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Supporting Information

for

A bis-NHC-CAAC dimer derived dicationic diradical

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General Considerations

All experiments were carried out either under nitrogen or argon atmosphere using standard Schlenk techniques, PL-HE-2GB Innovative Technology GloveBox, and MBraun Unilab SP GloveBox. Hexane, diethyl ether, THF, and toluene were dried with a PS-MD-5 Innovative Technology solvent purification system. Compounds 1^{Et} , S1 1^{Pr} , S1 and 2^{S2} were synthesized in accordance with the literature procedures. Compound 1^{Cy} was synthesized based on a similar procedure as for 1^{Et} and 1^{Pr} , S1 All other employed chemicals were purchased commercially (potassium bis(trimethylsilyl)amide - Sigma Aldrich, potassium - Sigma Aldrich, graphite - Sigma Aldrich, diisopropylamine - Avra Chemicals, *n*BuLi - Hychem Laboratories, and AgOTf - Sigma Aldrich) and used as received except for diisopropylamine which was distilled under N₂ over KOH before use. Benzene-d₆ and THF-d₈ were dried and distilled over potassium under argon. CD₃CN was dried and distilled over CaH₂ under argon. NMR spectra were referenced to the peaks of residual protons of the deuterated solvent (¹H) or the deuterated solvent itself (¹³C{¹H}). ¹⁹F{¹H} NMR spectra were referenced to external tol-CF₃.

Melting points were determined in closed NMR tubes under argon atmosphere and are uncorrected. Elemental analyses of 6^{Cy}, 7^{Cy}, 3^{Et}, 4^{Et}, 5^{Et}, 8^{Et} 9^{Et}, 10^{Et}, 8^{Pr} and 9^{Pr} were performed on a Perkin Elmer Analyser 240. Elemental analyses of 3^{Cy}, 4^{Cy}, 5^{Cy} 3^{Pr}, 4^{Pr} and 5^{Pr} were performed on an Elementar vario MICRO cube elemental analyzer. HRMS of 3^{Et}, 4^{Et}, 5^{Et}, 8^{Et}, 9^{Et}, and 10^{Et} were performed on an Exactive Plus Orbitrap-HRMS manufactured by Thermo Scientific. HRMS of 3^{cy}, 5^{cy}, 3^{Pr}, 5^{Pr}, and 8^{Pr} were performed on a Waters Xevo G2-XS QTOF (Waters Corporation) using electrospray ionization (ESI). EPR measurements at X-band (9.38 GHz) were carried out using a Bruker ELEXSYS E580 CW EPR spectrometer equipped with an Oxford Instruments helium cryostat (ESR900) and a MercuryiTC temperature controller. The spectral simulations were performed using MATLAB 9.8.0.1323502 (R2020a) and the EasySpin 5.2.28 toolbox.^{S3} The magnetic susceptibility measurements were performed with Quantum Design MPMS-XL EverCool SQUID magnetometer, between 2 K to 375 K for dc applied fields ranging from -5 to +5 T. Polycrystalline sample (21.5 mg) was introduced in a polypropylene bag and was subjected to the measurement. The temperature dependent data were measured using 1000 Oe and 10000 Oe dc magnetic field. The isothermal magnetization data were acquired at 1.9, 2.5, 5, and 6 K. M vs H measurements were performed at 100 K to check for the presence of impurities, where the sample was free from impurities. The magnetic data were corrected for the sample holder and the intrinsic diamagnetic contributions.

Experimental Details and Analytical Data

Synthesis of 3^{Cy}



About 80 mL of THF was added to a 100 mL Schlenk flask containing 1^{cy} (4.617 g, 7.320 mmol) and 2 (2 g, 16.104 mmol) at 0 °C. After stirring for 24 hours at room temperature, the reaction mixture was filtered and the white precipitate was washed with about 50 mL of diethyl ether and dried under vacuum. The ¹H NMR spectrum of the residue showed the formation of a mixture of two diastereomers (d/l- and meso-) of 3^{cy} in an about 59:41 ratio. Yield: 5.8 g (90 %). M.P.: > 180 °C. 3^{cy} was crystallized by layering diethyl ether over CH₃CN and THF solution of the crude compound. The obtained crystals were suitable for a single crystal X-ray diffraction study. We used the mixture of diastereomers for the next reaction. NMR data of the mixture of diastereomers: ¹H NMR (CD₃CN, 25 °C, 300 MHz): δ = 4.51 & 4.52 (s, 2H, CH), 3.94 & 3.96 (s, 6H, CH₃-N), 3.68 (s, 6H, CH₃-N), 2.51 (m, 2H, CH_{Cy}), 2.25 (s, 6H, CH₃-C=C), 2.20 (s, 6H, CH₃-C=C), 1.77-1.87 (m, 2H, CH_{2Cy}), 1.77-1.87 (m, 4H, CH₂), 1.66 (m, 2H, CH_{2Cy}), 1.46-1.49 & 1.18 (m, 2H, CH_{2Cy}), 1.38, (s, 6H, CH₃), 1.21 (s, 3H, CH₃), 1.18 (s, 6H, CH₃), 1.12 (s, 3H, CH₃), 0.67 (m, 2H, CH_{2CV} , 0.67 (s, 6H, CH_3) ppm. ¹³C{¹H} NMR (CD₃CN, 25 °C, 75 MHz): δ = 145.33 & 145.29 (*C*=N-CH₃), 128.40 (CH₃-C=C), 128.38 (CH₃-C=C), 122.125 (q, ¹J_{C-F} = 321 Hz, CF₃SO₃⁻), 64.42 & 64.45 (CH), 64.11 & 64.13 (C(CH₃)₂), 55.83 (CH₂), 54.33 (CH_{cy}), 43.52 (C(CH₃)₂), 34.67 & 34.70 (CH₃-N), 34.29 (48.95 (CH_{2Cy}), 34.02 (CH_{2Cy}), 33.16 (CH₃-N), 32.74 (C(CH₃)₂), 30.98 (CH_{2Cy}), 30.62 (CH_{2Cy}), 29.33 (C(CH₃)₂), 27.91 (C(CH₃)₂), 24.23 & 24.07 (C(CH₃)₂), 9.12 (CH₃-C=C), 8.59 (CH₃-C=C) ppm. ¹⁹F{¹H} NMR: (CD₃CN, 25 °C, 282 MHz): δ = -79.28 ppm. Elemental analysis: Calculated (%) for C₃₈H₆₄F₆N₆O₆S₂: C, 51.92; H, 7.34; N, 9.56; S, 7.29; Found: C, 51.84; H, 7.30; N, 9.17; S, 7.41. HRMS-ESI (m/z): Calculated for C₃₆H₆₄N₆ [M-2OTf]: 290.2591, Found: 290.2593.



Fig. S1 ¹H NMR spectrum of mixture of diastereomers of 3^{Cy} in CD₃CN at RT.



Fig. S2 ¹³C{¹H} NMR spectrum of mixture of diastereomers of 3^{Cy} in CD₃CN at RT.



Fig. S3 $^{19}F{^{1}H}$ NMR spectrum of mixture of diastereomers of 3^{Cy} in CD₃CN at RT.

Synthesis of 4^{Cy}



About 80 mL of toluene was added to a 100 mL Schlenk flask containing 3^{cy} (4.0 g, 4.55 mmol) and LDA (1.060 g, 9.895 mmol) at room temperature with stirring. Then the reaction mixture was stirred for 12 hours at room temperature. After that the reaction mixture was heated at 90 °C for three hours and filtered while heated to boiling temperature. The filtrate was evaporated and the white precipitate of 4^{cy} was washed with about 10 mL of pentane and dried. The washing pentane solution was kept at -35 °C to increase the amount of 4^{cy} . Yield: 2.19 g (83 %). M.P.: 175 °C. ¹H NMR (C₆D₆, 25 °C, 300 MHz): $\delta = 3.23$ (m, 2H, CH_{cy}), 2.98 (s, 6H, CH_3 -N), 2.70 (s, 6H, CH_3 -N), 2.22-2.25 (m, 4H, CH_{2cy}), 1.77-1.91 (m, 4H, CH_{2cy}), 1.67 (s, 4H, CH_2), 1.56 (s, 12H, CH_3 -C=C), 1.40 (s, 12H, CH_3), 1.35 (s, 12H, CH_3) ppm. ¹³C{¹H} NMR (C₆D₆, 25 °C, 75 MHz): $\delta = 144.82$ (NC=*C*NN), 121.73 (CH₃-C=*C*), 120.49 (CH₃-*C*=*C*), 109.37 (N*C*=CNN), 62.11 (*C*H₂), 60.47 (*C*(CH₃)₂), 57.55 (*C*H_{cy}), 42.31 (*C*H₃-N), 41.01 (*C*(CH₃)₂), 32.95 (*C*H_{2cy}), 32.26 (*C*H₃-N), 28.05 (C(*C*H₃)₂), 10.10 (*C*H₃-C=*C*), 9.76 (*C*H₃-C=*C*) ppm. Most likely due to high air and moisture sensitivity we were not able to get satisfactory elemental analysis data even after repeating measurements.



Fig. S4 ¹H NMR spectrum of 4^{Cy} in C₆D₆ at RT.



Fig. S6 Overlay of ¹H NMR spectra of a mixture of 4^{Cy} and *n*-Bu₄NPF₆ (Blue), 4^{Cy} (green) and *n*-Bu₄NPF₆ (red) in THF-d₈ at RT.



Fig. S7 Overlay of ¹H NMR spectra of a mixture of 4^{Cy} and *n*-Bu₄NPF₆ (Blue), 4^{Cy} (green) and *n*-Bu₄NPF₆ (red) in CD₃CN at RT.

Synthesis of 5^{Cy}



20 mL THF solution of 4^{Cy} (417 mg, 0.72 mmol) was added dropwise to a 10 mL THF solution of AgOTf (824 mg, 3.207 mmol) at room temperature while stirring. Immediately, black colored metallic silver precipitated out. After 1 hour all volatiles were removed under vacuum and the residue was dissolved in acetonitrile (20 mL) and filtered. The filtrate was evaporated and an oily sticky compound was obtained. After that 40 mL of THF was added to this oily compound and then sonicated. A white precipitate of 5^{cy} was obtained after sonication. This precipitate was filtered, washed with ether and dried. Yield: 750 mg (89 %). M.P.: > 180 °C. Acetonitrile solution of 5^{Cy} was kept for crystallization with DCM diffusion at room temperature for 24 hours. Colorless crystals of 5^{Cy} were obtained which were also suitable for X-ray structural analysis. ¹**H NMR** (CD₃CN, 25 °C, 300 MHz): δ = 3.98 (m, 2H, CH_{CV}), 3.78 (s, 12H, CH₃-N), 2.44 (s, 4H, CH₂), 2.41 (s, 12H, CH₃-C=C), 2.41 (br. 4H, CH_{2 CV}), 1.84 (s, 12H, CH₃), 1.45 (s, 12H, CH₃), 1.45 (br. 4H, $CH_{2 \text{ CV}}$) ppm. ¹³C{¹H} NMR (CD₃CN, 25 °C, 75 MHz): δ = 181.09 (C=N), 134.78 (CH₃-C=C), 128.21 (CNN), 121.83 (q, ${}^{1}J_{C-F}$ = 320.75 Hz, CF₃SO₃), 87.29 (C(CH₃)₂), 62.92 (CH_{Cy}), 57.03 (C(CH₃)₂), 48.09 (CH₂), 37.24 (CH₃-N), 31.24 (CH_{2Cy}), 27.89 (C(CH₃)₂), 27.33 (C(CH₃)₂), 9.37 (CH₃-C=C) ppm. ¹⁹F{¹H} NMR (CD₃CN, 25 °C, 282 MHz): $\delta = -79.27$ ppm. Elemental analysis: Calculated (%) for C40H62N6F12O12S4: C, 40.88; H, 5.32; N, 7. 15; S, 10.91; Found: C, 40.72; H, 5.55; N, 6.66; S, 10.11. HRMS-ESI (m/z): Calculated for $C_{39}H_{62}N_6F_9O_9S_3$ [M-1OTf]³⁺: 1025.3592, Found: 1025.3573.



