400	-2.63642500
H	-2.26121000	-1.43551800	-2.15261200
H	-3.85518400	-0.65923900	-2.29846300
H	-3.30278300	-0.89021700	1.43282800
H	-4.42150000	-1.31928700	0.11945100
H	-2.84171000	-2.12437500	0.24434500
H	-4.54004600	1.15476000	-0.58261400
H	-3.42476400	1.56733300	0.73954100
H	-3.03688300	2.04057500	-0.92594700
Na	0.70575700	0.22467400	0.43560900

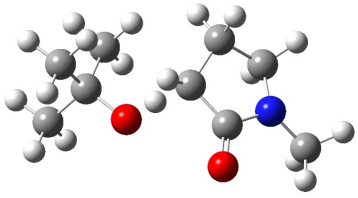
-1317.539804 [M06-2X/6-31++G(d,p)]

O	0.98562500	2.09008400	1.87401800
O	0.93336500	-0.43147900	2.98346400
O	0.86473200	-2.62642000	1.29814500
O	1.73410100	-2.36456700	-1.34862400
O	1.60426800	0.16650900	-2.51805800
O	1.70781300	2.39208500	-0.79832900
C	1.17959500	1.90581500	3.26256900
C	0.30919900	-1.64151800	3.37423100
C	1.41087700	-3.71219800	0.57497300
C	1.55551800	-2.18494500	-2.73953800
C	2.10981100	1.41934300	-2.92595000
C	1.15672900	3.45496100	-0.04597000
C	1.08402700	-3.52929500	-0.88302300
C	2.24998000	-0.91515300	-3.15475800
C	1.37340900	2.49318700	-2.16962500
C	1.56866000	3.28503400	1.39192800
C	0.40230600	0.68427900	3.67562600
C	1.01859300	-2.78197900	2.69449100
H	0.81264900	2.77986800	3.81859100
H	0.37437500	-1.76665000	4.46394900
H	0.97669100	-4.65828700	0.92854400
H	1.98132800	-3.03622500	-3.29080300
H	1.95758100	1.56071000	-4.00621100
H	1.52377100	4.42008800	-0.42352200
H	1.42653700	-4.41050500	-1.44514600
H	2.18977200	-0.80900800	-4.24794900
H	1.66487000	3.47940000	-2.55867800
H	1.21269300	4.14401600	1.97780700
H	0.49267700	0.53658000	4.76063300
H	0.57736500	-3.73339500	3.02427900
H	2.24868800	1.77177400	3.48225200
H	-0.75174900	-1.62636200	3.08371900
H	2.50061200	-3.75260800	0.71813200
H	0.48301200	-2.11654000	-2.97643000
H	3.18753400	1.48449100	-2.71426200
H	0.05878400	3.44152700	-0.12285800
H	-0.00470500	-3.43289600	-1.01538100
H	3.31106400	-0.94870200	-2.86595800
H	0.28728600	2.36952300	-2.30125300
H	2.66392500	3.23329100	1.47422500
H	-0.66131800	0.80916500	3.42261400
H	2.08551500	-2.77976700	2.96118800

O	-1.13635700	0.03458200	-0.02954500
C	-2.43542400	-0.11225700	-0.45837200
C	-2.47668600	-0.47447400	-1.95774500
C	-3.14654600	-1.23291100	0.32951700
C	-3.22574400	1.19745400	-0.25447200
H	-1.97539200	0.31028300	-2.53763600
H	-1.93745700	-1.41562000	-2.12186600
H	-3.49894500	-0.59004800	-2.34047300
H	-3.13244600	-0.99234900	1.39953400
H	-4.18979800	-1.37460100	0.01889500
H	-2.61145100	-2.18006500	0.18706500
H	-4.27236800	1.11814600	-0.57517500
H	-3.20729400	1.47317200	0.80704500
H	-2.74939100	2.00544900	-0.82330900
Na	0.92579200	-0.05903400	0.47014500

10.5.2. XYZ Co-ordinates of transition states

Deprotonation of NMP (19) with $^{-}$O*t*Bu anion T.S., solvent = DMSO



Charge = -1; Multiplicity = 1

30

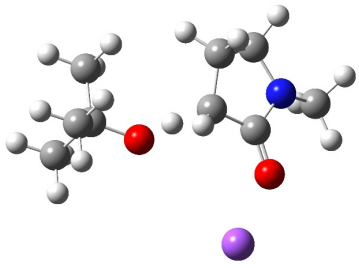
-558.943355 [B3LYP/6-31+G(d,p)]

C	-0.20333000	-0.14895200	0.65294200
O	0.88904100	0.45573400	0.80874400
C	-1.12283500	1.53749600	-0.93366900
H	-0.26585700	2.13929900	-0.62603400
H	-0.94990000	1.17835400	-1.96198700
H	-2.01766700	2.16921700	-0.94015700
C	-2.34704800	-0.54212700	-0.21915900
H	-3.33597800	-0.07356900	-0.15832900
H	-2.24830400	-0.99218900	-1.22269300
N	-1.28682800	0.44186600	-0.00110800
C	-2.08055000	-1.58572500	0.88319800
H	-2.61476400	-1.29507900	1.80177000
H	-2.45419800	-2.57405400	0.59116500
H	0.08372000	-2.37106100	0.09523600
O	0.70094900	-3.03846200	-0.72540800
C	0.52923600	-4.44070500	-0.67322500
C	1.62768100	-5.09098800	-1.53782800
H	2.61931600	-4.83034000	-1.14995100
H	1.54127100	-6.18516300	-1.55302600
H	1.56011900	-4.72754100	-2.56996900
C	0.65584400	-4.95786800	0.77842700
H	-0.11941000	-4.51724400	1.41452800
H	0.55754500	-6.04966400	0.82875400
H	1.63247800	-4.68320600	1.19387700
C	-0.85422500	-4.84072800	-1.23673400
H	-1.65562000	-4.38628700	-0.64350700
H	-0.95555300	-4.48910200	-2.27023900
H	-1.00114100	-5.92857100	-1.22917800
C	-0.55732100	-1.50706400	1.03502400
H	-0.14082600	-1.81902000	1.99727600

-558.666310 [M06-2X/6-31++G(d,p)]

C	-0.13383500	-0.13538400	0.64092800
O	0.89308800	0.56985600	0.66606300
C	-1.28308200	1.27915700	-1.03024700
H	-0.47279600	1.98068500	-0.82788800
H	-1.12643900	0.83058400	-2.02291500
H	-2.23333600	1.82093300	-1.04274200
C	-2.24991400	-0.82505600	-0.06814600
H	-3.27823500	-0.45352000	-0.01293400
H	-2.12890800	-1.36600800	-1.02245800
N	-1.29586300	0.27342700	0.00554600
C	-1.84011500	-1.70789900	1.11914500
H	-2.34799600	-1.35569600	2.02837900
H	-2.13562200	-2.75050900	0.95977000
H	0.30130700	-2.28142500	0.25077300
O	0.95698300	-2.96780200	-0.60111200
C	0.53077000	-4.29544200	-0.71068800
C	1.59054900	-5.09995200	-1.47579700
H	2.54372800	-5.06921800	-0.93627100
H	1.29566800	-6.14902000	-1.60109100
H	1.74479800	-4.66197300	-2.46835200
C	0.33877000	-4.92306700	0.68246000
H	-0.42389100	-4.37294200	1.24499200
H	0.02759100	-5.97244700	0.61535800
H	1.27808300	-4.87537100	1.24510500
C	-0.80055700	-4.37045400	-1.47949800
H	-1.57038900	-3.79826100	-0.94920700
H	-0.67755400	-3.93213500	-2.47655400
H	-1.15473800	-5.40224000	-1.59413100
C	-0.32898000	-1.48456100	1.16593700
H	0.16675900	-1.65700500	2.12431300

Deprotonation of NMP (19) with NaO*t*Bu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

31

-721.200806 [B3LYP/6-31+G(d,p)]

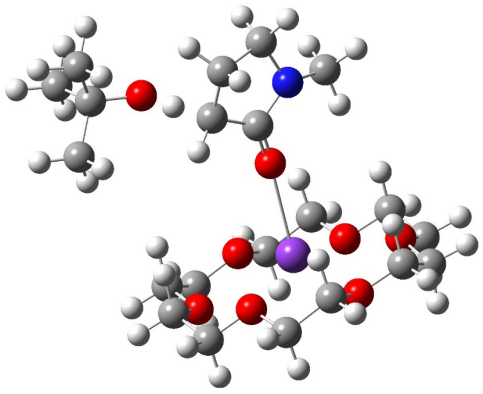
C	-0.24006800	-0.08552700	0.57044000
C	-1.26306300	1.55118500	-1.00182100
H	-0.39986800	2.16869800	-0.74884100
H	-1.14956500	1.19155400	-2.03693200
H	-2.16893400	2.16422400	-0.95026200
C	-2.40336900	-0.55296500	-0.19187300
H	-3.39282800	-0.09444900	-0.08813000
H	-2.35212100	-1.02542000	-1.18729500
N	-1.34681700	0.45269700	-0.06099400
C	-2.06043300	-1.56140300	0.92300300
H	-2.56430100	-1.26612500	1.85592200
H	-2.41209500	-2.56742400	0.66851700
H	0.10142000	-2.29502900	0.10735400

O	0.74690600	-2.97792400	-0.70824900
C	0.57070200	-4.37885300	-0.66148900
C	1.68830400	-5.03480200	-1.49746300
H	2.67102600	-4.77891100	-1.08432900
H	1.59749200	-6.12860500	-1.51509700
H	1.64898300	-4.67093100	-2.53092800
C	0.65744800	-4.89671000	0.79315700
H	-0.13284300	-4.45283800	1.40844700
H	0.55335800	-5.98806000	0.84167000
H	1.62397700	-4.62584100	1.23414300
C	-0.79952700	-4.77426100	-1.26004000
H	-1.61407300	-4.31848900	-0.68586700
H	-0.87367500	-4.41983800	-2.29483900
H	-0.95024300	-5.86160500	-1.25874400
C	-0.53463900	-1.43538200	1.01709800
H	-0.07832200	-1.69272500	1.97726200
O	0.84827300	0.55301300	0.66147200
Na	2.87988800	0.04914200	1.38969900

-720.886967 [M06-2X/6-31++G(d,p)]

C	-0.19954700	-0.11416900	0.57077100
C	-1.40383600	1.26655600	-1.09170300
H	-0.60261700	1.98451400	-0.91268400
H	-1.27458600	0.82823600	-2.09140300
H	-2.36539300	1.78646400	-1.06190600
C	-2.30938700	-0.85540900	-0.08434100
H	-3.33605700	-0.48475500	-0.00709800
H	-2.21270000	-1.41475900	-1.02930100
N	-1.35857500	0.25050800	-0.06648400
C	-1.86004800	-1.70588800	1.11302800
H	-2.35805400	-1.34778300	2.02437200
H	-2.13238700	-2.75755800	0.97815200
H	0.27065400	-2.23677600	0.24363900
O	0.93442400	-2.93501300	-0.63021600
C	0.53760700	-4.27251400	-0.71417100
C	1.60233800	-5.06767300	-1.48322500
H	2.56330400	-5.00628100	-0.96034100
H	1.32962200	-6.12525400	-1.58543700
H	1.73061400	-4.64401500	-2.48566500
C	0.38051000	-4.88337700	0.69109700
H	-0.38496300	-4.34123300	1.25776800
H	0.09117700	-5.94013000	0.64576800
H	1.32725400	-4.80655600	1.23793700
C	-0.80401000	-4.39104800	-1.46017700
H	-1.57769800	-3.82549600	-0.92823700
H	-0.70711700	-3.97007600	-2.46754900
H	-1.13772200	-5.43223900	-1.54894400
C	-0.35251600	-1.44966200	1.13535600
H	0.15772900	-1.58233500	2.09178300
O	0.81974000	0.61280200	0.57147000
Na	2.36750100	2.15525100	0.53668900

Reaction of NMP K^+/18-crown-6 complex with $^-$OtBu (3) T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

73

-2081.563254 [B3LYP/6-31+G(d,p)]

O	0.69492100	2.47841000	1.61356200
O	0.98546500	0.13668100	3.24497800
O	1.10443700	-2.44734800	2.00672400
O	2.09520400	-2.54288400	-0.68372300
O	1.80888200	-0.24616000	-2.37727800
O	1.67956000	2.30652000	-1.07452700
C	0.93339100	2.52381300	3.01929200
C	0.49362800	-1.05225000	3.86203900
C	1.86530000	-3.53653600	1.48733400
C	1.93106700	-2.62809200	-2.09877200
C	2.33890600	0.95243400	-2.94073200
C	0.98822400	3.44580600	-0.56456100
C	1.58883500	-3.68418600	0.00732900
C	2.54752900	-1.40889400	-2.74848900
C	1.51406400	2.13467100	-2.48153700
C	1.27070100	3.58130800	0.91561500
C	0.30562100	1.31449800	3.67700200
C	1.31905200	-2.23317100	3.40052400
H	0.48938600	3.43365100	3.44982300
H	0.57232700	-0.97150100	4.95617100
H	1.58583900	-4.47070500	1.99669400
H	2.43496300	-3.52651800	-2.48468200
H	2.30710800	0.90105100	-4.03914000
H	1.33262900	4.35729700	-1.07495500
H	2.08431700	-4.59681200	-0.35538800
H	2.52583300	-1.53888900	-3.84063200
H	1.85654900	3.03319200	-3.01561900
H	0.83634800	4.52581400	1.27542700
H	0.39034900	1.42173300	4.76845800
H	1.01707900	-3.12363600	3.97161200
H	2.01520200	2.54131900	3.21719200
H	-0.56475000	-1.20281700	3.60319300
H	2.93791900	-3.36003000	1.65503600
H	0.86331600	-2.69712400	-2.35297800
H	3.38647100	1.08219200	-2.63168500
H	-0.09289400	3.34224400	-0.73860100
H	0.50829600	-3.78476400	-0.17035200
H	3.59642300	-1.30421900	-2.43452900
H	0.45230700	1.97573300	-2.72078700
H	2.35605200	3.61218000	1.09094500
H	-0.76187400	1.25174300	3.41928600

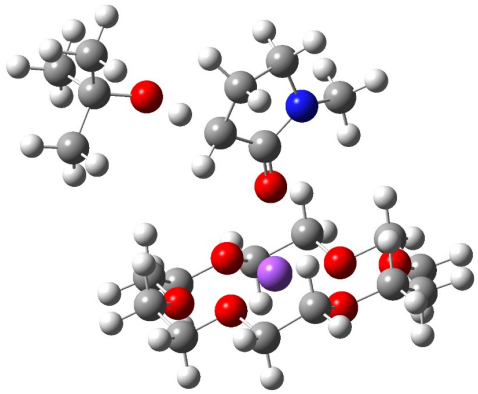
H	2.38565500	-2.04557300	3.59263900
C	-2.95645300	-0.65995600	-0.07096100
O	-1.73562000	-0.34500700	-0.10147200
C	-3.75682600	1.68029300	-0.36991100
H	-2.71250600	1.94592400	-0.19863600
H	-3.99334100	1.84708400	-1.43348800
H	-4.39525900	2.33887400	0.22858800
C	-5.27550200	-0.31989000	-0.15429500
H	-6.02681100	0.18630100	0.46215300
H	-5.59767400	-0.24644800	-1.20751300
N	-3.95991500	0.29871000	0.01377800
K	0.86662000	-0.10549200	0.34153100
C	-5.02115700	-1.78606100	0.24735200
H	-5.17626600	-1.90368900	1.33124600
H	-5.72045500	-2.46242100	-0.25673700
C	-3.55594000	-1.98087500	-0.16246700
H	-2.99513500	-2.75996100	0.36167800
H	-3.49151000	-2.36193300	-1.51944900
O	-3.43864700	-2.62172000	-2.72987100
C	-3.56085000	-3.98457000	-3.08191500
C	-3.46251200	-4.09806000	-4.61619100
H	-2.50187900	-3.70102700	-4.96474100
H	-3.54627800	-5.13925800	-4.95387800
H	-4.26265000	-3.51851600	-5.09133800
C	-2.42585900	-4.81700200	-2.44082300
H	-2.46912600	-4.74743300	-1.34830700
H	-2.49010300	-5.87715700	-2.71768600
H	-1.45050600	-4.43722100	-2.76669200
C	-4.92548900	-4.54710900	-2.62111900
H	-5.01940400	-4.47909500	-1.53167700
H	-5.74159600	-3.96757900	-3.06867500
H	-5.05302200	-5.59837000	-2.90950100

-2080.855504 [M06-2X/6-31++G(d,p)]

O	0.40050200	2.43412100	1.36372900
O	0.07401200	-0.00381600	2.78853700
O	0.47693700	-2.31437900	1.32039900
O	1.87895300	-2.39239600	-1.09795900
O	2.32696000	0.10537300	-2.37338200
O	2.09912500	2.48001800	-0.88200700
C	0.11481900	2.37840900	2.75007400
C	-0.65332700	-1.18985700	3.06143500
C	0.87174600	-3.53779500	0.73707500
C	1.99747200	-2.24096000	-2.50090900
C	3.13213000	1.24117000	-2.63106900
C	1.34216500	3.60692800	-0.47704400
C	0.89109500	-3.35130300	-0.75940400
C	2.93937400	-1.10121900	-2.79237400
C	2.34537900	2.47728800	-2.27698200
C	1.17199400	3.57052700	1.01999300
C	-0.71228500	1.15049100	3.02979700
C	0.19170900	-2.38699300	2.70155700
H	-0.44901500	3.27171000	3.05442100
H	-0.92162600	-1.23262500	4.12728800
H	0.14715600	-4.32851500	0.98483900
H	2.38687500	-3.16600900	-2.94950900
H	3.40425700	1.28045100	-3.69526700
H	1.86100700	4.53370100	-0.76036900
H	1.11116300	-4.31292400	-1.24653800

H	3.14572900	-1.06481100	-3.87131000
H	2.91937900	3.37014500	-2.56214500
H	0.66196800	4.48821600	1.34611000
H	-1.04155000	1.17040400	4.07893700
H	-0.38057400	-3.29846700	2.92768500
H	1.05093900	2.34356000	3.32649000
H	-1.57400000	-1.20175900	2.46069100
H	1.86153800	-3.84414000	1.10655000
H	1.01110400	-2.02919900	-2.94055100
H	4.05561500	1.19341700	-2.03594600
H	0.35771300	3.59257200	-0.96746300
H	-0.09341800	-2.99479500	-1.09561300
H	3.89010100	-1.24908500	-2.25957900
H	1.39253700	2.48318000	-2.82589900
H	2.15394200	3.52268900	1.51297500
H	-1.60201300	1.13396300	2.38225300
H	1.12284000	-2.40497600	3.28631800
C	-2.22916500	-0.79557300	-0.09970000
O	-1.19303400	-0.40500300	-0.67606800
C	-3.17503500	1.48325000	0.06017200
H	-2.15684700	1.81356900	-0.15292900
H	-3.80005500	1.64832300	-0.83003600
H	-3.57980100	2.08094200	0.88295400
C	-4.37720200	-0.59738400	0.79594200
H	-4.83616300	-0.13647300	1.67664600
H	-5.09712700	-0.53723100	-0.03738700
N	-3.14396600	0.08948400	0.43579200
K	1.22790700	0.03953300	0.19624600
C	-3.91106600	-2.04441100	1.02113600
H	-3.62337800	-2.17761900	2.07403000
H	-4.71743000	-2.75438900	0.80946700
C	-2.72260800	-2.16124900	0.06482100
H	-1.93332100	-2.86015800	0.35445800
H	-3.13266400	-2.54853400	-1.16673100
O	-3.53378200	-2.88529500	-2.33816800
C	-3.59547400	-4.27308100	-2.50205200
C	-4.17724300	-4.58709200	-3.88645600
H	-3.54289200	-4.14743500	-4.66446800
H	-4.24934300	-5.66681800	-4.06571900
H	-5.17918300	-4.15274800	-3.97641400
C	-2.19052600	-4.89504800	-2.39641200
H	-1.77349800	-4.71154500	-1.39943500
H	-2.20865300	-5.97826600	-2.56762400
H	-1.52289500	-4.43656400	-3.13550900
C	-4.49511700	-4.90518200	-1.42428100
H	-4.07988900	-4.71164900	-0.42865900
H	-5.49612600	-4.46063500	-1.46943000
H	-4.58978400	-5.99006900	-1.55453400

Reaction of NMP Na^+/18-crown-6 complex with $^-$OtBu (3) T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

73

-1643.949720 [B3LYP/6-31+G(d,p)]

O	0.76754600	2.51838500	1.58270000
O	0.86963400	0.10368600	3.11819200
O	1.07607800	-2.43302100	1.92397100
O	2.07418700	-2.41058000	-0.69377400
O	1.94426100	-0.06748600	-2.32224300
O	1.91789700	2.50628900	-1.04376800
C	0.91073900	2.50079100	2.99786500
C	0.37405300	-1.07355500	3.75612000
C	1.85696600	-3.51292200	1.41468400
C	1.97070000	-2.45543600	-2.11795700
C	2.50271000	1.11268700	-2.89444400
C	1.18344300	3.60219100	-0.51328900
C	1.62290800	-3.61558300	-0.07409400
C	2.64804700	-1.24231100	-2.71051500
C	1.71409600	2.31841800	-2.43846800
C	1.38605900	3.65350700	0.98362000
C	0.20493900	1.28849500	3.55921200
C	1.22160000	-2.24985900	3.33126300
H	0.46395000	3.40510400	3.43888900
H	0.43316000	-0.96618100	4.84861100
H	1.56009800	-4.45644400	1.89454700
H	2.46917800	-3.35779000	-2.50015700
H	2.46409800	1.05339100	-3.99267500
H	1.53204600	4.54831900	-0.95577000
H	2.18334700	-4.47608600	-0.46677700
H	2.65049800	-1.34144000	-3.80676600
H	2.05687800	3.20166300	-2.99950900
H	0.93794900	4.57955400	1.37482300
H	0.22998000	1.34380500	4.65705800
H	0.88898600	-3.14990100	3.86787700
H	1.97638600	2.47675300	3.27150200
H	-0.67752900	-1.23807300	3.48025200
H	2.92193100	-3.33593100	1.62343400
H	0.91364200	-2.49172600	-2.41721300
H	3.55578600	1.21647500	-2.59308700
H	0.11334800	3.49127800	-0.74397800
H	0.55573600	-3.77125000	-0.28547700
H	3.69256500	-1.18787200	-2.36866800
H	0.64424800	2.17246200	-2.65037400
H	2.46094100	3.66695100	1.21864700
H	-0.84631800	1.27224700	3.23732400

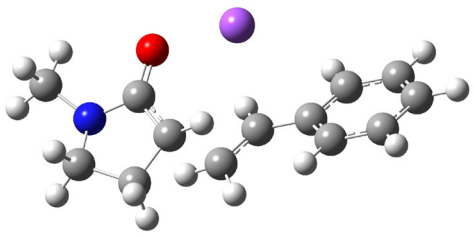
H	2.27734700	-2.06699100	3.57809500
C	-2.35866700	-0.65988000	-0.01736800
O	-1.14015900	-0.33622100	-0.08611500
C	-3.18046200	1.66364300	-0.38456300
H	-2.13381100	1.94057400	-0.25177300
H	-3.44922500	1.79493100	-1.44511400
H	-3.80590700	2.33637200	0.21178400
C	-4.68034800	-0.33820400	-0.05529300
H	-5.41427800	0.18856700	0.56459600
H	-5.03527500	-0.30698700	-1.09964800
N	-3.36379200	0.29330800	0.04696200
C	-4.40395800	-1.78575100	0.39582500
H	-4.52812600	-1.86262300	1.48706300
H	-5.11013700	-2.48600300	-0.06333200
C	-2.94863900	-1.98762600	-0.04537400
H	-2.36941400	-2.74392600	0.49131900
H	-2.92833300	-2.41031000	-1.38269500
O	-2.91890600	-2.70549500	-2.59360700
C	-3.11143100	-4.06642000	-2.91740200
C	-3.06750300	-4.20656600	-4.45206300
H	-2.10555600	-3.84673600	-4.83543900
H	-3.19731500	-5.24873200	-4.77174900
H	-3.86204700	-3.60577200	-4.91012100
C	-1.99295400	-4.93766200	-2.29905600
H	-2.00052400	-4.85231900	-1.20667800
H	-2.10946700	-5.99778800	-2.55855800
H	-1.01312500	-4.60276200	-2.65883700
C	-4.48331400	-4.56336800	-2.40490300
H	-4.53654600	-4.48615500	-1.31337100
H	-5.28688400	-3.94911200	-2.82808500
H	-4.66849200	-5.60918900	-2.68166000
Na	1.02142100	-0.37140100	0.52742700

-1643.226610 [M06-2X/6-31++G(d,p)]

O	0.33394500	2.28904100	1.53956300
O	0.20268800	-0.21571300	2.76925900
O	0.82139400	-2.33883200	1.16231000
O	1.99366100	-2.18750900	-1.31753700
O	2.45980100	0.40719000	-2.19722600
O	2.18250200	2.57248600	-0.51979800
C	-0.12783800	2.12415000	2.86567600
C	-0.27547200	-1.50958100	3.07680800
C	1.18022100	-3.51343000	0.46145900
C	1.94712700	-1.84147500	-2.68889400
C	3.32761200	1.51952200	-2.30975800
C	1.40957700	3.66567500	-0.06337100
C	1.06538100	-3.21200200	-1.00867400
C	2.92587000	-0.72101400	-2.91440800
C	2.57219200	2.74431100	-1.86822500
C	1.09795900	3.46849500	1.39520000
C	-0.78485900	0.77547200	2.98159500
C	0.72138600	-2.51628200	2.56329800
H	-0.84938800	2.91477500	3.11845500
H	-0.40732100	-1.62229200	4.16297300
H	0.49458100	-4.33391200	0.71952300
H	2.21926400	-2.70673000	-3.30978700
H	3.64511000	1.65230600	-3.35329700
H	1.96550700	4.60595200	-0.19135600
H	1.28634900	-4.11689200	-1.59380500

H	2.98871600	-0.48766700	-3.98628100
H	3.21121300	3.63320300	-1.97179300
H	0.53430500	4.33916500	1.76165500
H	-1.22222700	0.67167200	3.98530700
H	0.35867400	-3.52628600	2.79687800
H	0.71608400	2.18439700	3.56886100
H	-1.24264800	-1.67703400	2.58138800
H	2.20510700	-3.81858000	0.71861900
H	0.93015200	-1.51541100	-2.95022200
H	4.22163000	1.36534700	-1.68874000
H	0.47695700	3.73174000	-0.64279300
H	0.04743600	-2.86666700	-1.24024900
H	3.92452900	-1.01249400	-2.55778100
H	1.68189500	2.87772700	-2.50062700
H	2.02825400	3.38747900	1.97675100
H	-1.58595200	0.67024000	2.23284800
H	1.70412400	-2.37967100	3.03561100
C	-1.74460100	-0.56276200	-0.49151200
O	-0.61226000	-0.36086100	-0.98659200
C	-2.57155600	1.70231100	-1.05139200
H	-1.52773400	1.87195900	-1.31973000
H	-3.17958300	1.68986900	-1.96722900
H	-2.91795100	2.52303700	-0.41555200
C	-3.96371400	-0.08198200	0.05103100
H	-4.47838400	0.61266000	0.72281500
H	-4.59487500	-0.23038100	-0.84082100
N	-2.66592800	0.44756500	-0.34471800
C	-3.59952600	-1.42487000	0.70237000
H	-3.41218000	-1.27031000	1.77536000
H	-4.41991200	-2.14347700	0.60916000
C	-2.33724400	-1.82691700	-0.06350400
H	-1.62602600	-2.47467900	0.45424100
H	-2.67505300	-2.46698000	-1.19861900
O	-3.03016600	-3.05261000	-2.29816200
C	-3.21823200	-4.42841000	-2.13517500
C	-3.75314700	-5.02146400	-3.44546700
H	-3.04176700	-4.82981300	-4.25675200
H	-3.91117600	-6.10434300	-3.37036500
H	-4.70647000	-4.54850800	-3.70705100
C	-1.88749500	-5.11851800	-1.78211200
H	-1.49376400	-4.71086500	-0.84339500
H	-2.00548400	-6.20281600	-1.66477200
H	-1.14927700	-4.93192900	-2.57070000
C	-4.23024900	-4.70698600	-1.00839700
H	-3.84621500	-4.32415200	-0.05614000
H	-5.17601500	-4.19640400	-1.22468900
H	-4.43120200	-5.77901700	-0.89376800
Na	1.34262800	-0.14681600	0.05407500

Reaction of NMP Na enolate with styrene (**3**) **T.S.**, solvent = DMSO



Charge =0; Multiplicity = 1

32

-797.151944 [B3LYP/6-31+G(d,p)]

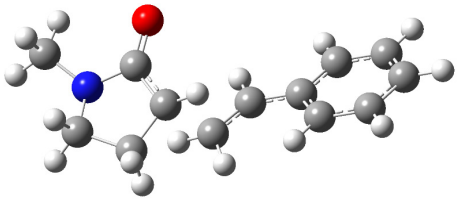
C	-4.78567700	-0.30284300	-0.52420500
C	-4.46078200	0.75708800	0.33584700
C	-3.18790800	0.85687000	0.89354500
C	-2.16982500	-0.10063900	0.62430500
C	-2.52031800	-1.15719400	-0.26303700
C	-3.79802000	-1.25455300	-0.81402900
H	-5.77789800	-0.38181500	-0.95846300
H	-5.20798900	1.51032000	0.57506000
H	-2.96167300	1.68481400	1.56298700
H	-1.77817200	-1.90694000	-0.52189600
H	-4.02415400	-2.08052400	-1.48472600
C	-0.86251200	0.02536300	1.23813700
H	-0.69049200	0.93544500	1.81341300
C	0.17151100	-0.90100500	1.14595000
H	-0.04715800	-1.92976300	0.86865000
H	1.01589500	-0.79853900	1.82257800
C	1.55039400	-0.86932000	-0.57717900
H	0.77857100	-0.97700400	-1.32984300
C	2.18746700	0.38243500	-0.37718900
O	1.73034800	1.54961600	-0.58485300
C	4.43141100	1.22145200	0.27187000
H	3.94145900	2.18607300	0.41325800
H	5.12908300	1.05316300	1.09852700
H	5.01357100	1.25779900	-0.66561500
C	3.86124600	-1.20373500	0.00631900
H	4.53016000	-1.23824700	-0.87147400
H	4.41887600	-1.59216900	0.86521000
N	3.42824200	0.17689100	0.24566400
C	2.54191600	-1.97237500	-0.26642900
H	2.66796400	-2.69945600	-1.07597800
H	2.24657500	-2.54863800	0.62814700
Na	-0.44077500	1.90918500	-0.90400800

-796.815503 [M06-2X/6-31++G(d,p)]

C	-4.65207200	-0.27213500	-0.56220100
C	-4.36288200	0.76794800	0.32662100
C	-3.10841300	0.86555200	0.91876700
C	-2.08315400	-0.07365900	0.65157800
C	-2.39208100	-1.10519300	-0.26811300
C	-3.65217700	-1.20306200	-0.85208900
H	-5.63155200	-0.35061100	-1.02283800
H	-5.12384700	1.50711600	0.56266700
H	-2.90431100	1.67735400	1.61421100
H	-1.63088100	-1.83516900	-0.52940000
H	-3.85236400	-2.01189400	-1.54992700
C	-0.77983500	0.04742000	1.28181900
H	-0.58551900	0.96588400	1.83322600
C	0.21826900	-0.90202000	1.18255400
H	-0.03145900	-1.92961600	0.92344800
H	1.10105200	-0.80431800	1.81184600
C	1.49062400	-0.92718900	-0.59712500
H	0.68653700	-1.05431400	-1.31184200
C	2.07674300	0.33163300	-0.36525700
O	1.59505000	1.48401800	-0.55547300
C	4.27994700	1.22101600	0.26026900
H	3.78004200	2.17165900	0.44893300

H	5.03751200	1.05719300	1.03118600
H	4.78698500	1.27657600	-0.71775400
C	3.78290200	-1.19648800	0.00557200
H	4.41836400	-1.17651600	-0.89673500
H	4.38086600	-1.58654200	0.83464700
N	3.30472300	0.15390200	0.29665600
C	2.49258100	-2.00294000	-0.25524500
H	2.64257200	-2.74852000	-1.04108600
H	2.20023800	-2.55366600	0.65652300
Na	-0.55312400	1.79833700	-0.92489600

Reaction of NMP "naked enolate" with styrene (**3**) **T.S.**, solvent = DMSO



Charge = -1; Multiplicity = 1

31

-634.894475 [B3LYP/6-31+G(d,p)]

C	-1.99389900	1.34137900	0.07652700
C	-1.80150000	2.68598000	0.43303800
C	-0.58361500	3.31893200	0.19734800
C	0.51675700	2.64353900	-0.40454900
C	0.28961600	1.28550700	-0.77135500
C	-0.93118500	0.65549100	-0.52932700
H	-2.94347500	0.84706300	0.25974000
H	-2.61086900	3.24403000	0.89900500
H	-0.45953300	4.36141000	0.48509500
H	1.08330700	0.72269300	-1.25450000
H	-1.05819900	-0.38413300	-0.82429400
C	1.77224800	3.32712400	-0.61124600
H	1.76907700	4.39683000	-0.40277800
C	2.92057100	2.76777400	-1.16186300
H	3.06387300	1.68955200	-1.12871400
H	3.84857400	3.33147700	-1.10140600
C	3.14535700	2.60377000	-3.33858000
H	2.22268800	2.06203100	-3.51109800
C	3.25153400	3.96527900	-3.74581400
O	2.34755100	4.83393000	-3.88879700
C	5.02362700	5.47544100	-4.60684800
H	4.34352900	6.29427700	-4.36571900
H	6.04142200	5.76547100	-4.32581000
H	5.00382000	5.31671300	-5.70033000
C	5.38105100	3.05740600	-4.11069500
H	5.50475500	2.89365100	-5.19654200
H	6.38222100	3.12240300	-3.66978200
N	4.62367800	4.28992700	-3.87707100
C	4.50402500	1.94644900	-3.47850400
H	4.50297400	1.04367300	-4.09981500
H	4.92007400	1.64895000	-2.49892500

-634.592611 [M06-2X/6-31++G(d,p)]

C	-1.91956100	1.39003100	0.01160600
C	-1.72438600	2.71804100	0.40735000
C	-0.50816500	3.35306100	0.18566700

C	0.57818100	2.69224400	-0.43862000
C	0.35113400	1.35522100	-0.84756300
C	-0.86745700	0.72098000	-0.61923500
H	-2.86921800	0.89378800	0.18422500
H	-2.52981100	3.26159000	0.89483700
H	-0.37603800	4.38535800	0.50373000
H	1.14021800	0.81132500	-1.35941400
H	-1.00047500	-0.30693900	-0.94755800
C	1.83917100	3.37305300	-0.64314500
H	1.84555100	4.44554400	-0.45861100
C	2.96521800	2.77605500	-1.17392100
H	3.08838200	1.69558500	-1.11067000
H	3.90434500	3.32718200	-1.17103100
C	3.12098400	2.51315700	-3.33071900
H	2.20300600	1.95132300	-3.45324900
C	3.18689100	3.88207300	-3.68065400
O	2.27066100	4.73092400	-3.79262200
C	4.88756200	5.43756800	-4.53496300
H	4.22055000	6.25119600	-4.24720700
H	5.91984200	5.73222300	-4.32581400
H	4.78922600	5.27051500	-5.62168300
C	5.32234900	3.04863800	-4.07929400
H	5.39226600	2.91816900	-5.17406900
H	6.33956600	3.12236300	-3.68141800
N	4.55325100	4.25281100	-3.77704300
C	4.49758400	1.90667800	-3.44994500
H	4.54465800	1.00101500	-4.06217700
H	4.91456600	1.64324600	-2.46040100

10.6. REACTION PROFILES FOR CYCLOHEXANONE (25) OR α-TETRALONE (27) WITH STYRENE

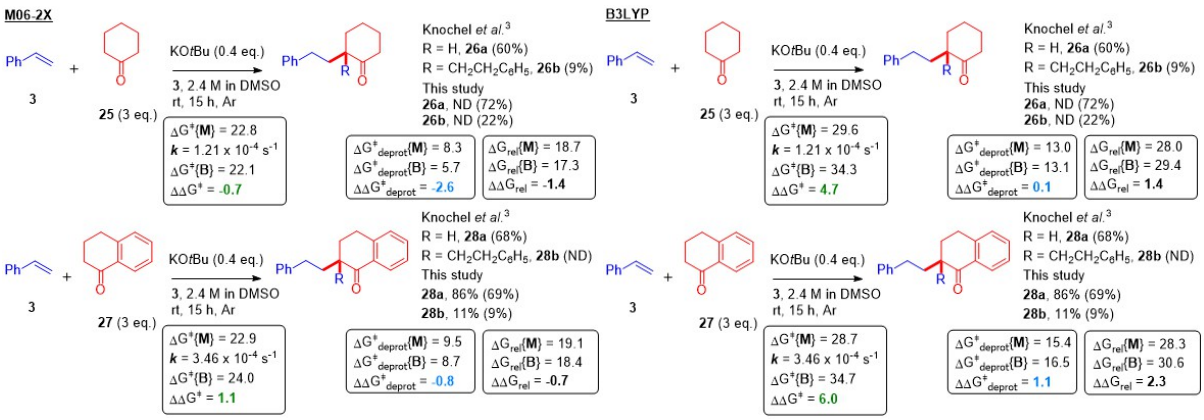
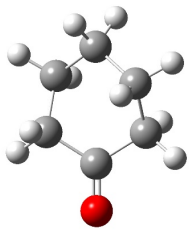


Figure S71. Application of the computational model to ketone CAKES. Comparison of B3LYP/6-31+G(d,p) and M06-2X/6-31++(d,p) methods.