Fig. S8 ¹H NMR spectrum of **5**^{Cy} in CD₃CN at RT.



Fig. S9 ¹³C{¹H} NMR spectrum of 5^{Cy} in CD₃CN at RT.



Fig. S10 $^{19}F\{^{1}H\}$ NMR spectrum of 5^{Cy} in CD_3CN at RT.

Reduction of 5^{Cy}



THF was added to the mixture of 5^{Cy} (70 mg, 0.059 mmol) and KC₈ (65 mg, 0.480 mmol) at -30 °C with stirring. After 6 hours stirring at room temperature, solvent and other volatiles were removed under vacuum and the ¹H NMR spectrum of the reaction mixture in C₆D₆ was measured which showed the formation of 4^{Cy} along with the residual THF solvent.



Fig. S11 Overlay of ¹H NMR spectra from the reaction mixture of 5^{cy} and excess KC₈ (red) and 4^{cy} (green) in C₆D₆ at RT.

Synthesis of 6^{Cy}



5 mL Acetonitrile was added to the mixture of 4^{Cy} (130 mg, 0.225 mmol) and 5^{Cy} (264 mg, 0.225 mmol) at -30 °C and then stirred for 6 hours at room temperature. Then the solvent and other volatiles were removed under reduced pressure and a deep red powder was obtained. Yield: 380 mg (96 %). After that about 2 mL of CH₃CN was added to the residue and kept for crystallization at -35 °C. After 24 hours, dark red colored crystals were collected. **M.P.:** Upto 120 °C there was no color change observed. At 130 °C the color changed from red to light yellow without melting (the UV/Vis spectrum of the light yellow colored sample reveals that decomposition of 6^{Cy} has occurred and the ¹H NMR spectrum shows the formation of an unidentified mixture of compounds). The resulting light yellow sample does not melt even at 170 °C. UV/Vis (CH₃CN): λ_{max} (nm)= 455, 375, 299. Elemental analysis: Calculated (%) for C₃₈H₆₂F₆N₆O₆S₂: C, 52.04; H, 7.13; N, 9.58; S, 7.31; Found: C, 49.62; H, 7.00; N, 9.18; S, 6.8.



Fig. S12 UV/Vis spectrum of 6^{Cy} in acetonitrile at room temperature.



Fig. S13 UV/Vis spectrum of the light-yellow solid, which was obtained after heating solid **6**^{Cy} at 130 °C for 10 minutes in a closed sealed NMR tube in acetonitrile measured at room temperature.



Fig. S14 ¹H NMR spectrum of the light-yellow solid, which was obtained after heating solid 6^{Cy} at 130 °C for 10 minutes in closed sealed NMR tube measured in CD₃CN at RT.

Synthesis of 7^{Cy}

Method I



About 6 mL of CH₃CN was added to the mixture of 5^{cy} (134 mg, 0.114 mmol) and 6^{cy} (100 mg, 0.114 mmol) at -30 °C and then the reaction mixture was warmed to room temperature over 15 minutes. The solvent and other volatiles from the reaction mixture were removed under vacuum and a red colored solid was obtained as compound 7^{cy} . Yield: 205 mg (88 %). UV/Vis (CH₃CN): λ_{max} (nm)= 451, 374, and 308.

Method II



About 6 mL of CH₃CN was added to the mixture of AgOTf (30 mg, 0.117 mmol) and 6^{cy} (100 mg, 0.114 mmol) at room temperature. Immediately the formation of the black precipitate of metallic silver was observed. The filtrate was evaporated and the red colored solid of compound 7^{cy} was obtained.





About 4 mL of CH₃CN was added to the mixture of 4^{Cy} (43 mg, 0.074 mmol) and 5^{Cy} (262 mg, 0.223 mmol) at -30 °C. The solution of the reaction mixture became dark red colored. It was stirred for 12 hours at room temperature. The filtrate was evaporated and red colored solid of compound 7^{Cy} was obtained. About 2 mL of THF was added to it and the solution kept for crystallization at -35 °C for 24 hours. In the first fraction we obtained 5^{Cy} , whereas in the second fraction we obtained red colored crystals of 7^{Cy}

(minor amount and suitable for single-crystal X-ray diffraction study) along with colorless crystals of **5**^{cy} (major amount).



Fig. S15 UV/Vis spectra of 7^{Cy} in acetonitrile at room temperature.

Synthesis of 3Et



About 250 mL of THF was added to a 500 mL Schlenk flask containing 1^{Et} (10 g, 17.343 mmol) and 2 (5 g, 40.260 mmol) at 0 °C. After stirring for 24 hrs at room temperature, about 150 mL of diethyl ether was added to the reaction mixture and then the reaction mixture was filtered. The white solid residue was washed with about 50 mL of diethyl ether and dried under vacuum. ¹H NMR spectrum of the solid residue showed the formation of a mixture of two diastereomers (*d/l-* and *meso-*) of **3^{Et}** in ca. 60:40 ratio. These two are diastereomers of each other. Yield: 13.2 g (92 %). M.P.: > 180 °C. The pure major diastereomer of 3^{Et} was obtained through fractional crystallization by layering diethyl ether over a saturated CH₃CN solution of the crude compound. The obtained crystals were suitable for a single crystal X-ray diffraction study and the analysis of single crystal data showed that it was the *meso*-isomer of **3**^{Et}. The pure major diastereomer of 3^{Et} was obtained up to the third consecutive fraction of fractional crystallization. In the fourth fraction of fractional crystallization we obtained mostly the minor diastereomer along with small amounts of the major diastereomer. It was not possible to isolate the pure minor diastereomer. We used the mixture of diastereomers for the next reaction. NMR data of the major diastereomer: ¹H NMR $(CD_3CN, 25 \ ^{\circ}C, 300 \ \text{MHz})$: $\delta = 4.24 \ (s, 2H, CH), 3.94 \ (s, 6H, CH_3-N), 3.68 \ (s, 6H, CH_3-N), 2.24 \ (s, 6H,$ CH₃-C=C), 2.21 (s, 6H, CH₃-C=C), 2.14-2.00 (m, 4H, CH₂CH₂), 1.87-1.76 (m, 4H, CH₂), 1.31 (s, 6H, CH₃), 1.01 (s, 6H, CH₃), 0.94 (s, 6H, CH₃), 0.78 (s, 6H, CH₃) ppm. ¹³C{¹H} NMR (CD₃CN, 25 °C, 75 MHz): δ = 144.68 (*C*=N-CH₃), 128.97 (CH₃-*C*=*C*), 128.15 (CH₃-*C*=*C*), 122.11 (q, ¹*J*_{C-F} = 320.02 Hz, *C*F₃SO₃⁻), 71.58 (CH), 62.90 (C(CH₃)₂), 55.94 (CH₂), 48.95 (CH₂CH₂), 43.33 (C(CH₃)₂), 35.14 (CH₃-N), 33.43 (CH₃-N), 31.65 (C(CH₃)₂), 29.58 (C(CH₃)₂), 27.72 (C(CH₃)₂), 22.18 (C(CH₃)₂), 9.03 (CH₃-C=C), 8.68 (CH₃-C=C) ppm. ¹⁹F{¹H} NMR: (CD₃CN, 25 °C, 282 MHz): $\delta = -79.23$ ppm. NMR data of the minor diastereomer: ¹**H NMR:** (CD₃CN, 25 °C, 300 MHz): δ = 4.18 (s, 2H, CH), 3.96 (s, 6H, CH₃-N), 3.60 (s, 6H, CH₃-N), 2.23 (s, 6H, CH₃-C=C), 2.20 (s, 6H, CH₃-C=C), 1.76-1.87 (m, 4H, CH₂CH₂), 1.66-1.73 (m, 4H, CH₂), 1.29 (s, 6H, CH₃), 1.15 (s, 6H, CH₃), 1.00 (s, 6H, CH₃), 0.74 (s, 6H, CH₃) ppm. Elemental analysis: Calculated (%) for C₃₄H₅₈F₆N₆O₆S₂: C, 49.50; H, 7.09; N, 10.19; S, 7.77; Found: C, 49.84; H, 6.87; N, 10.08; S, 7.60. **HRMS-ESI (m/z):** Calculated for C₃₃H₅₈N₆F₃SO₃ [M-OTf]⁺: 675.4238; Found: 675.4218.



Fig. S16 ¹H NMR spectrum of the major diastereomer of 3^{Et} in CD₃CN at RT.



Fig. S17 $^{13}C{^{1}H}$ NMR spectrum of the major diastereomer of 3^{Et} in CD₃CN at RT.





Fig. S19 ¹H NMR spectrum of the minor diastereomer of **3**^{Et} with small amounts of the major diastereomer in CD₃CN at RT.



Fig. S20 ¹H NMR spectrum of the crude compound of 3^{Et} (after work up) in CD₃CN at RT.



Fig. S21 ¹³C{¹H} NMR spectrum of the crude compound of 3^{Et} (after workup) in CD₃CN at RT.

Synthesis of LiTMP

Solid LiTMP (lithium 2,2,6,6-tetramethylpiperidide) was prepared based on the literature procedure.^{S4} *n*BuLi (50.5 mL, 80.80 mmol, 1.6 M in hexane) was added to the pentane solution of 2,2,6,6-tetramethylpiperidine (15 mL, 88.89 mmol) at 0 °C. After 2 hours, it was warmed to room temperature and stirred for another 12 hours. The solid residue was filtered and dried. The filtrate was concentrated and kept at -35 °C for crystallization. Both solid residues were collected after drying and stored inside a glove box. **Yield:** 11.8 g (99 %).

Synthesis of 4^{Et}

Method I



About 30 mL of toluene was added into a 50 mL Schlenk flask containing 3^{Et} (327 mg, 0.395 mmol) and LiTMP (168 mg, 1.141 mmol) at room temperature with stirring. Then the reaction mixture was stirred for 12 hours at room temperature. After that the reaction mixture was filtered while heated to boiling temperature (compound 4^{Et} is poorly soluble in toluene). Further 10 mL of toluene was added to the residue and filtered at boiling temperature. Both filtrates were combined and kept at -35 °C for crystallization. Light yellow colored crystals were obtained after 12 hours which were suitable for a single crystal X-ray diffraction study. Subsequently, the mother liquor was concentrated and kept at -35 °C to get a second crop of crystals. The combined crystals were washed with a small amount of pentane giving pure compound 4^{Et} . Yield: 130 mg (63 %).

Method II



About 80 mL of toluene was added into a 250 mL Schlenk flask containing **3**^{Et} (4 g, 4.836 mmol) and KHMDS (2.485 g, 12.457 mmol) at room temperature while stirring. The reaction mixture turned into a yellow colour and the reaction mixture was stirred for 72 hours at 90 °C. After that it was stirred for overnight at room temperature. Then the reaction mixture was filtered while heated to boiling temperature (compound **4**^{Et} is poor soluble in toluene). Further 20 mL of toluene was added to the residue and filtered

at boiling temperature. Both filtrates were combined and kept at -35 °C for crystallization. Light yellow colored crystals were obtained after 12 hours and collected. Subsequently, the mother liquor was concentrated and kept at -35 °C to get a second crop of crystals. The combined crystals were washed with a small amount of pentane giving pure compound **4**^{Et}. **Yield:** 2.31 g (91 %). **M.P.:** 162 °C (decomposed). ¹**H NMR** (THF-D₈, 25 °C, 300 MHz): $\delta = 2.69$ (br, 4H, CH₂CH₂), 2.67 (s, 6H, CH₃-N), 2.46 (s, 6H, CH₃-N), 1.74 (s, 6H, CH₃-C=C), 1.71 (s, 6H, CH₃-C=C), 1.61 (s, 4H, CH₂), 1.26 (s, 12H, CH₃), 1.10 (s, 12H, CH₃) ppm. ¹³C{¹H} **NMR** (THF-D₈, 25 °C, 75 MHz): $\delta = 138.76$ (NC=CNN), 122.75 (CH₃-C=C), 122.70 (CH₃-C=C), 112.80 (NC=CNN), 60.15 (CH₂), 59.46 (C(CH₃)₂), 41.94 (CH₃-N), 39.55 (C(CH₃)₂), 38.91 (CH₂CH₂), 33.72 (CH₃-N), 28.93 (C(CH₃)₂), 27.96 (C(CH₃)₂), 9.99 (CH₃-C=C), 9.75 (CH₃-C=C) ppm. Compound **4**^{Et} is not well soluble in THF. For the UV/Vis measurement 2 mg of compound **4**^{Et} was heated to reflux in THF to dissolve it and allowed to cool down to room temperature. Then the resulting solution was subsequently used for the UV/Vis study. **UV/Vis** (**THF**): λ_{max} (ϵ) = 290 (31879) nm (L mol⁻¹ cm⁻¹). **Elemental analysis:** Calculated (%) for C₃₂H₅₆N₆: C, 73.23; H, 10.76; N, 16.01; Found: C, 72.98; H, 10.825; N, 15.48. **HRMS-ASAP (m/z):** Calculated for C₃₂H₅₇N₆ [M+H]⁺: 525.4639, Found: 525.4625.



Fig. S22 ¹H NMR spectrum of 4^{Et} in THF-D₈ at RT.





Fig. S24 ¹³C{¹H} NMR spectrum of 4^{Et} in THF-D₈ at RT.

Synthesis of 5^{Et}



40 mL THF solution of 4^{Et} (210 mg, 0.4 mmol) was added dropwise to a 10 mL THF solution of AgOTf (511 mg, 1.989 mmol) at room temperature while stirring. Immediately, black colored metallic silver precipitated out. After 12 hours all volatiles were removed under vacuum and the residue was dissolved in acetonitrile (50 mL) and filtered. The yellowish green colored filtrate was concentrated and kept for crystallization with diethyl ether diffusion at room temperature for 24 hours and then kept at −30 °C. Yellow colored crystals of 5^{Et} were obtained after 12 hours which were also suitable for X-ray structural analysis. The obtained crystals were washed with diethyl ether to give pure compound 5^{Et}. The mother liquor was concentrated and again stored for crystallization. Yield: 340 mg (76 %). M.P.: > 180 °C. ¹H NMR (CD₃CN, 25 °C, 300 MHz): δ = 4.21 (s, 4H, CH₂CH₂), 3.87 (s, 12H, CH₃-N), 2.51 (s, 4H, CH₂), 2. 41 (s, 12H, CH₃-C=C), 1.67 (s, 12H, CH₃), 1.56 (s, 12H, CH₃) ppm. ¹³C{¹H} NMR (CD₃CN, 25 °C, 75 MHz): δ = 186.43 (C=N⁺), 136.12 (CH₃-C=C), 124.32 (CNN⁺), 121.7 (q, ¹J_{C-F} = 320.05 Hz, CF₃SO₃⁻), 86.18 (C(CH₃)₂), 57.19 (C(CH₃)₂), 47.77 (CH₂CH₂), 47.34 (CH₂), 36.77 (CH₃-N), 27.56 (C(CH₃)₂), 27.01 $(C(CH_3)_2)$, 9.47 $(CH_3-C=C)$ ppm. ¹⁹F{¹H} NMR $(CD_3CN, 25 \ ^{\circ}C, 282 \ MHz)$: $\delta = -79.25$ ppm. UV/Vis (CH_3CN) : λ_{max} (ϵ) = 350 (3474), 243 (23303) nm (L mol⁻¹ cm⁻¹). Elemental analysis: Calculated (%) for C₃₆H₅₆N₆F₁₂O₁₂S₄: C, 38.57; H, 5.04; N, 7. 50; S, 11.44; Found: C, 38.93; H, 5.07; N, 8.04; S, 11.20. **HRMS-ESI (m/z):** Calculated for C₃₄H₅₆N₆F₆S₃O₆ [M-2OTf]²⁺: 411.1798, Found: 411.1788.



 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

 Fig. S26 ¹³C{¹H} NMR spectrum of 5^{Et} in CD₃CN at RT.



Fig. S27 $^{19}\text{F}\{^{1}\text{H}\}$ spectrum of 5^{Et} in CD_3CN at RT.

Reaction of 5^{Et} and KC₈



THF was added to the mixture of 5^{Et} (104 mg, 0.093 mmol) and KC₈ (150 mg, 1.109 mmol) at room temperature with stirring. After 4 hours stirring at room temperature, solvent and other volatiles were removed under vacuum and a ¹H NMR spectrum of the reaction mixture in C₆D₆ was measured. There was no clear evidence of formation of 4^{Et} in the ¹H NMR spectrum of the reaction mixture.



Fig. S28 Overlay of the ¹H NMR spectra of reaction mixture of 5^{Et} and KC₈ (red) and 4^{Et} (green) in C₆D₆ at RT.

Synthesis of 8^{Et} Method I



20 mL of THF was added to the mixture of 4^{Et} (200 mg, 0.381 mmol) and AgOTf (196 mg, 0.763 mmol) at room temperature while stirring. After 6 hours of stirring, all volatiles were removed under vacuum. Then about 10 mL of acetonitrile was added into the residue, and the silver particles allowed to settle down for overnight. The clear yellow supernatant solution was collected with a pipette. Again 10 mL acetonitrile was added to the residue, shaken well, allowed to stand for 10 minutes and supernatant solution was taken out. Alternatively, THF solution of AgOTf (196 mg, 0.763 mmol, in 15 mL of THF) was added to a THF solution of 4^{Et} (200 mg, 0.381 mmol, in 30 mL of THF) dropwise at 0 °C. After 6 hours all volatiles were evaporated under reduced pressure. After that the workup was carried out as in the previous procedure. The ¹H NMR spectrum of the filtrate after extraction with CH₃CN showed the formation of two diastereomers of 8^{Et} (56 % & 19 %) along with the compound 3^{Et} (24 %). Then the combined supernatant solution was concentrated to about 4 mL and diethyl ether was added dropwise until a slightly yellow precipitate appeared. This was kept at -30 °C for 12 hours to obtain crystals/more precipitate. The ¹H NMR spectrum of the collected precipitate (90 mg) showed that it was the major diastereomer of 8^{Et}. Suitable single crystals for a single crystal X-ray diffraction study were obtained for the major diastereomer of 8^{Et} by diffusing diethyl ether into the concentrated CH₃CN/THF (1:2) solution. The analysis of the single crystal X-ray diffraction data showed that it was the meso-isomer. After collecting the first crop, diethyl ether was added to the mother liquor again dropwise until further precipitate appeared. The ¹H NMR spectrum of the collected precipitate shows that it was the major diastereomers of 8^{Et} along with compound 3^{Et}. Subsequently, after collecting the second crop, about 5 mL diethyl ether was added to the mother liquor and kept at -30 °C. After 7 days red colored small crystals formed. The ¹H NMR spectrum of the collected red colored crystalline compound (25 mg) showed that it was the minor diastereomer of 8^{Et}. We were unable to obtain single crystals suitable for XRD of the minor diastereomer

of 8^{Et}. Yield: 115 mg (36 %). M.P.: > 180 °C. NMR data of the major diastereomer: ¹H NMR (CD₃CN, 25 °C, 300 MHz): δ = 4.66 (s, 2H, CH=CH), 4.48 (s, 2H, CH), 3.78 (s, 6H, CH₃-N), 3.76 (s, 6H, CH₃-N), 2.25 (s, 6H, CH₃-C=C), 2.14 (s, 6H, CH₃-C=C), 1.89-1.78 (m, 4H, CH₂), 1.30 (s, 6H, CH₃), 1.10 (s, 6H, CH₃), 0.86 (s, 6H, CH₃), 0.64 (s, 6H, CH₃) ppm. ¹³C{¹H} NMR (CD₃CN, 25 °C, 75 MHz): δ = 142.89 (C=N-CH₃), 128.92 (CH₃-C=C), 128.23 (CH₃-C=C), 122.08 (q, ¹J_{C-F} = 320.95 Hz, CF₃SO₃⁻), 116.36 (HC=CH), 65.73 (CH), 62.69 (C(CH₃)₂), 54.85 (CH₂), 43.74 (C(CH₃)₂), 34.18 (CH₃-N), 33.61 (CH₃-N), 30.43 (C(CH₃)₂), 27.96 (C(CH₃)₂), 27.32 (C(CH₃)₂), 25.05 (C(CH₃)₂), 8.99 (CH₃-C=C), 8.70 (CH₃-C=C) ppm. ¹⁹F{¹H} NMR (CD₃CN, 25 °C, 282 MHz): δ = -79.33 ppm. NMR data of the minor diastereomer: ¹H NMR (CD₃CN, 25 °C, 300 MHz): δ = 4.88 (s, 2H, CH=CH), 4.39 (s, 2H, CH), 3.85 (s, 6H, CH₃-N), 3.68 (s, 6H, CH₃-N), 2.23 (s, 6H, CH₃-C=C), 2.17 (s, 6H, CH₃-C=C), 1.87-1.80 (m, 4H, CH₂), 1.28 (s, 6H, CH₃), 1.22 (s, 6H, CH₃), 0.85 (s, 6H, CH₃), 0.76 (s, 6H, CH₃) ppm. ¹³C{¹H} NMR (CD₃CN, 25 °C, 75 MHz): δ = 143.01 (C=N-CH₃), 128.54 (CH₃-C=C), 128.30 (CH₃-C=C), 121.33 (HC=CH), 68.02 (CH), 63.25 (C(CH₃)₂), 55.14 (CH₂), 43.55 (C(CH₃)₂), 34.40 (CH₃-N), 33.57 (CH₃-N), 30.71 (C(CH₃)₂), 28.90 (C(CH₃)₂), 27.41 (C(CH₃)₂), 24.39 (C(CH₃)₂), 9.08 (CH₃-C=C), 8.68 (CH₃-C=C) ppm. ¹⁹F{¹H} NMR (CD₃CN, 25 °C, 282 MHz): δ = -79.33 ppm. UV/Vis (CH₃CN): λ_{max} (ε) = 233 (31673) nm (L mol⁻¹ cm⁻¹). Elemental analysis: Calculated (%) for C₃₄H₅₆N₆F₆O₆S₂: C, 49.62; H, 6.86; N, 10.21; S, 7.79; Found: C, 49.71; H, 6.86; N, 10.11; S, 7.53. HRMS-LIFDI (m/z): Calculated for C₃₃H₅₆N₆F₃SO₃ [M-OTf]⁺: 673.4081, Found: 673.4067.



Fig. S29¹H NMR spectrum of the major diastereomer of 8^{Et} in CD₃CN at RT.



Fig. S30 ¹³C{¹H} NMR spectrum of the major diastereomer of 8^{Et} in CD₃CN at RT.



Fig. S31 ¹⁹F{¹H} spectrum of the major diastereomer of 8^{Et} in CD₃CN at RT.



Fig. S32 ¹H NMR spectrum of the minor diastereomer of 8^{Et} in CD₃CN at RT.



Fig. S33 ¹³C{¹H} NMR spectrum of the minor diastereomer of 8^{Et} in CD₃CN at RT.



Fig. S34 ¹⁹F{¹H} spectrum of the minor diastereomer of 8^{Et} in CD₃CN at RT.



Fig. S35 ¹H NMR spectrum of the crude reaction mixture of **8**^{Et} (containing both diastereomers of **8**^{Et} along with compound **3**^{Et} which has also two diastereomers) in CD₃CN at RT.