10.6.1. XYZ Co-ordinates of starting materials, intermediates, products

Cyclohexanone (**25**), solvent = DMSO



Charge = 0; Multiplicity = 1

17

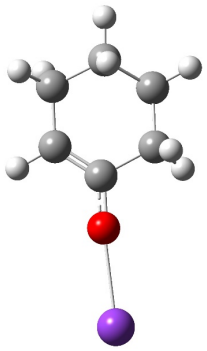
-309.800369 [B3LYP/6-31+G(d,p)]

C	1.17194800	-0.00001300	-0.00001300
O	2.39924200	0.00000900	0.00008000
C	-1.00200900	1.23880600	0.36208500
H	-1.54184300	2.15890300	0.11628900
H	-0.82868300	1.26704800	1.44481400
C	0.36328500	-1.23670000	0.34611100
H	0.95753400	-2.12528700	0.11193800
H	0.22226400	-1.22906400	1.43791300
C	-1.00205900	-1.23875500	-0.36210300
H	-1.54189000	-2.15887700	-0.11638700
H	-0.82881800	-1.26688200	-1.44485200
C	-1.85825700	0.00000100	0.00008600
H	-2.51460900	-0.23542800	0.84543300
H	-2.51480400	0.23541300	-0.84511400
C	0.36328700	1.23665400	-0.34623800
H	0.22216800	1.22888500	-1.43802600
H	0.95756600	2.12525800	-0.11221000

-309.644618 [M06-2X/6-31++G(d,p)]

C	-1.16459300	0.00003600	-0.00009800
O	-2.38369900	0.00003100	-0.00001500
C	0.98894300	1.22500900	-0.37691500
H	1.53136100	2.14984600	-0.16337400
H	0.79194000	1.22458400	-1.45519100
C	-0.35458600	-1.22795300	-0.35953700
H	-0.95190900	-2.11826500	-0.14685000
H	-0.18927600	-1.19830900	-1.44639600
C	0.98891700	-1.22498000	0.37696500
H	1.53130800	-2.14986100	0.16354000
H	0.79194600	-1.22440200	1.45524700
C	1.84671200	-0.00002500	-0.00006800
H	2.49996600	-0.24959400	-0.84224600
H	2.50016200	0.24948400	0.84197500
C	-0.35454000	1.22790700	0.35962400
H	-0.18919600	1.19802400	1.44647100
H	-0.95182100	2.11829200	0.14713100

Cyclohexanone K enolate, solvent = DMSO



Charge = 0; Multiplicity = 1

17

-909.175362 [B3LYP/6-31+G(d,p)]

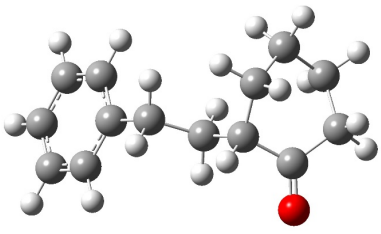
C	-0.17456300	-0.15273100	-0.05495600
O	1.13962400	-0.15787200	-0.04826100

K	3.64898700	0.01534600	0.04408300
C	-0.97256900	-1.26665600	-0.11036800
H	-0.48206700	-2.23949600	-0.18131300
C	-2.32815800	1.25614500	-0.28023100
H	-2.47912200	1.16845000	-1.36637200
H	-2.76414400	2.21862300	0.01857100
C	-0.82346700	1.23398500	0.03140700
H	-0.28171200	1.90428200	-0.64995400
H	-0.64396400	1.63075500	1.04332700
C	-2.48816000	-1.24943100	-0.08561700
H	-2.86958300	-2.06082500	0.55320300
H	-2.91326700	-1.45185900	-1.08643400
C	-3.04549400	0.09249800	0.41288700
H	-2.89091200	0.17270900	1.49912400
H	-4.12850800	0.14590800	0.23962300

-908.999976 [M06-2X/6-31++G(d,p)]

C	0.16223400	0.09722600	-0.02604600
O	-1.14378000	0.04776000	0.00699000
K	-3.61041000	0.00757600	0.02410600
C	0.90953000	1.23790300	-0.10875700
H	0.37563100	2.18625200	-0.17853100
C	2.35306300	-1.21143300	-0.29902100
H	2.46954200	-1.09056900	-1.38552000
H	2.83837900	-2.15715800	-0.03066900
C	0.86529700	-1.25701700	0.05202200
H	0.33048200	-1.94743100	-0.61227100
H	0.73013900	-1.65044200	1.07076900
C	2.42145000	1.28146300	-0.10155900
H	2.77531800	2.10900300	0.52893800
H	2.82514900	1.48778600	-1.10785300
C	3.02652600	-0.03143200	0.39837700
H	2.86516000	-0.11972200	1.48221600
H	4.10963400	-0.04401400	0.22889300

Cyclohexanone/styrene monoadduct (26a), solvent = DMSO



Charge = 0; Multiplicity = 1

33

-619.372406 [B3LYP/6-31+G(d,p)]

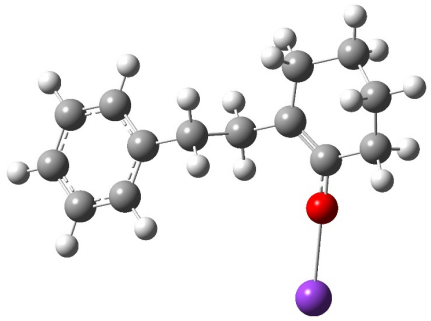
C	4.67479500	-0.09834200	-0.75160400
C	4.17243800	1.10539500	-0.24554900
C	2.91861600	1.13851100	0.37252600
C	2.14291000	-0.02561500	0.49725700
C	2.66084700	-1.22697800	-0.01233800
C	3.91414700	-1.26596800	-0.63203700
H	5.64997200	-0.12664500	-1.22919400
H	4.75777900	2.01710100	-0.32755700
H	2.53908800	2.07810600	0.76754000
H	2.07913900	-2.14115200	0.08109700
H	4.29699000	-2.20748500	-1.01615500

C	0.77031800	0.02086400	1.13647200
H	0.55015900	-0.95261300	1.58740600
H	0.76686000	0.75795900	1.94916600
C	-0.33471700	0.39305100	0.12525800
H	-0.34391100	-0.34464100	-0.68599900
H	-0.08548700	1.35859600	-0.32913900
C	-1.74428900	0.50535100	0.76531000
H	-1.66414600	1.21556000	1.59928600
C	-2.70671000	1.14566200	-0.23617500
O	-2.63776100	2.34005100	-0.51087300
C	-3.18414100	-1.17652300	-1.12608800
H	-2.39811000	-1.10171200	-1.88648200
H	-3.97167800	-1.79674600	-1.56549700
C	-2.62070000	-1.84297800	0.15765300
H	-3.33230600	-2.58279400	0.54043900
H	-1.71064400	-2.39840600	-0.09470400
C	-3.74204500	0.23563400	-0.86669500
H	-4.11729500	0.70560900	-1.78031900
H	-4.58720700	0.17906700	-0.16442000
C	-2.32493200	-0.82617900	1.28215500
H	-3.25344300	-0.60115400	1.82104200
H	-1.65289100	-1.27037400	2.02360900

-619.078384 [M06-2X/6-31++G(d,p)]

C	4.59757900	-0.11145000	-0.75150200
C	4.15801500	1.06227100	-0.13833500
C	2.91067500	1.10140800	0.48441400
C	2.08413600	-0.02763100	0.50566200
C	2.53512800	-1.19854200	-0.11328400
C	3.78136700	-1.24325100	-0.73755800
H	5.56958200	-0.14529600	-1.23385200
H	4.78756300	1.94701300	-0.14150400
H	2.57278500	2.01803100	0.96304600
H	1.90264900	-2.08374100	-0.10226200
H	4.11687800	-2.16208500	-1.20928400
C	0.71275700	0.02815700	1.13290600
H	0.45848100	-0.95962200	1.53265800
H	0.71285500	0.73056600	1.97539500
C	-0.34788500	0.46581000	0.11420600
H	-0.37366500	-0.26172900	-0.70755000
H	-0.05178700	1.42640300	-0.32340500
C	-1.75092400	0.62608900	0.73451600
H	-1.69290700	1.42440100	1.48560300
C	-2.70216700	1.11287000	-0.34910100
O	-2.66871500	2.26308000	-0.75303900
C	-3.00487300	-1.29477500	-1.01188100
H	-2.19926500	-1.23444700	-1.75152700
H	-3.73120700	-2.00729900	-1.41115800
C	-2.44821200	-1.79216800	0.34423100
H	-3.10680900	-2.55859800	0.76350300
H	-1.47725800	-2.27424400	0.18253900
C	-3.66554600	0.08761300	-0.90510200
H	-4.04092200	0.44287200	-1.86765100
H	-4.52011900	0.04010800	-0.21575300
C	-2.29977600	-0.65670900	1.36971700
H	-3.27696000	-0.43086900	1.81219100
H	-1.66181700	-0.97427200	2.19999800

Cyclohexanone/styrene monoadduct K enolate, solvent = DMSO



Charge = 0; Multiplicity = 1

33

-1218.752633 [B3LYP/6-31+G(d,p)]

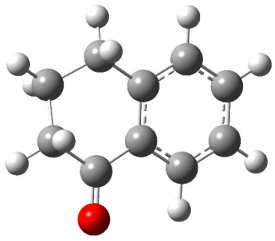
C	-1.36308000	-0.90516300	-0.25308400
C	-2.27741400	0.10068900	-0.03655200
O	-2.01358100	1.38995600	-0.06824700
K	-1.45276100	3.83277800	-0.23811600
C	0.08997700	-0.59005300	-0.51354300
H	0.46353700	-1.17809700	-1.36884100
H	0.19318800	0.46731500	-0.78146400
C	1.03474200	-0.87739200	0.69208300
H	0.93583400	-1.93154700	0.97891900
H	0.69530800	-0.28052000	1.54716100
C	2.48626200	-0.56939100	0.40184400
C	3.03613700	0.68646400	0.70959800
C	3.31596200	-1.51548400	-0.22446800
C	4.36695800	0.98964800	0.40369700
H	2.41484100	1.43284500	1.19978800
C	4.64701100	-1.21861000	-0.53426200
H	2.91517900	-2.49745800	-0.46623500
C	5.17896600	0.03716900	-0.22127800
H	4.76991000	1.96664100	0.65715600
H	5.26956100	-1.96874900	-1.01473400
H	6.21377600	0.26857300	-0.45729600
C	-4.01081900	-1.71270200	0.59779300
H	-5.08825100	-1.92358100	0.57069000
H	-3.67742000	-1.91381100	1.62663400
C	-1.73698900	-2.37792100	-0.23617400
H	-1.37512000	-2.87527800	0.68365700
H	-1.21477300	-2.89740700	-1.05724900
C	-3.24529000	-2.63112400	-0.35801300
H	-3.47407100	-3.68592300	-0.15559800
H	-3.57046400	-2.42605900	-1.38880100
C	-3.74452400	-0.24234900	0.24960200
H	-4.34111400	0.04645400	-0.63111200
H	-4.08619900	0.41147800	1.06406300

-1218.436218 [M06-2X/6-31++G(d,p)]

C	-1.52732700	-0.75571600	-0.28953200
C	-2.32610100	0.33757300	-0.08353600
O	-1.92109200	1.58200800	-0.11850200
K	-0.49281600	3.60949900	-0.13177600
C	-0.05382800	-0.58070800	-0.53505900
H	0.28959200	-1.26631600	-1.32678500
H	0.14426000	0.44102100	-0.88148500
C	0.82004500	-0.84096800	0.71467100

H	0.61905500	-1.85147200	1.09064200
H	0.52086700	-0.13559600	1.49938000
C	2.29085200	-0.69122900	0.42211900
C	2.89949100	0.56994400	0.44598900
C	3.06967700	-1.79519600	0.05549900
C	4.24577100	0.72521900	0.11743400
H	2.30885400	1.43862300	0.73017000
C	4.41730000	-1.64712400	-0.27429600
H	2.61292100	-2.78238600	0.03159400
C	5.01072500	-0.38497800	-0.24454300
H	4.69926300	1.71175300	0.14810000
H	5.00432100	-2.51764500	-0.55209800
H	6.05983600	-0.26695300	-0.49770500
C	-4.22019900	-1.27031500	0.56917000
H	-5.31163500	-1.37452100	0.55888300
H	-3.88831800	-1.49249000	1.59345800
C	-2.04377200	-2.17894900	-0.25521100
H	-1.74228300	-2.69247200	0.67559000
H	-1.57423100	-2.75739900	-1.06644200
C	-3.56394900	-2.26472800	-0.38444400
H	-3.90936800	-3.28607300	-0.18495700
H	-3.85767500	-2.01726500	-1.41451700
C	-3.81583700	0.15595700	0.19843900
H	-4.37393000	0.48452600	-0.69162600
H	-4.08637600	0.85541200	0.99936100

α-Tetralone (**27**), solvent = DMSO



Charge = 0; Multiplicity = 1

21

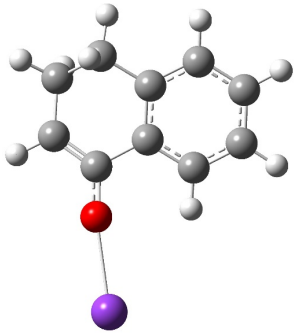
-462.224184 [B3LYP/6-31+G(d,p)]

C	1.22957100	1.06923500	0.05671800
O	1.43123000	2.28455600	0.01407800
C	2.38700600	0.09505800	0.16913200
H	3.26821600	0.56033900	-0.28226600
H	2.60051900	-0.01433800	1.24393600
C	2.07550800	-1.28015800	-0.43273800
H	2.91713400	-1.95991500	-0.26576400
H	1.94826600	-1.18695400	-1.51894400
C	0.79761000	-1.85375200	0.18758700
H	0.98193700	-2.07567300	1.24955700
H	0.52839200	-2.80532300	-0.28252800
C	-0.15022900	0.50616900	0.02720000
C	-0.36499500	-0.89022100	0.08470400
C	-1.68467200	-1.36473800	0.05605400
H	-1.86317600	-2.43621300	0.09088800
C	-1.24590700	1.38620500	-0.05604100
H	-1.05147000	2.45277900	-0.09953600
C	-2.54765900	0.89846700	-0.07898600
H	-3.38819100	1.58271000	-0.14228100
C	-2.76517000	-0.48560900	-0.02329200
H	-3.77784900	-0.87779100	-0.04770700

-462.013123 [M06-2X/6-31++G(d,p)]

C	-1.23156800	1.06478000	-0.05916800
O	-1.42717200	2.27018100	-0.00482300
C	-2.37849200	0.08842000	-0.18950200
H	-3.27224700	0.55543400	0.23150600
H	-2.55542500	-0.04507000	-1.26707500
C	-2.06268600	-1.26574100	0.44435700
H	-2.90501200	-1.94862200	0.30508300
H	-1.91718600	-1.14292000	1.52446400
C	-0.79739400	-1.84862100	-0.17993200
H	-0.98893100	-2.07081600	-1.23918100
H	-0.52492700	-2.79570300	0.29523800
C	0.15138900	0.50137300	-0.02640400
C	0.36390400	-0.88739100	-0.08519500
C	1.68030200	-1.36077500	-0.05913900
H	1.85806800	-2.43230900	-0.09513000
C	1.23743200	1.38369300	0.05675500
H	1.03752500	2.44974300	0.10096300
C	2.53753300	0.89869300	0.07793600
H	3.37695500	1.58334200	0.14122400
C	2.75613400	-0.48159500	0.02006200
H	3.76922800	-0.87154900	0.04287000

α-Tetralone K enolate, solvent = DMSO



Charge = 0; Multiplicity = 1

21

-1061.597361 [B3LYP/6-31+G(d,p)]

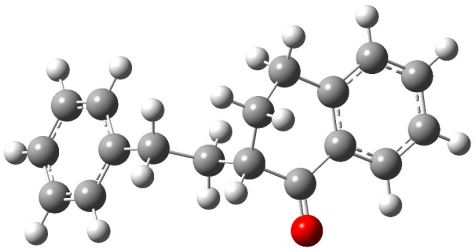
C	-0.45495600	0.93518000	-0.10724400
O	-1.71940200	0.59861800	-0.07196100
K	-4.03176200	-0.38275300	0.15953500
C	0.03067900	2.21639900	-0.22781000
H	-0.68297200	3.03135200	-0.34519400
C	1.50717500	2.52705900	-0.33449100
H	1.71322500	3.54405100	0.02299300
H	1.85455700	2.50692600	-1.38501100
C	2.34009300	1.52861500	0.47911400
H	2.17357700	1.72818500	1.55024100
H	3.41318700	1.65924800	0.29522200
C	0.56188500	-0.17663000	-0.05351800
C	1.92871500	0.10180800	0.18937900
C	2.85314500	-0.94884400	0.20754200
H	3.90214900	-0.72912800	0.39566400
C	0.16838800	-1.50866000	-0.25951700
H	-0.88331400	-1.71007700	-0.43772500
C	1.09989300	-2.55166300	-0.24162600
H	0.77417000	-3.57508400	-0.40998500

C	2.45005300	-2.27287100	-0.00945000
H	3.18370100	-3.07447300	0.00403100

-1061.368653 [M06-2X/6-31++G(d,p)]

C	-0.50498000	0.83658300	-0.03131900
O	-1.72811300	0.40312900	0.07622500
K	-4.05547700	-0.42814400	0.09000400
C	-0.12212400	2.13921300	-0.20495200
H	-0.89739900	2.89753400	-0.29991500
C	1.32139300	2.54465700	-0.38630000
H	1.46864000	3.58525400	-0.07594600
H	1.62625100	2.49906200	-1.44668100
C	2.24613900	1.64138000	0.42835900
H	2.08326600	1.84904600	1.49686300
H	3.30066200	1.84671100	0.21438300
C	0.59309600	-0.19466600	-0.01188000
C	1.93711400	0.18621100	0.17383500
C	2.93502900	-0.78903100	0.16210700
H	3.97088600	-0.48971000	0.30741800
C	0.28731300	-1.54695900	-0.19369800
H	-0.75512100	-1.82150100	-0.32563600
C	1.29113500	-2.51596700	-0.20604800
H	1.03772200	-3.56188600	-0.35456600
C	2.62137300	-2.13680500	-0.02945400
H	3.41112600	-2.88250100	-0.03969100

α-Tetralone/styrene monoadduct (28a), solvent = DMSO



Charge = 0; Multiplicity = 1

37

-771.798013 [B3LYP/6-31+G(d,p)]

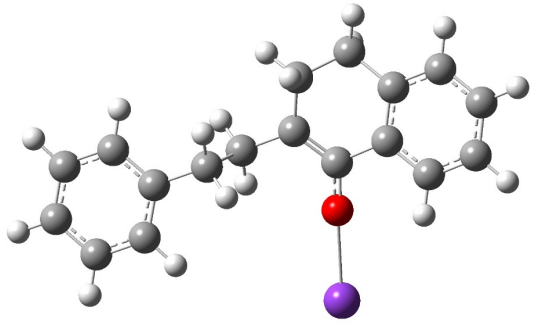
C	-5.40067700	0.67014800	-1.21926400
C	-5.09763800	-0.67033100	-0.95742500
C	-3.98525000	-0.99919600	-0.17662300
C	-3.15536400	0.00008700	0.35703400
C	-3.47266800	1.34111400	0.08824900
C	-4.58361700	1.67584800	-0.69267000
H	-6.26612800	0.92790700	-1.82292000
H	-5.72874200	-1.45947400	-1.35679400
H	-3.76108300	-2.04407900	0.02552900
H	-2.84697200	2.13036400	0.49857300
H	-4.81282000	2.72042000	-0.88479700
C	-1.93300600	-0.36078500	1.17579500
H	-1.73655300	0.43817600	1.89836700
H	-2.13201500	-1.27231300	1.75298800
C	-0.68602300	-0.59200900	0.29616900
H	-0.46283300	0.32388900	-0.26472100
H	-0.91856300	-1.36305700	-0.44735100
C	0.56223000	-1.05858800	1.09462000
H	0.28608500	-1.97964100	1.62198000

C	1.64730100	-1.45570800	0.09961200
O	1.64166100	-2.57767500	-0.41123400
C	1.68997800	1.20036300	1.41133400
H	2.15473400	1.86626700	2.14620500
H	0.88802800	1.78640500	0.94059500
C	1.10083700	-0.03101800	2.10658100
H	1.88289400	-0.51077100	2.70876500
H	0.31268800	0.26763600	2.80446300
C	2.68059600	-0.44395300	-0.26362300
C	2.70706800	0.82601500	0.35601300
C	3.69795100	1.73986100	-0.03315300
H	3.73349500	2.71661200	0.44233500
C	3.63692700	-0.76934300	-1.24523500
H	3.59431100	-1.75179100	-1.70369600
C	4.60986700	0.14932500	-1.62103300
H	5.34249300	-0.10787500	-2.37985000
C	4.63814200	1.41117000	-1.00947500
H	5.39776700	2.13471100	-1.29123200

-771.446339 [M06-2X/6-31++G(d,p)]

C	5.21850500	-1.14226700	-0.90380400
C	5.15199400	0.24767800	-0.81131100
C	4.05895100	0.85674000	-0.19319900
C	3.02033600	0.08959200	0.34288200
C	3.09797600	-1.30493400	0.24445800
C	4.18644500	-1.91831600	-0.37386500
H	6.06892900	-1.61821200	-1.38195200
H	5.95228400	0.85939500	-1.21696500
H	4.01274100	1.94090900	-0.12111100
H	2.29854400	-1.91427500	0.66181700
H	4.23185900	-3.00141400	-0.43800800
C	1.81639400	0.74160900	0.97827200
H	1.52394200	0.16694400	1.86414500
H	2.07204000	1.75244600	1.31762600
C	0.63753100	0.81890200	-0.00100200
H	0.35303100	-0.19847500	-0.30176200
H	0.95991100	1.33403900	-0.91356200
C	-0.58449800	1.57023600	0.57105300
H	-0.31938600	2.62825400	0.67576500
C	-1.68822000	1.49026700	-0.46489400
O	-1.79319500	2.32987700	-1.34690300
C	-1.51754700	-0.43857700	1.77203300
H	-1.95253200	-0.80228800	2.70769200
H	-0.64437500	-1.07559500	1.57158100
C	-1.08164700	1.01722700	1.91144700
H	-1.93521700	1.61869700	2.24700700
H	-0.30624400	1.11793600	2.67601900
C	-2.60548700	0.31169800	-0.40092900
C	-2.51918300	-0.61359200	0.65456700
C	-3.39148800	-1.70772600	0.65406600
H	-3.33954500	-2.42559900	1.46850700
C	-3.55111600	0.13717500	-1.42169800
H	-3.59373400	0.87089000	-2.22081200
C	-4.40883300	-0.95370600	-1.40784700
H	-5.13928900	-1.08661600	-2.19907300
C	-4.32422900	-1.88040700	-0.36352700
H	-4.99269800	-2.73563800	-0.34190700

α-Tetralone/styrene monoadduct K enolate, solvent = DMSO



Charge = 0; Multiplicity = 1

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-1371.177039 [B3LYP/6-31+G(d,p)]

C	-0.43017900	-0.84819300	-0.41813700
C	-1.31024500	0.20387100	-0.25739700
O	-0.98762500	1.47483500	-0.28840800
K	-0.45922600	3.92872800	-0.42571400
C	1.04496100	-0.60938500	-0.60484900
H	1.44815400	-1.29196600	-1.36963600
H	1.20882900	0.41268900	-0.96340800
C	1.88818900	-0.81074500	0.69099500
H	1.71726000	-1.82480300	1.07221600
H	1.52016800	-0.11503200	1.45428900
C	3.36941700	-0.59649200	0.47627600
C	3.94888300	0.67265900	0.64289000
C	4.20065600	-1.65119600	0.06214200
C	5.31067500	0.88369300	0.40406500
H	3.32641000	1.50304600	0.96886900
C	5.56294900	-1.44678900	-0.17929100
H	3.77635600	-2.64447300	-0.06671100
C	6.12449200	-0.17663400	-0.00933200
H	5.73615900	1.87371300	0.54498600
H	6.18592700	-2.27954400	-0.49467800
H	7.18311000	-0.01618100	-0.19264800
C	-0.89609400	-2.28482100	-0.27442100
H	-0.83269900	-2.62938100	0.77539800
H	-0.22978100	-2.95108800	-0.83994200
C	-2.33221100	-2.47603200	-0.77085800
H	-2.70140900	-3.48375900	-0.54556600
H	-2.33872200	-2.37312300	-1.86828700
C	-2.75234800	-0.12781700	0.02014700
C	-3.25721400	-1.43365500	-0.18705300
C	-3.62666500	0.86314700	0.49842800
H	-3.23323900	1.86433000	0.64378000
C	-4.59789900	-1.71290800	0.09878600
H	-4.97634000	-2.71994700	-0.06543600
C	-5.45666500	-0.71894100	0.58656800
H	-6.49422800	-0.95474100	0.80766300
C	-4.96545300	0.57506900	0.78364300
H	-5.62116200	1.35675300	1.15933100

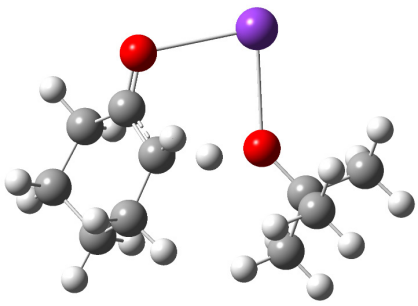
-1370.804659 [M06-2X/6-31++G(d,p)]

C	-0.45091700	-0.82517700	-0.43405200
C	-1.31626800	0.23009700	-0.29348500
O	-0.99107100	1.49302000	-0.34295200

K	-0.24428200	3.84362800	-0.34820300
C	1.02186900	-0.59555200	-0.61090900
H	1.43767300	-1.30996100	-1.33809300
H	1.19680200	0.41238000	-1.00406400
C	1.82022100	-0.74976200	0.70566800
H	1.61588100	-1.73863700	1.13415000
H	1.45706900	-0.00238200	1.42081600
C	3.30298700	-0.58814000	0.49167000
C	3.90240500	0.67647900	0.53104500
C	4.10471800	-1.69317700	0.18138100
C	5.26395300	0.83398600	0.27180400
H	3.29331700	1.54526100	0.77240500
C	5.46664500	-1.54259100	-0.07898700
H	3.65364800	-2.68270200	0.14625700
C	6.05166300	-0.27655700	-0.03481700
H	5.71079100	1.82311000	0.31318400
H	6.07122100	-2.41343800	-0.31495500
H	7.11205200	-0.15626800	-0.23415000
C	-0.91903100	-2.25172100	-0.24547500
H	-0.87352400	-2.55368800	0.81643200
H	-0.24601100	-2.93600300	-0.77917300
C	-2.34411400	-2.44785000	-0.75433200
H	-2.72329100	-3.44763800	-0.51587800
H	-2.33885000	-2.35478000	-1.85101800
C	-2.75875200	-0.09100500	-0.00876100
C	-3.26438500	-1.39348100	-0.19250400
C	-3.62015700	0.91086000	0.45238800
H	-3.21682600	1.91115400	0.57779200
C	-4.60192700	-1.66231800	0.09902000
H	-4.98410800	-2.67053700	-0.04657000
C	-5.45154400	-0.65789200	0.56984600
H	-6.48929100	-0.88449000	0.79659200
C	-4.95687300	0.63415900	0.74373400
H	-5.60958900	1.42337400	1.10634000

10.6.2. XYZ Co-ordinates of transition states

Deprotonation of cyclohexanone (25) by KOtBu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

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-1142.753394 [B3LYP/6-31+G(d,p)]

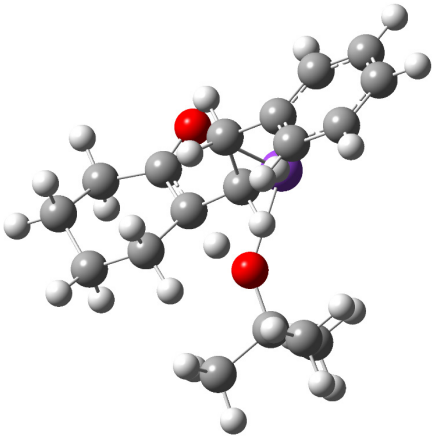
C	-1.78604800	0.92495300	0.26431600
O	-1.52990700	2.15224000	0.41669000
K	1.10408500	2.69443000	-0.07735100
H	0.04813900	-0.14840900	0.35586600
O	1.21886600	0.04311200	-0.24084500
C	2.19428700	-0.97082300	-0.13202500
C	3.51118600	-0.44749100	-0.74248200

H	3.84398800	0.45133700	-0.20995800
H	4.31305300	-1.19488700	-0.68696900
H	3.36089800	-0.18402900	-1.79596300
C	2.43656500	-1.33527600	1.35130000
H	1.51298500	-1.70467900	1.81100100
H	3.20444600	-2.11159600	1.46058100
H	2.76356600	-0.45002600	1.90947600
C	1.75158800	-2.23645300	-0.90113400
H	0.81889400	-2.63214800	-0.48358300
H	1.57483600	-1.99318600	-1.95538700
H	2.50827500	-3.03011500	-0.85489800
C	-1.11561600	-0.10998900	1.00897000
H	-0.76391200	0.25653600	1.98015000
C	-1.74066400	-1.50937100	1.07183100
H	-0.96754000	-2.24961300	1.31925000
H	-2.48082800	-1.56591600	1.88606400
C	-2.43219500	-1.90366300	-0.24098700
H	-1.67962600	-2.04133400	-1.03023300
H	-2.94581000	-2.86588500	-0.12180100
C	-3.42622600	-0.82015300	-0.67506100
H	-3.94486900	-1.11106100	-1.59670100
H	-4.19993300	-0.70991600	0.09814100
C	-2.71575500	0.52625400	-0.88131700
H	-2.09667200	0.48052200	-1.79033100
H	-3.42969200	1.34263700	-1.03596500

-1142.455146 [M06-2X/6-31++G(d,p)]

C	-1.76744800	0.91214100	0.31775200
O	-1.53106800	2.12383400	0.50649900
K	1.13512200	2.55417200	0.29606200
H	0.00447500	-0.13860500	0.32724500
O	1.16120700	0.05006900	-0.39404900
C	2.12062400	-0.94568600	-0.19159200
C	3.44985200	-0.49803000	-0.81668400
H	3.78323200	0.43797400	-0.35311500
H	4.23843200	-1.24882800	-0.68567600
H	3.31464200	-0.31955900	-1.88936100
C	2.33301100	-1.18690600	1.31411600
H	1.39818100	-1.52235300	1.77822500
H	3.10240400	-1.94495400	1.50277500
H	2.63904300	-0.25307000	1.80072200
C	1.67457400	-2.26227800	-0.84848700
H	0.73014500	-2.59892800	-0.40464800
H	1.50963700	-2.10404900	-1.92038900
H	2.41849600	-3.05827600	-0.72375700
C	-1.07590400	-0.13483500	1.03604500
H	-0.72022800	0.21751300	2.01014400
C	-1.67634100	-1.53880200	1.05510800
H	-0.89516700	-2.26838900	1.30610900
H	-2.44287600	-1.63021900	1.83897000
C	-2.31136700	-1.89853400	-0.28856500
H	-1.53174000	-1.95500700	-1.06147000
H	-2.78349600	-2.88558100	-0.23194600
C	-3.33713600	-0.83887100	-0.68753800
H	-3.84397600	-1.11292000	-1.61876800
H	-4.11058000	-0.77692900	0.08990000
C	-2.66518300	0.52620400	-0.84833900
H	-2.01853000	0.51489300	-1.73810500
H	-3.39167000	1.33081000	-0.99653700

Deprotonation of cyclohexanone/styrene monoadduct by KOtBu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

48

-1452.325409 [B3LYP/6-31+G(d,p)]

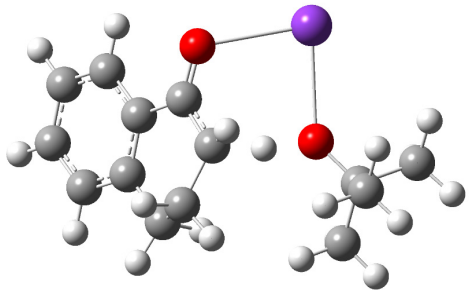
C	-1.69330800	1.02343400	0.21559100
O	-1.38003100	2.20573500	0.53023300
K	1.30946100	2.60140200	0.24841100
H	-0.03694100	-0.20526800	0.46034500
O	1.21888400	-0.03572800	0.03609400
C	2.11732700	-1.12270300	0.00424300
C	3.52223900	-0.58045600	-0.33598200
H	3.84176400	0.14506600	0.42164500
H	4.27142200	-1.38144600	-0.37892400
H	3.50681100	-0.07432300	-1.30848100
C	2.17224100	-1.83110000	1.37690900
H	1.18724700	-2.23223000	1.64031400
H	2.88955100	-2.66157600	1.37808300
H	2.46865300	-1.12089300	2.15747900
C	1.69749400	-2.14455100	-1.07685200
H	0.70209400	-2.54525100	-0.85568100
H	1.65808800	-1.65937500	-2.05925400
H	2.39756200	-2.98767600	-1.13917000
C	-1.26664800	-0.13001600	0.97759100
C	-1.96574100	-1.47363300	0.70686300
H	-1.28860200	-2.29026200	0.99581000
H	-2.85224900	-1.58291200	1.35232400
C	-2.40950200	-1.66378400	-0.74944500
H	-1.52981800	-1.77335100	-1.39816900
H	-2.99049500	-2.58973800	-0.84482100
C	-3.23275000	-0.46148600	-1.22032800
H	-3.58607800	-0.60371000	-2.24897300
H	-4.12848500	-0.36554900	-0.59039500
C	-2.39891300	0.82233200	-1.12646100
H	-1.61713900	0.81083200	-1.90117300
H	-3.00436500	1.71559200	-1.31556100
C	-0.97330000	0.12108000	2.46233900
H	-0.49006300	-0.77157200	2.88116400
H	-0.25166200	0.93835000	2.56911000
C	-2.21758000	0.46110100	3.32330800
H	-2.67465700	1.37456900	2.92655100
H	-2.95836000	-0.34054400	3.22401700
C	-1.88551900	0.65320800	4.78675400
C	-1.48014200	1.90618200	5.27670100
C	-1.93660100	-0.42259700	5.68879700

C	-1.13588300	2.08033900	6.62087400
H	-1.43932000	2.75500800	4.59772500
C	-1.59389000	-0.25525500	7.03449000
H	-2.25324100	-1.40065300	5.33325700
C	-1.19063000	0.99843400	7.50638600
H	-0.82976100	3.06032100	6.97711600
H	-1.64591700	-1.10184400	7.71387600
H	-0.92666000	1.13170200	8.55164400

-1451.893012 [M06-2X/6-31++G(d,p)]

C	-1.67501000	0.99593600	0.27170800
O	-1.37280300	2.15155600	0.63754800
K	1.29983000	2.54209200	0.48710800
H	-0.06452000	-0.19719600	0.44998800
O	1.21457700	0.02827500	-0.03932300
C	2.07692400	-1.06919100	-0.00704000
C	3.49049400	-0.60806200	-0.39236500
H	3.83743700	0.15646800	0.31275400
H	4.21009200	-1.43573400	-0.38588000
H	3.47697600	-0.16796600	-1.39604100
C	2.11427700	-1.68048600	1.40411000
H	1.11425100	-2.03349400	1.68221400
H	2.80882000	-2.52680900	1.46725900
H	2.42171100	-0.92084200	2.13221800
C	1.61080500	-2.14922200	-0.99746100
H	0.61194100	-2.50251300	-0.71508600
H	1.55213400	-1.72882700	-2.00795800
H	2.28801000	-3.01162700	-1.01692100
C	-1.23258500	-0.18388400	0.99018600
C	-1.92058400	-1.51541200	0.68558500
H	-1.23618400	-2.33330600	0.95290500
H	-2.81061500	-1.64681100	1.32190800
C	-2.34744500	-1.65072600	-0.77571200
H	-1.45840600	-1.69971700	-1.41948000
H	-2.90368200	-2.58338800	-0.92071700
C	-3.19158100	-0.44780600	-1.18966900
H	-3.56500900	-0.56004000	-2.21290500
H	-4.07020500	-0.37983300	-0.53371100
C	-2.36479700	0.83190000	-1.07456100
H	-1.56896500	0.82540200	-1.83418800
H	-2.96257400	1.73113000	-1.25174000
C	-0.95016800	0.04262100	2.47132800
H	-0.53582100	-0.87966000	2.90104600
H	-0.18168300	0.81504200	2.60138500
C	-2.19440500	0.45420200	3.28158900
H	-2.58715300	1.38647300	2.86057800
H	-2.96960500	-0.31265900	3.16858600
C	-1.87996500	0.64493900	4.74328300
C	-1.42090500	1.87952300	5.21851500
C	-1.98423600	-0.41802100	5.64786000
C	-1.07925700	2.05041600	6.55984000
H	-1.33587000	2.71489500	4.52646200
C	-1.64411300	-0.25374700	6.99080000
H	-2.33989000	-1.38322300	5.29360400
C	-1.19000700	0.98271700	7.45157600
H	-0.72965200	3.01716800	6.91009000
H	-1.73623200	-1.08948000	7.67825500
H	-0.92776800	1.11413100	8.49684300

Deprotonation of α-tetralone (27) by KOtBu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

36

-1452.325409 [B3LYP/6-31+G(d,p)]

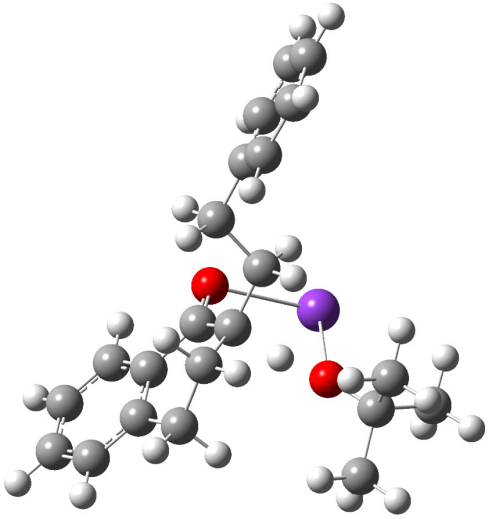
C	-1.72542200	0.91414400	0.08419300
O	-1.41363300	2.12985800	0.22719400
K	1.21051000	2.60567400	-0.35145000
H	0.11413000	-0.21637500	0.20515900
O	1.31088500	-0.05676800	-0.35242400
C	2.29797300	-1.02195400	-0.05766100
C	3.63786500	-0.54643700	-0.65727300
H	3.92510400	0.41939400	-0.22482000
H	4.44793700	-1.26136300	-0.46408100
H	3.54373700	-0.42048100	-1.74228900
C	2.45969200	-1.18432400	1.47164900
H	1.52169100	-1.52574400	1.92360300
H	3.24231700	-1.91115900	1.72313500
H	2.72580900	-0.22296200	1.92664700
C	1.92534700	-2.38789600	-0.67760100
H	0.97697300	-2.74962700	-0.26475800
H	1.80767600	-2.28976600	-1.76313900
H	2.69211100	-3.14874400	-0.48331600
C	-1.07040800	-0.14869700	0.80947900
H	-0.74269400	0.19225500	1.79743500
C	-1.76618200	-1.50942500	0.82139900
H	-1.08838100	-2.27631300	1.21615100
H	-2.64509500	-1.50345900	1.48616300
C	-2.21174600	-1.90366900	-0.59233100
H	-1.31946100	-2.09474300	-1.20646200
H	-2.78698700	-2.83637900	-0.58105700
C	-2.75779800	0.54533700	-0.94329500
C	-3.02234800	-0.80873900	-1.24932200
C	-3.48955200	1.55898400	-1.58505200
C	-4.01591600	-1.10723400	-2.19228300
C	-4.47603100	1.24824600	-2.51976500
H	-3.27044200	2.59117600	-1.33147100
C	-4.73997500	-0.09289200	-2.82414800
H	-4.22518200	-2.14739600	-2.43052600
H	-5.03801000	2.04076500	-3.00566500
H	-5.50989200	-0.34753000	-3.54726700

-1294.821713 [M06-2X/6-31+G(d,p)]

C	-1.71208400	0.94372100	0.10444400
O	-1.42741200	2.15108800	0.24290100
K	1.25611600	2.49179200	0.11126700
H	0.07956300	-0.17254500	0.17207300
O	1.28039200	-0.05000400	-0.48960800
C	2.22562400	-1.01566700	-0.13061900

C	3.59141700	-0.62448900	-0.71356600
H	3.89666200	0.35479100	-0.32635200
H	4.36988600	-1.35382900	-0.45871600
H	3.52480500	-0.55551200	-1.80519100
C	2.34241400	-1.10644500	1.40208500
H	1.38212400	-1.40811700	1.83660900
H	3.10319700	-1.83261600	1.71211100
H	2.61033300	-0.12638500	1.81482000
C	1.82282600	-2.39497800	-0.67797800
H	0.86207300	-2.70156200	-0.24762400
H	1.70979300	-2.34533100	-1.76698400
H	2.56652000	-3.16493100	-0.43956800
C	-1.02947600	-0.10991600	0.82673600
H	-0.70139800	0.24184400	1.81025500
C	-1.70262100	-1.47614600	0.83285800
H	-1.01908700	-2.22618300	1.24801400
H	-2.60204300	-1.48378500	1.46624400
C	-2.08942200	-1.87140100	-0.59184500
H	-1.17199400	-1.99999100	-1.18411000
H	-2.62170200	-2.82789800	-0.61248300
C	-2.73206300	0.54876800	-0.92334400
C	-2.93445700	-0.80506000	-1.24508300
C	-3.49270700	1.54205800	-1.55100300
C	-3.90418700	-1.13065300	-2.19821500
C	-4.45632000	1.20496400	-2.49510600
H	-3.31250900	2.57810200	-1.28110900
C	-4.66098700	-0.13874400	-2.81856400
H	-4.06860000	-2.17510000	-2.45133100
H	-5.04615700	1.97919700	-2.97566800
H	-5.41391700	-0.41328200	-3.55159900

Deprotonation of α-tetralone/styrene monoadduct by KOtBu T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

52

-1604.745534 [B3LYP/6-31+G(d,p)]

C	-1.79967700	0.89862600	0.18016000
O	-1.47380500	2.09324200	0.42935600
K	1.16851900	2.52246300	-0.06579300
H	-0.09301100	-0.31847200	0.40662100
O	1.13330800	-0.13560700	-0.07856500
C	2.11245500	-1.14935500	0.00211400
C	3.50474200	-0.49219400	-0.11804300
H	3.66113500	0.21769300	0.70302000

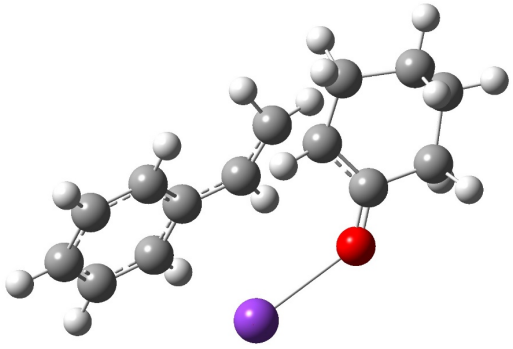
H	4.31250100	-1.23455100	-0.08576500
H	3.58353100	0.05642600	-1.06421000
C	2.02721500	-1.89687500	1.35146900
H	1.05048300	-2.38076000	1.46233300
H	2.80041700	-2.67101300	1.43306700
H	2.15515100	-1.19553500	2.18352500
C	1.93488200	-2.16392000	-1.15035400
H	0.95690500	-2.65302600	-1.07892800
H	1.98749000	-1.64878600	-2.11661300
H	2.70716700	-2.94363200	-1.13407300
C	-1.31091900	-0.22538900	0.95448900
C	-2.04880200	-1.55201800	0.73721000
H	-1.47136500	-2.36829000	1.19050400
H	-3.02746700	-1.55302200	1.24401800
C	-2.26316000	-1.85035900	-0.75007900
H	-1.28900800	-2.04904500	-1.21885100
H	-2.86489900	-2.75603100	-0.88718300
C	-0.98203900	0.07995700	2.42049200
H	-0.44561000	-0.77700600	2.84725900
H	-0.29650300	0.93227900	2.47674200
C	-2.21339000	0.38725400	3.31263800
H	-2.73504300	1.25832200	2.89980700
H	-2.91212300	-0.45603600	3.27244500
C	-1.83851700	0.65485200	4.75361800
C	-1.47887600	1.94498900	5.17836400
C	-1.80158600	-0.38499700	5.69746100
C	-1.09303700	2.18959800	6.50000600
H	-1.50659900	2.76666000	4.46609800
C	-1.41643400	-0.14712800	7.02086900
H	-2.08222900	-1.39074800	5.39260300
C	-1.05914200	1.14270100	7.42770800
H	-0.82330400	3.19686400	6.80597700
H	-1.39975900	-0.96717400	7.73375800
H	-0.76241200	1.33068800	8.45562800
C	-2.65474600	0.62982300	-1.02751900
C	-2.91198200	-0.68800700	-1.46379400
C	-3.22805700	1.71202200	-1.71747300
C	-3.73864400	-0.88566300	-2.57861200
C	-4.04944400	1.50301700	-2.82444800
H	-3.01921400	2.71640000	-1.36401300
C	-4.30599900	0.19612500	-3.25686400
H	-3.94035300	-1.89971000	-2.91567200
H	-4.49012200	2.34838100	-3.34529500
H	-4.94864800	0.02055000	-4.11519200

-1604.256128 [M06-2X/6-31++G(d,p)]

C	-1.87714400	0.82253300	0.18143100
O	-1.54161100	2.00191900	0.41680500
K	1.10882200	2.35151700	0.06600800
H	-0.23276700	-0.39334500	0.29590800
O	0.98821300	-0.23353700	-0.32564400
C	1.97835000	-1.16509400	-0.00125100
C	2.91126400	-0.58623300	1.07661300
H	2.32441300	-0.31250900	1.96179900
H	3.68780700	-1.29801500	1.38133100
H	3.40889300	0.31543600	0.69909700
C	1.35387900	-2.46522500	0.53531800
H	0.65293800	-2.87678100	-0.20017100
H	2.11778400	-3.22208700	0.74806800

H	0.80059600	-2.26742700	1.46028800
C	2.80177800	-1.49290100	-1.25610700
H	2.15110000	-1.92914100	-2.02241800
H	3.24086400	-0.57459400	-1.66222700
H	3.61194200	-2.20097400	-1.04348600
C	-1.35247800	-0.30807500	0.92655900
C	-2.13791200	-1.60665200	0.77120200
H	-1.58120800	-2.42662100	1.24118400
H	-3.11102900	-1.55269200	1.28423300
C	-2.37310000	-1.92592300	-0.70288000
H	-1.40377500	-2.12281300	-1.18254200
H	-2.98111100	-2.82832600	-0.82479200
C	-0.92253900	0.02117700	2.34965900
H	-0.35718200	-0.82586600	2.76284500
H	-0.23638800	0.87684100	2.34286400
C	-2.09420500	0.34601700	3.29608800
H	-2.67251200	1.17155300	2.86418500
H	-2.75971400	-0.52215600	3.36248700
C	-1.61627700	0.72373500	4.67484200
C	-1.28269100	2.04994900	4.97516200
C	-1.44234500	-0.24736200	5.66787400
C	-0.79466200	2.39930300	6.23392200
H	-1.41273500	2.81495400	4.21242500
C	-0.95320900	0.09549900	6.92857100
H	-1.69756400	-1.28213000	5.44931700
C	-0.62819500	1.42158600	7.21614600
H	-0.54744300	3.43462600	6.44986500
H	-0.82900900	-0.67159200	7.68721800
H	-0.25158700	1.69192300	8.19784700
C	-2.77276000	0.54770400	-0.99244500
C	-3.03160200	-0.76853400	-1.41144000
C	-3.35959900	1.62601200	-1.66553000
C	-3.88037600	-0.97254500	-2.50377500
C	-4.20415800	1.41071700	-2.74903200
H	-3.14137100	2.63114300	-1.31851700
C	-4.46407300	0.10379000	-3.16873900
H	-4.08709200	-1.98856800	-2.83113900
H	-4.66100100	2.25088000	-3.26256800
H	-5.12624200	-0.07651200	-4.01043800

Reaction of cyclohexanone (25) with styrene (3) T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

33

-1218.703714 [B3LYP/6-31+G(d,p)]

C	-4.32442800	-0.69639300	-0.58090900
C	-4.10146100	0.11505300	0.54408500

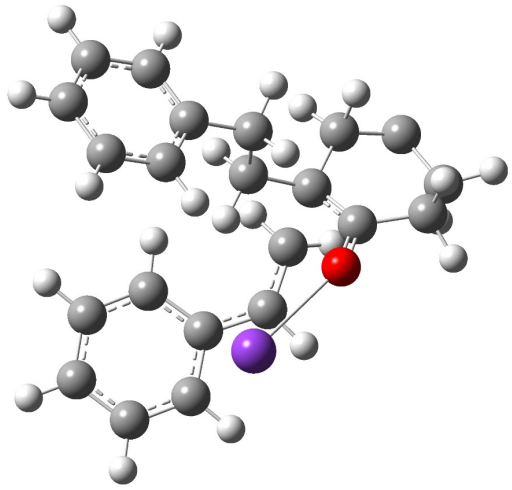
C	-2.85298300	0.16057600	1.15921800
C	-1.74254200	-0.61002900	0.69010400
C	-1.99675600	-1.41572700	-0.46399400
C	-3.25186200	-1.45731100	-1.07004600
H	-5.29792300	-0.73028200	-1.06064400
H	-4.91286700	0.71847200	0.94564300
H	-2.71277800	0.79313700	2.03438100
H	-1.19460400	-2.01688900	-0.88221400
H	-3.39422500	-2.08955200	-1.94415100
C	-0.46990300	-0.54251300	1.34961000
H	-0.37860600	0.19536800	2.14542900
C	0.67964100	-1.27276700	0.97969700
H	0.53530900	-2.24034800	0.49872000
H	1.48890000	-1.30468700	1.70717500
C	1.75719600	-0.63171300	-0.59441200
H	0.92715300	-0.62460300	-1.30013600
C	2.14650800	0.67383700	-0.17327500
O	1.36335200	1.66964900	-0.24625500
K	-1.14536800	2.12891500	-0.83768900
C	4.34244800	-0.39288400	0.65896900
H	5.38210400	-0.12293000	0.87997700
H	3.98870100	-0.99227700	1.50909800
C	3.49090800	0.87823900	0.51883600
H	3.29997200	1.34071500	1.49727100
H	4.03689500	1.63291300	-0.06553400
C	2.80800900	-1.71347500	-0.84469500
H	2.70477200	-2.10009100	-1.86686800
H	2.62505700	-2.57758400	-0.18368600
C	4.25217500	-1.23336300	-0.61917800
H	4.58163400	-0.62404800	-1.47292900
H	4.92841000	-2.09557500	-0.56558300

-1218.386273 [M06-2X/6-31++G(d,p)]

C	-4.12458700	-0.35026100	-0.55815000
C	-3.83177900	0.36646000	0.61162300
C	-2.61474200	0.20674800	1.26002300
C	-1.60796400	-0.67501600	0.77338100
C	-1.93808100	-1.40628400	-0.40231300
C	-3.16433900	-1.24402400	-1.04339400
H	-5.07288900	-0.21939400	-1.06805400
H	-4.56167900	1.06340800	1.01534200
H	-2.40492500	0.78524500	2.15718800
H	-1.21290400	-2.09539200	-0.82534400
H	-3.36846400	-1.81549200	-1.94539800
C	-0.33054000	-0.75255900	1.41873100
H	-0.14631600	-0.02983500	2.21092000
C	0.73891600	-1.52073100	0.95206500
H	0.53670700	-2.44655100	0.41347000
H	1.61666800	-1.59752400	1.59148600
C	1.73075200	-0.84259100	-0.71286400
H	0.90871900	-0.99252700	-1.41335100
C	1.88613900	0.49728300	-0.29391400
O	0.97065900	1.35750200	-0.41788100
K	-1.43166000	1.55376100	-1.33617400
C	4.12293200	-0.24417400	0.72218900
H	5.09339000	0.16756500	1.01903700
H	3.79066700	-0.88855900	1.54688200
C	3.11988700	0.89135000	0.50254800
H	2.76929500	1.30723800	1.45690200

H	3.59835400	1.72149100	-0.03432300
C	2.91697700	-1.77860300	-0.85370400
H	2.94568600	-2.20204800	-1.86457700
H	2.80415100	-2.63880600	-0.17100700
C	4.24954900	-1.08763700	-0.54523600
H	4.53017500	-0.43415800	-1.38261000
H	5.04408400	-1.83405300	-0.43747900

Reaction of cyclohexanone/styrene monoadduct K enolate with styrene (3) T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

47

-1528.273563 [B3LYP/6-31+G(d,p)]

C	-4.64808200	-0.93314900	0.51367700
C	-4.14229200	-0.17212600	1.57825200
C	-2.77207900	-0.10052500	1.82225900
C	-1.81163800	-0.78732200	1.01302200
C	-2.35965800	-1.55289300	-0.06405500
C	-3.73019200	-1.62226200	-0.29691300
H	-5.71532500	-0.98785600	0.32135600
H	-4.82488900	0.36997500	2.22958900
H	-2.41520200	0.48150700	2.67118200
H	-1.69227700	-2.09956500	-0.72346600
H	-4.09206200	-2.22193700	-1.12984900
C	-0.41301600	-0.70156500	1.32650800
H	-0.16125100	-0.07084800	2.17904700
C	0.66014700	-1.34098800	0.65695600
H	0.41556600	-2.20001700	0.02998400
H	1.54048800	-1.54182000	1.26503000
C	1.60294600	-0.38927000	-0.80705800
C	1.95309700	0.86462300	-0.18912000
O	1.13350500	1.80998300	-0.05477700
K	-1.40155600	2.44005600	0.22922200
C	3.91262600	-1.47176700	-0.17516600
C	4.07712100	-0.29377900	0.71442200
H	5.13011500	-0.11851700	0.96705900
H	3.66579400	-0.72937800	1.64992000
C	3.35760600	1.02561900	0.37672500
H	3.31629400	1.68602800	1.25018200
H	3.94419300	1.56337300	-0.38446300
C	2.77319200	-1.32710700	-1.08731900
H	3.43257300	-0.91715500	-1.90368000
H	2.43160400	-2.28410600	-1.50237900

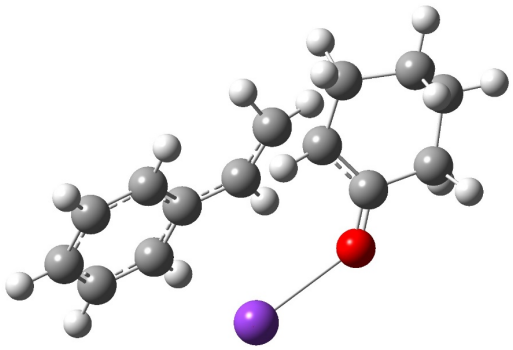
C	0.55498700	-0.33977000	-1.91146200
H	-0.35854400	0.11679400	-1.52033200
H	0.28903800	-1.36524000	-2.20120600
C	0.99583400	0.43096800	-3.18120600
H	1.89207200	-0.04139300	-3.60127900
H	1.27402200	1.45131300	-2.89493200
C	-0.08555400	0.47836700	-4.23960100
C	-0.18288100	-0.52070300	-5.22186100
C	-1.04236800	1.50677500	-4.24403500
C	-1.20420500	-0.49633900	-6.17722800
H	0.55189100	-1.32248000	-5.24092000
C	-2.06526800	1.53724800	-5.19690700
H	-0.98102100	2.29424400	-3.49615800
C	-2.15063300	0.53375100	-6.16809900
H	-1.25728400	-1.27798200	-6.93023800
H	-2.79133800	2.34562500	-5.18393900
H	-2.94233700	0.55676900	-6.91147500

-1527.822199 [M06-2X/6-31++G(d,p)]

C	-4.57158700	-0.76422900	0.20229200
C	-4.13344900	-0.00954000	1.29377900
C	-2.78740700	0.02502500	1.64457800
C	-1.79321300	-0.68709500	0.91727600
C	-2.26994500	-1.44860300	-0.18610300
C	-3.61646900	-1.48554900	-0.52499100
H	-5.62034400	-0.79035800	-0.07445500
H	-4.84913100	0.55738400	1.88422800
H	-2.47959600	0.60752700	2.51219100
H	-1.56438900	-2.01245300	-0.78917700
H	-3.92679800	-2.08276700	-1.37917600
C	-0.41255600	-0.61732200	1.31920400
H	-0.19850700	0.01802300	2.17796900
C	0.65609600	-1.31904400	0.74095500
H	0.42900100	-2.18886400	0.12150100
H	1.53636800	-1.47877600	1.36236300
C	1.67467900	-0.49812400	-0.81829700
C	1.97958000	0.71701600	-0.14255900
O	1.18744500	1.69631400	-0.12658400
K	-1.29508500	2.28972900	0.09478400
C	4.10962500	-0.43316800	0.73994300
H	5.10799400	-0.16948500	1.10435500
H	3.71744500	-1.19522600	1.42554800
C	3.20923500	0.80405100	0.74805600
H	2.85415600	1.03523100	1.76188400
H	3.77372600	1.68545700	0.41620000
C	2.78439900	-1.50375400	-1.09160700
H	2.79509000	-1.75408700	-2.16070800
H	2.56621900	-2.45078200	-0.56732600
C	0.59464400	-0.42615900	-1.87167200
H	-0.29641700	0.05376400	-1.45075700
H	0.29722900	-1.44491000	-2.16177100
C	1.01948400	0.34188800	-3.13736900
H	1.89030200	-0.15029600	-3.58761500
H	1.32542000	1.35166100	-2.84240800
C	-0.10267200	0.41728800	-4.14222300
C	-0.31073300	-0.60820400	-5.07242400
C	-1.00374800	1.48796600	-4.12141200
C	-1.38880900	-0.56579500	-5.95688200
H	0.38183800	-1.44676600	-5.10341000
C	-2.08453500	1.53582100	-5.00171200

H	-0.84882900	2.29739500	-3.41136400
C	-2.28131800	0.50651000	-5.92291800
H	-1.53100200	-1.36843100	-6.67453500
H	-2.76954800	2.37797800	-4.97157400
H	-3.12017700	0.54148900	-6.61108900
C	4.17323000	-1.02170700	-0.66687000
H	4.52549100	-0.24946700	-1.36499000
H	4.88959800	-1.84938200	-0.71122800

Reaction of α-tetralone (27) with styrene (3) T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

37

-1371.127188 [B3LYP/6-31+G(d,p)]

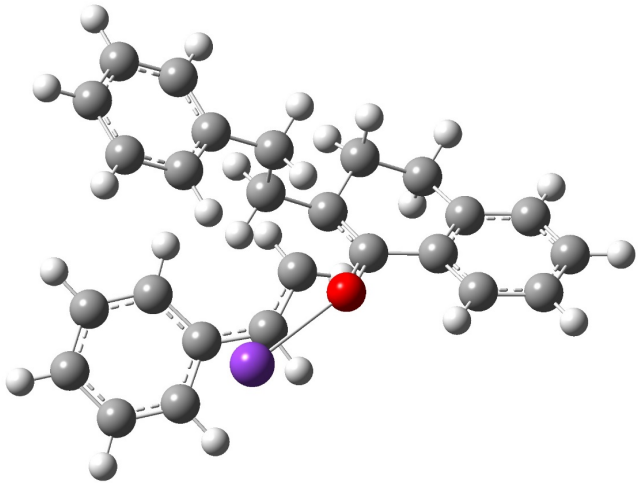
C	-4.33387900	-0.74674000	-0.60491500
C	-4.14201400	-0.12850200	0.64115600
C	-2.89261900	-0.13442600	1.25674900
C	-1.75742100	-0.76649500	0.66391900
C	-1.97907800	-1.37561900	-0.60807500
C	-3.23419600	-1.36702100	-1.21588500
H	-5.30763400	-0.74100600	-1.08525300
H	-4.97664100	0.36225500	1.13681100
H	-2.77299900	0.34598500	2.22630000
H	-1.15379500	-1.86388600	-1.11803400
H	-3.35537500	-1.84724700	-2.18446200
C	-0.48445400	-0.76097600	1.33386800
H	-0.42463500	-0.16297400	2.24189400
C	0.68913000	-1.37710100	0.86878800
H	0.59933300	-2.24922900	0.22185800
H	1.49914500	-1.47098500	1.58624400
C	1.72724000	-0.39173500	-0.61062600
H	0.87506800	-0.33844400	-1.28695800
C	2.07157000	0.85626300	-0.02454600
O	1.22190400	1.79660500	0.12199400
K	-1.29092200	2.24141400	-0.41178700
C	2.84108900	-1.32585000	-1.05050700
H	3.25318300	-0.99680500	-2.01828400
H	2.44564600	-2.33598200	-1.22142600
C	3.97279000	-1.39435400	-0.01527400
H	4.83747400	-1.92944800	-0.42365500
H	3.63486800	-1.98096400	0.85051300
C	4.39648400	-0.02502000	0.47231500
C	5.69724200	0.20167500	0.93898300
C	6.08062600	1.44954400	1.44248500
C	5.15097600	2.49476800	1.48496300
C	3.85311500	2.28377200	1.01867400
C	3.45756500	1.03361300	0.50857300

H	6.41996000	-0.61072000	0.90810400
H	7.09660500	1.60373000	1.79534100
H	5.43899300	3.46773500	1.87377900
H	3.12130900	3.08486700	1.03599300

-1370.754029 [M06-2X/6-31++G(d,p)]

C	-4.12503600	-0.44053200	-0.59719200
C	-3.91767100	0.09977500	0.67954800
C	-2.70569700	-0.07096700	1.33622700
C	-1.62724100	-0.78982200	0.75200900
C	-1.86782300	-1.34139000	-0.53529500
C	-3.08728900	-1.16760100	-1.18682600
H	-5.06908500	-0.30009600	-1.11259000
H	-4.71022100	0.66470200	1.16311400
H	-2.56315300	0.36802800	2.32137100
H	-1.08349800	-1.90332500	-1.03403500
H	-3.22423300	-1.59935700	-2.17487800
C	-0.35936200	-0.88224700	1.42304300
H	-0.24642800	-0.28845900	2.32705900
C	0.75774700	-1.52947100	0.90117400
H	0.62669700	-2.37832200	0.23036300
H	1.61907800	-1.63115600	1.55598400
C	1.69089700	-0.53181100	-0.66630400
H	0.81024500	-0.55596500	-1.30836100
C	1.93429000	0.71648400	-0.06328500
O	1.02771000	1.58621200	0.10410200
K	-1.37563400	1.82788600	-0.81942300
C	2.84907900	-1.40789900	-1.08761300
H	3.25634400	-1.06946000	-2.05247100
H	2.50331600	-2.43726800	-1.24780300
C	3.96620800	-1.41127500	-0.04161300
H	4.86879100	-1.88436900	-0.44189900
H	3.65697400	-2.01911600	0.81852700
C	4.29717900	-0.02369200	0.45719500
C	5.57276600	0.27679700	0.94052600
C	5.87049900	1.53879400	1.45547000
C	4.88096500	2.52225700	1.49529400
C	3.60676700	2.23552500	1.01257100
C	3.30206100	0.97247200	0.49077200
H	6.34321000	-0.49056700	0.91138300
H	6.87025400	1.75246200	1.82185200
H	5.10409400	3.50690300	1.89534200
H	2.82285100	2.98656600	1.02628000

Reaction of cyclohexanone/styrene monoadduct K enolate with styrene (3) T.S., solvent = DMSO



Charge = 0; Multiplicity = 1

53

-1680.697280 [B3LYP/6-31+G(d,p)]

C	-4.70143700	-0.83398000	0.25481700
C	-4.23483800	-0.07813400	1.34048800
C	-2.87890100	-0.04561900	1.66078700
C	-1.89692500	-0.76755500	0.91153000
C	-2.40517600	-1.53057600	-0.18559700
C	-3.76163600	-1.56062400	-0.49570100
H	-5.75723800	-0.85860900	0.00246800
H	-4.93658700	0.48985200	1.94772900
H	-2.55240200	0.53113700	2.52547600
H	-1.71764600	-2.10475200	-0.79897600
H	-4.09511400	-2.15909800	-1.34116100
C	-0.51539700	-0.72044500	1.30453600
H	-0.30012900	-0.09768300	2.17266700
C	0.57817700	-1.39590900	0.71141800
H	0.36141600	-2.26414500	0.08739400
H	1.42195900	-1.57287400	1.37192200
C	1.60781900	-0.48445400	-0.75746700
C	1.97274500	0.74569400	-0.10813100
O	1.15447600	1.70992500	0.00206500
K	-1.32302900	2.46660100	0.20968600
C	2.74434800	-1.44914800	-1.09077100
H	3.23536200	-1.13209800	-2.02407100
H	2.32695100	-2.44427500	-1.29806900
C	0.55659600	-0.37632800	-1.85453500
H	-0.34504100	0.09247900	-1.45240300
H	0.26759900	-1.38679600	-2.17333100
C	1.01218700	0.42041200	-3.10535500
H	1.90499800	-0.04938800	-3.53400900
H	1.29689000	1.43078200	-2.79231800
C	-0.06392700	0.50237200	-4.16659200
C	-0.18822900	-0.49279500	-5.15035300
C	-0.98817000	1.56008400	-4.17644000
C	-1.20319800	-0.43625100	-6.11088900
H	0.52118600	-1.31722200	-5.16655400
C	-2.00510600	1.62287400	-5.13437900
H	-0.90501300	2.34636500	-3.42959200
C	-2.11731400	0.62288800	-6.10626000
H	-1.27666600	-1.21554100	-6.86468200

H	-2.70514800	2.45398000	-5.12483100
H	-2.90403100	0.67086300	-6.85374800
C	3.80745800	-1.56796200	0.00906100
H	4.68775300	-2.09748700	-0.37257100
H	3.42252700	-2.18561900	0.83123500
C	3.31175000	0.85872800	0.54600000
C	4.21920600	-0.22516800	0.57015500
C	3.69388700	2.08528100	1.12270200
H	2.98678800	2.90773600	1.09212100
C	4.94776100	2.24619700	1.71090900
H	5.22636800	3.20124100	2.14781500
C	5.47697800	-0.04972100	1.16144700
H	6.17518100	-0.88364300	1.17690500
C	5.84714100	1.17342200	1.72910200
H	6.82991700	1.28858100	2.17778300

-1680.188356 [M06-2X/6-31++G(d,p)]

C	-4.55372100	-0.87094000	-0.01802500
C	-4.17360800	-0.07971700	1.06866000
C	-2.84263600	-0.01170300	1.46980100
C	-1.81198400	-0.72413900	0.79935800
C	-2.22971100	-1.52733800	-0.29608900
C	-3.56047800	-1.59731200	-0.68701300
H	-5.59018700	-0.92316200	-0.33455400
H	-4.92260000	0.48799600	1.61507200
H	-2.57922700	0.59416000	2.33598900
H	-1.48993500	-2.09736800	-0.85012600
H	-3.82921100	-2.22401900	-1.53390700
C	-0.44720000	-0.62036500	1.25475000
H	-0.28164000	0.03716600	2.10721700
C	0.65966400	-1.30640200	0.74186900
H	0.49518100	-2.19793200	0.13296800
H	1.51663500	-1.39615200	1.40398400
C	1.67847800	-0.43599500	-0.81921200
C	2.01489600	0.76958100	-0.15133900
O	1.20538200	1.73404000	-0.04453400
K	-1.26506000	2.35098700	0.11546800
C	2.79625400	-1.40741800	-1.14842300
H	3.31429000	-1.08406400	-2.06507400
H	2.36243100	-2.39042200	-1.37952900
C	0.58677300	-0.35018700	-1.85737000
H	-0.29756500	0.12490400	-1.41826200
H	0.28421800	-1.36427300	-2.15631200
C	0.99121300	0.43079600	-3.12333700
H	1.85305800	-0.05609400	-3.59442600
H	1.30057800	1.43981600	-2.82836000
C	-0.14916200	0.50688500	-4.10734800
C	-0.38107400	-0.52942600	-5.01996100
C	-1.04156800	1.58451400	-4.08526100
C	-1.47336300	-0.49074300	-5.88655100
H	0.30464300	-1.37354400	-5.05161800
C	-2.13694900	1.62852300	-4.94798300
H	-0.86873500	2.40281500	-3.38973800
C	-2.35732400	0.58871100	-5.85156600
H	-1.63363700	-1.30188400	-6.59070600
H	-2.81496900	2.47628700	-4.91762700
H	-3.20776800	0.62079800	-6.52547400
C	3.82223600	-1.56316500	-0.02490600
H	4.71683800	-2.07467300	-0.39485400

H	3.41172100	-2.20587400	0.76374300
C	3.32922500	0.85057200	0.56142100
C	4.21455200	-0.24233700	0.59436100
C	3.69050800	2.05108300	1.18744700
H	2.99141900	2.88039900	1.14531700
C	4.91387200	2.17884700	1.83861000
H	5.18298500	3.11610400	2.31638900
C	5.44121800	-0.10188500	1.24957700
H	6.12679700	-0.94590400	1.27275200
C	5.79539300	1.09646400	1.86785000
H	6.75598000	1.18658000	2.36631400

10.7. REACTION PROFILES FOR ALKYLPYRIDINES WITH STYRENE

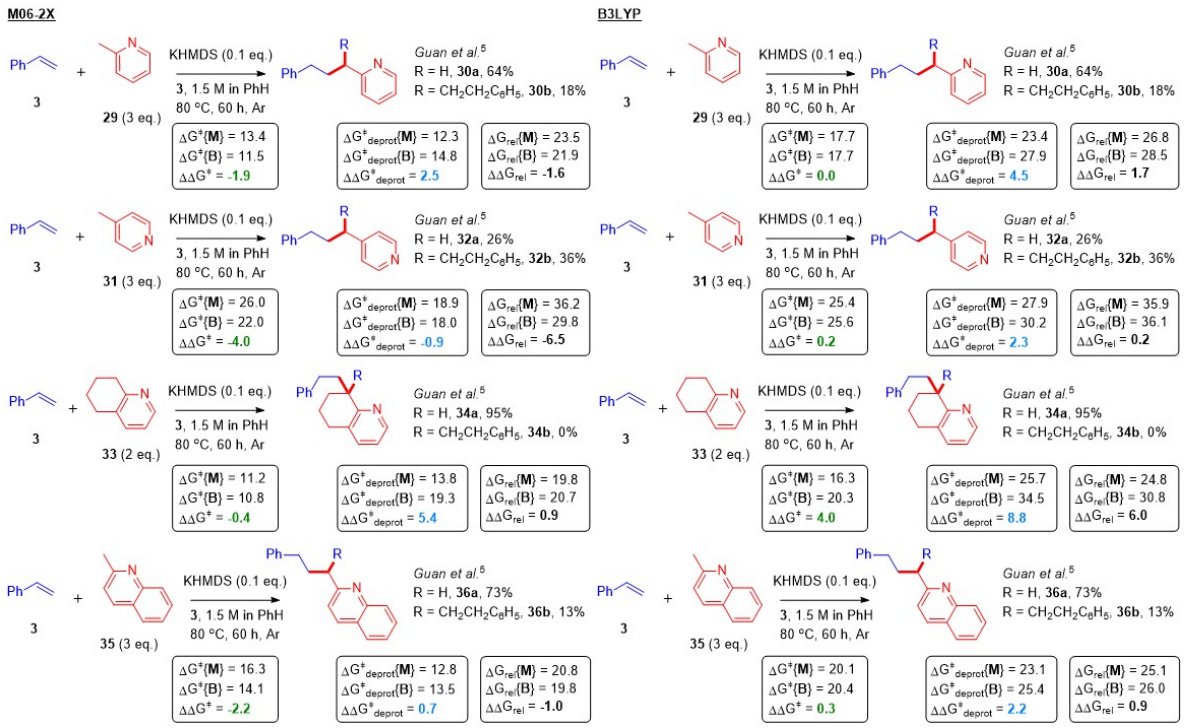
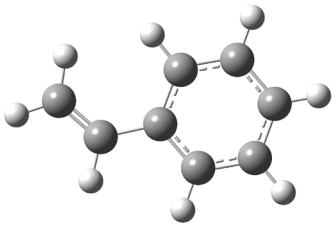


Figure S72. Application of the computational model to alkylpyridine CAKES. Comparison of B3LYP/6-31+G(d,p) and M06-2X/6-31++(d,p) methods.

10.7.1. XYZ Co-ordinates of starting materials, intermediates, products

Styrene, solvent = benzene



Charge = 0; Multiplicity = 1

16

-309.573885 [B3LYP/6-31+G(d,p)]

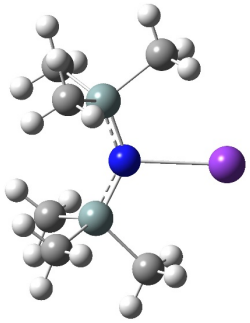
C	-2.26877900	0.26199700	-0.00002300
C	-1.78316600	-1.04791900	-0.00002000
C	-0.40640800	-1.28348500	0.00001100

C	0.51574800	-0.22039800	0.00001400
C	0.00912900	1.09422100	0.00002700
C	-1.36438200	1.33146900	0.00001100
H	-3.33834500	0.45038600	-0.00003800
H	-2.47379000	-1.88636900	-0.00003100
H	-0.03598300	-2.30569500	0.00002800
H	0.69158500	1.93849600	0.00007100
H	-1.73246700	2.35357800	0.00001800
C	1.95722300	-0.53041700	0.00002000
H	2.18946600	-1.59508800	0.00007200
C	2.98198900	0.33631100	-0.00003800
H	2.84427600	1.41384300	-0.00011300
H	4.00713400	-0.01982100	-0.00001600

-309.420049 [M06-2X/6-31++G(d,p)]

C	2.25937300	0.26585200	0.00001500
C	1.78068000	-1.04230600	0.00001700
C	0.40747700	-1.28185000	0.00000000
C	-0.51141000	-0.22452000	-0.00001600
C	-0.01524600	1.08790300	-0.00002300
C	1.35423700	1.32975000	-0.00000700
H	3.32763200	0.45804300	0.00002600
H	2.47403300	-1.87764700	0.00003200
H	0.03800100	-2.30427100	0.00000200
H	-0.70203400	1.92867600	-0.00004600
H	1.71897700	2.35235600	-0.00001300
C	-1.95462000	-0.53586600	-0.00002800
H	-2.19121600	-1.59921700	-0.00008900
C	-2.96439900	0.33969200	0.00003600
H	-2.80901000	1.41451500	0.00010700
H	-3.99292400	-0.00438600	0.00002000

Potassium bis(trimethylsilyl)amide, solvent = benzene



Charge = 0; Multiplicity = 1

28

-1473.145220 [B3LYP/6-31+G(d,p)]

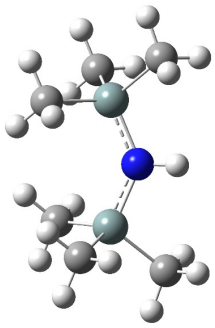
N	0.00001600	0.15257200	0.00003800
Si	1.56271300	-0.49274200	0.00051700
Si	-1.56246800	-0.49324400	-0.00052400
C	-2.84884200	0.93485900	-0.02808400
H	-3.87446300	0.54485000	-0.03005700
H	-2.75910300	1.58267200	0.85606700
H	-2.74625600	1.56019400	-0.92678100
C	-2.01543200	-1.53901100	1.53634300
H	-1.38040500	-2.43116900	1.60557500
H	-1.87259900	-0.96512900	2.46097200
H	-3.06028500	-1.87604700	1.50776600

C	-1.99658100	-1.58501200	-1.51058500
H	-3.04212800	-1.92015800	-1.48607200
H	-1.83986500	-1.04045000	-2.45050000
H	-1.36189900	-2.47952700	-1.54271200
C	2.01596200	-1.53859800	-1.53621600
H	1.38096900	-2.43077100	-1.60554300
H	1.87342400	-0.96482700	-2.46095800
H	3.06081200	-1.87563100	-1.50729000
C	2.84862600	0.93575700	0.02782300
H	2.74607200	1.56097500	0.92659800
H	3.87438300	0.54611700	0.02942100
H	2.75831000	1.58357900	-0.85626100
C	1.99726900	-1.58419100	1.51069600
H	3.04310200	-1.91847100	1.48653100
H	1.83982300	-1.03967400	2.45052000
H	1.36332400	-2.47923500	1.54273700
K	-0.00067200	2.79135200	-0.00000200

-1472.872044 [M06-2X/6-31++G(d,p)]

N	0.00000200	0.23729200	0.00004300
Si	1.52580400	-0.48171600	0.00713900
Si	-1.52575800	-0.48180000	-0.00711900
C	-2.85556400	0.84991700	-0.32559800
H	-3.85846000	0.41074700	-0.37682400
H	-2.87564700	1.59466800	0.48190900
H	-2.67929200	1.37242700	-1.27471500
C	-2.02642300	-1.30146900	1.63385200
H	-1.35066100	-2.13034800	1.87454200
H	-1.97411400	-0.58354300	2.46092100
H	-3.04751600	-1.70000100	1.59373400
C	-1.77799500	-1.81913400	-1.33510500
H	-2.81096800	-2.18685500	-1.35326400
H	-1.53185800	-1.43744700	-2.33273300
H	-1.12195000	-2.67612800	-1.13867300
C	2.02653100	-1.30110700	-1.63395500
H	1.35085200	-2.13001800	-1.87476800
H	1.97413700	-0.58305700	-2.46091200
H	3.04766600	-1.69953700	-1.59391300
C	2.85552800	0.85003500	0.32580300
H	2.67921100	1.37241700	1.27498100
H	3.85845500	0.41092900	0.37697400
H	2.87556100	1.59488700	-0.48161200
C	1.77810100	-1.81923200	1.33492800
H	2.81109600	-2.18689400	1.35304100
H	1.53193100	-1.43771300	2.33261100
H	1.12211100	-2.67623500	1.13835600
K	-0.00012000	2.82872700	0.00001100

Bis(trimethylsilyl)amide, solvent = benzene



Charge = 0; Multiplicity = 1

28

-873.801959 [B3LYP/6-31+G(d,p)]

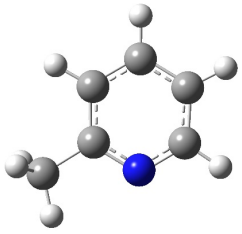
N	-0.00144100	-0.03248600	0.76484400
Si	-1.61747900	-0.01320100	0.07686300
Si	1.61571900	0.00681300	0.07967300
C	2.79661600	0.51196100	1.46734100
H	3.83340400	0.52369000	1.11111500
H	2.56083600	1.51248800	1.84776100
H	2.74535200	-0.19006500	2.30853100
C	1.70302100	1.25742700	-1.33786200
H	1.01096400	1.00581900	-2.14993800
H	1.45959100	2.26779800	-0.99050400
H	2.71275300	1.28071300	-1.76553100
C	2.13610900	-1.68743300	-0.58823300
H	3.14806700	-1.65155600	-1.01044400
H	2.12933000	-2.44150200	0.20768600
H	1.45690500	-2.03038000	-1.37715100
C	-1.66498900	-1.06592400	-1.49380400
H	-0.97348200	-0.69239500	-2.25779600
H	-1.40066100	-2.10798300	-1.28211600
H	-2.67082600	-1.05425900	-1.93076000
C	-2.79268500	-0.72253200	1.37728400
H	-2.75299900	-0.14249300	2.30748500
H	-3.82911300	-0.70079300	1.02027900
H	-2.54043100	-1.76178300	1.61706700
C	-2.17512200	1.74311200	-0.36205600
H	-3.18870300	1.74490400	-0.78201500
H	-2.17691900	2.38704500	0.52537600
H	-1.50567800	2.19778900	-1.10131600
H	-0.00136900	-0.04987800	1.78084100

-873.545425 [M06-2X/6-31++G(d,p)]

N	0.00076700	-0.03020300	0.84402100
Si	-1.57711500	-0.01246700	0.09447900
Si	1.57787500	0.00637700	0.09346700
C	2.82598300	0.51175200	1.40322300
H	3.83774400	0.53620100	0.98514300
H	2.59907600	1.50595700	1.80133200
H	2.82837600	-0.19764500	2.23789400
C	1.56667300	1.25067700	-1.31788800
H	0.83370100	0.98570400	-2.08802600
H	1.32476900	2.25402700	-0.95224700
H	2.54942900	1.28970800	-1.80033400
C	2.05825400	-1.67468400	-0.60510800
H	3.04552400	-1.63350100	-1.07878600

H	2.09166200	-2.43017500	0.18702000
H	1.33652900	-2.00889500	-1.35790600
C	-1.56970400	-1.14516500	-1.40951100
H	-0.83832800	-0.82053600	-2.15815200
H	-1.32804800	-2.17456800	-1.12541900
H	-2.55387600	-1.14385700	-1.89086600
C	-2.82263300	-0.62061300	1.36331000
H	-2.82156900	0.01640200	2.25433100
H	-3.83555700	-0.60918900	0.94753800
H	-2.59543300	-1.64494700	1.67574700
C	-2.06025300	1.71588100	-0.47591200
H	-3.05119700	1.71018300	-0.94368800
H	-2.08609500	2.41196900	0.36903600
H	-1.34397300	2.10265600	-1.20850400
H	0.00133100	-0.07990500	1.85782100

2-alkylpyridine (**29**), solvent = benzene



Charge = 0; Multiplicity = 1

14

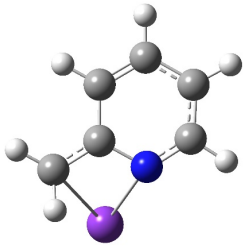
-287.543225 [B3LYP/6-31+G(d,p)]

C	-1.09084800	-1.20891500	0.00000500
C	0.88035900	-0.00839900	0.00005700
C	0.16917100	1.20369700	0.00001400
C	-1.22317400	1.17983100	-0.00002300
C	-1.87532100	-0.05648800	-0.00000700
H	-1.55664500	-2.19237100	0.00002300
H	0.70803900	2.14680100	0.00002500
H	-1.79014500	2.10639700	-0.00001200
H	-2.95814000	-0.12756300	0.00000100
N	0.25232200	-1.19739800	-0.00001300
C	2.38992000	-0.02292900	-0.00001300
H	2.78902700	0.48974800	-0.88278300
H	2.78914600	0.49074000	0.88212100
H	2.75182400	-1.05274400	0.00051900