Fig. S36 Overlay of the ¹H NMR spectra of the crude reaction mixture of **8**^{Et} (red), minor diastereomer of **8**^{Et} (navy), major diastereomer of **8**^{Et} (green), and two diastereomers **3**^{Et} (purple) in CD₃CN at RT.

Method II



 4^{Et} (14 mg, 0.027 mmol) and 5^{Et} (30 mg, 0.027 mmol) were taken into an NMR tube and about 0.6 mL of CD₃CN was added. The ¹H NMR spectrum of the reaction mixture was measured which showed the formation of two diastereomers of compound 8^{Et} .



Fig. S37 Overlay of the ¹H NMR spectra of the crude reaction mixture of 1:1 reaction of **4**^{Et} and **5**^{Et} (red) with minor diastereomer of **8**^{Et} (blue) and major diastereomer of **8**^{Et} (green) in CD₃CN at RT.

Method III



An acetonitrile (15 mL) solution of $Co(Cp)_2$ (27 mg, 0.143 mmol) was added dropwise to the acetonitrile solution (15 mL) of **5**^{Et} (80 mg, 0.071 mmol) at room temperature with stirring. After 12 hours, solvent and other volatiles were removed under vacuum and the residue was washed with THF (15 ml) and dried. Then the ¹H NMR spectrum of the remaining residue in CD₃CN showed the formation of two diastereomers of **8**^{Et} in ca. 89:11 ratio along with the cobaltocenium cation. The same outcome was obtained when we performed the reaction of **5**^{Et} with four equivalents of Co(Cp)₂ in a similar reaction condition.



Fig. S38 ¹H NMR spectrum after work up of the 1:2 reaction of 5^{Et} and Co(Cp)₂ in CD₃CN at RT.



Fig. S39 Overlay of the ¹H NMR spectra of the product of the 1:4 reaction of 5^{Et} and Co(Cp)₂ (blue), major diastereomer of 8^{Et} (red), minor diastereomer of 8^{Et} (green) in CD₃CN at RT.
Synthesis of 9^{Et}

Method I



Toluene (25mL) was added to the mixture of the major diastereomer of 8^{Et} (213 mg, 0.258 mmol) and LiTMP (95 mg, 0.645 mmol) at room temperature and stirred for twelve hours. Then the reaction mixture was filtered while heated to boiling temperature. The resulting filtrate was concentrated to about 5 mL and kept at -35 °C for crystallization. After 12 hrs dark yellow crystals of 9^{Et} were obtained which were suitable for an X-ray diffraction study. The obtained single crystals were washed with a small amount of pentane and the mother liquor was concentrated and again kept at -35 °C for crystallization. Yield: 56 mg (41 %).

Method II



A THF solution of AgOTf (196 mg, 0.763 mmol, in 15 mL of THF) was added to a THF solution of **4**^{Et} (200 mg, 0.381 mmol, in 30 mL of THF) dropwise at 0 °C. After 6 hours all volatiles were removed under vacuum and then CH₃CN (10 mL) was added and stirred for 5 minutes. The filtrate was evaporated to dryness to obtain a solid residue which was dried at 80 °C under vacuum for 4 hrs. Then KHMDS (170 mg, 0.852 mmol) and toluene (30 mL) were added to it at room temperature and stirred for 12 hours. The ¹H NMR spectrum of the crude reaction mixture showed the formation of compound **9**^{Et} along with a small amount of **4**^{Et}. The reaction mixture was filtered while heated to boiling temperature and the resulting

filtrate was concentrated to about 10 mL and kept at -30 °C for crystallization. After 12 hours, orange crystals were obtained and collected. Subsequently, the mother liquor was concentrated and kept again for crystallization at -30 °C. The ¹H NMR spectrum of the obtained crystals showed the presence of compound **4**^{Et} (6 %) along with compound **9**^{Et}. **Yield:** 90 mg (45 %). **M.P.:** 162 °C. ¹H **NMR** (C₆D₆, 25 °C, 300 MHz): δ = 4.91 (s, 2H, C*H*=C*H*), 2.79 (s, 6H, C*H*₃-N), 2.57 (s, 6H, C*H*₃-N), 1.80 (s, 4H, C*H*₂), 1.69 (s, 6H, C*H*₃-C=C), 1.65 (s, 6H, C*H*₃-C=C), 1.50 (s, 12H, C*H*₃), 1.37 (s, 12H, C*H*₃) ppm. ¹³C{¹H} **NMR** (C₆D₆, 25 °C, 75 MHz): δ = 140.77 (NC=CNN), 122.13 (CH₃-C=C), 120.16 (CH₃-C=C), 108.06 (NC=CNN), 105.87 (CH=CH), 59.91 (CH₂), 59.74 (C(CH₃)₂), 43.26 (CH₃-N), 40.11 (C(CH₃)₂), 31.75 (CH₃-N), 28.85 (C(CH₃)₂), 27.83 (C(CH₃)₂), 10.31 (CH₃-C=C), 9.60 (CH₃-C=C) ppm. **UV/Vis** (THF): λ_{max} (ε) = 320 (13087), 236 (26347) nm (L mol⁻¹ cm⁻¹). **Elemental analysis:** Calculated (%) for C₃₂H₅₄N₆: C, 73.51; H, 10.439; N, 15.32. Most likely due to high air and moisture sensitivity we were not able to get satisfactory elemental analysis data even after repeating measurements. **HRMS-ASAP (m/z):** Calculated for C₃₂H₅₅N₆ [M+H]⁺: 523.4483, Found: 523.4455.



Fig. S40 ¹H NMR spectrum of 9^{Et} in C₆D₆ at RT.



Fig. S42 ¹H NMR spectrum of the crude reaction mixture of 9^{Et} in C₆D₆ at RT (indicating the formation of only *E*-isomer).

Oxidation of 8^{Et}



5 mL CH₃CN was added to the mixture of 8^{Et} (56 mg, 0.068 mmol) and AgOTf (18 mg, 0.07 mmol) at room temperature. After 10 minutes of stirring the reaction mixture, all volatiles were removed under vacuum. Then about 10 mL of CH₃CN was added to the residue and filtered. The orange colored filtrate was concentrated to about 2 mL and then 3 mL of THF was added into it. The resulting solution was kept for crystallization with diethyl ether diffusion at room temperature. Orange colored crystalline compound 10^{Et} was obtained after 24 hours. The ¹H NMR spectrum of crystals showed the presence of compound 8^{Et} also. Amount of crystalline solids: 50 mg. Quantitative EPR measurement indicates a radical concentration of ca. 54% in the crystalline crude products considering TEMPO as standard. HRMS-ESI (m/z): Calculated for C₃₃H₅₆N₆F₃SO₃ [M-2OTf]⁺: 673.4081; Found: 673.4065.



Fig. S43 ¹H NMR spectrum of red crystals containing a mixture of 8^{Et} and 10^{Et} from the 1:1 reaction of 8^{Et} and AgOTf in CD₃CN at RT.

UV/Vis spectra



Fig. S44 UV/Vis spectra of 4^{Et} in THF at different concentrations.



Fig. S45 Linear regression of the concentration dependent absorbance of 4^{Et} at 290 nm.



Fig. S46 UV/Vis spectra of 5^{Et} in acetonitrile at different concentrations.



Fig. S47 Linear regression of the concentration dependent absorbance of 5^{Et} at 350 nm.



Fig. S48 Linear regression of the concentration dependent absorbance of $\mathbf{5}^{Et}$ at 243 nm



Fig. S49 UV/Vis spectra of the major diastereomer of 8^{Et} in acetonitrile in different concentrations at RT.



Fig. S50 Linear regression of the concentration dependent absorbance of 8^{Et} at 233 nm.



Fig. S51 UV/Vis spectra of 9^{Et} in THF at different concentrations.



Fig. S52 Linear regression of the concentration dependent absorbance of 9^{Et} at 320 nm.



Fig. S53 Linear regression of the concentration dependent absorbance of 9^{Et} at 236 nm.

Synthesis of 3^{Pr}



For the synthesis of 3^{Pr} we have used 1^{Pr} which contained LiOTf instead of crystalline 1^{Pr}. About 90 mL THF was added to the mixture of 1^{Pr} (considering the presence of two molecules of LiOTf) (6g, 6.647 mmol) and 2 (2.1 g, 16.91 mmol) at 0 °C with stirring. After two hours the reaction mixture was warmed to room temperature and stirred for 24 hours. After that the reaction mixture was filtered and the ¹H NMR spectrum was recorded for both residue and filtrate. The product 3^{Pr} was present in the residue as well as in the filtrate. The residue was isolated as colorless powder of pure 3^{Pr} of 2.1 g (37 %). The vellow colored filtrate was concentrated up to 30 mL and then about 60 mL of diethylether was added to it and left for 24 hours. Then 3.9 g of a separated sticky material of 3^{Pr} was isolated which contained LiOTf and trace amounts of 2.HOTf. M.P.: > 180 °C (sample from residue). Note: In compound 3^{Pr}, there are two chiral centers and we see the formation of two diastereomers: the residue contains one diastereomer as major component, while the filtrate contains another diastereomer as major component. Here we are providing the NMR data of the major diastereomer from the residue. ¹H NMR (CD₃CN, 25 °C, 300 MHz): δ = 4.25 (s, 2H, CH), 4.00 (s, 6H, CH₃-N), 3.65 (s, 6H, CH₃-N), 2.56-2.47 (m, 2H, CH₂-CH₂-CH₂), 2.21 (s, 6H, CH₃-C=C), 2.20 (s, 6H, CH₃-C=C), 2.15-2.05 (m, 2H, CH₂-CH₂-CH₂), 1.87-1.77 (m, 4H, CH₂), 1.26 (s, 6H, CH₃), 1.14 (s, 6H, CH₃), 1.10 (s, 6H, CH₃), 1.10-1.01 (m, 2H, CH₂-CH₂-CH₂), 0.80 (s, 6H, CH₃) ppm; ¹³C{¹H} NMR (CD₃CN, 25 °C, 75 MHz): δ = 144.08 (C=N-CH₃), 128.82 (CH₃-C=C), 127.96 (CH₃-C=C), 122.08 (g, ${}^{1}J_{C-F}$ = 321.03 Hz, CF₃SO₃⁻), 71.37 (CH), 62.12 (C(CH₃)₂), 56.88 (CH₂), 47.60 (CH₂-CH₂-CH₂), 43.41 (C(CH₃)₂), 34.59 (CH₃-N), 33.43 (CH₃-N), 30.94 (C(CH₃)₂), 30.42 (C(CH₃)₂), 29.40 (CH₂-CH₂-CH₂), 27.31 (C(CH₃)₂), 22.47 (C(CH₃)₂), 9.00 (CH₃-C=C), 8.68 (CH₃-C=C) ppm; ¹⁹F{¹H} NMR (CD₃CN, 25 °C, 282 MHz): $\delta = -79.24$ ppm. Elemental analysis: Calculated (%) for C₃₅H₆₀N₆F₆O₆S₂: C, 50.10; H, 7.21; N, 10.02; S, 7.64; Found: C, 49.84; H, 7.23; N, 9.70; S, 7.70. HRMS-ESI (m/z): Calculated for C₃₄H₆₀N₆F₃SO₃ [M-1OTf]⁺: 689.4395, Found: 689.4397.



Fig. S54 ¹H NMR spectrum of the residue of the reaction mixture yielding 3^{Pr} in CD₃CN at RT.



Fig. S55 ¹H NMR spectrum of the filtrate of the reaction mixture yielding 3^{Pr} in CD₃CN at RT.



Fig. S56 Overlay of ¹H NMR spectra (selected region) of residue (red) and filtrate (green) of the reaction mixture yielding **3**^{Pr} in CD₃CN at RT.



Fig. S57 ¹³C{¹H} NMR spectrum of the residue of the reaction mixture yielding 3^{Pr} in CD₃CN at RT.



Fig. S58 ¹⁹F{¹H} NMR spectrum of the residue of the reaction mixture yielding 3^{Pr} in CD₃CN at RT.

Synthesis of 4^{Pr}



About 40 mL of toluene was added into a 50 mL of Schlenk flask containing 3^{Pr} (2.04 g, 2.43 mmol) and LDA (662 mg, 6.18 mmol) at room temperature with stirring. The reaction mixture turned into a yellow color. After 24 hours stirring at room temperature the reaction mixture was filtered under hot condition and the filtrate was evaporated to yield a reddish brown oily type of liquid. Then pentane (30 mL) was added to it, stirred well and filtered and the filtrate was evaporated to yield a brownish oily liquid which transformed into crystalline solids after some time. The crystalline solid (875 mg) was collected and the filtrate was evaporated. The ¹H NMR spectra of crystalline solids and filtrate were measured which showed the presence of 4^{Pr} as pure compound. Yield: 1.15 g (88 %). M.P.: 105 °C. Compound 4^{Pr} can be obtained in a satisfactory yield using 3^{Pr} which contains LiOTf and traces of 2.HOTf in a similar procedure. ¹H NMR (C₆D₆, 25 °C, 300 MHz): δ = 2.84 (t, 4H, 7.62 Hz, CH₂-CH₂-CH₂), 2.73 (s, 6H, CH₃-N), 2.66 (s, 6H, CH₃-N), 1.84-1.75 (CH₂-CH₂-CH₂), 1.72 (s, 4H, CH₂), 1.63 (s, 12H, CH₃-C=C), 1.46 (s, 12H, CH₃), 1.25 (s, 12H, CH₃) ppm. ¹³C{¹H} NMR (C₆D₆, 25 °C, 75 MHz): δ = 140.03 (NC=CNN), 122.50 (CH₃-C=C), 121.92 (CH₃-C=C), 112.56 (NC=CNN), 59.95 (CH₂), 59.56 (C(CH₃)₂), 42.13 (CH₃-N), 40.85 (CH₂-CH₂-CH₂), 39.77 (C(CH₃)₂), 33.42 (CH₃-N), 29.05 (C(CH₃)₂), 28.29 (C(CH₃)₂), 10.21 (CH₃-C=C), 9.98 (CH₃-C=C) ppm. Elemental analysis: Calculated (%) for C₃₃H₅₈N₆: C, 73.55; H, 10.85; N, 15.60; Found: C, 70.22; H, 10.88; N, 15.35.



Fig. S59 ¹H NMR spectrum of crystals of 4^{Pr} in C₆D₆ at RT.



Fig. S60 ${}^{13}C{}^{1}H$ NMR spectrum of crystals of 4^{Pr} in C₆D₆ at RT.

Synthesis of 5^{Pr}



10 mL THF solution of 4^{Pr} (217 mg, 0.403 mmol) was added dropwise to 10 mL THF solution of AgOTf (524 mg, 2.039 mmol) at room temperature while stirring. Immediately, black colored metallic silver precipitated out. After 4 hours all volatiles were removed under vacuum and the residue was dissolved in about 7 mL acetonitrile and decanted from dropper (first part). Again about 50 mL acetonitrile was added to the residue, stirred well and allowed to stand for settling down the black particles and then filtered (second part). The filtrate (second part) was evaporated to obtain a precipitate of 5^{Pr} . The acetonitrile solution (first part) was evaporated to obtain a precipitate of 5^{Pr} and this precipitate was washed with 10 mL of THF to remove excess silver triflate. Finally, 5^{Pr} was washed with ether and dried under vacuum. The ¹H NMR spectrum of the precipitate was measured, which showed the formation of pure **5**^{Pr}. **Yield:** 406 mg (89 %). A concentrated solution of 5^{Pr} in acetonitrile was kept for crystallization with diethyl ether diffusion at room temperature. Colorless crystals of 5^{Pr} were obtained after 6 hours which were suitable for X-ray structural analysis. 5^{Pr} is an air stable compound. M.P.: > 180 °C. ¹H NMR (CD₃CN, 25 °C, 300 MHz): δ = 4.24-4.19 (t, 4H, 8.20 Hz, CH₂-CH₂-CH₂), 3.72 (s, 12H, CH₃-N), 2.47 (s, 4H, CH₂), 2.33 (s, 12H, CH₃-C=C), 2.33 (br. 2H, CH₂-CH₂-CH₂), 1.84 (s, 12H, CH₃), 1.49 (s, 12H, CH₃) ppm. ¹³C{¹H} NMR $(CD_3CN, 25 \circ C, 75 \text{ MHz}): \delta = 182.44 (C=N^+), 134.87 (CH_3-C=C), 124.90 (CNN^+), 121.69 (q, {}^1J_{C-F} = 12.44 (C=N^+))$ 320.43 Hz, CF₃SO₃⁻), 85.07 (C(CH₃)₂), 55.90 (C(CH₃)₂), 48.33 (CH₂-CH₂-CH₂), 47.81 (CH₂), 36.09 (CH₃-N), 31.21 (CH₂-CH₂-CH₂), 27.93 (C(CH₃)₂), 26.80 (C(CH₃)₂), 9.37 (CH₃-C=C) ppm. ¹⁹F{¹H} NMR (CD₃CN, 25 °C, 282 MHz): δ = -79.21 ppm. Elemental analysis: Calculated (%) for C₃₇H₅₈N₆F₁₂O₁₂S₄: C, 39.15; H, 5.15; N, 7. 40; S, 11.30; Found: C, 39.37; H, 5.23; N, 7.70; S, 11.29. HRMS-ESI (m/z): Calculated for C₃₆H₅₈N₆F₉O₉S₃ [M-1OTf]³⁺: 985.3279, Found: 985.3246.



Fig. S61 ¹H NMR spectrum of compound 5^{Pr} in CD₃CN at RT.



Fig. S62 ¹³C{¹H} NMR spectrum of compound 5^{Pr} in CD₃CN at RT.



Fig. S63 $^{19}F\{^{1}H\}$ NMR spectrum of compound 5^{Pr} in CD_3CN at RT.

Reduction of 5^{Pr}



THF was added to the mixture of 5^{Pr} (75 mg, 0.066 mmol) and KC₈ (72 mg, 0.532 mmol) at -30 °C with stirring. After 6 hours stirring at room temperature, solvent and other volatiles were removed under vacuum and the ¹H NMR spectrum of the reaction mixture in C₆D₆ was measured which showed the formation of mostly 4^{Pr} along with the residual THF solvent.



Fig. S64 Overlay of the ¹H NMR spectra of the reaction mixture of 5^{Pr} and KC₈ (red) and 4^{Pr} (green) in C₆D₆ at RT.

Synthesis of 8^{Pr} Method I



A THF (15 mL) solution of AgOTf (100 mg, 0.389 mmol) was added to the THF (30 mL) solution of 4^{Pr} (95 mg, 0.176 mmol) dropwise with stirring at 0 °C. After 2 hours the ¹H NMR spectrum of reaction mixture was measured which showed the formation of 8^{Pr} along with the starting dication 3^{Pr}. This NMR spectrum was overlapping with the NMR spectrum of the comproportionation reaction between 4^{Pr} and 5^{Pr}. Solvent and other volatiles of the reaction mixture were removed under vacuum and acetonitrile (10 mL) was added to the residue, stirred and allowed to stand for six hours to settle down the black silver particles. Then the solution was decanted and then evaporated under vacuum to obtain 8^{Pr}. Yield: 106 mg (72%).

Method II



An acetonitrile solution of $Co(Cp)_2$ (15 mg, 0.079 mmol) was added dropwise to the acetonitrile solution (15 mL) of **5**^{Pr} (46 mg, 0.040 mmol) at room temperature with stirring. After 12 hours, solvent and other volatiles were removed under vacuum and the ¹H NMR spectrum of the reaction mixture was measured in CD₃CN which showed the formation of **8**^{Pr} along with cobaltocenium triflate. It was not possible to separate the cobaltocenium triflate and, hence, impossible to calculate the yield of the formation of **8**^{Pr}.

Method III



Acetonitrile was added to the mixture of 4Pr (80 mg, 0.148 mmol) and 5Pr (160 mg, 0.141 mmol) at room temperature and stirred for 12 hours. After that the solvent and other volatiles were evaporated and a foam like solid residue was obtained. The ¹H NMR spectrum of this residue was measured which showed the formation of two diastereomers of compound 8^{Pr}. Yield: 210 mg (87 %). Due to its complex nature we were not able to assign the NMR spectra unambiguously. ¹H NMR (CD₃CN, 25 °C, 300 MHz): δ = 6.08-6.12 (d, 14.0 Hz, 1H, CH=CH-CH₂ of one diastereomer), 5.99-6.04 (d, 14.0 Hz, 1H, CH=CH-CH₂ of another diastereomer), 4.62, 4.52, 4.43, 4.33, 4.31, 4.26, 4.24, 4.19, 4.10, 3.99, 3.95, 3.85, 3.76, 3.71, 3.69, 3.66, 3.65, 3.63, 3.46, 3.08, 2.94, 2.91, 2.64, 2.63, 2.51, 2.24, 2.22, 1.86, 1.82, 1.81, 1.78, 1.76, 1.43, 1.39, 1.37, 1.34, 1.31, 1.26, 1.22, 1.15, 1.13, 1.11, 1.02, 1.00, 0.84, 0.82, 0.80, 0.77, 0.72 ppm. ¹³C{¹H} NMR (CD₃CN, 25 °C, 75 MHz): δ = 144.43, 143.05, 142.83, 133.26 (*C*H=CH-CH₂ of one diastereomer), 132.99 (CH=CH-CH₂ of another diastereomer), 128.96, 128.86, 128.56, 128.39, 128.27, 127.94, 127.76, 127.72, 124.21, 119.96, 102.58 (CH=CH-CH₂ of one diastereomer), 102.13 (CH=CH-CH₂ of another diastereomer), 70.38, 68.61, 66.48, 65.95, 65.00, 63.42, 63.09, 62.07, 61.41, 56.96, 56.87, 56.82, 56.54, 55.29, 55.24, 49.53, 47.61, 43.78, 43.65, 43.39, 43.33, 43.27, 43.18, 35.00, 34.74, 34.55, 34.51, 33.97, 33.93, 33.80, 33.69, 33.42, 31.76, 31.42, 31.12, 31.03, 30.55, 30.25, 29.62, 27.94, 27.87, 27.50, 27.44, 27.28, 27.22, 27.13, 23.81, 22.85, 22.41, 9.10, 9.05, 8.99, 8.97, 8.84, 8.78, 8.75, 8.72, 8.67 ppm. ¹⁹F{¹H} NMR (CD₃CN, 25 °C, 282 MHz): δ = -79.23 ppm. Elemental analysis: Calculated (%) for C35H58N6F6O6S2: C, 50.23; H, 6.98; N, 10.04; S, 7.66; Found: C, 50.08; H, 6.81; N, 10.34; S, 7.17. HRMS-ESI (m/z): Calculated for C₃₃H₅₈N₆ [M-2OTf]: 269.2356, Found: 269.2359.

S58



Fig. S65 ¹H NMR spectrum of 8^{Pr} in its crude reaction mixture in CD₃CN at RT.



Fig. S66 ${}^{13}C{}^{1}H$ NMR spectrum of 8^{Pr} in its crude reaction mixture in CD₃CN at RT.



Fig. S67 ¹⁹F{¹H} NMR spectrum of 8^{Pr} in its crude reaction mixture in CD₃CN at RT.