-287.404604 [M06-2X/6-31++G(d,p)]

C	1.07172600	-1.21210800	0.00000000
C	-0.87599000	0.00583100	0.00000000
C	-0.15923300	1.20706000	0.00000000
C	1.23177300	1.16896800	-0.00000100
C	1.86819100	-0.06840000	0.00000100
H	1.52925900	-2.19871400	0.00000000
H	-0.69053200	2.15327900	0.00000100
H	1.80754000	2.08941600	0.00000000
H	2.94916900	-0.15255300	0.00000200
N	-0.26302600	-1.18705700	-0.00000100
C	-2.38042700	-0.01498900	0.00000100
H	-2.74774000	-0.54756200	0.88161300
H	-2.79501100	0.99491700	0.00000300
H	-2.74774200	-0.54755500	-0.88161500

2-alkylpyridine K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

14

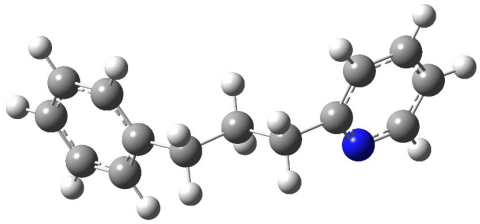
-886.872084 [B3LYP/6-31+G(d,p)]

C	1.04770100	-1.33601300	0.56553700
C	0.20332300	0.85467000	0.32509900
C	1.40972200	1.18989600	-0.40317200
C	2.39753700	0.25480400	-0.59889300
C	2.23890700	-1.06273600	-0.09700000
H	0.86982300	-2.33918400	0.95836700
H	1.52815300	2.20608000	-0.77120200
H	3.30494900	0.53028200	-1.13283000
H	3.00117800	-1.82433400	-0.22086900
N	0.05029400	-0.45882100	0.77163700
C	-0.82491800	1.77935000	0.54171800
H	-1.56042400	1.58648100	1.32130000
H	-0.68186900	2.81801900	0.25956700
K	-2.40250000	-0.51818000	-0.41134400

-886.715161 [M06-2X/6-31++G(d,p)]

C	1.05980000	-1.31462500	0.58897100
C	0.16981700	0.84739900	0.34543100
C	1.35031700	1.19681900	-0.41727500
C	2.34653600	0.28154200	-0.62294900
C	2.22642600	-1.03069800	-0.10126500
H	0.90946600	-2.31518500	0.99804500
H	1.43688300	2.20984300	-0.80078000
H	3.23373200	0.56674200	-1.18398600
H	2.99812700	-1.77932000	-0.23329000
N	0.05281700	-0.45719300	0.80715200
C	-0.86269200	1.75326800	0.57069300
H	-1.59981200	1.54393500	1.34291700
H	-0.74906400	2.78690400	0.26402800
K	-2.33369900	-0.53762100	-0.43256000

2-alkylpyridine/styrene monoadduct (30a), solvent = benzene



Charge = 0; Multiplicity = 1

30

-597.119718 [B3LYP/6-31+G(d,p)]

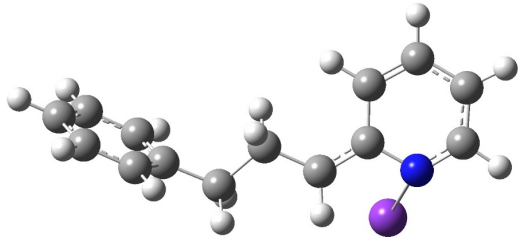
C	-4.85718900	0.37491000	1.00771700
C	-4.31301600	-0.91300700	1.01165600
C	-3.15933500	-1.18961100	0.27197200
C	-2.52663400	-0.18991300	-0.48320600
C	-3.08574700	1.09782400	-0.47971000
C	-4.23888800	1.38049200	0.25791300
H	-5.75527900	0.59159000	1.57898200
H	-4.78824100	-1.70350400	1.58604900
H	-2.74688800	-2.19608200	0.27651300
H	-2.61504400	1.88543600	-1.06371700
H	-4.65625500	2.38357300	0.24336300
C	-1.25674600	-0.48302900	-1.25402400
H	-1.25442700	-1.53445600	-1.56858300
H	-1.23579200	0.12049600	-2.17039900
C	0.02158400	-0.19797400	-0.44022500
H	0.00649600	-0.79418300	0.48144300
H	0.03508500	0.85476300	-0.13432400
C	1.30667600	-0.50750600	-1.23321500
H	1.31287900	-1.56563400	-1.52110400
H	1.30960700	0.08454200	-2.15627500
C	2.56115300	-0.18655300	-0.45419400
C	3.31747500	-1.19199200	0.16734100
N	2.90140700	1.11362300	-0.36560300
C	4.45209800	-0.84168500	0.89900200
H	3.01771700	-2.23148300	0.07297800
C	3.99285800	1.43964100	0.34047900
C	4.80216900	0.50611500	0.99150300
H	5.05177600	-1.60608200	1.38487400
H	4.23331500	2.50007100	0.38411600
H	5.67646200	0.82932300	1.54725600

-596.834839 [M06-2X/6-31++G(d,p)]

C	4.77828600	0.40350300	-1.03194800
C	4.17834000	-0.84981600	-1.15432700
C	3.04888600	-1.16114500	-0.39860500
C	2.50020600	-0.22978600	0.48982500
C	3.11054600	1.02341800	0.60304700
C	4.24064400	1.34034200	-0.14978800
H	5.65950800	0.64713900	-1.61707600
H	4.59176500	-1.58651900	-1.83663500
H	2.58670500	-2.14123600	-0.49575000
H	2.69572800	1.75645400	1.29120900
H	4.70262300	2.31743000	-0.04467300
C	1.24691600	-0.54934500	1.26690500
H	1.24096900	-1.61156800	1.54096600
H	1.23638500	0.02410500	2.20165000
C	-0.02189900	-0.22712100	0.46771200
H	-0.02335900	-0.80967900	-0.46281500
H	-0.01735400	0.83124200	0.18104100
C	-1.29889400	-0.52446800	1.26239100
H	-1.32047000	-1.58306700	1.54538000
H	-1.29566300	0.06815100	2.18438500
C	-2.53467400	-0.18094600	0.47219100
C	-3.32037300	-1.17330700	-0.12304500
N	-2.81449800	1.12369000	0.33937200
C	-4.42818000	-0.80085900	-0.87781300
H	-3.06152600	-2.21916800	0.01038900
C	-3.87992000	1.47039000	-0.38719700
C	-4.71881200	0.55303000	-1.01687300

H	-5.05405000	-1.55414300	-1.34674200
H	-4.07476600	2.53737000	-0.46834600
H	-5.57145300	0.89431300	-1.59343600

2-alkylpyridine/styrene monoadduct K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

30

-1196.445824 [B3LYP/6-31+G(d,p)]

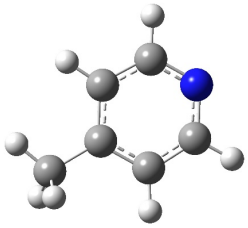
C	-4.42033800	-0.63725400	0.45011000
C	-2.07327900	-0.44025200	0.26211900
C	-2.07709900	-1.67693400	-0.49536800
C	-3.25414200	-2.34846000	-0.73909600
C	-4.48263600	-1.83716400	-0.25580100
H	-5.34112100	-0.19629500	0.83836700
H	-1.13590600	-2.08477400	-0.85034600
H	-3.23414000	-3.28304500	-1.29669100
H	-5.42646400	-2.34648000	-0.41741800
N	-3.30471100	0.05927000	0.70540200
C	-0.91053300	0.28552900	0.54021700
H	-0.97685400	1.01098900	1.35501000
K	-2.71223700	2.50004300	-0.30712800
C	0.47681200	-0.21447200	0.21405500
H	0.74336000	-1.12381200	0.78683200
H	0.55674700	-0.51186400	-0.84300800
C	1.56715200	0.84434800	0.49304400
H	1.35790100	1.73450300	-0.11490900
H	1.49177900	1.15566300	1.54337300
C	2.97247200	0.35816400	0.21310300
C	3.71366900	-0.31449500	1.19808100
C	3.56154400	0.53589100	-1.04888600
C	4.99863600	-0.79651800	0.93225900
H	3.27876900	-0.45934200	2.18440500
C	4.84654000	0.05699600	-1.32163000
H	3.00705900	1.05816200	-1.82556500
C	5.57085600	-0.61263000	-0.33054100
H	5.55347400	-1.31232200	1.71137500
H	5.28244700	0.20983500	-2.30531500
H	6.57052400	-0.98341700	-0.53848900

-1196.144410 [M06-2X/6-31++G(d,p)]

C	4.39135800	-0.64332900	-0.45427300
C	2.05651400	-0.41710200	-0.28232300
C	2.03863400	-1.64581900	0.48550200
C	3.20232800	-2.32760200	0.73558600
C	4.43725000	-1.83630900	0.25429700
H	5.31838000	-0.21516100	-0.84020700
H	1.08926600	-2.03721000	0.83674000
H	3.16879300	-3.25719800	1.29980600
H	5.37351200	-2.35445600	0.42220200
N	3.28906500	0.06390900	-0.71819400

C	0.90416500	0.30848100	-0.56680200
H	0.97066500	1.04337200	-1.37223900
K	2.68364700	2.44560800	0.33414000
C	-0.47556500	-0.17992600	-0.21570800
H	-0.75357100	-1.09637800	-0.76932800
H	-0.54648200	-0.45358600	0.84854900
C	-1.55234300	0.87894800	-0.50033100
H	-1.34323800	1.77004600	0.10547500
H	-1.47911600	1.18256800	-1.55243500
C	-2.94693200	0.38122400	-0.21609200
C	-3.68081900	-0.28604600	-1.20307500
C	-3.51980100	0.52576700	1.05236700
C	-4.95071700	-0.79374800	-0.93381300
H	-3.24788200	-0.40745200	-2.19359900
C	-4.78989400	0.02079800	1.32854900
H	-2.96201900	1.04194200	1.83091800
C	-5.51054400	-0.64145100	0.33491200
H	-5.50393100	-1.30690700	-1.71483100
H	-5.21834300	0.14678300	2.31855900
H	-6.50059600	-1.03359200	0.54631400

4-alkylpyridine (**31**), solvent = benzene



Charge = 0; Multiplicity = 1

14

-287.543730 [B3LYP/6-31+G(d,p)]

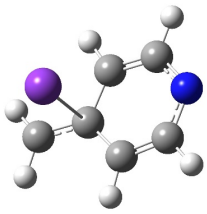
C	-1.22792900	1.13892300	0.00001700
C	-1.21836900	-1.14418200	0.00001400
C	0.17544100	-1.19085100	-0.00001300
C	0.90743800	0.00561400	-0.00003300
C	0.16803000	1.19446900	-0.00002700
H	-1.80989100	2.05823000	0.00001800
H	0.68277100	-2.15187200	-0.00002400
H	0.66960400	2.15816200	-0.00005600
N	-1.92849800	-0.00431500	0.00004000
C	2.41582200	0.00370200	-0.00001000
H	2.80619200	-0.51647200	0.88211300
H	2.80624800	-0.51763200	-0.88141700
H	2.81674300	1.02073100	-0.00065000
H	-1.79477600	-2.06699200	0.00004600

-287.404498 [M06-2X/6-31++G(d,p)]

C	-1.22582000	1.13407300	0.00001200
C	-1.21330400	-1.14173800	0.00002500
C	0.17707600	-1.18708300	-0.00001600
C	0.90316900	0.00784200	-0.00003400
C	0.16740800	1.19292200	-0.00002300
H	-1.80933200	2.05165300	0.00002100
H	0.68795900	-2.14578700	-0.00003700
H	0.66832600	2.15636500	-0.00004700
N	-1.92120700	-0.00584200	0.00003800
C	2.40815700	0.00361500	-0.00001200

H	2.79172600	-0.51695200	0.88238600
H	2.79177900	-0.51815100	-0.88167200
H	2.80716100	1.01990500	-0.00067200
H	-1.78928200	-2.06392400	0.00003400

4-alkylpyridine K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

14

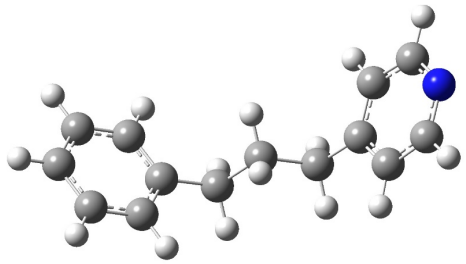
-886.870233 [B3LYP/6-31+G(d,p)]

C	-1.55982200	-0.32638800	-1.13781500
C	0.06138800	1.14979700	-0.00048300
C	-0.55308700	0.62042600	1.20263400
C	-1.56050200	-0.32492200	1.13776100
H	-1.98969100	-0.70338200	-2.06680100
H	-0.21984300	0.97753400	2.17562400
H	-1.99087500	-0.70076200	2.06697600
C	1.17995200	1.97354300	-0.00065300
H	1.54865300	2.40539800	-0.92793300
H	1.54815100	2.40633000	0.92639500
K	1.78009100	-1.14114700	0.00065100
C	-0.55240500	0.61891200	-1.20330000
H	-0.21859300	0.97480600	-2.17654200
N	-2.08466900	-0.84947700	0.00015000

-886.714848 [M06-2X/6-31++G(d,p)]

C	0.64256700	1.13561000	1.13772100
C	-1.33121000	0.19323300	0.00000600
C	-0.62041500	0.59535100	-1.20550200
C	0.64255000	1.13565900	-1.13769500
H	1.15533200	1.39546300	2.06429200
H	-1.08904900	0.44840100	-2.17545500
H	1.15530200	1.39555200	-2.06426300
C	-2.49449400	-0.53100100	0.00000200
H	-2.99515300	-0.78218800	0.92964500
H	-2.99518300	-0.78214100	-0.92963700
K	1.00486600	-1.60200000	-0.00002500
C	-0.62039700	0.59529800	1.20552100
H	-1.08901300	0.44829600	2.17547500
N	1.35053000	1.36710100	0.00001300

4-alkylpyridine/styrene monoadduct (32a), solvent = benzene



Charge = 0; Multiplicity = 1

30

-597.118486 [B3LYP/6-31+G(d,p)]

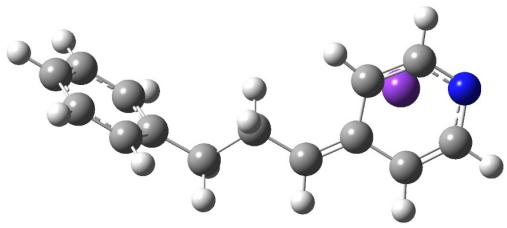
C	4.86712800	-0.00986100	-1.08167000
C	4.25284700	-1.21609600	-0.73066500
C	3.10152000	-1.21271600	0.06177300
C	2.54053800	-0.00923500	0.51734500
C	3.16919200	1.19344400	0.15956200
C	4.32125800	1.19632500	-0.63240700
H	5.76378900	-0.01033700	-1.69465300
H	4.67217300	-2.15951400	-1.06925000
H	2.63465100	-2.15647300	0.33462500
H	2.75521400	2.13670200	0.50875500
H	4.79373800	2.13907800	-0.89409800
C	1.27193200	-0.00788300	1.34407100
H	1.25635300	-0.89114500	1.99528500
H	1.26435600	0.86965600	2.00277100
C	-0.00794500	0.00074300	0.48382800
H	-0.01409200	-0.87920900	-0.17148400
H	0.00008900	0.87863400	-0.17421000
C	-1.29136300	0.01201200	1.34076100
H	-1.28977900	-0.86431800	2.00039900
H	-1.28206100	0.89870800	1.98669900
C	-2.55060200	0.01080700	0.50607000
C	-3.18944800	-1.18140400	0.13984500
C	-4.33216600	-1.13280000	-0.66044100
H	-2.80722400	-2.14121000	0.47696500
C	-4.26431400	1.14823900	-0.76346300
H	-4.83712100	-2.05291600	-0.94716300
H	-4.71482000	2.06688000	-1.13348300
N	-4.87587600	0.00649100	-1.11528200
C	-3.11919500	1.20121100	0.03249800
H	-2.68042800	2.16331700	0.28316500

-596.834577 [M06-2X/6-31++G(d,p)]

C	-4.78241300	0.01225500	-1.12116100
C	-4.15810900	1.21486900	-0.79007600
C	-3.03317700	1.21481000	0.03299700
C	-2.51288300	0.01802900	0.53773500
C	-3.14731100	-1.18093900	0.19868600
C	-4.27348300	-1.18699400	-0.62383700
H	-5.66108300	0.01034500	-1.75842300
H	-4.54966900	2.15383300	-1.16974200
H	-2.55181600	2.15554400	0.29159300
H	-2.75597200	-2.11880900	0.58651000
H	-4.75547600	-2.12764700	-0.87279300
C	-1.26297400	0.01925800	1.38330900

H	-1.24995900	0.90819100	2.02575600
H	-1.26269700	-0.85556100	2.04459900
C	0.00879500	0.00176800	0.52576200
H	0.01939600	0.88058600	-0.13130800
H	-0.00364300	-0.87949500	-0.12797100
C	1.28354800	-0.01255300	1.38092600
H	1.28950600	0.86569500	2.03685200
H	1.27640900	-0.90048100	2.02411300
C	2.52374000	-0.01550500	0.52666500
C	3.17082600	1.16985900	0.17306500
C	4.28553700	1.11679900	-0.66088100
H	2.81486300	2.12698000	0.54411400
C	4.16627100	-1.15183400	-0.81790900
H	4.80152800	2.03202700	-0.94142000
H	4.58553800	-2.06867800	-1.22547200
N	4.78827500	-0.01790200	-1.15725000
C	3.04725200	-1.20271400	0.00911400
H	2.59144100	-2.15985000	0.24798000

4-alkylpyridine/styrene monoadduct K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

30

-1196.444952 [B3LYP/6-31+G(d,p)]

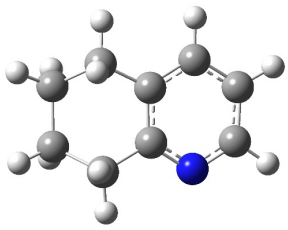
C	4.34805300	-0.97550500	-0.25996100
C	1.87796100	-0.82634400	-0.22027900
C	2.08644100	-0.46581100	1.18058800
C	3.36059400	-0.34137100	1.70171200
H	5.26550100	-1.20790300	-0.80211800
H	1.23474900	-0.30658500	1.83570900
H	3.47438100	-0.05904500	2.74964800
C	0.65374000	-0.85395600	-0.84977700
H	0.61670200	-1.19078700	-1.88592200
K	3.35466800	1.90599600	-0.35918500
C	-0.66427100	-0.57815000	-0.17045100
H	-0.96062600	-1.39726600	0.50958600
H	-0.60060300	0.31402600	0.47380800
C	-1.81539400	-0.36322800	-1.17878300
H	-1.55463300	0.47346700	-1.83924400
H	-1.89185000	-1.25390600	-1.81576300
C	-3.15090100	-0.09474900	-0.52061900
C	-3.97487900	-1.15198300	-0.10138800
C	-3.58730400	1.21745000	-0.27848300
C	-5.19128400	-0.90798700	0.54266500
H	-3.66017200	-2.17673100	-0.28518400
C	-4.80310800	1.46885300	0.36482800
H	-2.96870500	2.05168800	-0.60236100
C	-5.61028400	0.40518700	0.77967900
H	-5.81298400	-1.74248500	0.85564000
H	-5.12121800	2.49354300	0.53761600
H	-6.55673300	0.59695700	1.27716400
C	3.13643700	-1.13703300	-0.89297400

H	3.11481600	-1.50399800	-1.91750700
N	4.52684100	-0.52530400	1.02184300

-1196.148778 [M06-2X/6-31++G(d,p)]

C	4.35287100	-0.89948400	-0.19310300
C	1.88894300	-0.83406600	-0.20737900
C	2.05341500	-0.43793000	1.18711700
C	3.30932300	-0.23704200	1.71847800
H	5.28914600	-1.11490100	-0.70835500
H	1.18340600	-0.29807600	1.82175200
H	3.39335000	0.08663900	2.75668600
C	0.68537400	-0.86681700	-0.85919100
H	0.65821300	-1.21248900	-1.89207900
K	3.16851800	1.82929300	-0.42226800
C	-0.62720900	-0.56031800	-0.19055500
H	-0.89882600	-1.32463900	0.55830900
H	-0.57453100	0.38622000	0.37329700
C	-1.78115800	-0.45298000	-1.19859800
H	-1.54171900	0.32733200	-1.93170700
H	-1.85689300	-1.39777000	-1.75058800
C	-3.09865300	-0.14336500	-0.53398200
C	-3.92316200	-1.17054800	-0.06224700
C	-3.50217800	1.17997900	-0.32603100
C	-5.11729300	-0.88535500	0.59864500
H	-3.62397800	-2.20473900	-0.21815800
C	-4.69499500	1.47233800	0.33411400
H	-2.87297800	1.98960700	-0.68997000
C	-5.50733700	0.43857800	0.79944300
H	-5.74487800	-1.69726400	0.95408400
H	-4.99201300	2.50645500	0.48230800
H	-6.43802800	0.66252800	1.31143000
C	3.16640500	-1.14149800	-0.83941400
H	3.17788000	-1.55197000	-1.84642500
N	4.48770500	-0.38320900	1.06267600

5,6,7,8-tetrahydroquinoline (**33**), solvent = benzene



Charge = 0; Multiplicity = 1

21

-404.224813 [B3LYP/6-31+G(d,p)]

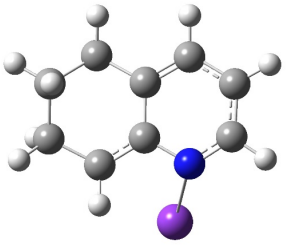
C	-1.03473000	-1.17539300	0.31886400
C	0.88346900	-0.00151700	-0.15741600
C	0.18989000	1.22630700	-0.17267600
C	-1.18122300	1.20705900	0.08103400
C	-1.81086100	-0.01639200	0.32759800
H	-1.48914400	-2.14505600	0.51070500
H	-1.75052900	2.13372400	0.08598100
H	-2.87642600	-0.07161900	0.52722200
N	0.28853000	-1.17892100	0.08637500
C	2.36477300	0.04132200	-0.43030100
H	2.80546600	-0.93748900	-0.22325000

H	2.51696700	0.24047400	-1.50157300
C	0.99738100	2.46941300	-0.44887500
H	0.39718200	3.36841600	-0.27191500
H	1.28065300	2.48681200	-1.51153600
C	2.27907100	2.49691900	0.41573700
H	1.98959600	2.73180300	1.44608400
H	2.91862400	3.31970800	0.07837400
C	3.06416200	1.15171800	0.39222400
H	3.19424000	0.79050300	1.41815700
H	4.07095300	1.30424600	-0.01096600

-404.033509 [M06-2X/6-31++G(d,p)]

C	2.41621800	-0.74740800	-0.19013700
C	0.16762300	-0.68901600	0.22579500
C	0.15035100	0.71711200	0.22500100
C	1.34662800	1.38569400	-0.00546700
C	2.50733600	0.64097200	-0.21400800
H	3.30015600	-1.35935300	-0.35173000
H	1.37251700	2.47265400	-0.02106000
H	3.46182200	1.12288200	-0.39552800
N	1.27207500	-1.41092100	0.02057600
C	-1.14675700	-1.38118200	0.45494100
H	-1.03036300	-2.45382700	0.28509600
H	-1.44100600	-1.24414900	1.50474000
C	-1.17917800	1.37892000	0.46088300
H	-1.10731400	2.45884400	0.30045800
H	-1.47021800	1.23108900	1.50976200
C	-2.25812900	0.76534600	-0.45308800
H	-2.09428200	1.13678600	-1.46939100
H	-3.23930200	1.13338300	-0.13937000
C	-2.23598000	-0.78618300	-0.45939400
H	-2.05627500	-1.14405100	-1.47778800
H	-3.20892900	-1.18333700	-0.15638400

5,6,7,8-tetrahydroquinoline K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

21

-1003.554479 [B3LYP/6-31+G(d,p)]

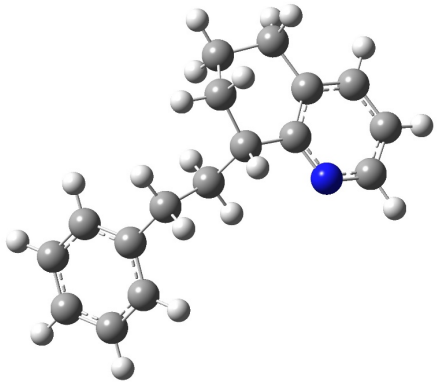
C	1.27083600	1.95993300	0.58995700
C	-0.04220000	0.00921500	0.38988600
C	-1.06913300	0.80050200	-0.28059100
C	-0.88385300	2.15341500	-0.43105000
C	0.31089200	2.78259100	0.01400800
H	2.21656500	2.38970400	0.92705000
H	-1.66667500	2.74800900	-0.90184200
H	0.47395400	3.84959000	-0.09422200
N	1.14649800	0.63473800	0.77694000
C	-0.21680900	-1.35704000	0.61580500
H	0.47419500	-1.84188400	1.30755200
K	2.55501000	-1.27408700	-0.50955600

C	-1.53442500	-2.06000100	0.33949300
H	-1.50413200	-2.67946700	-0.57523300
H	-1.76331200	-2.76399900	1.15306200
C	-2.69641300	-1.06063200	0.19769400
H	-2.93211100	-0.63326700	1.18171400
H	-3.60098700	-1.56768300	-0.16169200
C	-2.30746000	0.07794500	-0.76060900
H	-2.12266900	-0.36102400	-1.75558400
H	-3.13411000	0.78895000	-0.88537500

-1003.346445 [M06-2X/6-31++G(d,p)]

C	1.47643100	1.80115700	0.62997200
C	-0.02676600	0.00627900	0.43294400
C	-0.93634000	0.88515500	-0.29282200
C	-0.60489500	2.20104700	-0.46284000
C	0.63315800	2.70885300	0.01325500
H	2.45316600	2.13296600	0.98672600
H	-1.30193100	2.86056500	-0.97970900
H	0.91551900	3.74756900	-0.10897200
N	1.20708800	0.50416000	0.83800300
C	-0.35685400	-1.32058400	0.67439800
H	0.28357500	-1.87558400	1.36107600
K	2.30567400	-1.48943500	-0.55646300
C	-1.73561400	-1.87780200	0.38692600
H	-1.75655100	-2.52663900	-0.50490100
H	-2.06268700	-2.51550300	1.21917300
C	-2.76037700	-0.75649700	0.18326000
H	-2.95141400	-0.25945400	1.14292800
H	-3.71284600	-1.16392000	-0.17404400
C	-2.21408600	0.27642900	-0.80824600
H	-2.02244900	-0.23721900	-1.76431800
H	-2.94974900	1.06313100	-1.01226400

5,6,7,8-tetrahydroquinoline/styrene monoadduct (34a), solvent = benzene



Charge = 0; Multiplicity = 1

37

-713.801338 [B3LYP/6-31+G(d,p)]

C	-4.83838200	0.49582600	1.05159400
C	-4.45702700	-0.83158100	0.83393800
C	-3.33142700	-1.11977500	0.05630800
C	-2.56515700	-0.09316800	-0.51726100
C	-2.96185500	1.23470400	-0.29245500
C	-4.08633000	1.52913500	0.48380800
H	-5.71411200	0.72249200	1.65294000
H	-5.03712400	-1.64280100	1.26535200

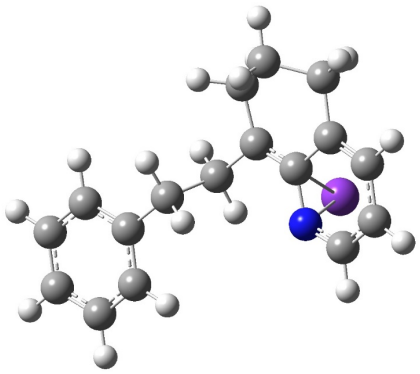
H	-3.04585300	-2.15588500	-0.11150700
H	-2.38608700	2.04533800	-0.73321200
H	-4.37694700	2.56420100	0.64135000
C	-1.32467000	-0.40723000	-1.32735900
H	-1.45132000	-1.38168400	-1.81268500
H	-1.21185700	0.33342300	-2.12941100
C	-0.04119000	-0.40393800	-0.46977700
H	-0.14697300	-1.12895700	0.34770000
H	0.06256800	0.58066300	-0.00139200
C	1.25245400	-0.69644000	-1.27344900
H	1.22894300	-0.04461600	-2.15718200
C	2.47538900	-0.27107100	-0.46927500
C	3.37931700	-1.20202000	0.08045000
N	2.62537300	1.05892700	-0.30848000
C	4.45512400	-0.69905500	0.82417800
C	3.66335500	1.51417500	0.39960700
C	4.60857600	0.67400000	0.99292100
H	5.16910700	-1.38959100	1.26787900
H	3.74364100	2.59510600	0.49653000
H	5.43379100	1.08614700	1.56508100
C	3.22996200	-2.69489700	-0.14357200
H	3.49876800	-3.23122600	0.77449600
H	3.96336800	-3.00637000	-0.90220300
C	1.82668800	-3.09185600	-0.61507700
H	1.83140300	-4.13367200	-0.95487900
H	1.12395600	-3.04026900	0.22641400
C	1.36450000	-2.16164300	-1.74374700
H	2.08805400	-2.22037200	-2.56849800
H	0.40641100	-2.49944500	-2.15268300

-713.469972 [M06-2X/6-31++G(d,p)]

C	-5.17504900	-0.58271200	-0.98291600
C	-4.53495200	0.63195500	-1.23003400
C	-3.38518300	0.97180500	-0.51976100
C	-2.85448100	0.10945500	0.44593600
C	-3.50435000	-1.10557200	0.68398300
C	-4.65633200	-1.45065200	-0.02275400
H	-6.07209200	-0.84928100	-1.53295500
H	-4.93363100	1.31640500	-1.97281900
H	-2.89074200	1.92171400	-0.71249900
H	-3.10345000	-1.78666500	1.43118900
H	-5.14918600	-2.39731000	0.17761900
C	-1.57838400	0.46724600	1.16789500
H	-1.56241500	1.54738800	1.35152600
H	-1.55174000	-0.02666600	2.14675900
C	-0.34041900	0.04653000	0.36305800
H	-0.38471600	0.49957600	-0.63652000
H	-0.37112700	-1.03922800	0.21647600
C	0.99273600	0.40717900	1.04596300
H	0.93652100	0.03586900	2.07787500
C	2.12525200	-0.35469300	0.38096900
C	3.08108800	0.27780200	-0.42952400
N	2.13386700	-1.67798800	0.60741600
C	4.06663600	-0.52400300	-1.01083600
C	3.08563600	-2.42077500	0.04651600
C	4.07961500	-1.89196200	-0.77614600
H	4.82067200	-0.06682200	-1.64818300
H	3.05550600	-3.48611000	0.26335900
H	4.83315500	-2.53683900	-1.21500600

C	3.07748900	1.77405200	-0.65482000
H	3.34763900	1.98371900	-1.69560000
H	3.86715800	2.21928200	-0.03375000
C	1.73998300	2.41835200	-0.29680600
H	1.84326600	3.50779700	-0.29155700
H	0.99360300	2.17374400	-1.06249200
C	1.27208000	1.91637000	1.06907900
H	2.05558300	2.12688400	1.80912600
H	0.38074000	2.46020400	1.39672200

5,6,7,8-tetrahydroquinoline/styrene monoadduct K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

37

-1313.127878 [B3LYP/6-31+G(d,p)]

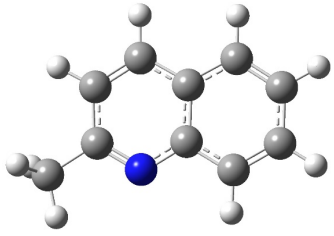
C	-2.30615400	-2.10875000	-1.13607300
C	-1.75186300	-0.00759000	-0.20270700
C	-3.11891100	0.43785300	-0.48079700
C	-3.98357000	-0.40430400	-1.13438400
C	-3.58957300	-1.72293400	-1.50017800
H	-1.96572300	-3.12268600	-1.35927300
H	-4.99027400	-0.05565100	-1.36467600
H	-4.25662200	-2.39906200	-2.02428600
N	-1.40534900	-1.33237100	-0.50799600
C	-0.82057400	0.83291900	0.40988800
K	-1.30166000	-1.63103900	2.21578300
C	-1.13247500	2.30404100	0.64544300
H	-1.30582700	2.52424700	1.71573400
H	-0.25661300	2.91483900	0.37487500
C	-2.34129600	2.80140800	-0.16175300
H	-2.06524900	2.87590300	-1.22224900
H	-2.63726000	3.80583700	0.16645700
C	-3.51491400	1.82098100	-0.02224500
H	-3.81223300	1.79353100	1.04034000
H	-4.39349000	2.16860700	-0.58026900
C	0.62905800	0.43451800	0.55895800
H	1.08881100	0.97255900	1.40315400
H	0.74795600	-0.63792200	0.76650000
C	1.49786300	0.71517300	-0.70978400
H	1.42589700	1.78140000	-0.95507900
H	1.05622400	0.15730600	-1.54210900
C	2.94636700	0.32653700	-0.53223900
C	3.38030400	-0.98106700	-0.81042400
C	3.88927600	1.24047800	-0.03265900
C	4.70809400	-1.36302900	-0.59772400
H	2.66908200	-1.70224100	-1.20704500
C	5.21867900	0.86464200	0.18249700

H	3.57801800	2.26040400	0.18287300
C	5.63416400	-0.44095600	-0.09869200
H	5.02133300	-2.37800200	-0.82816500
H	5.93054000	1.59216900	0.56354200
H	6.66756600	-0.73441700	0.06301800

-1312.780847 [M06-2X/6-31++G(d,p)]

C	-2.11235000	-2.14454100	-1.09684700
C	-1.69822000	-0.01423900	-0.18932500
C	-3.07762600	0.35145600	-0.50180300
C	-3.88018300	-0.54425200	-1.15079700
C	-3.40587100	-1.84294300	-1.48385100
H	-1.70964800	-3.13901100	-1.29955400
H	-4.90050100	-0.25555100	-1.40235700
H	-4.02278800	-2.56689700	-2.00243800
N	-1.26736000	-1.31036800	-0.47102900
C	-0.84180900	0.87558100	0.44624000
K	-1.25321700	-1.50339800	2.23388100
C	-1.20866800	2.33909000	0.60647800
H	-1.41513700	2.60437000	1.65789100
H	-0.34741500	2.96190700	0.31807200
C	-2.41169000	2.73907300	-0.25080300
H	-2.11410600	2.75567800	-1.30723600
H	-2.75550600	3.74593400	0.01088200
C	-3.53920200	1.71843300	-0.07420900
H	-3.81840600	1.70119800	0.99225200
H	-4.43630500	2.00654200	-0.63412500
C	0.61707900	0.53993000	0.61295400
H	1.07419100	1.18206600	1.38096500
H	0.78683600	-0.49963000	0.93126600
C	1.41942700	0.70750400	-0.70214800
H	1.33569200	1.74901400	-1.03520600
H	0.94190600	0.07371200	-1.45713400
C	2.86590600	0.32630100	-0.53596100
C	3.26952100	-1.00505200	-0.69482000
C	3.82575500	1.26856200	-0.14994100
C	4.59404200	-1.38407800	-0.48142400
H	2.53227900	-1.74643500	-0.99740800
C	5.15223100	0.89575500	0.06552500
H	3.52761800	2.30731500	-0.02317900
C	5.54125100	-0.43345400	-0.09982400
H	4.88878900	-2.42061100	-0.61801400
H	5.88331400	1.64379900	0.35868600
H	6.57427200	-0.72501000	0.06344000

2-methylquinoline (**35**), solvent = benzene



Charge = 0; Multiplicity = 1

20

-441.155719 [B3LYP/6-31+G(d,p)]

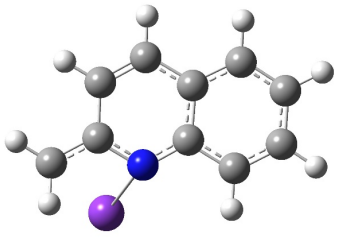
C	-2.02815500	-0.19265000	-0.00000400
C	-1.81555200	1.21988100	0.00000800

C	-0.53453100	1.71342800	0.00001100
H	-2.67099500	1.88885800	0.00001100
H	-0.34849300	2.78457400	0.00001600
N	-1.02857900	-1.05843700	-0.00001700
C	-3.43406200	-0.73837500	0.00004900
H	-3.98718600	-0.39471800	0.88214800
H	-3.98760600	-0.39388600	-0.88145400
H	-3.41295000	-1.82952500	-0.00044700
C	0.25710700	-0.58674500	-0.00001300
C	0.56303100	0.81132500	0.00000200
C	2.93817600	0.29618000	-0.00001100
H	3.97454900	0.62058200	-0.00001100
C	2.63546700	-1.08916300	-0.00002700
H	3.44479300	-1.81358700	-0.00003800
C	1.32520300	-1.52289700	-0.00002800
H	1.07847500	-2.58009200	-0.00004000
C	1.92074700	1.22815400	0.00000200
H	2.14487800	2.29202400	0.00001100

-440.952308 [M06-2X/6-31++G(d,p)]

C	-2.01797600	-0.19650900	0.00001000
C	-1.81085600	1.21705300	0.00001900
C	-0.53630000	1.71044000	0.00001900
H	-2.67148000	1.87886200	0.00002400
H	-0.34702700	2.78097400	0.00002500
N	-1.02535300	-1.05737600	-0.00000900
C	-3.42223700	-0.73663200	0.00004100
H	-3.96897700	-0.38956300	0.88257100
H	-3.96933900	-0.38879800	-0.88196000
H	-3.40029300	-1.82661700	-0.00041900
C	0.25671500	-0.58189200	-0.00001100
C	0.55935500	0.80608000	0.00000400
C	2.92849800	0.29806700	-0.00002300
H	3.96410800	0.62278400	-0.00002800
C	2.62709900	-1.08702000	-0.00003600
H	3.43730200	-1.80955900	-0.00005100
C	1.32251000	-1.51873700	-0.00003100
H	1.07106500	-2.57469100	-0.00004200
C	1.91448500	1.22551900	-0.00000400
H	2.13434600	2.29001800	0.00000500

2-methylquinoline K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

20

-1040.491086 [B3LYP/6-31+G(d,p)]

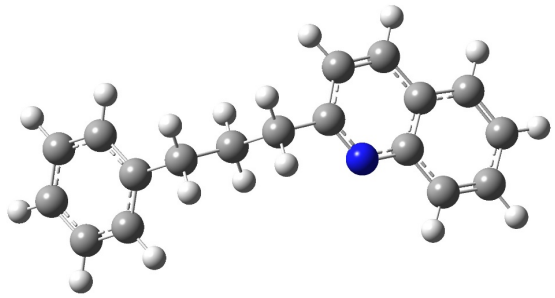
C	0.63286600	-0.23227500	0.38171600
C	-1.35853300	1.05341800	0.45262500
C	-0.63261400	2.16774800	-0.15450600
C	0.68772200	2.06361900	-0.45451300
C	1.39874700	0.84007800	-0.19079800

H	-1.17346300	3.09172300	-0.34268600
H	1.22548700	2.90260700	-0.89235600
N	-0.69312300	-0.13476900	0.67406200
C	-2.71112600	1.17845300	0.75424200
H	-3.20164500	0.44932300	1.39585400
H	-3.21969700	2.12520300	0.60649900
K	-2.60681200	-1.49550400	-0.64482000
C	3.40811300	-0.54374100	-0.21621400
H	4.46396800	-0.66691900	-0.43759400
C	2.66631100	-1.60402300	0.34434500
H	3.15850100	-2.54996400	0.55818000
C	1.31779700	-1.45602200	0.63628500
H	0.75639200	-2.27129900	1.08684600
C	2.76599200	0.66312600	-0.47558900
H	3.32011500	1.49500000	-0.90715600

-1040.271889 [M06-2X/6-31++G(d,p)]