Synthesis of 9^{Pr}



About 40 mL of toluene was added into a 50 mL Schlenk flask containing 8^{Pr} (prepared by comproportionation reaction between 5^{Pr} and 4^{Pr}) (630 mg, 0.753 mmol) and solid LDA (200 mg, 1.864 mmol) at room temperature with stirring. After 18 hours stirring at room temperature the reaction mixture was filtered and the filtrate was evaporated to obtain a reddish brown oily type of liquid. The ¹H, ⁷Li and ¹⁹F NMR spectrum of this oily compound showed the presence of **9**^{Pr} along with lithium triflate compound. Then pentane (2 x 20 mL) was added to it, stirred well and filtered and the filtrate was concentrated up to 5 mL and kept for crystallization at -35 °C. After 24 hours, colorless crystals (150 mg + 70 mg) were collected which were suitable for single crystal X-ray diffraction. Yield: 220 mg (54 %). M.P.: 121 °C. ¹H NMR (C₆D₆, 25 °C, 300 MHz): δ = 6.15-6.19 (d, 1H, 12.90 Hz, CH=CH-CH₂), 3.80-3.89 (m, 1H, CH=CH-CH₂), 3.68-3.70 (d, 2H, 5.50 Hz, CH=CH-CH₂), 2.80 (s, 3H, CH₃-N), 2.78 (s, 3H, CH₃-N), 2.76 (s, 3H, CH₃-N), 2.44 (s, 3H, CH₃-N), 1.78 (s, 2H, CH₂), 1.68 (s, 2H, CH₂), 1.68 (s, 3H, CH₃-C=C), 1.66 (s, 3H, CH₃-C=C), 1.63 (s, 3H, CH₃-C=C), 1.60 (s, 3H, CH₃-C=C), 1.50 (s, 6H, C(CH₃)₂), 1.40 (s, 6H, C(CH₃)₂), 1.38 (s, 6H, C(CH₃)₂), 1.28 (s, 6H, C(CH₃)₂) ppm. ¹³C{¹H} NMR (C₆D₆, 25 °C, 75 MHz): δ = 143.06 (NC=CNN), 140.01 (NC=CNN), 127.41 (CH=CH-CH₂), 122.40 (CH₃-C=C), 121.87 (CH₃-C=C), 121.25 (CH₃-C=C), 119.73 (CH₃-C=C), 114.47 (NC=CNN), 102.80 (NC=CNN), 97.68 (CH=CH-CH₂), 60.85 (CH₂), 60.16 (CH₂), 59.85 (C(CH₃)₂), 59.29 (C(CH₃)₂), 44.88 (CH=CH-CH₂), 42.59 (CH₃-N), 42.31 (CH₃-N), 39.93 (C(CH₃)₂), 39.89 (C(CH₃)₂), 32.74 (CH₃-N), 32.21 (CH₃-N), 29.55 (C(CH₃)₂), 28.33 (C(CH₃)₂), 10.30 (CH₃-C=C), 10.06 (CH₃-C=C), 10.02 (CH₃-C=C), 9.56 (CH₃-C=C) ppm. Most likely due to high air and moisture sensitivity we were not able to get satisfactory elemental analysis data even after repeating measurements.



Fig. S68 ¹H NMR spectrum of compound 9^{Pr} in C₆D₆ at RT.



Fig. S69 $^{13}C\{^{1}H\}$ NMR spectrum of compound 9^{Pr} in C_6D_6 at RT.

Molecular Structures of 3^{Cy}, 5^{Cy}, 3^{Et}, 4^{Et}, 5^{Et}, 8^{Et}, 9^{Et}, 10^{Et}, 3^{Pr}, 4^{Pr}, 5^{Pr}, and 9^{Pr}



Fig. S70 Molecular structure of 3^{Cy} (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C2, C4 and C5 are omitted for clarity.



Fig. S71 Molecular structure of 5^{cy} in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, and C1' are omitted for clarity.



Fig. S72 Molecular structure of **3**^{Et} (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C1', C2 and C2' are omitted for clarity.



Fig. S73 Molecular structure of 4^{Et} in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1 and C1' are omitted for clarity.



Fig. S74 Molecular structure of 5^{Et} in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms are omitted for clarity.



Fig. S75 Molecular structure of **8**^{Et} (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1 and C1'are omitted for clarity.



Fig. S76 Molecular structure of 9^{Et} in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1 and C1' are omitted for clarity.



Fig. S77 Molecular structure of **10**^{Et} (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1 and C1'are omitted for clarity.



Fig. S78 Molecular structure of 3^{Pr} (*meso*-isomer) in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C2, C4, C5 and C7 are omitted for clarity.



Fig. S79 Molecular structure of 4^{Pr} in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C4 and C7 are omitted for clarity.



Fig. S80 Molecular structure of 5^{Pr} in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C4 and C7 are omitted for clarity.



Fig. S81 Molecular structure of **9**^{Pr} in the solid state with thermal ellipsoids at the 50 % probability level. All hydrogen atoms except on C1, C2 and C5 are omitted for clarity.

Crystallographic Details

Single-crystal X-ray diffraction data of 3^{Cy}, 5^{Cy}, 6^{Cy}, 7^{Cy}, 3^{Et}, 4^{Et}, 5^{Et}, 8^{Et}, 9^{Et}, 10^{Et}, 3^{Pr}, 4^{Pr}, and 9^{Pr} were collected using a Rigaku diffractometer with graphite-monochromated molybdenum Ka radiation, $\lambda =$ 0.71073 Å. For 5^{Pr} diffraction data was collected using a STOE-IPDS 2T diffractometer with graphitemonochromated molybdenum Ka radiation, $\lambda = 0.71073$ Å. Data integration and reduction were processed with CrysAlisPro (Rigaku) or XArea (STOE) software.^{S5} An empirical absorption correction was applied to the collected reflections with SCALE3 ABSPACK integrated with CrysAlisPro. The applied absorption correction for the STOE measurement was numerical (face indexed) using X-Shape and X-Red32 as implemented in XArea. The structures were solved by direct methods using SHELXT^{S6} and refined by full matrix least-squares method based on P² by using SHELXL^{S7} through the Olex2^{S8} interface. All non-hydrogen-atoms were refined with anisotropic displacement parameters. The hydrogen atoms, unless stated otherwise, were refined isotropically on calculated positions using a riding model with their $U_{\rm iso}$ values constrained to 1.5 $U_{\rm eq}$ of their pivot atoms for terminal sp³ carbon atoms and 1.2 times for the aromatic carbon atoms. Crystal and structure refinement data of all these compounds are summarized in Tables S1-S14. Individual reflexes which were clear outliers were removed from the refinements with OMIT instructions. The crystal of 3^{cy} was of minor quality (weak diffraction, some thermal motion). This results in some reflexes missing from the data set and generating a B-alert. One pyrrolidine moiety is disordered comprising one iPr and a methylene group. For the pyrrolidine disorder only SAME was used as constraint; occupancies are 52% and 48%. One of the triflate anions is also disordered, which was modelled with SAME, SIMU and DELU constraints; occupancies are 77% and 23%. There is also some motion in the second triflate and in the imidazol moiety. Modelling this as disorder did not improve the refinement and was abandoned. In the structure of 5^{Cy} approximately ten very mobile water molecules per formula are co-crystallized. The respective diffuse electron density was SQUEEZED^[S9] from the refinement. The two triflate anions in the asymmetric unit are disordered entirely over two orientations. Occupancies are 66% vs. 34% and 77% vs. 23%. These disorders were treated with SAME, SIMU and DELU constraints. In addition there is a disorder of a methylene carbon in the nonaromatic fivefold ring (ring pucker). Occupancies are 54% vs. 46%. The model was refined without any constraints or restraints. In the structure of 6^{Cy} one C(CH₃)₂ moiety is disordered over two orientations. This was modelled with three SADI constraints plus SIMU and DELU. Occupancies are 80% vs. 20%. The two triflate anions are disordered entirely. This was modelled with SAME, SIMU and DELU constraints. Occupancies are 65% vs. 35% for one and 63% vs. 37% for the other anion. The two isopropyl hydrogen atoms were found and refined freely. The structure was further refined as inversion twin with roughly 26% of the minor domain being part of the data set. In the structure of 7^{Cy} two of the triflates are disordered entirely with occupancies of 62% and 38% and of 51% and 49%, respectively. One triflate has a disorder only in the SO₃ moiety with occupancies of 65% and 35%. All disorders were modelled with SAME, SIMU and DELU constraints. In the structure of 3^{Et} the triflate anion is disordered over two positions which are both well refined and have occupancies of 89% and 11%. Only for the CF3 moiety of the minor occupancy constraints had to be used (SIMU and DELU). All other atoms of the disorder are refined freely. Half of the cation is refined in the asymmetric unit. The second half is generated by symmetry operation (inversion centre). This renders the diastereomer necessarily to be the meso-isomer. Symmetry generation and meso-isomer form are the same also for the structures of 8^{Et} and 10^{Et}. The refinements of 4^{Et}, 4^{Pr} and 5^{Et} were unremarkable. In the structure of 8^{Et} two disorder problems are present. The triflate anion is disordered by a rotation over two orientations with occupancies of 70% and 30%. The disorder was treated with SAME, SIMU and DELU constraints for all atoms of this disorder. Secondly the CAAC rings are disordered with a distinct ring pucker which extends to all of the associated methyl substituents with occupancies of 79% and 21%. This disorder was treated only with a SAME constraint; i.e. thermal displacement parameters are refined freely. The H-atom of the ethenyl bridge was located and refined freely (no constraints or restraints) proving that it is indeed an ethenyl bridge (only one H was refined, the second is symmetry generated). In the structure of **10^{Et}** also two disorder problems are present. One of the two triflate anions is located directly on a two-fold rotoinversion axis (this axis and the C-S molecule axis are aligned). Therefore, all respective occupancies are fixed at 50% while all else was refined freely. PART -1 was used for all O and F atoms so that they do not bind their symmetry generated direct neighbors. The CAAC ring exhibits the exact same disorder as found for 8^{Et}. For **10**^{Et} occupancies of 50% and 50% were observed. The disorder was treated again only with a SAME constraint. The H-atom of the ethenyl bridge (similar to 8^{Et}) and the methine H-atom on the CAAC carbon atom bound to the NHC ring were both located and refined freely (no constraints or restraints). In the refinement of 9^{Et} the H-atom of the ethenyl bridge was located and refined freely (no constraints or restraints; similar to the structures of 8^{Et} and 10^{Et}). In the structure of 3^{Pr} two triflate anions are disordered; one in its entirely with occupancies of 60% and 40%, the other only with its O and F atoms (while C and S are not disordered) and occupancies of 54% and 46%. All atoms of the entirely disordered anion are constrained with SAME, SIMU and DELU commands. For the second anion only SAME was used for the O and F atoms. The methane hydrogen atoms on C4 and C19 were found and refined freely. The refinement of the data for 9^{Pr} was unremarkable. The hydrogen atoms on the central ene-moiety (C1 and C17) were found and refined freely. The checkcif-file for the structure of 5^{Pr} contains one B-alert. This refers to the proximity of one O and one N without them being in a hydrogen bond interaction for the absence of H. Based on spectroscopic data it is certain that the N is not protonated and neither is the triflate. The proximity therefore goes back to crystal packing. Isolated electron density indicative of an actual atom site was refined as half a molecule (fixed to 0.5) of water per formula after the electron count was established using the SQUEEZE routine in PLATON. The reported structure is unsqueezed. The hydrogen atoms were located but had to be constrained. All O-H and H-H distances are fixed to the ideal water geometry (DFIX). The displacement factors of H were constrained to the parent oxygen atom with a factor of 1.2. One fivefold ring is slightly disordered with a small ring pucker. This was modelled with SADI, SIMU and DELU constraints. Occupancies are 84% and 16%. One of the triflate anions is disordered entirely, which was modelled with SAME, SIMU and DELU constraints. Occupancies are 75% and 25%.