C	0.63248400	-0.22839800	0.40435700
C	-1.38515800	0.99615500	0.48227200
C	-0.69502800	2.12640700	-0.14384700
C	0.61770300	2.05344000	-0.45543300
C	1.36000600	0.84765600	-0.18735000
H	-1.26562200	3.03116600	-0.33591600
H	1.13163900	2.89836300	-0.90984800
N	-0.68887800	-0.16439800	0.71421300
C	-2.73419700	1.08678900	0.77541100
H	-3.20901900	0.33880200	1.40588600
H	-3.26887400	2.01467900	0.61047400
K	-2.52553900	-1.47924100	-0.68218300
C	3.39610800	-0.48056700	-0.23487600
H	4.44980300	-0.58169800	-0.47271600
C	2.68917200	-1.55002700	0.34673100
H	3.20598600	-2.48221700	0.55956100
C	1.34738500	-1.43098800	0.65864400
H	0.80975500	-2.25233700	1.12599800
C	2.72283600	0.70351000	-0.49248600
H	3.24585300	1.54574500	-0.94199500

2-methylquinoline/styrene monoadduct (36a), solvent = benzene



Charge = 0; Multiplicity = 1

36

-750.729885 [B3LYP/6-31+G(d,p)]

C	5.88103100	0.86164700	-1.23235300
C	5.51578100	-0.48790400	-1.24796100
C	4.47374400	-0.94225400	-0.43422200
C	3.77699300	-0.06214400	0.40834300
C	4.15604100	1.28951800	0.41505000

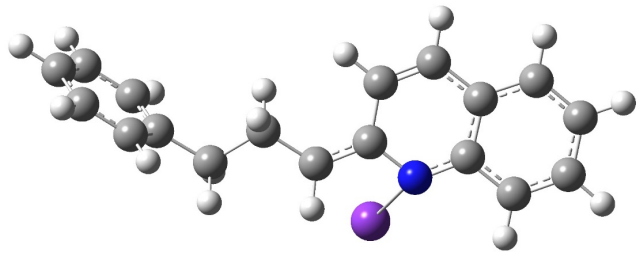
C	5.19697800	1.74975300	-0.39641100
H	6.69260900	1.21655500	-1.86100200
H	6.04430700	-1.18787200	-1.88929700
H	4.20088600	-1.99509700	-0.44859000
H	3.63348500	1.98694300	1.06579700
H	5.47603900	2.79956700	-0.37232000
C	2.62639600	-0.55062900	1.26288400
H	2.79877100	-1.59687600	1.54581500
H	2.59034900	0.02661700	2.19534600
C	1.26044200	-0.44073900	0.55570400
H	1.28940200	-1.01257400	-0.38080800
H	1.07351500	0.60426100	0.27999700
C	0.09983200	-0.94502600	1.43786100
H	0.28201600	-1.99266100	1.70912500
H	0.06752900	-0.36181300	2.36416000
C	-1.24160300	-0.82423300	0.75237100
C	-1.70967400	-1.87044500	-0.09793600
N	-1.93026400	0.28866600	0.95035600
C	-2.91550700	-1.73309000	-0.74198700
H	-1.10952500	-2.76656400	-0.22379000
C	-3.13278400	0.44585000	0.31794200
C	-3.67861100	-0.55102500	-0.55233900
H	-3.29496800	-2.51788000	-1.39165700
C	-5.62532900	0.85024100	-0.94335000
H	-6.58523100	1.02087900	-1.42154400
C	-5.08502800	1.83858700	-0.08081200
H	-5.63864000	2.75689900	0.09214500
C	-3.86722900	1.64257500	0.53716700
H	-3.44070900	2.38900900	1.20002600
C	-4.93552000	-0.32172400	-1.17378500
H	-5.34369600	-1.08380200	-1.83288100

-750.384409 [M06-2X/6-31++G(d,p)]

C	5.78508500	0.96819600	-1.20270400
C	5.54429000	-0.40448700	-1.16736900
C	4.52681300	-0.91528400	-0.36165800
C	3.73700500	-0.06739500	0.42076000
C	3.98789300	1.30863100	0.37601200
C	5.00254900	1.82482500	-0.42768700
H	6.57777000	1.36792500	-1.82743800
H	6.15061400	-1.07841100	-1.76518100
H	4.34454200	-1.98722700	-0.33483000
H	3.38249300	1.97918000	0.98213500
H	5.18533200	2.89503800	-0.44651700
C	2.60832700	-0.61348400	1.26027400
H	2.80408500	-1.66488700	1.50295000
H	2.55633500	-0.06899700	2.21112100
C	1.25364000	-0.50213400	0.54990100
H	1.30024600	-1.03537300	-0.40867100
H	1.04681300	0.54991800	0.31781900
C	0.10756900	-1.06210300	1.40274900
H	0.28934600	-2.12462600	1.60460900
H	0.07236400	-0.53490100	2.36123900
C	-1.22134600	-0.88902900	0.71517800
C	-1.64913600	-1.84649000	-0.25302900
N	-1.92103400	0.18515600	1.00964900
C	-2.83357600	-1.65384800	-0.90925800
H	-1.02887100	-2.71497000	-0.45367900
C	-3.10715700	0.39322700	0.36443400

C	-3.61281700	-0.50511700	-0.61309200
H	-3.18985300	-2.36547600	-1.64983200
C	-5.56125700	0.90283800	-0.91450900
H	-6.50913400	1.11276700	-1.39955300
C	-5.05788100	1.79977000	0.06160900
H	-5.62754900	2.68869500	0.31369800
C	-3.86030600	1.55235300	0.68829900
H	-3.45876500	2.22735500	1.43746400
C	-4.85282900	-0.22710500	-1.24382200
H	-5.22972600	-0.92227200	-1.98941100

2-methylquinoline/styrene monoadduct K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

36

-1350.064101 [B3LYP/6-31+G(d,p)]

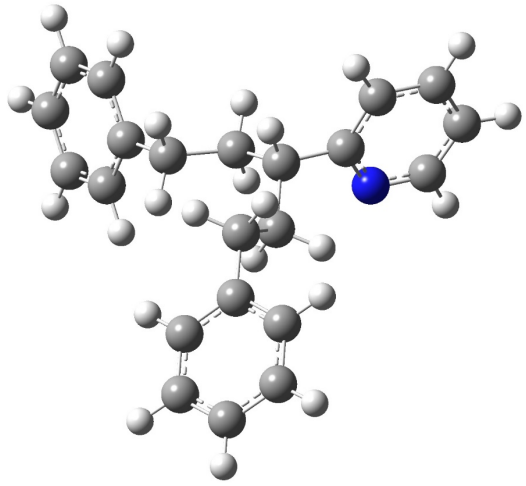
C	-3.35007000	-0.05143300	0.36634300
C	-0.97586700	-0.13123700	0.28529200
C	-1.06936400	-1.43558100	-0.36956600
C	-2.27621200	-2.00939200	-0.62079900
C	-3.49500800	-1.33894500	-0.25901000
H	-0.15589300	-1.95805300	-0.63525900
H	-2.33378300	-2.98813900	-1.09396300
N	-2.14994000	0.52883400	0.61685600
C	0.25068800	0.46791500	0.55243300
H	0.23837600	1.32043200	1.23537300
K	-1.37592500	2.77521500	-0.61963400
C	1.60155600	-0.16192500	0.30863800
H	1.82864000	-0.96114200	1.03779100
H	1.64609600	-0.64786400	-0.67642300
C	2.75251200	0.86783300	0.38150900
H	2.57915900	1.64606500	-0.37333000
H	2.71639000	1.36422800	1.36022700
C	4.12217700	0.25848800	0.17545800
C	4.83613400	-0.29382800	1.25119700
C	4.70139800	0.19806900	-1.10187100
C	6.08577600	-0.88992600	1.05826900
H	4.40907100	-0.25250300	2.25065500
C	5.95131300	-0.39581200	-1.30182200
H	4.16767000	0.62366300	-1.94891400
C	6.64871400	-0.94368400	-0.22080900
H	6.62072900	-1.30834300	1.90653000
H	6.38073100	-0.42788000	-2.29955200
H	7.62111600	-1.40348000	-0.37247600
C	-5.79910900	0.08252100	0.47236600
H	-6.69245000	0.63141400	0.76169300
C	-4.55138500	0.63484000	0.72016100
H	-4.46196900	1.60097500	1.21192800
C	-4.77476900	-1.87628300	-0.49476000
H	-4.84951700	-2.85480200	-0.96638300
C	-5.92735100	-1.18282100	-0.13941600

H	-6.90898700	-1.60829100	-0.32450300

-1349.780847 [M06-2X/6-31++G(d,p)]

C	-3.33295700	-0.04692000	0.38050400
C	-0.96914000	-0.11220100	0.34874200
C	-1.03890800	-1.40287400	-0.34118000
C	-2.23224100	-1.96884400	-0.63533200
C	-3.45978500	-1.30570300	-0.28455300
H	-0.11478100	-1.91356100	-0.59273600
H	-2.28093500	-2.93475000	-1.13496000
N	-2.14504600	0.52932200	0.67952400
C	0.24846300	0.47795700	0.63260200
H	0.24149800	1.32671100	1.31951600
K	-1.32269000	2.68921900	-0.60984900
C	1.59084700	-0.14024500	0.34008000
H	1.81222400	-0.99953700	0.99728200
H	1.63813300	-0.53508700	-0.68532700
C	2.73455300	0.87359900	0.50412800
H	2.55942100	1.72017000	-0.17193800
H	2.71123600	1.26982800	1.52725100
C	4.08698200	0.26880300	0.22301100
C	4.76631100	-0.45021200	1.21315200
C	4.66976700	0.36556100	-1.04485100
C	5.99313100	-1.05520500	0.94565300
H	4.32590100	-0.53469700	2.20429700
C	5.89766700	-0.23640800	-1.31889300
H	4.15418300	0.92071400	-1.82550900
C	6.56383100	-0.94980700	-0.32316100
H	6.50545700	-1.60657100	1.72845000
H	6.33495600	-0.14544800	-2.30883400
H	7.52079100	-1.41778900	-0.53230100
C	-5.77599700	0.08529800	0.42393100
H	-6.67655100	0.62524500	0.70506600
C	-4.54072800	0.62677400	0.72307700
H	-4.46117500	1.57700000	1.24575700
C	-4.72793600	-1.83532800	-0.57407200
H	-4.78510800	-2.79773900	-1.07973000
C	-5.88669800	-1.15741400	-0.23098500
H	-6.86180100	-1.57590800	-0.45693400

2-methylpyridine/styrene bisadduct (32b), solvent = benzene



Charge = 0; Multiplicity = 1

46

-906.687528 [B3LYP/6-31+G(d,p)]

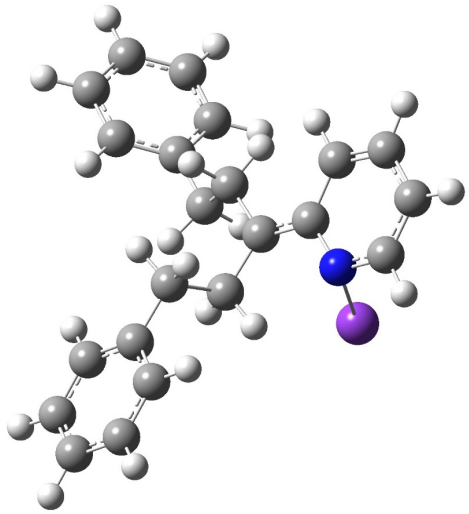
C	5.53722900	-2.35392200	0.47871200
C	5.35767200	-1.67135200	-0.72841200
C	4.08706200	-1.21978000	-1.09688200
C	2.97369300	-1.43862400	-0.27057800
C	3.16847800	-2.12756400	0.93674600
C	4.43665100	-2.58138200	1.31065400
H	6.52298100	-2.70852700	0.76576900
H	6.20490100	-1.49435200	-1.38529900
H	3.95627900	-0.69435200	-2.04025600
H	2.31775100	-2.31240600	1.58866200
H	4.56387000	-3.11534300	2.24834200
C	1.60465100	-0.91580900	-0.65491800
H	1.50141100	-0.93128900	-1.74756500
H	0.83889500	-1.58846800	-0.25307700
C	1.35794400	0.51796700	-0.14276900
H	2.15918300	1.16555600	-0.52143900
H	1.43456500	0.53503000	0.95117700
C	-0.00777300	1.12757100	-0.54836500
H	-0.06026700	1.12021900	-1.64587300
C	-0.04808400	2.58442000	-0.11677500
C	0.00287000	3.62433600	-1.05722700
N	-0.11688900	2.82958000	1.20521700
C	-0.01787300	4.94806200	-0.61718500
H	0.05548000	3.39410800	-2.11721200
C	-0.13527200	4.10372100	1.61842700
C	-0.08741700	5.19946400	0.75354000
H	0.01803900	5.76607700	-1.33109200
H	-0.19226200	4.25541400	2.69464100
H	-0.10656500	6.21109200	1.14589700
C	-1.22541500	0.32770100	0.00066500
H	-0.91326700	-0.29034900	0.85125000
H	-1.97203600	1.02240900	0.39928400
C	-1.90736100	-0.56166000	-1.06245100
H	-1.17453200	-1.25219000	-1.49479500
H	-2.25489600	0.07896200	-1.88318100
C	-3.07613900	-1.34995200	-0.50923800
C	-2.89980100	-2.65165700	-0.01480600
C	-4.36050000	-0.78636500	-0.44831900
C	-3.97074700	-3.36852500	0.52723600
H	-1.91473300	-3.11054700	-0.05892300
C	-5.43519400	-1.49796600	0.09232700
H	-4.52093100	0.21879600	-0.83186500
C	-5.24378200	-2.79331400	0.58334800
H	-3.81139500	-4.37648300	0.90040800
H	-6.42139300	-1.04307900	0.12561400
H	-6.07821900	-3.34956000	1.00062700

-906.266027 [M06-2X/6-31++G(d,p)]

C	5.33743300	-2.46472300	0.52388500
C	5.15596600	-1.93423400	-0.75291200
C	3.90396200	-1.45739800	-1.14058000
C	2.81599900	-1.50372700	-0.26370200
C	3.01061400	-2.03790900	1.01474800
C	4.25963500	-2.51505900	1.40797400
H	6.31037100	-2.83837000	0.82743400
H	5.98863400	-1.89386800	-1.44880200

H	3.76672600	-1.04535600	-2.13788900
H	2.17181100	-2.08043400	1.70639400
H	4.39096400	-2.92952900	2.40301000
C	1.47209100	-0.94259800	-0.66055800
H	1.34675300	-1.01223100	-1.74856100
H	0.68154100	-1.54841500	-0.20235000
C	1.32420100	0.51891500	-0.21855400
H	2.15477400	1.10074400	-0.63962800
H	1.41768100	0.57784600	0.87378000
C	-0.00763400	1.17830900	-0.62347300
H	-0.06013200	1.19218600	-1.72175000
C	0.00934200	2.61652400	-0.15264600
C	0.19427700	3.67481100	-1.04788200
N	-0.13500500	2.81667900	1.16472900
C	0.22785300	4.97792800	-0.56063800
H	0.30697700	3.47234800	-2.10862200
C	-0.10135900	4.06998600	1.62244700
C	0.07674000	5.18594800	0.80698300
H	0.36721900	5.81520300	-1.23787400
H	-0.22424600	4.18930900	2.69664400
H	0.09444300	6.18177500	1.23580700
C	-1.23736700	0.41538800	-0.08407800
H	-0.95568400	-0.16302300	0.80537900
H	-1.99877700	1.12741100	0.25319600
C	-1.87572500	-0.51457900	-1.12799800
H	-1.12393100	-1.19827600	-1.53722400
H	-2.23820600	0.09469400	-1.96518800
C	-3.01708600	-1.30860100	-0.54251900
C	-2.79988200	-2.57867200	0.00165300
C	-4.30524500	-0.76693100	-0.47957200
C	-3.84195800	-3.29130700	0.59368800
H	-1.80362500	-3.01385100	-0.04324800
C	-5.35098300	-1.47440400	0.11130000
H	-4.48789000	0.21954100	-0.90044100
C	-5.12166200	-2.74013400	0.65056200
H	-3.65578400	-4.27750800	1.00845900
H	-6.34504800	-1.03892500	0.14933100
H	-5.93481600	-3.29321300	1.11028400

2-methylpyridine/styrene bisadduct K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

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-1506.014522 [B3LYP/6-31+G(d,p)]

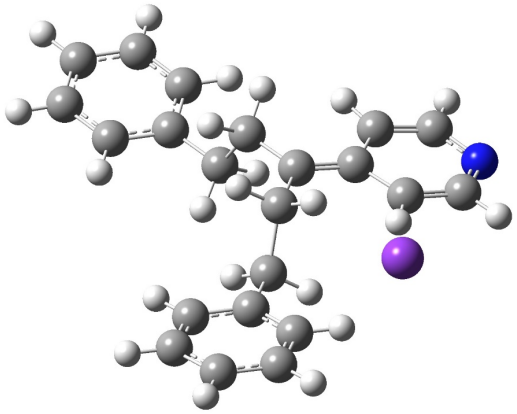
C	-2.04575700	3.88948600	-0.48580500
C	-0.38616600	2.19421000	-0.45899800
C	0.48689500	3.12665800	-1.15614700
C	0.05902700	4.39194800	-1.48406400
C	-1.25067700	4.81883900	-1.14982900
H	-3.06671000	4.16130600	-0.20667800
H	1.48128400	2.81441400	-1.45459400
H	0.73006600	5.05951400	-2.02156000
H	-1.62644100	5.80252600	-1.40954100
N	-1.67503700	2.64973800	-0.13534100
C	-0.00605200	0.89673400	-0.06993200
K	-1.02363800	2.16842600	2.47893800
C	1.37231800	0.35526600	-0.39899200
H	1.39209800	-0.18773200	-1.36371300
H	2.08570700	1.17653200	-0.51961900
C	1.97289600	-0.60071800	0.66751100
H	1.97190000	-0.08699000	1.63831000
H	1.33355200	-1.48407900	0.77710500
C	3.37919100	-1.04706400	0.33255000
C	3.60747900	-2.17486300	-0.47259200
C	4.49458700	-0.32340300	0.78431200
C	4.90454800	-2.56593400	-0.81801700
H	2.75904200	-2.75412400	-0.82962600
C	5.79433400	-0.70977300	0.44423200
H	4.34238800	0.55215000	1.41188100
C	6.00464700	-1.83395000	-0.36055800
H	5.05561000	-3.44357300	-1.44077800
H	6.64140800	-0.13531100	0.80952600
H	7.01348100	-2.13786900	-0.62485900
C	-1.07186500	-0.12994900	0.26708000
H	-0.75033000	-0.81342700	1.06902100
H	-1.98419800	0.36454800	0.61812800
C	-1.50022700	-1.01943300	-0.94501400
H	-0.61915800	-1.54318200	-1.33375200
H	-1.85598900	-0.35427800	-1.73984900
C	-2.57207700	-2.02188100	-0.58865700
C	-3.93314700	-1.68051700	-0.66634500
C	-2.24098600	-3.30365600	-0.11793700
C	-4.92868900	-2.58638500	-0.28951400
H	-4.21261300	-0.69550600	-1.03358300
C	-3.23208000	-4.21382100	0.26213200
H	-1.19437800	-3.59432300	-0.05826800
C	-4.58203600	-3.85844200	0.17831400
H	-5.97466300	-2.30140700	-0.36653700
H	-2.95043000	-5.20189400	0.61657100
H	-5.35421300	-4.56566900	0.46761300

-1505.578428 [M06-2X/6-31++G(d,p)]

C	-2.39228400	3.81087600	-0.49370800
C	-0.61799100	2.25679000	-0.42493400
C	0.20782700	3.25813500	-1.07900400
C	-0.30317800	4.48744000	-1.40281500
C	-1.65000100	4.80746000	-1.10907400
H	-3.44060100	3.99803200	-0.25174900
H	1.22981300	3.01848600	-1.34948800
H	0.33181300	5.21258200	-1.90756400
H	-2.09053800	5.76354200	-1.36418300
N	-1.94336100	2.59978200	-0.14932800

C	-0.13846900	1.00252500	-0.03946400
K	-1.39582800	1.98798400	2.42410700
C	1.29187100	0.60418300	-0.32228500
H	1.43320500	0.22915300	-1.35465600
H	1.95676200	1.47205000	-0.23688800
C	1.84706600	-0.47215100	0.63144000
H	1.75770500	-0.11244200	1.66524200
H	1.24610300	-1.38658300	0.55900000
C	3.28541000	-0.80317000	0.32446600
C	3.60165400	-1.73529800	-0.67034500
C	4.33447300	-0.14905200	0.97889100
C	4.92760800	-2.00839900	-1.00282700
H	2.79546600	-2.25196700	-1.18752900
C	5.66333000	-0.41879200	0.65242300
H	4.10560300	0.57963000	1.75371600
C	5.96443000	-1.35005400	-0.34084700
H	5.15118900	-2.73684600	-1.77668600
H	6.46370000	0.09724700	1.17450100
H	6.99806300	-1.56316700	-0.59532900
C	-1.10233300	-0.12555800	0.24428200
H	-0.80568800	-0.72869100	1.12050900
H	-2.10439200	0.26852600	0.45037100
C	-1.25628200	-1.10717000	-0.94628200
H	-0.26810500	-1.48337000	-1.23897300
H	-1.65374100	-0.54493600	-1.79906100
C	-2.15918900	-2.26320200	-0.60729400
C	-3.54569500	-2.16434700	-0.77331600
C	-1.63954700	-3.43822000	-0.05185000
C	-4.38885500	-3.21083000	-0.40213100
H	-3.96373600	-1.25662100	-1.20343700
C	-2.47766100	-4.48784400	0.32288100
H	-0.56311400	-3.53216800	0.07928300
C	-3.85702400	-4.37754100	0.14805300
H	-5.46132700	-3.11762400	-0.54653400
H	-2.05378300	-5.39418700	0.74532300
H	-4.51110600	-5.19548900	0.43383700

4-methylpyridine/styrene bisadduct, solvent = benzene



Charge = 0; Multiplicity = 1

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-906.684786 [B3LYP/6-31+G(d,p)]

C	5.51593000	-2.40323000	0.47308900
C	5.34979400	-1.67329900	-0.70804500
C	4.08253900	-1.21243000	-1.07574000

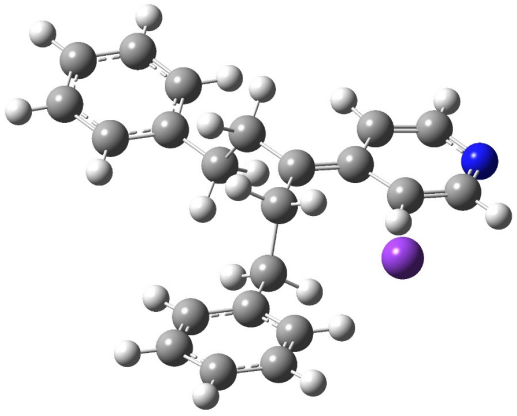
C	2.95919400	-1.46929800	-0.27415900
C	3.14014100	-2.20604200	0.90654800
C	4.40531100	-2.66933300	1.27957400
H	6.49933500	-2.76480700	0.75929200
H	6.20512700	-1.46641200	-1.34528300
H	3.96259000	-0.64977600	-1.99882500
H	2.28125100	-2.42224000	1.53791900
H	4.52210100	-3.24076600	2.19625100
C	1.59362400	-0.93529300	-0.65615200
H	1.49308900	-0.93387100	-1.74900900
H	0.82361200	-1.60975000	-0.26603600
C	1.35438200	0.49332700	-0.12596100
H	2.16235000	1.14057300	-0.48855900
H	1.43217500	0.48700700	0.96908200
C	-0.00381900	1.12313500	-0.53203600
H	-0.05182600	1.11642500	-1.62962000
C	-0.02835100	2.58094800	-0.10327000
C	0.05063900	3.61808600	-1.04090500
C	0.04382700	4.94595700	-0.60731900
H	0.11376000	3.39903800	-2.10339700
C	-0.10624700	4.31360500	1.58128700
H	0.10080700	5.75632900	-1.33124800
H	-0.16735900	4.61619000	2.62456600
C	-1.23395300	0.33148900	0.00578500
H	-0.93922800	-0.28042400	0.86811000
H	-1.99036100	1.03172300	0.37649100
C	-1.90244800	-0.56944000	-1.05659700
H	-1.16593800	-1.26712700	-1.46957400
H	-2.23519100	0.06347000	-1.88903800
C	-3.08183200	-1.34627200	-0.50931400
C	-2.91988200	-2.64799000	-0.01026000
C	-4.36143700	-0.77095600	-0.45942000
C	-4.00087700	-3.35385500	0.52636600
H	-1.93891800	-3.11622400	-0.04729300
C	-5.44588200	-1.47165600	0.07584500
H	-4.51090000	0.23392200	-0.84808000
C	-5.26897400	-2.76710500	0.57208000
H	-3.85319900	-4.36227800	0.90293300
H	-6.42835700	-1.00838700	0.10038000
H	-6.11118000	-3.31484300	0.98487000
N	-0.03213600	5.30784500	0.68143300
C	-0.10883600	2.95992500	1.24562700
H	-0.17584600	2.21567500	2.03389900

-906.262878 [M06-2X/6-31++G(d,p)]

C	5.18792100	-2.71293600	0.52659600
C	5.04013300	-2.12960700	-0.73161700
C	3.81040200	-1.59528100	-1.11427400
C	2.71159000	-1.63552800	-0.25047700
C	2.87193600	-2.22322500	1.00887400
C	4.09911200	-2.75812500	1.39701000
H	6.14380300	-3.13124400	0.82608700
H	5.88184800	-2.09328900	-1.41663900
H	3.69858400	-1.14322200	-2.09738000
H	2.02395400	-2.26289100	1.68942200
H	4.20503800	-3.21286700	2.37736900
C	1.39429900	-1.01096000	-0.64177300
H	1.26569600	-1.06376800	-1.73023500
H	0.57663200	-1.58411200	-0.18897100

C	1.31572200	0.45291000	-0.18883500
H	2.17750400	0.99632300	-0.59679100
H	1.40967100	0.49429400	0.90534300
C	0.02217200	1.18553300	-0.60051400
H	-0.02006400	1.19730600	-1.69936000
C	0.12827300	2.62355000	-0.14216700
C	0.52854800	3.63484300	-1.01647000
C	0.65817500	4.93890500	-0.54298100
H	0.73641100	3.41366600	-2.05977700
C	0.04268400	4.32413800	1.56043900
H	0.96467000	5.73603300	-1.21631200
H	-0.14608200	4.62506700	2.58828200
C	-1.24864400	0.48157200	-0.07570100
H	-1.00814500	-0.11381600	0.81604800
H	-1.98772000	1.22562000	0.24350700
C	-1.91349400	-0.42100100	-1.12760800
H	-1.18089400	-1.12247500	-1.54046800
H	-2.25456600	0.20671700	-1.95985400
C	-3.07831600	-1.18667300	-0.55042600
C	-2.90080800	-2.47525600	-0.03643700
C	-4.34670600	-0.60278800	-0.46702800
C	-3.96277700	-3.16550900	0.54668100
H	-1.92068300	-2.94354500	-0.09955500
C	-5.41196900	-1.28784100	0.11541300
H	-4.49943200	0.39756100	-0.86644100
C	-5.22241400	-2.57256500	0.62464600
H	-3.80762800	-4.16676900	0.93720000
H	-6.39061700	-0.82041700	0.16948300
H	-6.05122100	-3.10824300	1.07686000
N	0.42246000	5.29532500	0.72286000
C	-0.11630600	2.99371200	1.18359000
H	-0.43118200	2.25958700	1.92051800

4-methylpyridine/styrene bisadduct K enolate, solvent = benzene



Charge = 0; Multiplicity = 1

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-1506.016429 [B3LYP/6-31+G(d,p)]

C	-1.13978200	4.00526500	-0.69446300
C	0.00034700	1.80688300	-0.87605000
C	1.20791200	2.63291900	-0.82581900
C	1.14179600	4.00454700	-0.69439700
H	-2.06909100	4.57619100	-0.66604900
H	2.18763100	2.17375300	-0.91409000
H	2.07146900	4.57486600	-0.66565800

C	-0.00012800	0.42583500	-0.96096500
K	0.00096400	3.19638100	1.99853200
C	1.29264200	-0.35980200	-1.01933300
H	1.11588900	-1.32020600	-1.52230300
H	2.04676200	0.15690600	-1.63003900
C	1.94656100	-0.67063900	0.36433500
H	2.14426400	0.27997900	0.87583900
H	1.22377900	-1.22010400	0.97863700
C	3.22913300	-1.46439600	0.25914100
C	3.21653700	-2.86792200	0.30691700
C	4.46328200	-0.82258500	0.06336400
C	4.39458400	-3.60707800	0.16521100
H	2.27279600	-3.38647200	0.46078400
C	5.64482900	-1.55568300	-0.07931100
H	4.49890600	0.26404900	0.02605100
C	5.61518600	-2.95301100	-0.02905800
H	4.35942100	-4.69230000	0.20949200
H	6.58788300	-1.03620800	-0.22678600
H	6.53234700	-3.52485000	-0.13737600
C	-1.20672700	2.63368200	-0.82579300
H	-2.18670100	2.17509800	-0.91427700
N	0.00124700	4.74565500	-0.57043600
C	-1.29334300	-0.35903200	-1.01931700
H	-2.04731300	0.15823000	-1.62974700
H	-1.11719700	-1.31936500	-1.52264000
C	-1.94712200	-0.66998700	0.36435500
H	-1.22436600	-1.21973500	0.97845100
H	-2.14455200	0.28056200	0.87609700
C	-3.22990400	-1.46341400	0.25918100
C	-4.46390600	-0.82125000	0.06367800
C	-3.21766400	-2.86695700	0.30669400
C	-5.64566700	-1.55401500	-0.07898900
H	-4.49925600	0.26540000	0.02658100
C	-4.39591700	-3.60577700	0.16499100
H	-2.27404000	-3.38578200	0.46034900
C	-5.61637800	-2.95135500	-0.02901500
H	-6.58859900	-1.03425800	-0.22624400
H	-4.36103300	-4.69101600	0.20905700
H	-6.53369400	-3.52294300	-0.13733300

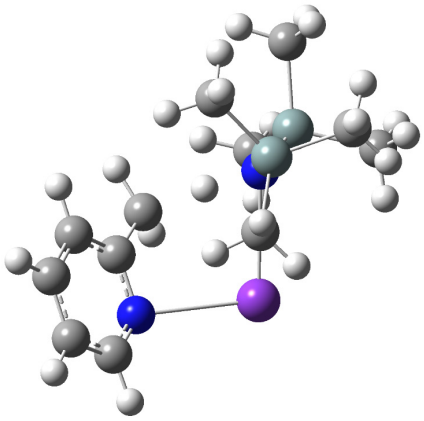
-1505.580533 [M06-2X/6-31++G(d,p)]

C	-1.13607300	3.86223700	-0.51022600
C	0.00007500	1.69907600	-0.89007400
C	1.20772000	2.51793500	-0.79518200
C	1.13680700	3.86197700	-0.51050000
H	-2.06375400	4.42962000	-0.42817500
H	2.18632200	2.07224200	-0.94681000
H	2.06463800	4.42914500	-0.42867100
C	-0.00007300	0.33122100	-1.01978200
K	0.00052800	2.62365000	1.95464600
C	1.29527800	-0.43916400	-1.06787200
H	1.12945500	-1.42897700	-1.51260800
H	2.03377000	0.05728500	-1.71431100
C	1.95174600	-0.64796100	0.32011900
H	2.08523000	0.33623700	0.78916200
H	1.26626300	-1.22378000	0.95322300
C	3.28416800	-1.34575000	0.23223100
C	3.38860500	-2.73159300	0.38885200
C	4.44287300	-0.62179600	-0.07358100

C	4.61647500	-3.37843700	0.24890900
H	2.49714000	-3.30848000	0.62509300
C	5.67235600	-1.26214100	-0.21571000
H	4.37715400	0.45738300	-0.19957400
C	5.76318600	-2.64497300	-0.05372700
H	4.67770100	-4.45505000	0.37768700
H	6.55997900	-0.68274000	-0.45167500
H	6.72019700	-3.14568500	-0.16247300
C	-1.20736500	2.51821000	-0.79488600
H	-2.18610700	2.07275000	-0.94627300
N	0.00047500	4.57524300	-0.28968200
C	-1.29555500	-0.43895800	-1.06781300
H	-2.03393500	0.05749100	-1.71437200
H	-1.12987100	-1.42886800	-1.51238700
C	-1.95214700	-0.64743700	0.32016700
H	-1.26672800	-1.22311000	0.95347200
H	-2.08568600	0.33687200	0.78896400
C	-3.28456300	-1.34524000	0.23230800
C	-4.44322600	-0.62135300	-0.07382000
C	-3.38902200	-2.73104600	0.38923400
C	-5.67269300	-1.26172600	-0.21595500
H	-4.37748500	0.45779500	-0.20006800
C	-4.61687700	-3.37791900	0.24928500
H	-2.49758800	-3.30788100	0.62571400
C	-5.76354800	-2.64452100	-0.05366500
H	-6.56028300	-0.68237900	-0.45217700
H	-4.67812200	-4.45450200	0.37830000
H	-6.72054500	-3.14525600	-0.16242100

10.7.2. XYZ Co-ordinates of transition states

Deprotonation of 2-methylpyridine (29) by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

42

-1760.651171 [B3LYP/6-31+G(d,p)]

C	-0.66849200	1.07157100	-0.33467300
C	-2.83540900	0.34425400	0.17364000
C	-2.90746600	1.34225500	1.18961800
C	-1.83535500	2.18465400	1.42469900
H	0.21024800	0.93536300	-0.96528000
H	-3.81145400	1.41930100	1.78691100
H	-1.89353000	2.93559800	2.20881600
C	-3.95501000	-0.51967300	-0.14382900
H	-4.69354700	-0.58654700	0.65958000

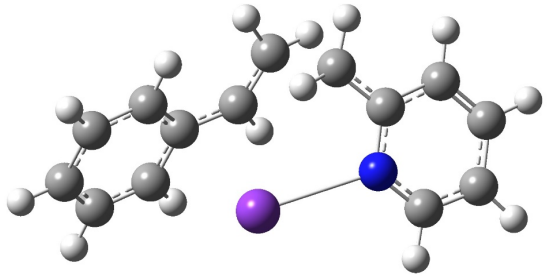
H	-4.76401800	-0.04707100	-1.28136400
H	-3.64472300	-1.52220700	-0.45841100
N	-5.44209900	0.27441300	-2.33719400
Si	-6.59564000	-0.93904300	-2.78862300
Si	-5.63890700	1.99361100	-2.47156600
C	-3.93441500	2.82676000	-2.66285400
H	-4.03782500	3.91873900	-2.64197500
H	-3.24760800	2.55208300	-1.85354100
H	-3.46136200	2.57319000	-3.62177300
C	-6.45331900	2.75664500	-0.93244800
H	-7.46263900	2.35529200	-0.78296500
H	-5.87066300	2.53330000	-0.03096500
H	-6.53378700	3.84768700	-1.01853400
C	-6.66261700	2.53298200	-3.98249700
H	-6.71791000	3.62854500	-4.02279400
H	-6.21231600	2.18888900	-4.92109300
H	-7.69027700	2.15397800	-3.94709000
C	-6.71552200	-1.15951100	-4.67828900
H	-7.07827000	-0.25108100	-5.17201300
H	-5.73751700	-1.40381600	-5.11343300
H	-7.40365400	-1.97545200	-4.93455200
C	-6.05769200	-2.62377100	-2.08681800
H	-6.00109900	-2.60888700	-0.99297900
H	-6.78161500	-3.39598800	-2.37508700
H	-5.07700300	-2.94118400	-2.46368900
C	-8.36271300	-0.62172200	-2.15476800
H	-9.03645000	-1.43989400	-2.43984500
H	-8.37777100	-0.54067700	-1.06115900
H	-8.78074600	0.30697500	-2.56101700
K	-2.78592400	-0.43734700	-3.06164900
N	-1.69866200	0.24578300	-0.58807000
C	-0.66806400	2.05308800	0.65090400
H	0.19938600	2.68539000	0.80695300

-1760.257113 [M06-2X/6-31++G(d,p)]

C	-0.79486500	1.31396700	-0.43556900
C	-2.74239800	0.17456600	0.21823400
C	-3.09948900	1.33260700	1.00863500
C	-2.27968900	2.42896300	1.05488700
H	0.11969400	1.27777900	-1.02955100
H	-4.01953500	1.30142300	1.58636600
H	-2.55794500	3.28570400	1.66456400
C	-3.56629900	-0.94705800	0.13624600
H	-4.42822900	-1.02406100	0.79205800
H	-5.01339300	-0.14006700	-1.39800800
H	-3.16747100	-1.88014100	-0.25617900
N	-5.45401400	0.18946600	-2.27541300
Si	-6.70001100	-0.92367300	-2.80504200
Si	-5.48360300	1.94269000	-2.35828000
C	-3.71632100	2.57474100	-2.49828400
H	-3.69872300	3.66942000	-2.45401100
H	-3.08789900	2.21246700	-1.67515500
H	-3.26107200	2.28572600	-3.45410100
C	-6.28691400	2.67248900	-0.82535100
H	-7.31912600	2.31976500	-0.72528300
H	-5.73344800	2.36941700	0.06993900
H	-6.29890600	3.76710200	-0.86152000
C	-6.44121800	2.47197300	-3.88920400
H	-6.43396500	3.56554800	-3.95667200

H	-5.98931700	2.07790100	-4.80542600
H	-7.48799100	2.15114800	-3.85863800
C	-6.80043900	-0.94836400	-4.68493200
H	-7.22603500	-0.02524800	-5.08897500
H	-5.80902400	-1.08795900	-5.12994800
H	-7.43593000	-1.77889700	-5.01220100
C	-6.19545500	-2.62911700	-2.19235500
H	-6.04668200	-2.62823100	-1.10750800
H	-6.96598900	-3.36976700	-2.43160900
H	-5.26017100	-2.96212700	-2.65723800
C	-8.39605800	-0.49051600	-2.11205700
H	-9.15195800	-1.20704500	-2.45233400
H	-8.38130500	-0.50564700	-1.01698500
H	-8.71655800	0.50789900	-2.42911800
K	-2.76094700	-0.65336700	-2.76884300
N	-1.56844800	0.22282500	-0.51754200
C	-1.07212500	2.44381900	0.31698300
H	-0.39418300	3.28835600	0.33370500

Reaction of 2-methylpyridine K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

30

-1196.417723 [B3LYP/6-31+G(d,p)]

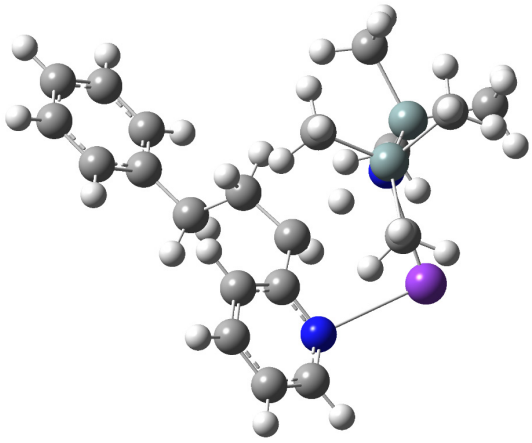
C	-4.46069600	-1.24868500	0.94388900
C	-4.19320500	0.09167900	1.26336000
C	-2.94665600	0.65367500	0.99757000
C	-1.89079200	-0.09692500	0.40327400
C	-2.19215700	-1.45247200	0.07961300
C	-3.44233900	-2.00892200	0.35274000
H	-5.43091700	-1.68756300	1.15512700
H	-4.96367300	0.70162800	1.72920800
H	-2.75959600	1.69152500	1.26650100
H	-1.42855700	-2.07483900	-0.37817200
H	-3.62415200	-3.05089000	0.09938000
C	-0.61910800	0.52856700	0.12001600
H	-0.56125900	1.59798100	0.31920400
C	0.49374600	-0.09439900	-0.42570100
H	0.58737900	-1.17604400	-0.39736100
H	1.43752500	0.43947400	-0.42379900
C	0.64373200	-0.25950700	-2.70684300
H	1.53877400	-0.87551000	-2.70012300
H	-0.27677000	-0.80814600	-2.89212000
C	0.75732700	1.06491000	-3.19215900
C	2.03442000	1.70486800	-3.33427500
C	-0.26569700	3.06923400	-3.85224600
C	2.12108200	3.01620800	-3.75028800
H	2.93276700	1.13097100	-3.12341900
C	0.93938500	3.73802500	-4.03136400
H	-1.20342800	3.59122100	-4.04958200

H	3.09379200	3.48808800	-3.86700900
H	0.96069600	4.76851200	-4.36897500
N	-0.38848200	1.79301300	-3.44617700
K	-2.67563600	0.71798600	-2.39575700

-1196.113825 [M06-2X/6-31++G(d,p)]

C	-4.30379700	-0.78749300	0.43871100
C	-3.95382600	0.55492900	0.63947300
C	-2.62853500	0.96395800	0.55021300
C	-1.58276800	0.05523000	0.24722400
C	-1.95754800	-1.30154000	0.06856100
C	-3.28638900	-1.70825800	0.16852100
H	-5.33733400	-1.10894000	0.51232600
H	-4.72457100	1.28668100	0.86629800
H	-2.37769000	2.01171200	0.69828000
H	-1.19652000	-2.04213200	-0.15811300
H	-3.53145600	-2.75764400	0.02657900
C	-0.23352900	0.53420300	0.05698800
H	-0.09462300	1.61123100	0.11684600
C	0.80582100	-0.24364500	-0.38100200
H	0.78191700	-1.32584500	-0.30197200
H	1.79647900	0.19093600	-0.46724600
C	0.70230100	-0.54510300	-2.70273000
H	1.64771300	-1.05813000	-2.84534000
H	-0.19018100	-1.16529700	-2.67997600
C	0.59574500	0.81147900	-3.02759200
C	1.76229000	1.62024800	-3.25839800
C	-0.70791800	2.74514900	-3.19241400
C	1.64810800	2.97209300	-3.45525000
H	2.73475600	1.13549100	-3.27433100
C	0.37055600	3.57831600	-3.42794000
H	-1.71292400	3.17149300	-3.15943900
H	2.53620200	3.57317800	-3.63429400
H	0.23237400	4.64166700	-3.58300100
N	-0.63803900	1.41877700	-2.99447600
K	-2.93910800	0.12091600	-2.45199600

Deprotonation of 2-methylpyridine/styrene monoadduct (30a) by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

58

-2070.220510 [B3LYP/6-31+G(d,p)]

C	-0.58917200	1.46438300	-0.72235800
C	-2.78389900	1.37737500	0.10183500

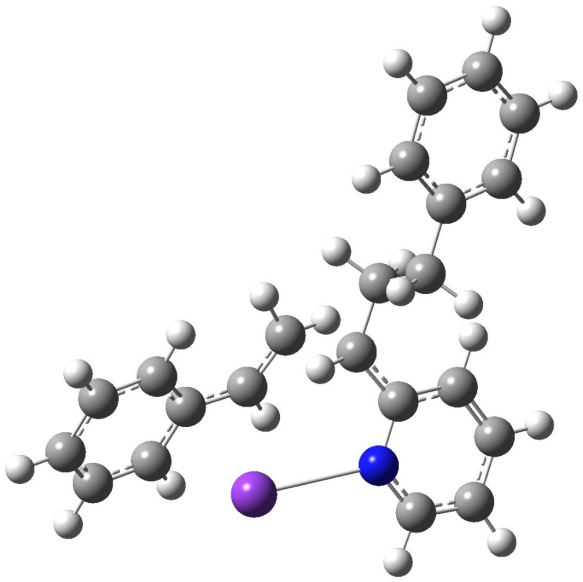
C	-2.64786000	2.73231900	0.52788200
C	-1.46344000	3.41995000	0.32204800
H	0.21167600	0.92440000	-1.22844500
H	-3.47542900	3.22359900	1.02755600
H	-1.36886100	4.44914700	0.65982000
C	-4.00895900	0.60978600	0.23500900
H	-4.77001700	0.62713400	-1.02746500
H	-3.77672700	-0.46165700	0.30708200
N	-5.44420000	0.52593700	-2.13614100
Si	-6.70822900	-0.65991700	-2.06854700
Si	-5.46944400	2.03957500	-2.98863100
C	-3.70820000	2.47523300	-3.57551200
H	-3.69032400	3.46957700	-4.03872900
H	-2.99103000	2.49139600	-2.74617300
H	-3.34651400	1.76628000	-4.33342100
C	-6.06456600	3.47897400	-1.90003200
H	-7.09514500	3.31374000	-1.56367300
H	-5.43814600	3.58703600	-1.00723200
H	-6.03727900	4.43065100	-2.44580100
C	-6.55992400	2.03718500	-4.54749600
H	-6.49359600	3.01504400	-5.04176700
H	-6.24077300	1.27758500	-5.27022500
H	-7.61644000	1.85798800	-4.31744400
C	-7.06237800	-1.46887800	-3.75741600
H	-7.49221300	-0.76067100	-4.47349900
H	-6.14758800	-1.87807100	-4.20547200
H	-7.77318500	-2.29760400	-3.64262200
C	-6.18126200	-2.08755900	-0.92147600
H	-5.94248900	-1.74275900	0.08995800
H	-6.99826600	-2.81522500	-0.84082900
H	-5.30783900	-2.63365100	-1.30276000
C	-8.36849900	-0.00317900	-1.41129100
H	-9.11538800	-0.80473300	-1.34752200
H	-8.25424600	0.42991000	-0.41059900
H	-8.77630000	0.77787900	-2.06416900
K	-2.94987300	-0.77220800	-2.49424500
C	-5.03157000	1.02168000	1.28775500
H	-5.30507600	2.07901600	1.17201900
H	-5.96516700	0.46895700	1.11654100
C	-4.59946200	0.77908600	2.76000500
H	-3.66871100	1.32499900	2.95463700
H	-4.37082100	-0.28755500	2.87997000
C	-5.65093500	1.19097700	3.76615400
C	-6.66426400	0.30101600	4.15878500
C	-5.67065500	2.48917000	4.30159500
C	-7.66490400	0.69287800	5.05277500
H	-6.66536500	-0.71209700	3.76257100
C	-6.66827200	2.88756900	5.19625100
H	-4.89165200	3.19341000	4.01787400
C	-7.67147900	1.99008400	5.57538900
H	-8.43611500	-0.01530500	5.34387900
H	-6.65955300	3.89651700	5.59996300
H	-8.44626100	2.29633600	6.27248400
N	-1.72672100	0.77612500	-0.53954400
C	-0.38682200	2.77994400	-0.31418200
H	0.56110400	3.27851300	-0.48544500

-2069.684486 [M06-2X/6-31++G(d,p)]

C	-0.67107300	1.55277800	-0.82479300

C	-2.79933100	1.25592600	0.08274700
C	-2.79856200	2.62115200	0.47927000
C	-1.71474900	3.43006500	0.19338900
H	0.16604200	1.08579700	-1.34265700
H	-3.65214000	3.02623900	1.01284400
H	-1.72226200	4.47343900	0.49723900
C	-3.94681000	0.38214500	0.23934900
H	-4.67245900	0.42848300	-1.00079800
H	-3.62929800	-0.66349200	0.35322000
N	-5.34744000	0.43266000	-2.11907400
Si	-6.69241900	-0.63738500	-2.03773000
Si	-5.33395100	2.00689500	-2.82055100
C	-3.56523000	2.44433800	-3.34558200
H	-3.51521200	3.47306400	-3.72037900
H	-2.86569100	2.37196900	-2.50248600
H	-3.20976100	1.79044000	-4.15272100
C	-5.89944400	3.34822900	-1.61580700
H	-6.89195000	3.11534600	-1.21290100
H	-5.20483600	3.42754400	-0.77262400
H	-5.94915700	4.32827300	-2.10461800
C	-6.42922800	2.13911000	-4.35746800
H	-6.33874100	3.13763500	-4.80072300
H	-6.14527600	1.40386100	-5.11858900
H	-7.48590100	1.97901400	-4.11401000
C	-7.22336200	-1.29791700	-3.73117300
H	-7.65468700	-0.51312200	-4.36063700
H	-6.37032300	-1.72726600	-4.26984500
H	-7.97758700	-2.08510500	-3.61358900
C	-6.18416300	-2.15360200	-1.01817700
H	-5.83191700	-1.87678500	-0.01892000
H	-7.03228700	-2.83727800	-0.89970300
H	-5.38316700	-2.71856900	-1.51237100
C	-8.22556400	0.12400300	-1.23424700
H	-9.03950300	-0.60510400	-1.14912600
H	-7.99709000	0.49972000	-0.23054200
H	-8.59443600	0.96850500	-1.82861400
K	-2.92952000	-0.84669200	-2.43867700
C	-5.02012800	0.76834100	1.23905800
H	-5.41443200	1.76986600	1.01081900
H	-5.88213100	0.09611600	1.12321400
C	-4.58093100	0.72978600	2.71777300
H	-3.68958200	1.35653100	2.84465300
H	-4.28823000	-0.29707900	2.96807800
C	-5.67049100	1.19920900	3.64674200
C	-6.58669400	0.29889900	4.20180600
C	-5.82859600	2.56218400	3.92361600
C	-7.62958100	0.74535800	5.01295300
H	-6.47683700	-0.76396200	3.99720500
C	-6.86852400	3.01501000	4.73337600
H	-5.12231300	3.27456900	3.50159900
C	-7.77401800	2.10607600	5.28193800
H	-8.32828300	0.03011500	5.43694200
H	-6.97104700	4.07641200	4.93933700
H	-8.58362500	2.45500300	5.91541700
N	-1.71220500	0.75280800	-0.57078500
C	-0.60788600	2.89597300	-0.47741900
H	0.26529300	3.49176500	-0.71557500

Reaction of 2-methylpyridine/styrene monoadduct K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

46

-1505.991442 [B3LYP/6-31+G(d,p)]

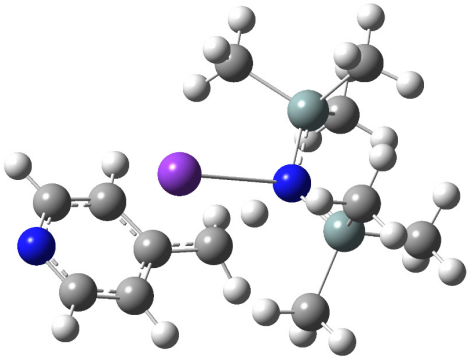
C	-4.71859200	-0.78019000	0.72402700
C	-4.21413400	0.43995000	1.20251300
C	-2.87684000	0.78211600	1.01702200
C	-1.96052800	-0.07973600	0.34461700
C	-2.49977500	-1.31188800	-0.13303700
C	-3.84012600	-1.64870700	0.06095400
H	-5.75999700	-1.04840100	0.87239700
H	-4.87112400	1.12801600	1.72947600
H	-2.50853900	1.72939000	1.40585500
H	-1.85201700	-2.01335100	-0.65120700
H	-4.20423700	-2.60363700	-0.31142800
C	-0.59289700	0.32980300	0.13475600
H	-0.34257900	1.33500700	0.47049900
C	0.39100400	-0.41083000	-0.50453900
H	0.28064600	-1.48608000	-0.61689300
H	1.41928700	-0.06983000	-0.43837700
C	0.54055400	-0.30753600	-2.77530200
H	-0.48381700	-0.62629600	-2.97148200
C	0.79480900	1.06966500	-3.01474700
C	2.11898200	1.61478100	-3.10584600
C	-0.05822300	3.24604900	-3.22914600
C	2.31176900	2.97238100	-3.26606200
H	2.97547600	0.95095000	-3.05601200
C	1.19770600	3.83402700	-3.33853500
H	-0.94937500	3.87486100	-3.27406600
H	3.32043600	3.37166000	-3.34159200
H	1.30398200	4.90506000	-3.47226900
N	-0.28449700	1.93184300	-3.07170900
K	-2.77149300	1.06894100	-2.30894300
C	1.57872700	-1.37612300	-3.00823600
H	2.52713400	-1.11344000	-2.51836100
H	1.25391900	-2.30946900	-2.52765200
C	1.87287800	-1.69196700	-4.50362100
H	2.20600100	-0.77341600	-5.00034800
H	0.93441200	-1.99136000	-4.98634900

C	2.90999900	-2.77777600	-4.68600700
C	4.27790700	-2.46572800	-4.75070700
C	2.53867000	-4.13073300	-4.74906800
C	5.24337600	-3.46932600	-4.87158400
H	4.58871100	-1.42402900	-4.71208500
C	3.49916600	-5.13927700	-4.87027300
H	1.48437500	-4.39588900	-4.70872900
C	4.85747600	-4.81220200	-4.93073300
H	6.29551800	-3.20245800	-4.92371200
H	3.18670500	-6.17886900	-4.92139400
H	5.60563400	-5.59379000	-5.02736700

-1505.547750 [M06-2X/6-31++G(d,p)]

C	-4.59080200	-0.44450600	0.43918300
C	-4.04570100	0.75811300	0.90680100
C	-2.67404900	0.98149000	0.85718300
C	-1.77948700	0.01822700	0.32931600
C	-2.35020000	-1.20011500	-0.11728500
C	-3.72436700	-1.42262100	-0.05841800
H	-5.66051900	-0.62055900	0.47907200
H	-4.69843700	1.52572900	1.31331800
H	-2.26888700	1.92458800	1.21631300
H	-1.70874400	-1.97364000	-0.52867400
H	-4.12411100	-2.36911900	-0.41248800
C	-0.37428700	0.33196100	0.17599100
H	-0.07931900	1.34846200	0.42639500
C	0.53751800	-0.49825700	-0.41168800
H	0.35796800	-1.56433300	-0.51809500
H	1.57839300	-0.19440400	-0.47635500
C	0.42285400	-0.50511800	-2.78029800
H	-0.60765900	-0.85995800	-2.80869500
C	0.61599700	0.87206700	-2.93596800
C	1.92196400	1.45859000	-3.08982500
C	-0.28406400	3.03236000	-2.88894500
C	2.07228500	2.82254500	-3.14126700
H	2.79035500	0.81150800	-3.16958800
C	0.94119100	3.66118600	-3.04375800
H	-1.18726200	3.64162400	-2.80804300
H	3.06320500	3.25339600	-3.26241900
H	1.01542300	4.74103000	-3.08806300
N	-0.47651600	1.70861600	-2.83197700
K	-2.98207600	0.87833400	-2.27357300
C	1.49306700	-1.52338600	-3.03872600
H	2.42676000	-1.25383900	-2.51978200
H	1.19188200	-2.49029700	-2.61114500
C	1.82564600	-1.74684200	-4.53310700
H	2.12933800	-0.78986900	-4.97406000
H	0.91296800	-2.06474800	-5.05053500
C	2.91198500	-2.77367200	-4.72294300
C	4.26028600	-2.39909200	-4.73877300
C	2.60062600	-4.13475100	-4.81790700
C	5.26946300	-3.35508400	-4.85007500
H	4.51841800	-1.34434200	-4.66717300
C	3.60462300	-5.09561000	-4.92887300
H	1.55683600	-4.44169400	-4.80794800
C	4.94446000	-4.70815700	-4.94566300
H	6.30970600	-3.04319100	-4.86515300
H	3.34153600	-6.14658500	-5.00546700
H	5.72820500	-5.45387400	-5.03612300

Deprotonation of 4-methylpyridine (31) by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

42

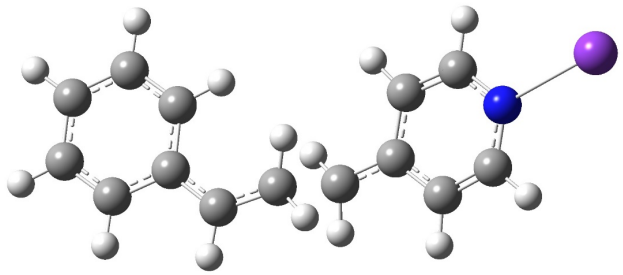
-1760.644544 [B3LYP/6-31+G(d,p)]

C	-0.92731400	-0.68711800	-0.02668700
C	-3.07540300	0.40152800	0.42027500
C	-2.30243300	1.60006300	0.47907900
C	-0.92968300	1.57354100	0.26345900
H	-0.35555300	-1.59524100	-0.21452400
H	-2.78822700	2.54648500	0.70327400
H	-0.36040500	2.50112000	0.31272800
C	-4.51513700	0.39555400	0.45579300
H	-4.95939600	1.25260200	0.96927600
H	-5.02466200	0.51684500	-0.88862400
H	-4.95995100	-0.54801000	0.78150000
N	-5.49654100	0.64969300	-2.11598800
Si	-6.16466800	-0.82162700	-2.75089400
Si	-6.16831200	2.23890300	-2.31216500
C	-4.78430500	3.54125000	-2.13323600
H	-5.20889600	4.55239900	-2.10864700
H	-4.21102700	3.40812700	-1.20797800
H	-4.08238900	3.51939900	-2.97881800
C	-7.48054500	2.65217600	-1.00152900
H	-8.32853500	1.96020600	-1.06504200
H	-7.06502600	2.57252600	0.00980000
H	-7.86714400	3.67134300	-1.12723700
C	-6.95321600	2.54118000	-4.01883900
H	-7.31482500	3.57540700	-4.08495700
H	-6.23280600	2.38923500	-4.83137000
H	-7.80873600	1.88251700	-4.20580800
C	-5.86703100	-1.00053500	-4.62658800
H	-6.34542600	-0.19482500	-5.19447500
H	-4.79646100	-0.98776900	-4.87100900
H	-6.27278600	-1.95214800	-4.99347600
C	-5.32166300	-2.31705400	-1.93352900
H	-5.51580300	-2.35044300	-0.85606700
H	-5.70293000	-3.24823700	-2.37060900
H	-4.23338000	-2.31119400	-2.07195000
C	-8.03606700	-1.03019700	-2.46952700
H	-8.38602400	-1.99057200	-2.86913800
H	-8.27693300	-1.00619400	-1.39991200
H	-8.61720200	-0.23868000	-2.95732200
K	-2.71040300	0.80830900	-2.65455700
C	-2.29945200	-0.77170200	0.17541400
H	-2.78367200	-1.74430500	0.14818300
N	-0.21468300	0.46082300	-0.01071700

-1760.246470 [M06-2X/6-31++G(d,p)]

C	-1.29157500	-0.52226600	0.04795700
C	-3.53749700	0.29013600	0.53983700
C	-2.93521200	1.57798300	0.53244200
C	-1.58404900	1.72364000	0.25858500
H	-0.61026200	-1.35170900	-0.13512200
H	-3.54067100	2.45897600	0.73143600
H	-1.14243100	2.71901000	0.24175400
C	-4.95905100	0.11356000	0.57065400
H	-5.51804000	0.89425200	1.08851400
H	-5.21376400	0.35616400	-0.79715500
H	-5.30450800	-0.89240300	0.81495300
N	-5.35385300	0.61432900	-2.10214800
Si	-6.01809600	-0.81433100	-2.79613700
Si	-5.89766600	2.22991000	-2.33635600
C	-4.42135300	3.39927600	-2.60370100
H	-4.76564400	4.43854200	-2.65503500
H	-3.70288100	3.34481900	-1.77553500
H	-3.89637300	3.19507600	-3.54617500
C	-6.81918000	2.88872000	-0.82435400
H	-7.63474100	2.21316300	-0.54246600
H	-6.15267200	2.98175200	0.03991200
H	-7.24681700	3.87728300	-1.02626600
C	-7.01881200	2.46724800	-3.84129500
H	-7.36405800	3.50677900	-3.88636100
H	-6.48876700	2.25021600	-4.77496800
H	-7.90448400	1.82343100	-3.79900800
C	-6.00659000	-0.81208600	-4.68989800
H	-6.74553400	-0.11929800	-5.10419000
H	-5.02301400	-0.52555800	-5.08187700
H	-6.23811600	-1.81393200	-5.07047300
C	-4.95983100	-2.28688400	-2.25013800
H	-4.94391400	-2.37096400	-1.15841800
H	-5.35767600	-3.22425000	-2.65484200
H	-3.92065300	-2.19924300	-2.59198300
C	-7.78753600	-1.15862600	-2.22851900
H	-8.18095800	-2.08898000	-2.65351000
H	-7.82294900	-1.24092200	-1.13601100
H	-8.45866800	-0.34319600	-2.52153300
K	-2.61856800	0.69207000	-2.53215600
C	-2.62928900	-0.77842300	0.30792800
H	-2.98441600	-1.80499800	0.32656000
N	-0.74488300	0.70711300	-0.01734200

Reaction of 4-methylpyridine K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

30

-1196.403421 [B3LYP/6-31+G(d,p)]

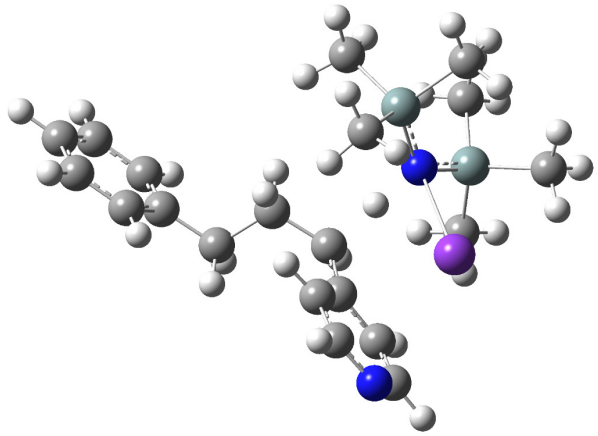
C	-2.90933300	-3.19039100	1.78527100
C	-1.64159300	-3.71281000	2.08826100
C	-0.48499200	-3.08278000	1.64080100
C	-0.52432500	-1.88654200	0.86670400
C	-1.82387400	-1.38629500	0.56084000
C	-2.97876100	-2.02082100	1.01549100
H	-3.81263900	-3.68307500	2.13307600
H	-1.55818600	-4.62221900	2.67977100
H	0.48577700	-3.50604100	1.89193100
H	-1.92198100	-0.48835300	-0.04265900
H	-3.94951300	-1.60080600	0.75932500
C	0.69489500	-1.25022600	0.44523200
H	1.61268900	-1.80635900	0.63499300
C	0.78282300	-0.07969300	-0.32104800
H	-0.03378800	0.64054700	-0.26989200
H	1.75875300	0.39860500	-0.38352800
C	0.59139800	-0.38297800	-2.33656300
H	1.45740600	-1.02269400	-2.48675500
H	-0.35705900	-0.91429600	-2.31843300
C	0.61240000	0.89247600	-2.95354200
C	1.82405200	1.55035500	-3.34666600
C	-0.46773900	3.00426800	-3.55471300
C	1.80598300	2.85025900	-3.80881400
H	2.77052600	1.01838200	-3.29001600
H	-1.37565800	3.60113500	-3.64981900
H	2.74146800	3.32300800	-4.10987500
N	0.68750000	3.61839700	-3.93331900
K	0.72828400	6.20841600	-4.64689000
C	-0.55745500	1.71192000	-3.07999200
H	-1.53047500	1.31021000	-2.80888400

-1196.093405 [M06-2X/6-31++G(d,p)]

C	-2.93193800	-2.99042400	1.63788000
C	-1.71168400	-3.51236500	2.08518700
C	-0.50884800	-2.94677000	1.68793200
C	-0.45620200	-1.82320700	0.82331900
C	-1.70419800	-1.32452900	0.36809600
C	-2.90777500	-1.89265000	0.77522100
H	-3.87283000	-3.43375600	1.94797900
H	-1.70290100	-4.37164900	2.75123600
H	0.42773400	-3.36470100	2.05141200
H	-1.72444400	-0.48286900	-0.31921000
H	-3.84201200	-1.47804600	0.40369400
C	0.80504000	-1.24785700	0.43768300
H	1.69903500	-1.81769300	0.68240200
C	0.92125700	-0.12113200	-0.37158700
H	0.11923500	0.61994200	-0.35661800
H	1.90812200	0.32536500	-0.48597000
C	0.65807400	-0.51120900	-2.36077500
H	1.54639700	-1.11095200	-2.53777900
H	-0.26921500	-1.07275700	-2.27430600
C	0.60268100	0.77418200	-2.92846600
C	1.76668600	1.49280800	-3.34655600
C	-0.57093800	2.87379900	-3.33615100
C	1.67724500	2.81177800	-3.72864600
H	2.73100300	0.99218700	-3.36931000
H	-1.49903800	3.44603200	-3.33768100
H	2.57824600	3.33485500	-4.05038700
N	0.53455000	3.54167100	-3.74435000

K	0.48357600	6.11534800	-4.38544800
C	-0.59481000	1.55755400	-2.93370300
H	-1.53546600	1.10864700	-2.62481000

Deprotonation of 4-methylpyridine/styrene monoadduct (32a) by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-2070.215542 [B3LYP/6-31+G(d,p)]

C	-0.78668900	-0.27537600	-0.54610800
C	-2.95772100	0.53282400	0.26161000
C	-2.31056500	1.80497500	0.31573100
C	-0.98736300	1.94757100	-0.08798800
H	-0.15381300	-1.09990100	-0.87236000
H	-2.84476600	2.68192100	0.66736200
H	-0.51981700	2.93076900	-0.04773900
C	-4.37137500	0.32820400	0.47004800
H	-4.98089100	0.50243800	-0.82613900
H	-4.60303300	-0.72758000	0.64894300
N	-5.54304100	0.63490500	-2.02361200
Si	-6.09290600	-0.87031700	-2.69821000
Si	-6.32910200	2.16293500	-2.28404200
C	-5.12168700	3.59136100	-1.90592900
H	-5.66048200	4.54684000	-1.91401300
H	-4.65065300	3.49009400	-0.92238700
H	-4.32385500	3.68055200	-2.65651800
C	-7.86780000	2.44765500	-1.20485100
H	-8.62898700	1.68149100	-1.39153300
H	-7.62186800	2.41853900	-0.13756700
H	-8.31805200	3.42550300	-1.41799300
C	-6.87589500	2.42963900	-4.09095000
H	-7.30010900	3.43543800	-4.20594000
H	-6.03477900	2.34481200	-4.78995900
H	-7.64268800	1.71381500	-4.40793800
C	-5.56711300	-1.06464300	-4.52471300
H	-5.96518400	-0.25982600	-5.15275600
H	-4.47423400	-1.06705700	-4.63909600
H	-5.93120500	-2.01586500	-4.93379700
C	-5.31974400	-2.34136800	-1.77835700
H	-5.65417800	-2.39548700	-0.73663100
H	-5.60944600	-3.27796500	-2.27079100
H	-4.22458000	-2.29508000	-1.77301100
C	-7.97782200	-1.12754800	-2.64494500
H	-8.24349400	-2.11251000	-3.04952000
H	-8.35079400	-1.07798900	-1.61500500

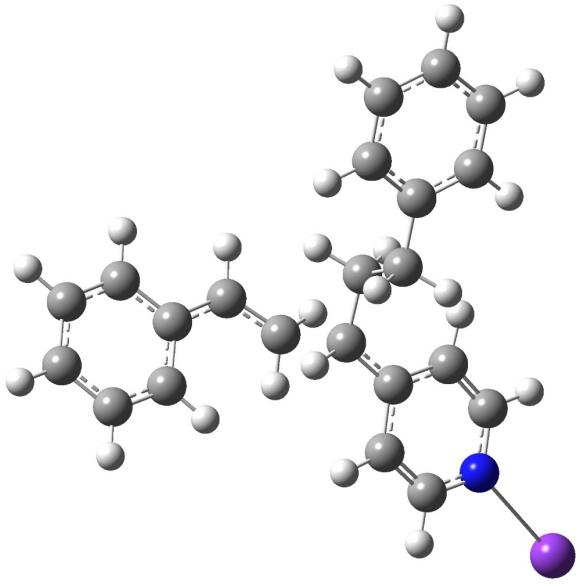
H	-8.51855700	-0.37467500	-3.22979500
K	-2.82838300	1.07674400	-2.83806900
C	-2.09839400	-0.52601900	-0.16756200
H	-2.47407800	-1.54550900	-0.19448000
N	-0.20511500	0.94608700	-0.54431100
C	-5.13368100	1.23984900	1.42473800
H	-4.99438900	2.29719900	1.16210900
H	-6.20921400	1.05129400	1.31314700
C	-4.76229100	1.05403000	2.92050300
H	-3.69290000	1.25938200	3.04945000
H	-4.91555600	0.00028300	3.18508800
C	-5.56664900	1.93432400	3.85118400
C	-6.81670700	1.51655800	4.33676700
C	-5.10697500	3.20802500	4.22272400
C	-7.58357900	2.34198500	5.16387600
H	-7.18985400	0.53076900	4.06784900
C	-5.86890900	4.03858100	5.05010600
H	-4.13765100	3.54897400	3.86561300
C	-7.11240900	3.60866200	5.52367100
H	-8.54575400	1.99459000	5.53056900
H	-5.48951500	5.01823400	5.32818100
H	-7.70482700	4.25071200	6.16926900

-2069.677957 [M06-2X/6-31++G(d,p)]

C	-1.47032300	3.90828800	-0.64275800
C	-0.01922300	1.94678700	-0.68243900
C	0.47128700	2.44241300	0.55744000
C	-0.06944300	3.59222600	1.11901800
H	-2.23541500	4.52204800	-1.11530000
H	1.26767700	1.92597600	1.08501200
H	0.30544000	3.94661900	2.07792700
C	0.29726500	0.64595300	-1.20599200
H	-0.72197500	-0.10669000	-0.60325900
H	0.09145100	0.55749800	-2.27748300
N	-1.69898100	-0.79677400	0.01708900
Si	-2.89493300	-1.30011000	-1.11871700
Si	-1.13094300	-1.79198100	1.30595400
C	-0.42627400	-0.69282700	2.68442500
H	0.14184500	-1.29367000	3.40344100
H	0.25173300	0.07081400	2.28614100
H	-1.21726900	-0.18743800	3.25468000
C	0.22224700	-3.01745000	0.81519100
H	-0.07971700	-3.59399700	-0.06646200
H	1.16505300	-2.51414400	0.58036500
H	0.41317600	-3.72328300	1.63200500
C	-2.50730600	-2.81840900	2.10819400
H	-2.11276400	-3.35518300	2.97909400
H	-3.33744000	-2.18832600	2.44767700
H	-2.91559600	-3.56484100	1.41735300
C	-4.63016300	-1.41746000	-0.35944300
H	-4.70862100	-2.22697100	0.37255600
H	-4.91246300	-0.48430700	0.14442700
H	-5.37360700	-1.60166600	-1.14402700
C	-3.03824200	-0.01340100	-2.49685400
H	-2.09764000	0.11140000	-3.04256400
H	-3.80991200	-0.31439400	-3.21455200
H	-3.32351800	0.96685700	-2.09542500
C	-2.52679900	-2.97068000	-1.92492100
H	-3.28105900	-3.22362400	-2.67897000

H	-1.54748600	-2.94941700	-2.41681000
H	-2.50979600	-3.77902900	-1.18450900
K	-2.51198400	1.56653300	1.23765200
C	-1.00038400	2.77877000	-1.29057400
H	-1.39869700	2.51412300	-2.26602600
N	-1.05620500	4.32249800	0.57225700
C	1.59387300	-0.01689200	-0.78602600
H	1.65031500	-0.09879900	0.31027200
H	1.60611400	-1.05036300	-1.15550900
C	2.86549100	0.69726500	-1.28817500
H	2.81467800	1.75700200	-1.00987200
H	2.88081300	0.65458400	-2.38388200
C	4.12152200	0.08540000	-0.72280000
C	4.71085300	-1.03667800	-1.31624800
C	4.69045300	0.59196300	0.45082800
C	5.83868500	-1.63430700	-0.75502800
H	4.28229800	-1.44170500	-2.23052100
C	5.81860100	-0.00036700	1.01650800
H	4.24498000	1.46615300	0.92152000
C	6.39686600	-1.11738000	0.41433300
H	6.28472300	-2.50164700	-1.23273700
H	6.24795100	0.41173000	1.92491800
H	7.27706200	-1.57952200	0.85032900

Reaction of 4-methylpyridine/styrene monoadduct K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-1505.978676 [B3LYP/6-31+G(d,p)]

C	3.60339200	-4.97763800	-0.77164000
C	4.24627700	-4.25138200	0.24427400
C	3.56651200	-3.27197600	0.96055400
C	2.19796300	-2.96014000	0.70910300
C	1.57403300	-3.70277600	-0.33649000
C	2.26050700	-4.68589900	-1.04774400
H	4.13469200	-5.74093700	-1.33268600
H	5.28977600	-4.45368500	0.47675100
H	4.08675100	-2.72518400	1.74478200

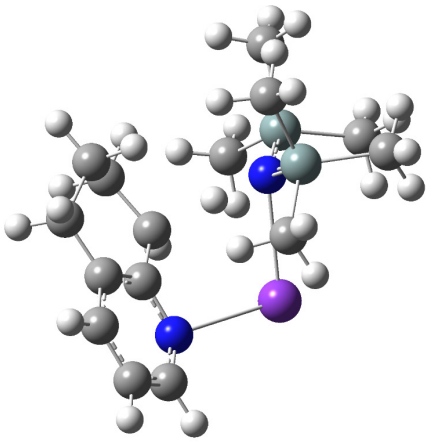
H	0.53703300	-3.50102200	-0.58926700
H	1.74187500	-5.22887800	-1.83559300
C	1.52116000	-1.95877800	1.48830800
H	2.14265000	-1.38828900	2.17707200
C	0.18103300	-1.56852700	1.32480800
H	-0.24971600	-0.95681000	2.11763200
H	-0.52679700	-2.30007800	0.93324500
C	-0.12392300	-0.22826900	-0.16603100
H	0.27014000	-0.84903700	-0.97293300
C	-1.53997800	-0.07136400	-0.20995500
C	-2.27234600	0.90818300	0.53627400
C	-3.74917600	-0.93123700	-0.82453800
C	-3.65396300	0.89990700	0.54804400
H	-1.75235200	1.67667300	1.09917400
H	-4.35604700	-1.65632800	-1.36760400
H	-4.18449600	1.66152100	1.12042400
C	0.78200300	0.92909000	0.18976800
H	0.43603400	1.42800700	1.10590600
H	1.77564600	0.52697600	0.42714300
C	0.92965200	1.99079100	-0.93084900
H	-0.05746500	2.40376700	-1.17044400
H	1.29199900	1.48997000	-1.83740900
C	1.87198100	3.11578600	-0.56009400
C	1.38826500	4.31536900	-0.01432400
C	3.26098300	2.97424200	-0.71524000
C	2.25963500	5.34102300	0.36559000
H	0.31560100	4.44815200	0.10917100
C	4.13736000	3.99507200	-0.33724200
H	3.65817900	2.05492800	-1.13945300
C	3.63975900	5.18432400	0.20590600
H	1.86072900	6.26216000	0.78229200
H	5.20791800	3.86331100	-0.46951200
H	4.31942800	5.97988400	0.49796800
C	-2.37420500	-1.01076900	-0.89898900
N	-4.43624600	0.00695100	-0.11520200
K	-7.11633700	-0.07676200	0.09846500
H	-1.91901300	-1.79546300	-1.49803600

-1505.533798 [M06-2X/6-31++G(d,p)]

C	3.25695400	-5.16378200	-0.52335200
C	3.86162700	-4.52120100	0.56334700
C	3.23479000	-3.45649200	1.19546200
C	1.96750200	-2.98112300	0.77790000
C	1.38527900	-3.63151700	-0.33742900
C	2.01525100	-4.70400600	-0.96384800
H	3.74813300	-5.99481000	-1.01900400
H	4.83209100	-4.85732700	0.91890400
H	3.71819400	-2.97265500	2.04134400
H	0.43218800	-3.28304500	-0.72696700
H	1.53534400	-5.17773600	-1.81649900
C	1.32516900	-1.89141600	1.47309600
H	1.92902800	-1.33350700	2.18479200
C	0.05230200	-1.42922100	1.15951700
H	-0.38801800	-0.69834900	1.84478600
H	-0.65911400	-2.14195700	0.72569300
C	-0.06139300	-0.17986300	-0.44744100
H	0.35116000	-0.86419200	-1.19084900
C	-1.46029600	0.00613500	-0.51634800
C	-2.16405800	1.03263300	0.19147800

C	-3.69066700	-0.87298400	-1.00723900
C	-3.54844900	1.02486000	0.24548100
H	-1.62548300	1.84472300	0.67079900
H	-4.32336800	-1.61772600	-1.48794400
H	-4.06561700	1.82094700	0.77936900
C	0.85244300	0.94344900	-0.04121100
H	0.52406200	1.37571000	0.91698000
H	1.85212800	0.53034400	0.14767300
C	0.95742800	2.07686100	-1.07955100
H	-0.04762200	2.45883100	-1.29670200
H	1.35392500	1.66569300	-2.01510100
C	1.83490400	3.20252600	-0.59282600
C	1.29251700	4.25631900	0.15101600
C	3.21576800	3.18827200	-0.81627900
C	2.10424300	5.27060900	0.65682300
H	0.21914600	4.28266600	0.32908900
C	4.03305700	4.19970100	-0.31327200
H	3.65255400	2.37530700	-1.39218000
C	3.47958500	5.24482600	0.42621800
H	1.66265300	6.08273100	1.22703800
H	5.10237500	4.17327700	-0.50078900
H	4.11459200	6.03437600	0.81591000
C	-2.31631300	-0.96588400	-1.12636000
N	-4.34296100	0.08588400	-0.31067100
K	-3.14481000	-1.49853900	1.90966600
H	-1.88131800	-1.77449000	-1.70913900

Deprotonation of 5,6,7,8-tetrahydroquinoline (33) by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-1877.329150 [B3LYP/6-31+G(d,p)]

C	0.45780300	3.34292700	-1.65662700
C	0.05912600	2.02796000	0.24469600
C	-0.40755200	3.18983900	0.94619400
C	-0.43859800	4.40540700	0.27923700
H	0.82245100	3.36704200	-2.68399900
H	-0.79125300	5.29200000	0.80413900
C	0.04281400	0.70564100	0.84331700
H	-1.06350100	-0.16923700	0.30874200
N	-1.87778000	-1.03743800	-0.16251400
Si	-1.50689200	-2.67386700	0.28996300
Si	-3.45889500	-0.40694600	-0.52114500
C	-3.29032300	1.28331100	-1.37783900
H	-4.27788400	1.74913200	-1.48478600

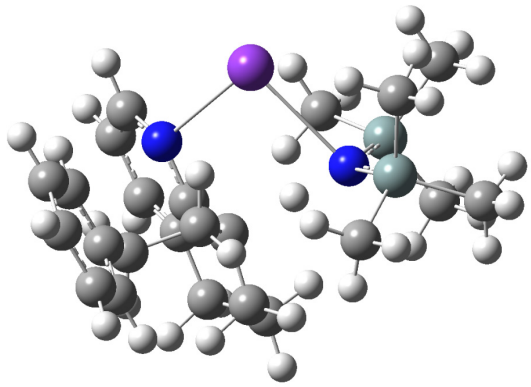
H	-2.65614900	1.97228400	-0.81004400
H	-2.87086000	1.19684500	-2.38915700
C	-4.57013000	-0.14528900	1.00130400
H	-4.72525800	-1.08161200	1.54958800
H	-4.13677200	0.57875100	1.70043900
H	-5.55565700	0.23220800	0.69967200
C	-4.45389200	-1.51367300	-1.71099800
H	-5.37134200	-0.99577600	-2.01959900
H	-3.88671300	-1.75510800	-2.61791200
H	-4.75400900	-2.45936700	-1.24520500
C	-1.80483200	-3.92298500	-1.12090200
H	-2.86090800	-3.98947200	-1.40216200
H	-1.23987400	-3.65835200	-2.02443200
H	-1.47924400	-4.92514200	-0.81309800
C	0.34216900	-2.83025600	0.71562000
H	0.62959100	-2.19454000	1.55900200
H	0.56497600	-3.86934600	0.98840100
H	0.99462400	-2.57377100	-0.12913000
C	-2.47551100	-3.31406700	1.79675900
H	-2.14310800	-4.32167500	2.07710400
H	-2.33255500	-2.65922800	2.66443000
H	-3.55175800	-3.36534000	1.59403900
K	-0.06204900	-0.27854600	-2.23139400
C	0.00054100	4.50777600	-1.05217000
H	-0.00748200	5.45131300	-1.58765200
N	0.48683900	2.14343600	-1.05384400
C	-1.18532600	1.66754300	2.82742800
H	-2.15126300	1.40819600	2.37732000
H	-1.31739900	1.62224800	3.91553500
C	-0.79377500	3.09069000	2.41097000
H	0.06157600	3.41404900	3.02370000
H	-1.60517200	3.79689800	2.62872100
C	-0.12641100	0.65835200	2.36224100
H	-0.42435000	-0.35107200	2.67752800
H	0.81736200	0.87315000	2.89380000
H	0.89790100	0.10838700	0.50179900