Identification code	aj1925r
Empirical formula	$C_{38}H_{64}N_6O_6F_6S_2$
Formula weight	879.07
Temperature/K	250(2)
Crystal system	monoclinic
Space group	P21/c
a/Å	9.1161(4)
b/Å	46.1464(16)
c/Å	11.2799(6)
α/°	90
β/°	105.642(5)
γ/°	90
Volume/ų	4569.4(4)
Z	4
ρ _{calc} g/cm ³	1.278
µ/mm ⁻¹	0.189
µ/mm ⁻¹ F(000)	0.189 1872.0
µ/mm ⁻¹ F(000) Crystal size/mm ³	0.189 1872.0 0.106 × 0.094 × 0.092
µ/mm ⁻¹ F(000) Crystal size/mm ³ Radiation	0.189 1872.0 0.106 × 0.094 × 0.092 ΜοΚα (λ = 0.71073)
µ/mm ⁻¹ F(000) Crystal size/mm ³ Radiation 2Θ range for data collection/°	0.189 1872.0 0.106 × 0.094 × 0.092 ΜοΚα (λ = 0.71073) 5.344 to 52.744
µ/mm ⁻¹ F(000) Crystal size/mm ³ Radiation 2Θ range for data collection/° Index ranges	0.189 1872.0 0.106 × 0.094 × 0.092 MoKa (λ = 0.71073) 5.344 to 52.744 -11 ≤ h ≤ 11, -57 ≤ k ≤ 47, -12 ≤ l ≤ 14
µ/mm ⁻¹ F(000) Crystal size/mm ³ Radiation 2Θ range for data collection/° Index ranges Reflections collected	0.189 1872.0 0.106 × 0.094 × 0.092 MoKa (λ = 0.71073) 5.344 to 52.744 -11 ≤ h ≤ 11, -57 ≤ k ≤ 47, -12 ≤ ≤ 14 32348
µ/mm ⁻¹ F(000) Crystal size/mm ³ Radiation 2Θ range for data collection/° Index ranges Reflections collected Independent reflections	0.189 1872.0 0.106 × 0.094 × 0.092 MoKa (λ = 0.71073) 5.344 to 52.744 -11 ≤ h ≤ 11, -57 ≤ k ≤ 47, -12 ≤ l ≤ 14 32348 9288 [R _{int} = 0.0469, R _{sigma} = 0.0557]
μ/mm ⁻¹ F(000) Crystal size/mm ³ Radiation 2Θ range for data collection/° Index ranges Reflections collected Independent reflections Data/restraints/parameters	0.189 1872.0 0.106 × 0.094 × 0.092 MoKa (λ = 0.71073) 5.344 to 52.744 -11 ≤ h ≤ 11, -57 ≤ k ≤ 47, -12 ≤ l ≤ 14 32348 9288 [Rint = 0.0469, R _{sigma} = 0.0557] 9288/579/651
µ/mm ⁻¹ F(000) Crystal size/mm ³ Radiation 2Θ range for data collection/° Index ranges Reflections collected Independent reflections Data/restraints/parameters Goodness-of-fit on F ²	0.189 1872.0 0.106 × 0.094 × 0.092 MoK α (λ = 0.71073) 5.344 to 52.744 -11 ≤ h ≤ 11, -57 ≤ k ≤ 47, -12 ≤ I ≤ 14 32348 9288 [Rint = 0.0469, R _{sigma} = 0.0557] 9288/579/651 1.054
μ /mm ⁻¹ F(000) Crystal size/mm ³ Radiation 2 Θ range for data collection/° Index ranges Reflections collected Independent reflections Data/restraints/parameters Goodness-of-fit on F ² Final R indexes [I>=2 σ (I)]	0.189 1872.0 0.106 × 0.094 × 0.092 MoKa (λ = 0.71073) 5.344 to 52.744 -11 ≤ h ≤ 11, -57 ≤ k ≤ 47, -12 ≤ I ≤ 14 32348 9288 [Rint = 0.0469, R _{sigma} = 0.0557] 9288/579/651 1.054 R ₁ = 0.0756, wR ₂ = 0.2015
µ/mm ⁻¹ F(000) Crystal size/mm ³ Radiation 2Θ range for data collection/° Index ranges Reflections collected Independent reflections Data/restraints/parameters Goodness-of-fit on F ² Final R indexes [I>=2σ (I)] Final R indexes [all data]	0.189 1872.0 0.106 × 0.094 × 0.092 MoKa (λ = 0.71073) 5.344 to 52.744 -11 ≤ h ≤ 11, -57 ≤ k ≤ 47, -12 ≤ I ≤ 14 32348 9288 [Rint = 0.0469, R _{sigma} = 0.0557] 9288/579/651 1.054 R ₁ = 0.0756, wR ₂ = 0.2015 R ₁ = 0.1226, wR ₂ = 0.2238

 Table S1. Crystal data and structure refinement for 3^{Cy} (CCDC 2161956)

Identification code	aj1944r_sq
Empirical formula	$C_{40}H_{82}N_6O_{22}F_{12}S_4$
Formula weight	1355.35
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.1305(3)
b/Å	11.4290(3)
c/Å	13.7220(4)
α/°	92.322(2)
β/°	99.653(2)
γ/°	113.256(2)
Volume/ų	1570.03(8)
Z	1
ρ _{calc} g/cm ³	1.433
µ/mm ⁻¹	0.260
F(000)	712.0
Crystal size/mm ³	0.376 × 0.237 × 0.219
Radiation	ΜοΚα (λ = 0.71073)
2O range for data collection/°	5.088 to 57.844
Index ranges	$-13 \le h \le 14$, $-14 \le k \le 13$, $-17 \le l \le 18$
Reflections collected	27333
Independent reflections	7324 [$R_{int} = 0.0336$, $R_{sigma} = 0.0350$]
Data/restraints/parameters	7324/1180/498
Goodness-of-fit on F ²	1.043
Final R indexes [I>=2σ (I)]	$R_1 = 0.0636, wR_2 = 0.1887$
Final R indexes [all data]	$R_1 = 0.0937$, $wR_2 = 0.2043$
Largest diff. peak/hole / e Å ⁻³	0.37/-0.24

Table S2. Crystal data and structure refinement for 5^{Cy} (CCDC2161957).
Identification code	aj2007
Empirical formula	$C_{42}H_{68}N_8O_6F_6S_2$
Formula weight	959.16
Temperature/K	297(2)
Crystal system	orthorhombic
Space group	Pna21
a/Å	27.5528(14)
b/Å	8.4292(5)
c/Å	22.0477(12)
α/°	90
β/°	90
γ/°	90
Volume/ų	5120.5(5)
Z	4
ρ _{calc} g/cm ³	1.244
µ/mm ⁻¹	0.176
F(000)	2040.0
Crystal size/mm ³	0.518 × 0.357 × 0.21
Radiation	ΜοΚα (λ = 0.71073)
2Θ range for data collection/°	5.174 to 54.204
Index ranges	$-35 \le h \le 35, -10 \le k \le 10, -28 \le l \le 22$
Reflections collected	62744
Independent reflections	10191 [$R_{int} = 0.0555$, $R_{sigma} = 0.0426$]
Data/restraints/parameters	10191/1525/780
Goodness-of-fit on F ²	1.026
Final R indexes [I>=2σ (I)]	$R_1 = 0.0741, wR_2 = 0.2041$
Final R indexes [all data]	$R_1 = 0.1046, wR_2 = 0.2258$
Largest diff. peak/hole / e Å-3	0.53/-0.31
Flack parameter	0.26(19)

 Table S3. Crystal data and structure refinement for 6^{Cy} (CCDC 2161958)

Identification code	aj2030
Empirical formula	C41H65F9N7O9S3
Formula weight	1067.18
Temperature/K	250(2)
Crystal system	monoclinic
Space group	P21/n
a/Å	13.7065(5)
b/Å	11.8374(5)
c/Å	32.3229(16)
α/°	90
β/°	91.669(4)
γ/°	90
Volume/ų	5242.1(4)
Z	4
ρ _{calc} g/cm ³	1.352
µ/mm ⁻¹	0.229
F(000)	2244.0
Crystal size/mm ³	0.058 × 0.037 × 0.022
Radiation	ΜοΚα (λ = 0.71073)
2Θ range for data collection/°	5.044 to 50.052
Index ranges	$-15 \le h \le 16, -14 \le k \le 14, -34 \le l \le 38$
Reflections collected	39048
Independent reflections	9249 [$R_{int} = 0.1234, R_{sigma} = 0.0948$]
Data/restraints/parameters	9249/1296/822
Goodness-of-fit on F ²	1.068
Final R indexes [I>=2σ (I)]	$R_1 = 0.0641, wR_2 = 0.1779$
Final R indexes [all data]	$R_1 = 0.1031, wR_2 = 0.1938$
Largest diff. peak/hole / e Å ⁻³	0.80/-0.39

 Table S4. Crystal data and structure refinement for 7^{Cy} (CCDC 2161959).

Identification code	AJ0064
Empirical formula	$C_{34}H_{58}F_6N_6O_6S_2$
Formula weight	824.98
Temperature/K	127.15
Crystal system	monoclinic
Space group	P21/c
a/Å	9.4465(5)
b/Å	20.4280(8)
c/Å	11.4500(7)
α/°	90
β/°	112.936(7)
γ/°	90
Volume/ų	2034.9(2)
Z	2
p _{calc} g/cm ³	1.346
µ/mm ⁻¹	0.208
F(000)	876.0
Crystal size/mm ³	0.44 × 0.37 × 0.10
Radiation	ΜοΚα (λ = 0.71073)
2 Θ range for data collection/°	5.17 to 53
Index ranges	$-11 \le h \le 11, -25 \le k \le 25, -13 \le l \le 14$
Reflections collected	17318
Independent reflections	4206 [$R_{int} = 0.0350, R_{sigma} = 0.0300$]
Data/restraints/parameters	4206/24/325
Goodness-of-fit on F ²	1.047
Final R indexes [I>=2σ (I)]	$R_1 = 0.0410, wR_2 = 0.1081$
Final R indexes [all data]	$R_1 = 0.0487$, $wR_2 = 0.1127$
Largest diff. peak/hole / e Å ⁻³	0.95/-0.32

 Table SS5. Crystal data and structure refinement for 3^{Et} (CCDC 2047110).

Identification code	AJ0381
Empirical formula	C ₃₂ H ₅₆ N ₆
Formula weight	524.82
Temperature/K	120(2)
Crystal system	monoclinic
Space group	P21/n
a/Å	7.9568(4)
b/Å	18.1921(10)
c/Å	11.2323(7)
α/°	90
β/°	107.697(6)
٧/°	90
Volume/Å ³	1548.94(16)
Z	2
ρ _{calc} g/cm ³	1.125
µ/mm ⁻¹	0.067
<i>F</i> (000)	580.0
Crystal size/mm ³	0.316 × 0.142 × 0.127
Radiation	ΜοΚα (λ = 0.71073)
2O range for data collection/°	5.562 to 52.726
Index ranges	$-8 \le h \le 9, -21 \le k \le 22, -14 \le l \le 12$
Reflections collected	10872
Independent reflections	$3153 [R_{int} = 0.0332, R_{sigma} = 0.0358]$
Data/restraints/parameters	3153/0/180
Goodness-of-fit on F ²	1.051
Final R indexes [I>=2σ (I)]	$R_1 = 0.0473$, w $R_2 = 0.1096$
Final R indexes [all data]	$R_1 = 0.0611, wR_2 = 0.1146$
l argest diff_peak/hole / e Å ⁻³	0.23/-0.20

Table S6. Crystal data and structure refinement for 4^{Et} (CCDC 2047111).