-1876.883482 [M06-2X/6-31++G(d,p)]

C	0.26507100	3.34298500	-1.75933300
C	0.10260200	1.96688800	0.11594600
C	-0.52462900	3.02373600	0.84367800
C	-0.73712100	4.23123500	0.20550300
H	0.59525100	3.43218900	-2.79363700
H	-1.22207800	5.04148300	0.74795600
C	0.26557600	0.64439400	0.68530800
H	-0.86942000	-0.17682700	0.22860800
N	-1.77387000	-0.98910900	-0.15418600
Si	-1.55813400	-2.55701500	0.52923800
Si	-3.30148900	-0.32844100	-0.60607300
C	-3.20019100	1.55306000	-0.72828400
H	-4.12577700	1.94293900	-1.16824600
H	-3.07293200	2.01708600	0.25550700
H	-2.36236300	1.89165100	-1.35095200
C	-4.70600800	-0.74147300	0.59281300
H	-4.90994900	-1.81785200	0.62810200
H	-4.45912300	-0.41405800	1.60923400
H	-5.63089700	-0.23735700	0.28895300
C	-3.84383500	-0.95008100	-2.31553800
H	-4.82316800	-0.54010200	-2.58911600

H	-3.13348200	-0.64657300	-3.09509400
H	-3.91703900	-2.04285800	-2.33824000
C	-2.43686600	-3.90151900	-0.47381900
H	-3.52326100	-3.75560100	-0.47310200
H	-2.10186700	-3.90317300	-1.51758600
H	-2.23622300	-4.89349700	-0.05238700
C	0.28960000	-2.97558900	0.53168600
H	0.87371300	-2.21651100	1.06313000
H	0.46219300	-3.93869200	1.02493200
H	0.68856800	-3.05985700	-0.48718500
C	-2.18369000	-2.71682500	2.30784200
H	-1.88034700	-3.67458900	2.74669100
H	-1.79272200	-1.91311300	2.94122300
H	-3.27713800	-2.66359500	2.34192600
K	0.05102000	-0.37451100	-2.16925800
C	-0.33553000	4.41878400	-1.12438900
H	-0.48840400	5.35889500	-1.64166300
N	0.47831700	2.15463100	-1.17937500
C	-1.11851000	1.33437500	2.63777700
H	-2.00178300	0.93100300	2.12339200
H	-1.29121500	1.22929300	3.71462400
C	-0.93931800	2.81268600	2.28513700
H	-0.16995500	3.23923700	2.94419700
H	-1.86030300	3.37446000	2.48338200
C	0.10989800	0.53839700	2.19388300
H	-0.01010900	-0.51490000	2.48271200
H	0.99121100	0.90887700	2.74375300
H	1.16902600	0.14871200	0.30740900

Deprotonation of 5,6,7,8-tetrahydroquinoline/styrene monoadduct by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-2186.891607 [B3LYP/6-31+G(d,p)]

C	-1.07122300	0.41487100	-0.22996000
C	-3.24179500	0.77235500	0.59273700
C	-2.81807700	2.03382000	1.13313600
C	-1.50201900	2.43449400	0.95332700
H	-0.40611400	-0.25858800	-0.77237700
H	-1.17608900	3.38785300	1.36630500
C	-4.61630800	0.29009300	0.69675200
H	-5.27662600	0.49213500	-0.66759900
N	-5.84619900	0.58627200	-1.81770500
Si	-7.29319700	-0.33396900	-2.13732900
Si	-5.45361200	2.00100600	-2.76142700
C	-3.64242200	2.52264400	-2.51688600

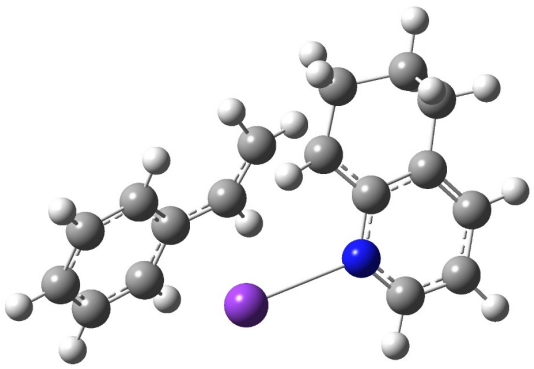
H	-3.46130300	3.44082100	-3.08992900
H	-3.39379000	2.72639200	-1.47179200
H	-2.92561100	1.77732300	-2.88508600
C	-6.50963000	3.53556300	-2.37493200
H	-7.56692500	3.36834200	-2.60596400
H	-6.44200400	3.81359000	-1.31717700
H	-6.16934800	4.39419400	-2.96791600
C	-5.61368700	1.69445600	-4.64034900
H	-5.32574200	2.60221600	-5.18635600
H	-4.95082100	0.88749900	-4.97859000
H	-6.63140800	1.43565000	-4.95097100
C	-6.98496000	-1.68323500	-3.45941600
H	-6.60144500	-1.26308700	-4.39671500
H	-6.27172200	-2.44286800	-3.10961000
H	-7.91557400	-2.21595600	-3.69345000
C	-7.95396700	-1.26642100	-0.62250300
H	-8.09235200	-0.60984100	0.24328400
H	-8.93220000	-1.69375200	-0.87697800
H	-7.30423600	-2.09316800	-0.31978800
C	-8.77127400	0.69647200	-2.75834600
H	-9.62479500	0.03145600	-2.94225900
H	-9.08046000	1.43092300	-2.00539800
H	-8.57012700	1.23762000	-3.68864800
K	-3.59901600	-1.12538700	-2.29076600
C	-0.58787300	1.61928600	0.26546000
H	0.44775100	1.91007400	0.12370100
N	-2.33947300	-0.00378700	-0.09022400
C	-5.24227200	2.60977700	1.55389400
H	-5.43521300	2.96792600	0.53574600
H	-5.91494700	3.16361400	2.22035600
C	-3.78400800	2.89128800	1.92779100
H	-3.64795300	2.68699800	3.00067100
H	-3.53820800	3.95159400	1.78764900
C	-5.52191500	1.10584100	1.62870000
H	-6.57273600	0.91498100	1.36932200
H	-5.41624400	0.79172800	2.68321900
C	-4.75043300	-1.21612500	0.96736000
H	-5.81287700	-1.45515000	1.07733300
H	-4.39901000	-1.83374600	0.12932000
C	-4.01194900	-1.73509700	2.23492700
H	-2.94366700	-1.51811800	2.13220500
H	-4.37327100	-1.17976200	3.10835000
C	-4.21002800	-3.21645100	2.45921700
C	-3.30570500	-4.15354200	1.93178100
C	-5.32624000	-3.70242900	3.16067700
C	-3.50764100	-5.52740600	2.09611700
H	-2.42725100	-3.79923200	1.39652400
C	-5.53367800	-5.07436000	3.32925900
H	-6.03685700	-2.99584000	3.58378100
C	-4.62493200	-5.99426300	2.79550000
H	-2.78955600	-6.23213200	1.68491100
H	-6.40206500	-5.42500200	3.88058200
H	-4.78262600	-7.06080900	2.92831200

-2186.311333 [M06-2X/6-31++G(d,p)]

C	0.26507100	3.34298500	-1.75933300
C	0.10260200	1.96688800	0.11594600
C	-0.52462900	3.02373600	0.84367800
C	-0.73712100	4.23123500	0.20550300
H	0.59525100	3.43218900	-2.79363700

H	-1.22207800	5.04148300	0.74795600
C	0.26557600	0.64439400	0.68530800
H	-0.86942000	-0.17682700	0.22860800
N	-1.77387000	-0.98910900	-0.15418600
Si	-1.55813400	-2.55701500	0.52923800
Si	-3.30148900	-0.32844100	-0.60607300
C	-3.20019100	1.55306000	-0.72828400
H	-4.12577700	1.94293900	-1.16824600
H	-3.07293200	2.01708600	0.25550700
H	-2.36236300	1.89165100	-1.35095200
C	-4.70600800	-0.74147300	0.59281300
H	-4.90994900	-1.81785200	0.62810200
H	-4.45912300	-0.41405800	1.60923400
H	-5.63089700	-0.23735700	0.28895300
C	-3.84383500	-0.95008100	-2.31553800
H	-4.82316800	-0.54010200	-2.58911600
H	-3.13348200	-0.64657300	-3.09509400
H	-3.91703900	-2.04285800	-2.33824000
C	-2.43686600	-3.90151900	-0.47381900
H	-3.52326100	-3.75560100	-0.47310200
H	-2.10186700	-3.90317300	-1.51758600
H	-2.23622300	-4.89349700	-0.05238700
C	0.28960000	-2.97558900	0.53168600
H	0.87371300	-2.21651100	1.06313000
H	0.46219300	-3.93869200	1.02493200
H	0.68856800	-3.05985700	-0.48718500
C	-2.18369000	-2.71682500	2.30784200
H	-1.88034700	-3.67458900	2.74669100
H	-1.79272200	-1.91311300	2.94122300
H	-3.27713800	-2.66359500	2.34192600
K	0.05102000	-0.37451100	-2.16925800
C	-0.33553000	4.41878400	-1.12438900
H	-0.48840400	5.35889500	-1.64166300
N	0.47831700	2.15463100	-1.17937500
C	-1.11851000	1.33437500	2.63777700
H	-2.00178300	0.93100300	2.12339200
H	-1.29121500	1.22929300	3.71462400
C	-0.93931800	2.81268600	2.28513700
H	-0.16995500	3.23923700	2.94419700
H	-1.86030300	3.37446000	2.48338200
C	0.10989800	0.53839700	2.19388300
H	-0.01010900	-0.51490000	2.48271200
H	0.99121100	0.90887700	2.74375300
H	1.16902600	0.14871200	0.30740900

Reaction of 5,6,7,8-tetrahydroquinoline K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

37

-1313.102373 [B3LYP/6-31+G(d,p)]

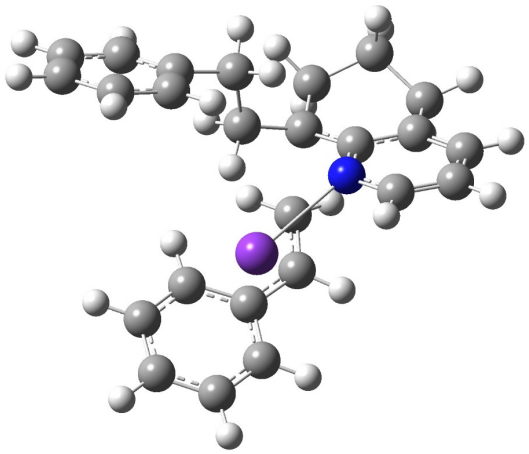
C	-4.50157600	-1.17726400	0.80034100
C	-4.26141500	0.17639300	1.08685400
C	-3.00083900	0.73564000	0.89119500
C	-1.90094400	-0.02910100	0.40108300
C	-2.17322600	-1.40083200	0.11601000
C	-3.43824500	-1.95374600	0.31840100
H	-5.48315200	-1.61366500	0.95705200
H	-5.06571100	0.79913100	1.47173600
H	-2.83805500	1.78463000	1.13095600
H	-1.37559900	-2.03679800	-0.25703700
H	-3.59640100	-3.00671800	0.09618400
C	-0.62010500	0.59482900	0.17167600
H	-0.57846500	1.66972100	0.34128700
C	0.52109200	-0.03970400	-0.29752000
H	0.61990000	-1.11950900	-0.22694700
H	1.46412300	0.49556600	-0.26349800
C	0.79079400	-0.32855100	-2.54400600
H	-0.15757900	-0.85001300	-2.65987900
C	0.82656000	1.00035400	-3.04358900
C	2.08357800	1.67395900	-3.25787800
C	-0.31176000	2.94645900	-3.68142000
C	2.07752500	2.97949000	-3.70602900
C	0.85642100	3.65628100	-3.92355900
H	-1.27805400	3.42817200	-3.84061700
H	3.02279500	3.48534700	-3.89604600
H	0.82500300	4.68331600	-4.27153900
N	-0.35864200	1.66813300	-3.26438600
K	-2.71870700	0.57218900	-2.42694500
C	3.35925100	0.89807700	-3.01687600
H	4.18590200	1.35457000	-3.57472000
H	3.63569400	0.94985400	-1.95254300
C	2.03214000	-1.20414900	-2.58800300
H	2.40969600	-1.40711700	-1.56854300
H	1.78528900	-2.18985900	-3.00522400
C	3.17782300	-0.57836700	-3.40213700
H	2.95062600	-0.64182400	-4.47474300
H	4.10976200	-1.13233700	-3.23593300

-1312.748657 [M06-2X/6-31++G(d,p)]

C	-4.38501100	-0.77774200	0.37364700
C	-4.05930300	0.57483100	0.54273400
C	-2.73496200	0.99552800	0.50705000
C	-1.66701800	0.08863000	0.29133000
C	-2.01770000	-1.27812000	0.14693500
C	-3.34598200	-1.69629800	0.19179800
H	-5.41782400	-1.10821200	0.40624400
H	-4.84724800	1.30554800	0.70359100
H	-2.50192300	2.05066800	0.62955300
H	-1.23820200	-2.01811400	-0.00755100
H	-3.57312200	-2.75314700	0.07856400
C	-0.31412700	0.57905200	0.15358100
H	-0.18909000	1.65796200	0.21082500
C	0.75203100	-0.18895900	-0.22565400
H	0.74008700	-1.27306700	-0.15547300
H	1.74230000	0.25399700	-0.27685800
C	0.82306700	-0.58133900	-2.54518500

H	-0.09008100	-1.17476700	-2.52131100
C	0.69412300	0.76958700	-2.89367100
C	1.86776000	1.59149500	-3.08183100
C	-0.64733900	2.65850600	-3.19431400
C	1.71463500	2.92723100	-3.35311800
C	0.42347100	3.50437100	-3.41195600
H	-1.66219100	3.06127000	-3.22439100
H	2.59752200	3.54393600	-3.51618000
H	0.27298900	4.55755900	-3.61758300
N	-0.55392700	1.34112200	-2.94851500
K	-2.86861900	0.05068100	-2.47477100
C	3.21577000	0.92486200	-2.96580400
H	3.97123200	1.51350700	-3.49864800
H	3.52428000	0.89556000	-1.90980200
C	2.13239900	-1.32008100	-2.68502400
H	2.57230000	-1.54909500	-1.69566500
H	1.97504800	-2.29316600	-3.16762400
C	3.15808800	-0.51338200	-3.48866000
H	2.86533100	-0.49672300	-4.54615100
H	4.14673000	-0.98113300	-3.42695500

Reaction of 5,6,7,8-tetrahydroquinoline/styrene monoadduct K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-1622.669470 [B3LYP/6-31+G(d,p)]

C	-4.48480000	-0.39501600	1.15762400
C	-3.95005900	0.89314400	1.32437100
C	-2.61956400	1.16381000	1.01165200
C	-1.73414900	0.15990700	0.50628000
C	-2.29988800	-1.14676100	0.37271700
C	-3.63069000	-1.40843300	0.69038200
H	-5.52064200	-0.60674200	1.40346500
H	-4.57843800	1.69444000	1.70732600
H	-2.23111900	2.16989300	1.15802900
H	-1.67972800	-1.95942600	0.00721500
H	-4.01163800	-2.42019500	0.56980000
C	-0.38612900	0.50366100	0.14728900
H	-0.12770800	1.55413400	0.27583100
C	0.60009900	-0.33552500	-0.37736300
H	0.50180200	-1.41600000	-0.28331800
H	1.62721400	0.01133900	-0.31712300

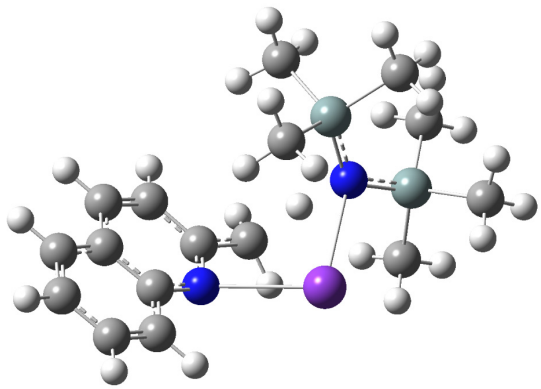
C	0.78835400	-0.56715200	-2.55727700
C	0.67494100	0.80856700	-2.95590800
C	1.84155600	1.64523800	-3.06790300
C	-0.67243300	2.66089100	-3.44559500
C	1.68902500	2.97778800	-3.40107600
C	0.40286800	3.52138300	-3.60096600
H	-1.68557500	3.04359800	-3.59154800
H	2.57092200	3.60560700	-3.51427600
H	0.25429200	4.56253700	-3.86732200
N	-0.57510500	1.35388700	-3.13476400
K	-3.11904900	0.79394700	-2.10507800
C	3.20439300	1.03172500	-2.84699700
H	3.97405800	1.64568000	-3.32981300
H	3.44239900	1.02276700	-1.77281800
C	2.15338000	-1.24899700	-2.67005900
H	2.52295000	-1.52571200	-1.66669500
H	2.04635400	-2.20268300	-3.20548700
C	3.23153600	-0.40906800	-3.37042200
H	3.04974300	-0.39675600	-4.45344800
H	4.22113200	-0.85572400	-3.21524500
C	-0.38015900	-1.49470400	-2.83349300
H	-0.21336800	-2.44916300	-2.31549100
H	-1.30138800	-1.09134500	-2.40846000
C	-0.62296700	-1.79218200	-4.33995500
H	-0.72107800	-0.84021700	-4.87138200
H	0.26123600	-2.29860100	-4.74687300
C	-1.85275300	-2.63804700	-4.58541500
C	-1.85810800	-4.01320000	-4.29478800
C	-3.03723600	-2.06621400	-5.07798500
C	-3.00617800	-4.78697500	-4.48242600
H	-0.95033200	-4.48271500	-3.92284700
C	-4.19010500	-2.83559000	-5.26961100
H	-3.04848200	-1.00829600	-5.33343700
C	-4.17979800	-4.20061500	-4.96919500
H	-2.98391200	-5.84905600	-4.25373300
H	-5.09109200	-2.37137600	-5.66220800
H	-5.07154400	-4.80227600	-5.11941100

-1622.183707 [M06-2X/6-31++G(d,p)]

C	-4.31545300	-0.98790900	0.49821500
C	-3.98071900	0.37042900	0.55507200
C	-2.66124400	0.78578500	0.40700500
C	-1.59967200	-0.13341100	0.19033400
C	-1.95898100	-1.50917400	0.19275100
C	-3.27951500	-1.91849800	0.33368100
H	-5.34372500	-1.31499100	0.60904500
H	-4.75810200	1.11393600	0.71103200
H	-2.42612600	1.84728600	0.43834500
H	-1.18716700	-2.26145100	0.05549800
H	-3.50834400	-2.98120000	0.31126300
C	-0.26349500	0.35839200	-0.03804500
H	-0.15965500	1.44198500	-0.01548000
C	0.84216400	-0.38152000	-0.40076600
H	0.86552500	-1.46394400	-0.28018600
H	1.81835700	0.09465200	-0.37099900
C	1.07430300	-0.72989200	-2.61698000
C	0.68434600	0.57859500	-2.98870600
C	1.65842000	1.63672000	-3.06436200
C	-1.00444700	2.13318700	-3.39604000

C	1.24194300	2.91710100	-3.33504600
C	-0.13211100	3.19709500	-3.51076600
H	-2.07515800	2.31333800	-3.52474300
H	1.97855300	3.71518900	-3.41087700
H	-0.49281200	4.19623300	-3.72556600
N	-0.64845300	0.86045100	-3.14681600
K	-3.10619100	-0.24165900	-2.47413000
C	3.10590500	1.28027300	-2.84258400
H	3.75205100	2.04700800	-3.28436100
H	3.32308100	1.26396200	-1.76458100
C	2.52269500	-1.15656600	-2.74258500
H	2.94344000	-1.38850400	-1.74583000
H	2.58441900	-2.09603300	-3.31088900
C	3.40487500	-0.10481200	-3.41980500
H	3.19650000	-0.09053400	-4.49730300
H	4.46403900	-0.35332900	-3.29345600
C	0.03960600	-1.81565600	-2.72369100
H	0.40654200	-2.72483900	-2.22694400
H	-0.84081200	-1.50440000	-2.15537100
C	-0.39972400	-2.15500200	-4.17453100
H	-0.17578100	-1.30279400	-4.82322000
H	0.18176800	-3.00603100	-4.55049400
C	-1.87569900	-2.45759400	-4.27390400
C	-2.50395800	-3.29279200	-3.33701200
C	-2.67484400	-1.83885900	-5.24376100
C	-3.88447900	-3.49174200	-3.36055600
H	-1.90718600	-3.77553600	-2.56651700
C	-4.05722100	-2.03725200	-5.27459400
H	-2.20769000	-1.17793800	-5.96988900
C	-4.66930200	-2.85937600	-4.32754100
H	-4.34813800	-4.13626100	-2.61951500
H	-4.65526400	-1.54297800	-6.03450600
H	-5.74402300	-3.00996000	-4.34452200

Deprotonation of 2-methylquinoline (35) by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-1914.264121 [B3LYP/6-31+G(d,p)]

C	-0.68419300	-0.02864400	-0.34030000
C	-2.96211700	-0.22204300	0.21173100
C	-2.83206900	0.89881800	1.11392400
C	-1.63122600	1.52839800	1.27431100
H	-3.70731800	1.22265200	1.66911500
H	-1.52929500	2.36754400	1.95885900
C	-4.25203900	-0.83804600	-0.00792200

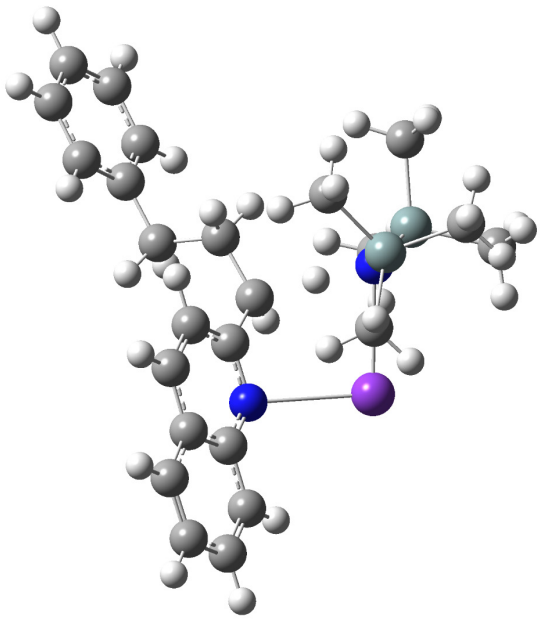
H	-4.96931400	-0.65910400	0.79660100
H	-4.91880700	-0.30688400	-1.16277400
H	-4.18888200	-1.90501600	-0.24285900
N	-5.51451600	0.07002600	-2.28667300
Si	-6.90622500	-0.89420300	-2.65730700
Si	-5.33336100	1.77252900	-2.56578400
C	-3.49452500	2.19254400	-2.85323000
H	-3.35654600	3.27842500	-2.92698800
H	-2.85559000	1.84265200	-2.03353300
H	-3.11958700	1.76358300	-3.79309500
C	-5.91186800	2.81983300	-1.08784900
H	-6.97784300	2.65831700	-0.88775900
H	-5.36012900	2.55575300	-0.17810500
H	-5.76253200	3.89138200	-1.27139600
C	-6.26198000	2.40701200	-4.10104700
H	-6.07017400	3.47948500	-4.23417000
H	-5.93606200	1.89498600	-5.01398000
H	-7.34662000	2.27644800	-4.01416100
C	-7.10619100	-1.20344800	-4.52790200
H	-7.27464600	-0.27236700	-5.08018900
H	-6.21306800	-1.68164300	-4.95115300
H	-7.95906200	-1.86616400	-4.72375800
C	-6.72997100	-2.61013300	-1.85266000
H	-6.67686600	-2.54402900	-0.76052900
H	-7.59697600	-3.23208300	-2.10773600
H	-5.83506400	-3.14566100	-2.19490600
C	-8.55584200	-0.17395600	-2.03504900
H	-9.39322400	-0.84156200	-2.27564100
H	-8.53798000	-0.03975200	-0.94662800
H	-8.77287800	0.80241900	-2.48448900
K	-3.07740600	-1.23290300	-2.95488200
N	-1.89471500	-0.64496400	-0.50023100
C	-0.48823100	1.08033000	0.54378000
C	1.67745800	0.09911900	-0.94924600
H	2.52052000	-0.28067100	-1.52022800
C	1.86304200	1.19704600	-0.07760800
H	2.84156200	1.65818700	0.01563100
C	0.43692000	-0.50022600	-1.07762000
C	0.79082500	1.67404800	0.65698600
H	0.29808500	-1.35422400	-1.73563800
H	0.91884800	2.51590800	1.33375700

-1913.803960 [M06-2X/6-31++G(d,p)]

C	-0.81657600	0.11303800	-0.37263200
C	-3.04103700	-0.23835600	0.25551800
C	-3.02068600	0.99316700	1.00939900
C	-1.89690300	1.75776200	1.04942800
H	-3.91887000	1.28801700	1.54322100
H	-1.87083000	2.68651000	1.61467300
C	-4.27879300	-0.97064300	0.11252400
H	-5.00859500	-0.77260500	0.89963800
H	-4.88604500	-0.49429100	-1.06484200
H	-4.13941000	-2.04566300	-0.03762800
N	-5.40316900	-0.12301900	-2.24247300
Si	-6.90929700	-0.91389700	-2.50210400
Si	-5.09014800	1.52939000	-2.61201400
C	-3.22438000	1.81564900	-2.79825100
H	-3.02172200	2.88122700	-2.95578900
H	-2.66570300	1.50831000	-1.90603800

H	-2.81192600	1.28579400	-3.66723900
C	-5.69503700	2.70399300	-1.26024300
H	-6.78349200	2.63874600	-1.15112300
H	-5.24521800	2.44091900	-0.29615800
H	-5.43526500	3.74538100	-1.48262400
C	-5.87976500	2.08012700	-4.24249500
H	-5.63265000	3.12713300	-4.45341100
H	-5.51847100	1.47295900	-5.08032600
H	-6.97210900	1.99552700	-4.21603100
C	-7.18226000	-1.37981300	-4.31756700
H	-7.21482900	-0.49074700	-4.95635300
H	-6.37191000	-2.02310700	-4.68137000
H	-8.12569500	-1.92293100	-4.44720400
C	-6.92530900	-2.52390600	-1.50729300
H	-6.82462700	-2.32579600	-0.43487500
H	-7.86254800	-3.06860900	-1.66672000
H	-6.10224400	-3.18773400	-1.79942100
C	-8.41250300	0.09957900	-1.95385800
H	-9.34436900	-0.45675700	-2.10765100
H	-8.33802000	0.34861900	-0.88906500
H	-8.49046100	1.04087800	-2.51032200
K	-3.11984400	-1.57744500	-2.72878000
N	-1.95381700	-0.64359300	-0.41231500
C	-0.72881600	1.33697100	0.34358900
C	1.49296400	0.40495800	-1.07904600
H	2.35979800	0.04696900	-1.62682500
C	1.57442600	1.62108400	-0.36420700
H	2.49746400	2.19129300	-0.36695900
C	0.32844600	-0.33176800	-1.08400100
C	0.47673600	2.07414000	0.33529600
H	0.26410800	-1.27480100	-1.62056100
H	0.52172900	3.00706200	0.89219600

Deprotonation of 2-methylquinoline/styrene monoadduct by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-2223.834702 [B3LYP/6-31+G(d,p)]

C	-0.53874800	0.25647000	-0.56305400

C	-2.69292000	0.90092300	0.14381800
C	-2.21628400	2.25416600	0.31799900
C	-0.91474600	2.57674600	0.05521400
H	-2.90127400	3.01788400	0.66834000
H	-0.55831500	3.59516300	0.19379200
C	-4.08262100	0.54327600	0.34914700
H	-4.77360700	0.55724600	-0.91222400
H	-4.16727500	-0.52457500	0.58926400
N	-5.44421100	0.44642300	-2.05432900
Si	-6.96823300	-0.36393900	-1.89176600
Si	-5.07951900	1.76607500	-3.12227800
C	-3.25586700	1.66905400	-3.67297000
H	-2.98346000	2.55529800	-4.25941300
H	-2.56779500	1.62326400	-2.82039100
H	-3.06978400	0.79717300	-4.31550300
C	-5.31531000	3.46203900	-2.29660000
H	-6.35729500	3.60530300	-1.98682000
H	-4.68871800	3.55972100	-1.40268400
H	-5.05217000	4.27871600	-2.98075900
C	-6.11171400	1.78021200	-4.72078000
H	-5.80970900	2.62946900	-5.34720100
H	-5.96855200	0.86673800	-5.30944900
H	-7.18429900	1.88493000	-4.52161300
C	-7.42544200	-1.39529700	-3.42900400
H	-7.59638700	-0.76850700	-4.31052600
H	-6.63301000	-2.11200700	-3.68192000
H	-8.34283200	-1.97010700	-3.24717700
C	-6.88490900	-1.60948100	-0.45251000
H	-6.67214400	-1.12337400	0.50522500
H	-7.84782800	-2.12629800	-0.35604200
H	-6.12110300	-2.38261100	-0.60840900
C	-8.44282100	0.78697900	-1.54059000
H	-9.37134700	0.21458200	-1.41945700
H	-8.28320300	1.36432000	-0.62220100
H	-8.59977500	1.50220000	-2.35696100
K	-3.35391500	-1.47038200	-2.16019900
N	-1.84288400	-0.05389700	-0.30449300
C	-0.00528400	1.57536700	-0.39895700
C	1.67255200	-0.49367800	-1.28197300
H	2.32855800	-1.29292100	-1.61658200
C	2.19048800	0.81304400	-1.12287900
H	3.23513100	1.01417300	-1.33966900
C	0.34433400	-0.76740900	-1.00894600
C	1.35717700	1.82773600	-0.68431800
H	-0.04629900	-1.77672300	-1.11209000
H	1.74065400	2.83710400	-0.55307600
C	-4.95211000	1.38895100	1.27420200
H	-4.93035700	2.44546400	0.97679500
H	-5.99976900	1.08395400	1.15263200
C	-4.59571500	1.28748800	2.78162800
H	-4.66629100	0.23438500	3.08248200
H	-3.54987300	1.58513900	2.92251000
C	-5.48697100	2.13233900	3.66502800
C	-6.72893400	1.65084900	4.11089200
C	-5.11630400	3.43655500	4.02997700
C	-7.57386900	2.44474500	4.89154800
H	-7.03442400	0.64057900	3.84747300
C	-5.95638100	4.23573200	4.81129900
H	-4.15532500	3.82774800	3.70320200
C	-7.19083100	3.74272300	5.24477000

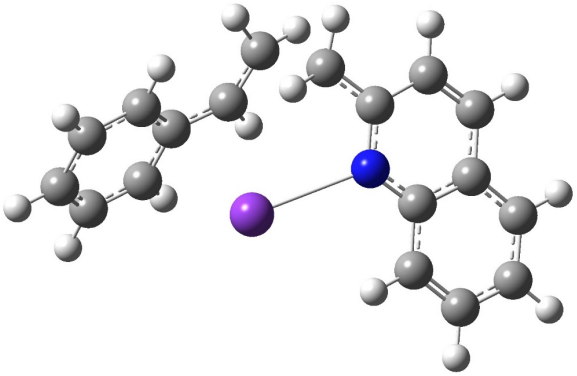
H	-8.52853300	2.04865700	5.22727000
H	-5.64489000	5.24042500	5.08426500
H	-7.84454000	4.36034600	5.85402300\

-2223.234925 [M06-2X/6-31++G(d,p)]

C	-0.58764200	0.26248600	-0.56517600
C	-2.73903600	0.74615500	0.22706400
C	-2.36025300	2.13170100	0.38453700
C	-1.10787000	2.54789100	0.04963700
H	-3.08172100	2.84003700	0.77748800
H	-0.81839300	3.59008300	0.16432200
C	-4.10102100	0.30534600	0.44413100
H	-4.71100100	0.32607500	-0.81938800
H	-4.13125100	-0.75495000	0.72791100
N	-5.31956500	0.29122900	-2.01278800
Si	-6.92363100	-0.31327500	-1.86623800
Si	-4.83950000	1.64706400	-2.95951600
C	-3.00392100	1.49037800	-3.41098000
H	-2.66096200	2.38727200	-3.93959200
H	-2.37418700	1.38136800	-2.51848800
H	-2.81733800	0.63703800	-4.07604200
C	-5.03621200	3.28491300	-2.03607300
H	-6.07141000	3.42143000	-1.70253900
H	-4.39336100	3.30776500	-1.14951000
H	-4.76516600	4.13725800	-2.66976200
C	-5.80008000	1.80512200	-4.58150300
H	-5.41270200	2.64615400	-5.16838900
H	-5.71365200	0.89823600	-5.19014500
H	-6.86550800	1.98885900	-4.40103000
C	-7.56695400	-1.11194300	-3.45890500
H	-7.69562800	-0.37517800	-4.25840700
H	-6.87419200	-1.88067400	-3.82136500
H	-8.53795300	-1.59036600	-3.28424500
C	-6.93743900	-1.67744700	-0.55147600
H	-6.58917600	-1.31445100	0.42102500
H	-7.95092800	-2.07252200	-0.41947400
H	-6.29781500	-2.52059700	-0.84255100
C	-8.18608500	1.00227900	-1.36187200
H	-9.18034800	0.56841600	-1.20523200
H	-7.88154800	1.50199700	-0.43525200
H	-8.27604700	1.77106900	-2.13894600
K	-3.34721700	-1.62451100	-1.99163700
N	-1.84624700	-0.14377800	-0.23466700
C	-0.15663200	1.61223400	-0.45266500
C	1.61582000	-0.32707000	-1.41290700
H	2.31060400	-1.07565400	-1.78226400
C	2.03667000	1.01824900	-1.30203600
H	3.04584300	1.29579600	-1.58780900
C	0.33926900	-0.69810400	-1.05302300
C	1.15951600	1.96807400	-0.82593900
H	0.01771300	-1.73431300	-1.11973600
H	1.46662400	3.00688000	-0.73084300
C	-5.03154400	1.15585300	1.28931600
H	-5.11174000	2.17136300	0.87528500
H	-6.04877400	0.74611400	1.22124700
C	-4.65169900	1.25010900	2.78079700
H	-4.65410200	0.23928800	3.20640600
H	-3.62621900	1.63006400	2.86915200
C	-5.59387700	2.13904800	3.55135900

C	-6.74368600	1.61859700	4.15474000
C	-5.37156100	3.51887300	3.62485400
C	-7.64618300	2.45105700	4.81578800
H	-6.93002500	0.54782600	4.10708100
C	-6.26975300	4.35652900	4.28402200
H	-4.47986100	3.93861700	3.16329600
C	-7.41167400	3.82418400	4.88269800
H	-8.53131000	2.02699800	5.28068500
H	-6.07690100	5.42414500	4.33337600
H	-8.11138500	4.47397700	5.39917400

Reaction of 2-methylquinoline K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-1350.032921 [B3LYP/6-31+G(d,p)]

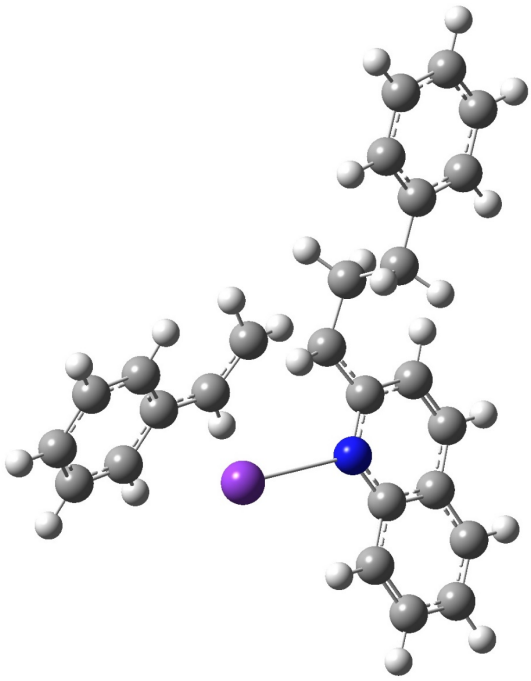
C	-4.43087600	-1.27930200	0.93770700
C	-4.16619200	0.05803700	1.27260200
C	-2.92243800	0.62737100	1.01026300
C	-1.86483100	-0.11252700	0.40349700
C	-2.16360400	-1.46588500	0.06540400
C	-3.41133000	-2.02922400	0.33530400
H	-5.39914100	-1.72363700	1.14628400
H	-4.93717600	0.66004900	1.74783600
H	-2.73812100	1.66254700	1.29096700
H	-1.39982400	-2.08140100	-0.40128900
H	-3.59040600	-3.06874900	0.07020000
C	-0.59933500	0.52056800	0.12197700
H	-0.54351800	1.58793100	0.33103000
C	0.51550600	-0.09555600	-0.43985200
H	0.61878100	-1.17641600	-0.38935700
H	1.45915400	0.43887200	-0.41101400
C	0.60118800	-0.25289900	-2.64046900
H	1.50034300	-0.86216700	-2.66958500
H	-0.31842400	-0.81141700	-2.79887400
C	0.69071800	1.06296600	-3.15531900
C	1.99263800	1.68070700	-3.29828200
C	-0.32360600	3.07225900	-3.85101700
C	2.11208000	2.97212700	-3.71437800
H	2.87410800	1.08745000	-3.07130700
C	0.93748400	3.73453200	-4.01984900
H	3.09001100	3.43472700	-3.82762200
N	-0.43774600	1.78083300	-3.41589600
K	-2.75217800	0.73457700	-2.34271800
C	-1.42781600	5.12423700	-4.60777900
H	-2.34359400	5.66031800	-4.84318900

C	-1.49756600	3.81257400	-4.16657500
H	-2.46455000	3.32455100	-4.07173900
C	0.98147700	5.07127000	-4.46980500
H	1.95151000	5.54992900	-4.58648200
C	-0.18214600	5.76926000	-4.76062500
H	-0.13690300	6.79739400	-5.10641500

-1349.665907 [M06-2X/6-31++G(d,p)]

C	-4.30490300	-0.44359800	0.09124600
C	-3.92621900	0.90768500	0.08932800
C	-2.58642100	1.27174100	0.05553400
C	-1.54448500	0.30532500	0.01436300
C	-1.95208800	-1.05634300	0.03425600
C	-3.29793400	-1.41466400	0.07912600
H	-5.35128100	-0.72764900	0.12758100
H	-4.68820600	1.68260800	0.11395900
H	-2.31434500	2.32461700	0.03776900
H	-1.20068500	-1.84047600	0.02099800
H	-3.56487000	-2.46834700	0.10208300
C	-0.17453100	0.72020100	-0.11093200
H	-0.00537100	1.79274000	-0.17079800
C	0.86886400	-0.13275500	-0.42160200
H	0.81507700	-1.19209300	-0.18480100
H	1.87886400	0.26657400	-0.43397500
C	0.83407300	-0.61323400	-2.55299900
H	1.76749800	-1.15197500	-2.68630000
H	-0.05883500	-1.23147600	-2.48970800
C	0.72706800	0.69420900	-3.05736600
C	1.93291100	1.42934300	-3.38438600
C	-0.53224100	2.65042700	-3.34465600
C	1.87801400	2.74993400	-3.68563300
H	2.87932000	0.89561400	-3.37527300
C	0.61365000	3.42985300	-3.67356300
H	2.77714700	3.30859000	-3.93537500
N	-0.47421500	1.31686500	-3.05758400
K	-2.74114500	-0.14004600	-2.76785400
C	-1.89556700	4.66212200	-3.59507600
H	-2.86958000	5.14171300	-3.55592100
C	-1.78691200	3.31434200	-3.31169400
H	-2.67329900	2.74655400	-3.03866000
C	0.47921000	4.80030300	-3.96350000
H	1.37246400	5.36881500	-4.21308100
C	-0.75702300	5.42038400	-3.92932900
H	-0.85032500	6.47800300	-4.15254100

Reaction of 2-methylquinoline/styrene monoadduct K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-1659.605550 [B3LYP/6-31+G(d,p)]

C	-4.67110000	-0.95027600	0.69725100
C	-4.23001300	0.29614600	1.17076200
C	-2.90863300	0.70026600	0.99714300
C	-1.94414400	-0.12276100	0.34188300
C	-2.42041300	-1.38264000	-0.13220700
C	-3.74523900	-1.78100400	0.05039600
H	-5.70016500	-1.26641200	0.83689700
H	-4.92465600	0.95647900	1.68477200
H	-2.59001900	1.66675700	1.38248000
H	-1.73475200	-2.05741800	-0.63677200
H	-4.05955200	-2.75490600	-0.31820700
C	-0.59626100	0.34702900	0.14525000
H	-0.39326500	1.36426900	0.47590300
C	0.42906400	-0.35847500	-0.48069100
H	0.37024800	-1.44219800	-0.54936300
H	1.44171400	0.01980300	-0.37782400
C	0.54895800	-0.27919800	-2.67228800
H	-0.47162800	-0.61192400	-2.86692400
C	0.78041500	1.09790000	-2.94851400
C	2.12494900	1.62878700	-3.01140600
C	-0.07174000	3.27849300	-3.23892500
C	2.34430200	2.96306400	-3.18714600
H	2.96717100	0.95221000	-2.91661500
C	1.23726200	3.85989300	-3.31682600
H	3.35663100	3.35803600	-3.23618600
N	-0.28611500	1.94249900	-3.05068200
K	-2.77747100	0.99267500	-2.30719300
C	1.58599900	-1.34718400	-2.93652600
H	2.54683700	-1.08936800	-2.47093600
H	1.27108700	-2.28042900	-2.45044500

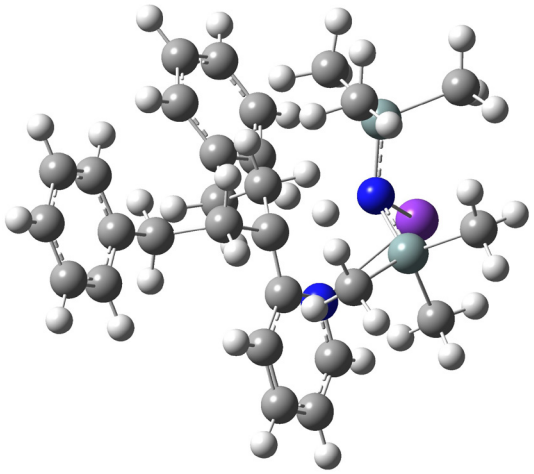
C	1.83366800	-1.65537200	-4.43985000
H	2.16662900	-0.73859000	-4.94001600
H	0.87857200	-1.93757300	-4.89995700
C	2.84991100	-2.75506500	-4.65756500
C	4.21967600	-2.46123800	-4.75576000
C	2.45698800	-4.10153600	-4.72378400
C	5.16706600	-3.47712800	-4.91164900
H	4.54617100	-1.42443900	-4.71574300
C	3.39942800	-5.12223400	-4.88005500
H	1.40041300	-4.35205300	-4.65810200
C	4.76017000	-4.81360100	-4.97326400
H	6.22115400	-3.22475100	-4.98924600
H	3.07090500	-6.15671900	-4.93297800
H	5.49412400	-5.60469600	-5.09728400
C	0.28313300	6.07922300	-3.64017600
H	0.40899500	7.14678700	-3.79192800
C	-1.01041000	5.51760200	-3.57344000
H	-1.88130200	6.15927200	-3.67886600
C	-1.18376300	4.15747400	-3.37879300
H	-2.18836600	3.74342700	-3.34502900
C	1.38752400	5.24969000	-3.51450400
H	2.39264400	5.66276600	-3.56671500

-1659.099469 [M06-2X/6-31++G(d,p)]

C	-4.52819300	-0.12624000	0.16900600
C	-3.96824000	1.13918200	0.39964600
C	-2.59116200	1.32164200	0.38716000
C	-1.69354600	0.25019600	0.13131600
C	-2.28307700	-1.02610400	-0.07809300
C	-3.66463300	-1.20450700	-0.05177000
H	-5.60317300	-0.27039200	0.18852700
H	-4.61675100	1.99002300	0.59177400
H	-2.17664600	2.31344600	0.55278900
H	-1.64573100	-1.88621000	-0.26172900
H	-4.07378900	-2.19935500	-0.20904600
C	-0.28076800	0.49718000	0.02405400
H	0.03472300	1.53026000	0.14868800
C	0.62908500	-0.41933300	-0.46304500
H	0.43042700	-1.48787400	-0.41573600
H	1.68606700	-0.16398900	-0.45510700
C	0.53717100	-0.55985300	-2.65298600
H	-0.47711800	-0.96297700	-2.65049400
C	0.64873400	0.81546700	-2.93149800
C	1.94635300	1.41803000	-3.16872100
C	-0.31747400	2.95473100	-2.87590100
C	2.07863300	2.76549100	-3.25445300
H	2.81617200	0.77711800	-3.27495200
C	0.92849400	3.60778500	-3.10384300
H	3.04917300	3.22249800	-3.43446500
N	-0.45160500	1.60063800	-2.80805500
K	-2.92992500	0.49121000	-2.64211800
C	1.62209300	-1.55626100	-2.95600900
H	2.58441200	-1.22904000	-2.53622300
H	1.39248600	-2.50401300	-2.45015100
C	1.82089000	-1.84936500	-4.45962900
H	2.06098000	-0.91139700	-4.97460300
H	0.87306400	-2.21018000	-4.87619200
C	2.90933800	-2.86450100	-4.69913700
C	4.24672000	-2.46750700	-4.80758500

C	2.61551300	-4.23121400	-4.75492100
C	5.26323700	-3.40800900	-4.96958200
H	4.49087200	-1.40767200	-4.76937200
C	3.62736800	-5.17681200	-4.91681700
H	1.58033700	-4.55594200	-4.67387400
C	4.95608100	-4.76767100	-5.02484500
H	6.29456600	-3.07893200	-5.05596700
H	3.37826800	-6.23294500	-4.96142300
H	5.74517600	-5.50181400	-5.15394900
C	-0.13781800	5.78925100	-3.00645400
H	-0.07766000	6.87134100	-3.05539600
C	-1.37453700	5.15623500	-2.77207100
H	-2.26951500	5.75702700	-2.63596600
C	-1.46332600	3.77998200	-2.71017800
H	-2.42476900	3.31091500	-2.51519100
C	0.99451200	5.01245600	-3.16868100
H	1.96131200	5.47936000	-3.34437600

Deprotonation of 2-methylpyridine/styrene bisadduct (30b) by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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N/A (structural optimization only) [B3LYP/6-31+G(d,p)]

C	-0.97433200	0.20241400	-0.30826000
C	-3.11962900	0.77474500	0.45651100
C	-2.64213200	2.09822600	0.69883600
C	-1.32369100	2.43493800	0.44086100
H	-0.33759600	-0.58330400	-0.71731800
H	-3.31027000	2.84681600	1.10645500
H	-0.97358100	3.44410900	0.64370800
C	-4.50158500	0.35974800	0.67104100
H	-5.10837000	0.44671800	-0.67460500
N	-5.64882400	0.50644600	-1.88174600
Si	-7.24736600	-0.16069400	-2.06619900
Si	-5.10216900	1.87880200	-2.80872600
C	-3.23524700	1.75521800	-3.18678300
H	-2.90079600	2.67904100	-3.67526100
H	-2.62109600	1.62619600	-2.28976200
H	-3.00908900	0.93951100	-3.88840100
C	-5.37811200	3.54065500	-1.93016700
H	-6.43993200	3.68914900	-1.70123200
H	-4.82425300	3.59674700	-0.98686600
H	-5.04938200	4.37586900	-2.56153500

C	-5.91170700	2.03834700	-4.52689600
H	-5.50355800	2.92464400	-5.02970200
H	-5.69532100	1.17149900	-5.16202400
H	-6.99918800	2.15832200	-4.48426400
C	-7.45105100	-1.11492200	-3.70781500
H	-7.33279500	-0.47092600	-4.58511500
H	-6.71734400	-1.92817600	-3.79072100
H	-8.44800400	-1.57107000	-3.76228300
C	-7.65234100	-1.43403500	-0.71695900
H	-7.70820000	-0.98140000	0.27812900
H	-8.63281300	-1.87612000	-0.93453700
H	-6.92383800	-2.25132600	-0.67187700
C	-8.65144300	1.12589900	-1.99035500
H	-9.62875900	0.63380000	-2.07729200
H	-8.63534300	1.66483800	-1.03523500
H	-8.58658500	1.87137100	-2.79085500
K	-3.58458000	-1.41773700	-2.19235000
C	-5.41726400	1.33889300	1.41608800
H	-5.36659800	2.32737400	0.94315300
H	-6.45631700	1.01363800	1.26898600
C	-5.20575900	1.52849300	2.94712000
H	-4.15558000	1.77232100	3.14523500
H	-5.41259800	0.58226400	3.45809600
C	-6.09512400	2.60692700	3.52544100
C	-7.40112700	2.31483700	3.95210600
C	-5.65577600	3.93805600	3.61285300
C	-8.24137500	3.31671000	4.44620800
H	-7.76075700	1.28945800	3.90104200
C	-6.49069100	4.94469000	4.10660000
H	-4.64508100	4.18677700	3.29696100
C	-7.78933700	4.63789700	4.52449600
H	-9.24669500	3.06523500	4.77341900
H	-6.12578900	5.96644200	4.16858600
H	-8.43953400	5.41764000	4.91078800
C	-4.68869100	-1.10936900	1.09254900
H	-5.74274700	-1.26035100	1.34781700
H	-4.50607800	-1.80312300	0.25942700
C	-3.82947200	-1.63288400	2.27998300
H	-2.77259400	-1.47390000	2.04734700
H	-4.05390000	-1.04906900	3.17790000
C	-4.07140300	-3.10016900	2.55636900
C	-5.12747200	-3.51980500	3.38239900
C	-3.27217100	-4.08853700	1.95810200
C	-5.37928800	-4.87704300	3.60180400
H	-5.75539500	-2.77318000	3.86342700
C	-3.51874500	-5.44827400	2.17267200
H	-2.43910600	-3.78579900	1.32717700
C	-4.57613200	-5.84856100	2.99535800
H	-6.19941200	-5.17589400	4.24911700
H	-2.88134400	-6.19388900	1.70455500
H	-4.76806000	-6.90380500	3.16742600
C	-0.44373400	1.46650800	-0.06908800
H	0.59930400	1.68345100	-0.27292200
N	-2.24883200	-0.14809000	-0.07446000

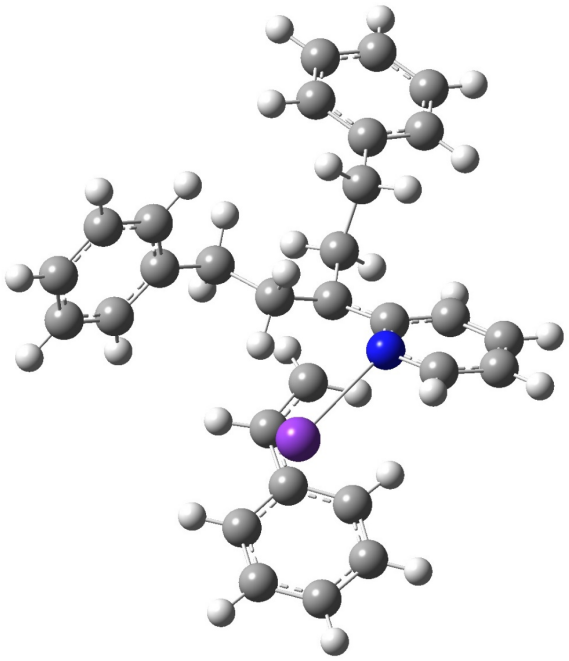
-2379.111681 [M06-2X/6-31++G(d,p)]

C	-0.99411600	0.19104300	-0.35024400
C	-3.14328300	0.68606600	0.42064600
C	-2.72379400	2.02576700	0.65106800

C	-1.42954900	2.41523000	0.36206000
H	-0.32825400	-0.57477200	-0.74796700
H	-3.41744100	2.74421900	1.07279600
H	-1.11913800	3.44026700	0.54659500
C	-4.50911400	0.22709700	0.61778200
H	-5.06625000	0.33909200	-0.70055500
N	-5.60447200	0.48067000	-1.89659500
Si	-7.25429600	-0.02219900	-1.98403400
Si	-5.01512300	1.87592100	-2.72873800
C	-3.16285000	1.69002200	-3.10053800
H	-2.77730500	2.62719300	-3.51866500
H	-2.57207900	1.47524100	-2.20202700
H	-2.96864300	0.91151900	-3.85053100
C	-5.21557700	3.48753000	-1.76120900
H	-6.25060600	3.61901200	-1.42564500
H	-4.57072900	3.50055800	-0.87655400
H	-4.94668800	4.34819000	-2.38483000
C	-5.84452600	2.14397300	-4.41058200
H	-5.40356700	3.01972000	-4.90117000
H	-5.69764400	1.28077500	-5.06923500
H	-6.92194900	2.32088700	-4.32269800
C	-7.69489300	-0.77694300	-3.66584700
H	-7.61291100	-0.05166500	-4.48067700
H	-7.03125200	-1.61900300	-3.89834400
H	-8.72314800	-1.15726700	-3.65610000
C	-7.60388800	-1.38308600	-0.71849800
H	-7.60452800	-1.00218800	0.30747500
H	-8.59282400	-1.81431800	-0.91276800
H	-6.86912700	-2.19526100	-0.77203500
C	-8.48575400	1.37509600	-1.64369100
H	-9.51763600	1.00546900	-1.65468000
H	-8.29548200	1.81909000	-0.65932400
H	-8.41005900	2.17551300	-2.38875600
K	-3.63377100	-1.41287600	-2.15235200
C	-5.46852000	1.18994300	1.30372100
H	-5.42481600	2.17224800	0.81377800
H	-6.49651900	0.83949000	1.12591500
C	-5.30546300	1.39454900	2.82653300
H	-4.26036900	1.63849500	3.05620100
H	-5.53903000	0.45657700	3.34347100
C	-6.21408800	2.48570200	3.33140300
C	-7.50767500	2.19552000	3.77739300
C	-5.80836700	3.82500600	3.29644300
C	-8.37296700	3.21250200	4.17991400
H	-7.83777500	1.15930100	3.80990800
C	-6.66801400	4.84605900	3.69788700
H	-4.80404100	4.06729700	2.95404600
C	-7.95527900	4.54248400	4.14154300
H	-9.37273700	2.96597200	4.52510000
H	-6.33251700	5.87852800	3.66713100
H	-8.62609800	5.33582500	4.45635000
C	-4.64964500	-1.22415600	1.08222200
H	-5.69415000	-1.39611600	1.37118100
H	-4.46408200	-1.95246700	0.27616500
C	-3.75121200	-1.65422800	2.26459200
H	-2.70394600	-1.49527500	1.99079300
H	-3.96205000	-1.02051800	3.13205300
C	-3.97428600	-3.10147200	2.61878600
C	-5.00729700	-3.47892100	3.48453100
C	-3.19730900	-4.10841000	2.03517000

C	-5.25561500	-4.82206600	3.76331300
H	-5.61977900	-2.70708300	3.94662600
C	-3.44087800	-5.45431000	2.30872100
H	-2.38575300	-3.82804800	1.36629900
C	-4.47276400	-5.81558500	3.17448300
H	-6.05945300	-5.09383400	4.44116800
H	-2.82192200	-6.22065600	1.85105200
H	-4.66330600	-6.86195200	3.39209900
C	-0.52149500	1.48131300	-0.15146100
H	0.50512100	1.74039500	-0.38234100
N	-2.24463400	-0.20746800	-0.09118300

Reaction of 2-methylpyridine/styrene bisadduct K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-1815.555271 [B3LYP/6-31+G(d,p)]

C	-1.54547600	3.69287900	1.50710400
C	-2.26667800	2.50890300	1.73173600
C	-1.78941100	1.28249800	1.27348400
C	-0.55926200	1.16405500	0.55605400
C	0.16463500	2.38039200	0.36407100
C	-0.31860200	3.60193500	0.82813200
H	-1.91392600	4.64820700	1.86759800
H	-3.20859100	2.54335500	2.27480900
H	-2.36598600	0.37990400	1.46689700
H	1.11064600	2.35853600	-0.16808900
H	0.27004800	4.50037900	0.65673900
C	-0.13049200	-0.11790200	0.05942900
H	-0.79884800	-0.94898000	0.28241000
C	1.01619700	-0.39340600	-0.68493900
H	1.34041300	-1.42889000	-0.73185000
H	1.83337900	0.32301200	-0.71745400
C	0.80155600	-0.39471300	-2.90249900
C	1.09636000	0.97708500	-3.23009700
C	2.43816100	1.46396100	-3.36634000
C	0.33396000	3.15391200	-3.65303500

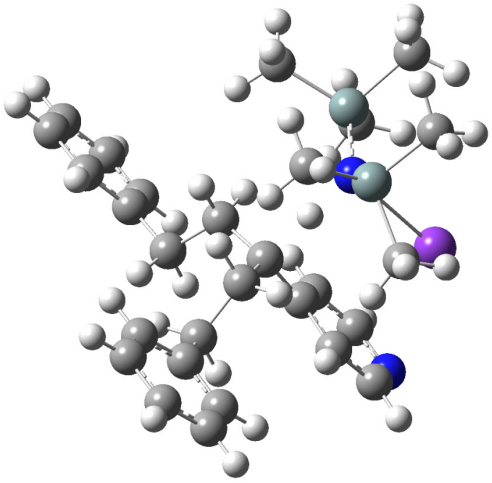
C	2.68779000	2.79431100	-3.64121200
H	3.27258900	0.78264400	-3.25090400
C	1.61012700	3.68643500	-3.79989500
H	-0.53000500	3.81151900	-3.77711500
H	3.71237600	3.14452500	-3.73944000
H	1.75612000	4.73590400	-4.03160400
N	0.05489900	1.87105900	-3.37329400
K	-2.23083000	2.15889900	-1.78975500
C	1.87091700	-1.42952900	-3.21581700
H	2.82273900	-1.15909100	-2.73953300
H	1.59978400	-2.39142700	-2.76640000
C	2.13807900	-1.66961400	-4.73021000
H	2.43107500	-0.72170100	-5.19535200
H	1.20309000	-1.98007400	-5.21171800
C	3.20653200	-2.71102300	-4.97916900
C	4.56030600	-2.34862900	-5.07187000
C	2.88066900	-4.07349300	-5.08039700
C	5.55585200	-3.31245400	-5.25663400
H	4.83621200	-1.29853500	-5.00545800
C	3.87132600	-5.04225900	-5.26515600
H	1.83823500	-4.37816800	-5.01983300
C	5.21511900	-4.66531500	-5.35275500
H	6.59604000	-3.00644700	-5.32957800
H	3.59330900	-6.08981200	-5.34439600
H	5.98663500	-5.41590600	-5.49877800
C	-0.65300400	-0.80588400	-3.06426700
H	-1.24178300	-0.29457300	-2.28575800
H	-1.05890500	-0.45138700	-4.02484600
C	-0.97568400	-2.30929300	-2.92067100
H	-0.46168900	-2.88291800	-3.69999500
H	-0.60305800	-2.67596600	-1.95754200
C	-2.46395200	-2.57539200	-3.01591900
C	-3.25816700	-2.68217500	-1.86307900
C	-3.09527200	-2.69174400	-4.26530700
C	-4.63785800	-2.89530800	-1.95247300
H	-2.78845400	-2.60668400	-0.88518200
C	-4.47352400	-2.90405100	-4.36171400
H	-2.49829600	-2.62174700	-5.17185100
C	-5.25183400	-3.00525400	-3.20377200
H	-5.22999100	-2.98305000	-1.04543300
H	-4.93816800	-2.99734700	-5.33962400
H	-6.32208100	-3.17657700	-3.27625500

-1814.982081 [M06-2X/6-31++G(d,p)]

C	-1.86201800	3.48691800	0.92310300
C	-2.49425500	2.28201500	1.24801000
C	-1.87598200	1.06245000	0.98362300
C	-0.59988700	0.98674000	0.36980700
C	0.03649800	2.22167100	0.08185700
C	-0.58268800	3.43605300	0.35082700
H	-2.33918100	4.43878700	1.13123500
H	-3.47619000	2.29303500	1.71395000
H	-2.38613700	0.13628500	1.24053500
H	1.00903700	2.22333200	-0.40412300
H	-0.06430000	4.35816300	0.10063300
C	-0.03123700	-0.29936800	0.02998500
H	-0.64059800	-1.16696700	0.27882600
C	1.13928600	-0.49877600	-0.66320200
H	1.52290100	-1.51193000	-0.75181600

H	1.89083000	0.28233100	-0.75001400
C	0.86534300	-0.41978800	-2.94303700
C	1.17494700	0.95222500	-3.13465700
C	2.52515700	1.43634200	-3.19877200
C	0.44204100	3.16883500	-3.23049500
C	2.78625500	2.78696800	-3.23457200
H	3.34995500	0.73197800	-3.20346400
C	1.72075800	3.70653700	-3.24081300
H	-0.41258800	3.85062400	-3.26489600
H	3.81461700	3.13796100	-3.26349100
H	1.87881700	4.77780100	-3.27525700
N	0.14643000	1.86756100	-3.18221200
K	-2.31440400	1.94626800	-1.98888900
C	1.90625800	-1.45586300	-3.28380200
H	2.86452900	-1.22971100	-2.79382100
H	1.61330800	-2.43491500	-2.88359900
C	2.16140000	-1.61755600	-4.79988200
H	2.46914000	-0.64963400	-5.21355300
H	1.21755400	-1.89032900	-5.28880000
C	3.21062700	-2.66037500	-5.08386700
C	4.56356500	-2.31229800	-5.16213000
C	2.86465200	-4.01111500	-5.20245700
C	5.54442600	-3.28412500	-5.35746600
H	4.84804000	-1.26571400	-5.07240200
C	3.84043700	-4.98769400	-5.39748400
H	1.81639300	-4.29767300	-5.14384900
C	5.18551000	-4.62661700	-5.47579100
H	6.58888800	-2.99281900	-5.41903100
H	3.55068800	-6.03026200	-5.49051900
H	5.94707000	-5.38480900	-5.62926300
C	-0.59125000	-0.78360300	-3.02739900
H	-1.10126700	-0.28700100	-2.18333900
H	-1.06383900	-0.39505900	-3.94608800
C	-0.93094800	-2.27235000	-2.88464600
H	-0.48564900	-2.85408000	-3.70025800
H	-0.50326300	-2.64720200	-1.94551300
C	-2.42680600	-2.47239600	-2.88121300
C	-3.18304400	-2.13876800	-1.74920800
C	-3.10081700	-2.93574400	-4.01469600
C	-4.57093300	-2.26677600	-1.74948900
H	-2.66966900	-1.78285100	-0.85741000
C	-4.49051200	-3.06588100	-4.02141900
H	-2.52918200	-3.19987300	-4.90134800
C	-5.23080200	-2.73125100	-2.88876400
H	-5.13768300	-2.01330100	-0.85811900
H	-4.99365300	-3.43193500	-4.91156200
H	-6.31123000	-2.83687800	-2.89029700

Deprotonation of 4-methylpyridine/styrene bisadduct (32b) by KO*t*Bu T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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N/A (structural optimization only) [B3LYP/6-31+G(d,p)]

C	-0.95359000	-0.62155600	-0.25836000
C	-3.06539900	0.39100400	0.48376100
C	-2.33019100	1.61595200	0.41356600
C	-1.00556000	1.63849500	-0.00517700
H	-0.38268900	-1.51325800	-0.51440900
H	-2.79683900	2.55632900	0.68264300
H	-0.47733900	2.58992800	-0.05456400
C	-4.49603200	0.33326200	0.72763900
H	-5.00497300	0.48885700	-0.62596000
N	-5.48289600	0.63944100	-1.90130200
Si	-6.06418900	-0.85039400	-2.59314300
Si	-6.17704600	2.21263400	-2.18565900
C	-4.88006600	3.57776700	-1.86705900
H	-5.37083100	4.55902900	-1.87215200
H	-4.35752700	3.47999300	-0.91139800
H	-4.12293100	3.60697900	-2.66367700
C	-7.70751200	2.59004500	-1.12170000
H	-8.49501400	1.84969500	-1.30942200
H	-7.48876000	2.57489200	-0.04954200
H	-8.11596000	3.57885000	-1.36647200
C	-6.72509700	2.54911700	-3.98060200
H	-6.94178700	3.62075200	-4.07977100
H	-5.94925900	2.29963900	-4.71358300
H	-7.63299200	2.00516500	-4.25836400
C	-6.55922600	-0.75653600	-4.43259100
H	-7.50371200	-0.22835400	-4.59481200
H	-5.79584400	-0.27107900	-5.05181100
H	-6.68782700	-1.78015200	-4.80827900
C	-4.67762100	-2.16398700	-2.58579000
H	-4.15942600	-2.25333800	-1.62717000
H	-5.10120700	-3.14783200	-2.82298100
H	-3.92374700	-1.95871500	-3.35924100
C	-7.57752600	-1.58632600	-1.70759600
H	-7.89764000	-2.51597000	-2.19515800
H	-7.37829900	-1.81203500	-0.65536200
H	-8.42148200	-0.88636000	-1.74254400
K	-2.74025800	0.80690000	-2.68488700
C	-2.27489600	-0.75318900	0.15093700

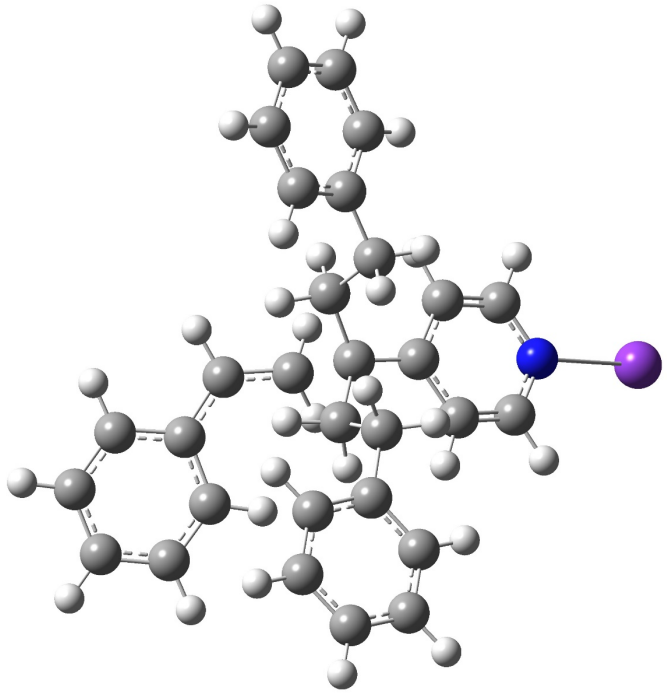
H	-2.69487300	-1.75075500	0.20786700
N	-0.29313500	0.55132400	-0.37274500
C	-5.12093000	1.53632200	1.45055900
H	-4.96964800	2.44869500	0.86239600
H	-6.20795100	1.39220100	1.47678300
C	-4.64324400	1.84337100	2.90077800
H	-3.54831900	1.87704500	2.92457400
H	-4.94594000	1.02994500	3.56633400
C	-5.19931000	3.14804600	3.42910500
C	-6.46334800	3.19996100	4.03913000
C	-4.48339800	4.34841300	3.29299700
C	-6.99645600	4.40876700	4.49542100
H	-7.03291000	2.28153500	4.16300900
C	-5.01064000	5.56090300	3.74741100
H	-3.49672500	4.33167300	2.83520000
C	-6.27180900	5.59611900	4.35001500
H	-7.97480200	4.42273700	4.96815400
H	-4.43446600	6.47552600	3.63596700
H	-6.68269400	6.53609300	4.70711000
C	-5.08041900	-1.02738500	1.13343900
H	-6.17356500	-0.93626200	1.14420200
H	-4.86451400	-1.77657100	0.36274100
C	-4.64146100	-1.63647800	2.49674800
H	-3.54754500	-1.68246000	2.54313700
H	-4.96281900	-0.98037300	3.31083600
C	-5.21771400	-3.01833200	2.71930200
C	-6.52530800	-3.18041200	3.20666200
C	-4.48154700	-4.17318700	2.41067700
C	-7.08145900	-4.45106500	3.37622700
H	-7.11179900	-2.30020100	3.46059900
C	-5.03192800	-5.44781700	2.57855000
H	-3.46292100	-4.07361300	2.04234700
C	-6.33616100	-5.59195400	3.06083200
H	-8.09404800	-4.55045000	3.75784500
H	-4.44047500	-6.32694700	2.33718400
H	-6.76512000	-6.58093000	3.19441400

-2379.104934 [M06-2X/6-31++G(d,p)]

C	-1.02531500	-0.66905600	-0.25722200
C	-3.09924100	0.34512400	0.54729000
C	-2.36687400	1.56502800	0.47651900
C	-1.06262900	1.58460100	0.00437600
H	-0.46391700	-1.55885000	-0.53668500
H	-2.82090100	2.50261500	0.77961400
H	-0.53218500	2.53319800	-0.06121500
C	-4.52298800	0.29423800	0.78112500
H	-4.98091300	0.45995600	-0.52508000
N	-5.47366000	0.65174300	-1.79595200
Si	-6.05717200	-0.82184400	-2.47728000
Si	-6.09721300	2.24097400	-2.05191700
C	-4.68029700	3.50087900	-1.89114800
H	-5.08238400	4.51132600	-1.75392600
H	-4.02174000	3.29345000	-1.04032600
H	-4.06672100	3.52975900	-2.80192500
C	-7.47797900	2.76907200	-0.86787000
H	-8.19038100	1.94978000	-0.71703600
H	-7.10658800	3.07698300	0.11367900
H	-8.02640500	3.61618000	-1.29696700
C	-6.80245000	2.54302100	-3.78469300
H	-6.96237700	3.62077500	-3.91112000

H	-6.12715900	2.20686700	-4.57837200
H	-7.76735500	2.04742600	-3.92997400
C	-6.62198600	-0.70451600	-4.28263300
H	-7.57405000	-0.17836700	-4.39708300
H	-5.88188700	-0.20283500	-4.91594100
H	-6.75754300	-1.72188900	-4.66980400
C	-4.63593900	-2.08473600	-2.52649600
H	-4.02392100	-2.07624700	-1.61890600
H	-5.03262500	-3.09959400	-2.64502300
H	-3.97702600	-1.90573400	-3.38729400
C	-7.50581500	-1.60252000	-1.54522700
H	-7.90989300	-2.44994200	-2.11165200
H	-7.21797200	-1.96800400	-0.55512300
H	-8.31191400	-0.87137400	-1.41330700
K	-2.78218900	0.75562400	-2.54754000
C	-2.32656200	-0.80148500	0.20433500
H	-2.74862700	-1.79798100	0.28539800
N	-0.37818800	0.50136800	-0.40418800
C	-5.15680800	1.50859900	1.44411900
H	-4.96974700	2.40481000	0.83515900
H	-6.24700300	1.37821900	1.43027400
C	-4.72514400	1.83707000	2.89090200
H	-3.63026100	1.84943100	2.95531700
H	-5.07714000	1.05359300	3.56902900
C	-5.28179300	3.16860600	3.32727400
C	-6.56136100	3.26011900	3.88584500
C	-4.56322400	4.35021400	3.11461300
C	-7.10752300	4.49634300	4.22748800
H	-7.13208200	2.34976000	4.05690600
C	-5.10344300	5.58971600	3.45480300
H	-3.56471300	4.29493400	2.68488700
C	-6.37935200	5.66647100	4.01292700
H	-8.10083100	4.54703200	4.66361400
H	-4.52759800	6.49517300	3.28716100
H	-6.80162200	6.62996400	4.28110500
C	-5.11916500	-1.05224100	1.16720700
H	-6.21150700	-0.94482200	1.19874100
H	-4.92731500	-1.79546500	0.37967700
C	-4.65726100	-1.66782600	2.50702000
H	-3.56154100	-1.68574500	2.54717300
H	-4.99695200	-1.03970900	3.33639100
C	-5.20117400	-3.06431800	2.67312700
C	-6.50953900	-3.26836900	3.12656700
C	-4.44254800	-4.18123000	2.30701700
C	-7.04607500	-4.55166400	3.21333700
H	-7.11103900	-2.40910300	3.41564700
C	-4.97347600	-5.46823700	2.39236200
H	-3.42288300	-4.03906400	1.95447400
C	-6.27850300	-5.65736200	2.84548800
H	-8.06202700	-4.68961500	3.57135600
H	-4.36726500	-6.32322400	2.10800000
H	-6.69369500	-6.65794800	2.91539500

Reaction of 4-methylpyridine/styrene bisadduct K enolate with styrene (3) T.S., solvent = benzene



Charge = 0; Multiplicity = 1

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-1815.540258 [B3LYP/6-31+G(d,p)]

C	-3.68932700	-3.45844600	1.19600900
C	-2.46770900	-4.13053800	1.36771600
C	-1.28021200	-3.59539600	0.88113100
C	-1.22930100	-2.34431900	0.18917900
C	-2.48933500	-1.68879600	0.02333400
C	-3.67327800	-2.23039700	0.51671900
H	-4.61770700	-3.87827500	1.57195300
H	-2.44465100	-5.08636600	1.88794500
H	-0.34924100	-4.13886400	1.03355000
H	-2.53218300	-0.74007000	-0.50401500
H	-4.60451800	-1.68766000	0.36381700
C	0.02817000	-1.81205700	-0.24348100
H	0.89909800	-2.43343700	-0.03664700
C	0.24745100	-0.59585600	-0.95378600
H	1.22276800	-0.13148700	-0.78123700
H	-0.55204100	0.14748100	-0.88938800
C	0.39961700	-0.72876900	-2.85103800
C	0.60142300	0.66021300	-3.22939000
C	1.87079700	1.30847000	-3.12243800
C	-0.23804400	2.90407000	-3.73254500
C	1.99759300	2.67141300	-3.32177500
H	2.76276500	0.74312400	-2.87771300
H	-1.07598700	3.55464900	-3.98296800
H	2.98110300	3.13276400	-3.23283500
C	1.61471000	-1.65766500	-2.99359700
H	2.41200600	-1.32529100	-2.31500600
H	1.31830200	-2.64546600	-2.62020900
C	2.24513500	-1.81851500	-4.40238300
H	2.52398900	-0.83393000	-4.79502400
H	1.51037800	-2.23468300	-5.09667100
C	3.46739800	-2.71272600	-4.38108600

C	4.75431600	-2.17748300	-4.21271300
C	3.34309100	-4.10698100	-4.49484800
C	5.88055900	-3.00428600	-4.15710100
H	4.87595100	-1.09959700	-4.13045100
C	4.46445600	-4.93935800	-4.43989700
H	2.35657000	-4.54429500	-4.63067400
C	5.73967400	-4.39069400	-4.26973700
H	6.86668700	-2.56568400	-4.02937900
H	4.34260500	-6.01520300	-4.53231900
H	6.61275100	-5.03573600	-4.22863300
C	-0.46627600	1.55234400	-3.54900500
N	0.97467400	3.50700700	-3.63198600
K	1.20618100	6.19903900	-3.69104500
H	-1.48103100	1.18795300	-3.65725900
C	-0.93839300	-1.36035500	-3.25110600
H	-1.75914900	-0.73557400	-2.88075500
H	-1.03232300	-2.30519300	-2.70438900
C	-1.18978100	-1.62678200	-4.75925800
H	-0.95318900	-0.72899700	-5.34226200
H	-0.51709400	-2.41632700	-5.10920700
C	-2.61872700	-2.04289100	-5.04185800
C	-3.05321400	-3.35204700	-4.77590900
C	-3.55432800	-1.12754500	-5.54836300
C	-4.37761800	-3.73306200	-5.00498300
H	-2.34629400	-4.07929600	-4.38360900
C	-4.88162200	-1.50281000	-5.78093100
H	-3.23785800	-0.11027900	-5.76847700
C	-5.29897100	-2.80857900	-5.50853300
H	-4.69036100	-4.75129300	-4.79033000
H	-5.58685400	-0.77669700	-6.17671000
H	-6.32880600	-3.10404100	-5.68808300

-1814.960783 [M06-2X/6-31++G(d,p)]

C	-3.67707400	-3.63292300	0.78532000
C	-2.46685900	-4.29861500	1.01152200
C	-1.25443200	-3.70667000	0.68559500
C	-1.17294900	-2.41055500	0.10816300
C	-2.41677000	-1.75649100	-0.10676700
C	-3.62755800	-2.35230500	0.22618200
H	-4.62558600	-4.09750900	1.03447100
H	-2.47108500	-5.29568800	1.44576100
H	-0.32839300	-4.24698800	0.87189600
H	-2.43011800	-0.76280400	-0.54643700
H	-4.55140400	-1.80912400	0.03856000
C	0.10865400	-1.83498700	-0.19946500
H	0.97493400	-2.45745700	0.01943300
C	0.32678700	-0.61391400	-0.85961700
H	1.31303700	-0.15888100	-0.73577300
H	-0.47664600	0.12840700	-0.83467200
C	0.44513200	-0.75478400	-2.82516500
C	0.61237900	0.62505400	-3.16125200
C	1.87285200	1.28978500	-3.06890600
C	-0.27641600	2.85850800	-3.57638300
C	1.96487400	2.65705200	-3.22442800
H	2.78085300	0.73004800	-2.86823300
H	-1.13030100	3.50137000	-3.79115100
H	2.93989200	3.13677400	-3.14291900
C	1.65402800	-1.66216600	-2.97988800
H	2.46330100	-1.33659500	-2.30873100

H	1.37234300	-2.66350900	-2.62676700
C	2.23980100	-1.77022200	-4.40291200
H	2.49341300	-0.76788600	-4.76892800
H	1.48812000	-2.17625400	-5.08614600
C	3.46875600	-2.64410100	-4.42903600
C	4.74241400	-2.09571500	-4.24366600
C	3.35888000	-4.03045100	-4.58361000
C	5.87676400	-2.90655400	-4.21719200
H	4.84376000	-1.01872400	-4.12321900
C	4.48869500	-4.84679600	-4.55833700
H	2.37495600	-4.47211000	-4.72664000
C	5.75325600	-4.28655400	-4.37557000
H	6.85705300	-2.46066700	-4.07615500
H	4.38196800	-5.92037000	-4.68326700
H	6.63470200	-4.91995800	-4.35848700
C	-0.47979800	1.50188400	-3.43371700
N	0.92155300	3.47711500	-3.47955100
K	1.01275700	6.13527800	-3.43068100
H	-1.48733300	1.11630400	-3.54719200
C	-0.89474100	-1.39582400	-3.13397900
H	-1.69452900	-0.78000400	-2.70317800
H	-0.93495400	-2.34286400	-2.58228000
C	-1.22616700	-1.64238400	-4.61071600
H	-0.97090400	-0.75638800	-5.20756000
H	-0.60206800	-2.45786400	-4.99814200
C	-2.67769400	-1.99967700	-4.86859000
C	-3.51840700	-2.48200500	-3.85860600
C	-3.20450800	-1.86640700	-6.16024600
C	-4.84338400	-2.82474800	-4.13593300
H	-3.14655600	-2.59186000	-2.84282800
C	-4.52539300	-2.20742500	-6.44088500
H	-2.56479900	-1.48756100	-6.95483200
C	-5.35280900	-2.69030300	-5.42564800
H	-5.47643700	-3.19687500	-3.33542600
H	-4.91108600	-2.09341800	-7.44988000
H	-6.38396400	-2.95521400	-5.63900500

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