Identification code	AJ1406
Empirical formula	$C_{36}H_{56}F_{12}N_6O_{12}S_4$
Formula weight	1121.10
Temperature/K	101.15
Crystal system	monoclinic
Space group	P21/n
a/Å	12.7027(3)
b/Å	13.3266(3)
c/Å	14.3241(3)
α/°	90
β/°	93.044(2)
γ/°	90
Volume/ų	2421.42(9)
Z	2
ρ _{calc} g/cm ³	1.538
µ/mm ⁻¹	0.306
F(000)	1164.0
Crystal size/mm ³	0.32 × 0.23 × 0.15
Radiation	ΜοΚα (λ = 0.71073)
2O range for data collection/°	5.696 to 52.744
Index ranges	$-15 \le h \le 15, -16 \le k \le 16, -17 \le l \le 17$
Reflections collected	29135
Independent reflections	$4938 \; [R_{int} = 0.0288, R_{sigma} = 0.0189]$
Data/restraints/parameters	4938/0/324
Goodness-of-fit on F ²	1.030
Final R indexes [I>=2σ (I)]	$R_1 = 0.0309, wR_2 = 0.0763$
Final R indexes [all data]	$R_1 = 0.0338$, $wR_2 = 0.0778$
Largest diff. peak/hole / e Å ⁻³	0.38/-0.42

 Table SS7. Crystal data and structure refinement for 5^{Et} (CCDC 2047114).

Identification code	AJ1408
Empirical formula	$C_{42}H_{72}F_6N_6O_8S_2$
Formula weight	967.17
Temperature/K	100.15
Crystal system	monoclinic
Space group	P21/c
a/Å	10.2368(4)
b/Å	11.7148(5)
c/Å	20.4531(8)
α/°	90
β/°	92.856(3)
γ/°	90
Volume/Å ³	2449.73(17)
Z	2
$ ho_{calc}g/cm^3$	1.311
µ/mm ⁻¹	0.186
F(000)	1032.0
Crystal size/mm ³	0.24 × 0.19 × 0.15
Radiation	ΜοΚα (λ = 0.71073)
2O range for data collection/°	5.292 to 52.746
Index ranges	$-11 \le h \le 12, -13 \le k \le 14, -25 \le l \le 25$
Reflections collected	18267
Independent reflections	5003 [$R_{int} = 0.0643$, $R_{sigma} = 0.0556$]
Data/restraints/parameters	5003/381/424
Goodness-of-fit on F ²	1.028
Final R indexes [I>=2σ (I)]	$R_1 = 0.0607, wR_2 = 0.1635$
Final R indexes [all data]	$R_1 = 0.0734, wR_2 = 0.1747$
Largest diff. peak/hole / e Å ⁻³	0.75/-0.55

Table S8. Crystal data and structure refinement for 8^{Et} (CCDC 2047112).

Identification code	AJ1445
Empirical formula	C ₃₂ H ₅₄ N ₆
Formula weight	522.81
Temperature/K	120.15
Crystal system	triclinic
Space group	P-1
a/Å	8.4164(4)
b/Å	9.9098(3)
c/Å	10.3761(4)
α/°	101.120(3)
β/°	111.201(4)
γ/°	93.802(3)
Volume/ų	782.89(6)
Z	1
ρ _{calc} g/cm ³	1.109
µ/mm ⁻¹	0.066
F(000)	288.0
Crystal size/mm ³	0.26 × 0.21 × 0.19
Radiation	ΜοΚα (λ = 0.71073)
2O range for data collection/°	5.378 to 52.738
Index ranges	$-10 \le h \le 10, -12 \le k \le 10, -11 \le l \le 12$
Reflections collected	14448
Independent reflections	$3204 [R_{int} = 0.0414, R_{sigma} = 0.0321]$
Data/restraints/parameters	3204/0/184
Goodness-of-fit on F ²	1.064
Final R indexes [I>=2σ (I)]	$R_1 = 0.0441, wR_2 = 0.1144$
Final R indexes [all data]	$R_1 = 0.0518$, $wR_2 = 0.1189$
Largest diff. peak/hole / e Å ⁻³	0.38/-0.19

Table S9. Crystal data and structure refinement for 9^{Et} (2047115).

Identification code	AJ1512
Empirical formula	C35H56F9N6O9S3
Formula weight	972.03
Temperature/K	100.15
Crystal system	monoclinic
Space group	l2/a
a/Å	11.2729(4)
b/Å	20.2466(7)
c/Å	19.5699(6)
α/°	90
β/°	92.742(3)
γ/°	90
Volume/ų	4461.5(3)
Z	4
ρ _{calc} g/cm ³	1.447
µ/mm ⁻¹	0.261
F(000)	2036.0
Crystal size/mm ³	0.23 × 0.19 × 0.14
Radiation	ΜοΚα (λ = 0.71073)
2O range for data collection/°	5.736 to 52.742
Index ranges	$-13 \le h \le 14, -25 \le k \le 19, -24 \le l \le 24$
Reflections collected	28001
Independent reflections	4552 [$R_{int} = 0.0328$, $R_{sigma} = 0.0239$]
Data/restraints/parameters	4552/6/374
Goodness-of-fit on F ²	1.064
Final R indexes [I>=2σ (I)]	$R_1 = 0.0477, wR_2 = 0.1245$
Final R indexes [all data]	$R_1 = 0.0542, wR_2 = 0.1281$
Largest diff. peak/hole / e Å-3	0.61/-0.50

 Table S10. Crystal data and structure refinement for 10^{Et} (CCDC 2047113).

Identification code	aj0161rt
Empirical formula	$C_{35}H_{60}N_6O_6F_6S_2$
Formula weight	839.01
Temperature/K	190(2)
Crystal system	monoclinic
Space group	P21/c
a/Å	16.4086(4)
b/Å	22.9375(7)
c/Å	11.3222(3)
α/°	90
β/°	97.679(2)
γ/°	90
Volume/Å ³	4223.1(2)
Z	4
p _{calc} g/cm ³	1.320
µ/mm ⁻¹	0.201
F(000)	1784.0
Crystal size/mm ³	0.42 × 0.307 × 0.269
Radiation	ΜοΚα (λ = 0.71073)
2Θ range for data collection/°	5.004 to 57.886
Index ranges	$-21 \le h \le 19, -25 \le k \le 30, -15 \le l \le 15$
Reflections collected	56617
Independent reflections	9882 [$R_{int} = 0.0868, R_{sigma} = 0.0483$]
Data/restraints/parameters	9882/567/648
Goodness-of-fit on F ²	1.035
Final R indexes [I>=2σ (I)]	$R_1 = 0.0577, wR_2 = 0.1588$
Final R indexes [all data]	$R_1 = 0.0775, wR_2 = 0.1709$
Largest diff. peak/hole / e Å ⁻³	0.35/-0.33

 Table S11. Crystal data and structure refinement for 3^{Pr} (CCDC 2161952).

Table S12. Crystal	data and structure	refinement for 4Pr	(CCDC 2161953).
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Identification code	aj1872
Empirical formula	C33H58N6
Formula weight	538.85
Temperature/K	250(2)
Crystal system	monoclinic
Space group	P21/c
a/Å	11.5251(10)
b/Å	28.9745(15)
c/Å	11.6064(9)
α/°	90
β/°	119.306(11)
γ/°	90
Volume/Å ³	3379.7(5)
Z	4
p _{calc} g/cm ³	1.059
µ/mm ⁻¹	0.063
F(000)	1192.0
Crystal size/mm ³	0.27 × 0.23 × 0.18
Radiation	ΜοΚα (λ = 0.71073)
2Θ range for data collection/°	5.83 to 58.088
Index ranges	$-14 \le h \le 15, -37 \le k \le 38, -15 \le l \le 15$
Reflections collected	58618
Independent reflections	8242 [$R_{int} = 0.0388$, $R_{sigma} = 0.0295$]
Data/restraints/parameters	8242/0/368
Goodness-of-fit on F ²	1.046
Final R indexes [I>=2σ (I)]	$R_1 = 0.0529, wR_2 = 0.1333$
Final R indexes [all data]	$R_1 = 0.0805, wR_2 = 0.1449$
Largest diff. peak/hole / e Å ⁻³	0.29/-0.20

Identification code	mk645
Empirical formula	C37H59F12N6O12.5S4
Formula weight	1144.14
Temperature/K	170(2)
Crystal system	monoclinic
Space group	P21/c
a/Å	14.521(3)
b/Å	11.291(2)
c/Å	30.821(6)
α/°	90
β/°	93.80(3)
γ/°	90
Volume/Å ³	5042.4(18)
Z	4
ρ _{calc} g/cm ³	1.507
µ/mm⁻¹	0.296
F(000)	2380.0
Crystal size/mm ³	0.31 × 0.102 × 0.057
Radiation	ΜοΚα (λ = 0.71073)
29 range for data collection/°	3.988 to 59.022
Index ranges	-20 ≤ h ≤ 20, -15 ≤ k ≤ 13, -42 ≤ l ≤ 42
Reflections collected	56832
Independent reflections	13960 [$R_{int} = 0.1030, R_{sigma} = 0.0738$]
Data/restraints/parameters	13960/423/755
Goodness-of-fit on F ²	1.040
Final R indexes [I>=2σ (I)]	$R_1 = 0.0548$, $wR_2 = 0.1153$
Final R indexes [all data]	$R_1 = 0.1276, wR_2 = 0.1442$
Largest diff. peak/hole / e Å-3	0.41/-0.53

Table S13. Crystal data and structure refinement for 5^{Pr} (CCDC 2204009)

Table S14.	Crystal data	and structure	refinement for	r 9^{Pr} (CCDC 2	161955).

Identification code	aj1992
Empirical formula	C ₃₃ H ₅₆ N ₆
Formula weight	536.83
Temperature/K	297(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.4000(5)
b/Å	10.3658(7)
c/Å	20.0368(13)
α/°	78.183(5)
β/°	79.823(5)
γ/°	82.783(5)
Volume/Å ³	1673.56(19)
Z	2
ρ _{calc} g/cm ³	1.065
µ/mm ⁻¹	0.064
F(000)	592.0
Crystal size/mm ³	0.423 × 0.352 × 0.274
Radiation	ΜοΚα (λ = 0.71073)
2⊝ range for data collection/°	5.066 to 57.788
Index ranges	$-11 \le h \le 10, -13 \le k \le 13, -26 \le l \le 22$
Reflections collected	29087
Independent reflections	7703 [$R_{int} = 0.0721, R_{sigma} = 0.0687$]
Data/restraints/parameters	7703/0/376
Goodness-of-fit on F ²	1.082
Final R indexes [I>=2σ (I)]	$R_1 = 0.0602, wR_2 = 0.1675$
Final R indexes [all data]	R ₁ = 0.0873, wR ₂ = 0.1818
Largest diff. peak/hole / e Å ⁻³	0.24/-0.28

EPR Spectroscopy



Fig. S82 Variable temperature X-band EPR spectra of 6^{Cy} in a 1:1 toluene/acetonitrile mixture between 10 and 140 K for the g = 2.



Fig. S83 Three different representations of the temperature dependence of the double integral EPR intensity (*A*) of 6^{Cy} in a 1:1 toluene/acetonitrile mixture. Circles (°) represent the experimental results and the red line corresponds to the fit with the Bleaney-Bowers equation.



Fig. S84 Experimental EPR spectrum of 6^{Cy} in acetonitrile. The signal is centered around $g_{iso} = 2.0029$.



Fig. S85 EPR spectra of a solid sample of 6^{Cy}, before (blue) and after heating at 80 °C for 1 h (red).



Fig. S86 EPR spectra of **6**^{Cy} in a mixture of acetonitrile and toluene, before (blue) and after heating at 80 °C for 1 h (red).



Fig. S87 Experimental (black) and simulated (red) X-band EPR spectra of 10^{Et} in acetonitrile. The simulation parameters are: $g_{iso} = 2.0034$, $a(^{14}N) = 22.3$ MHz (2N), $a(^{1}H) = 36.7$ MHz (2H), and $a(^{1}H) = 11.7$ MHz (2H).

Magnetic Study of 6^{Cy}



Fig. S88 Plot of magnetic susceptibility versus temperature for 6^{Cy}.

As we know curie Weiss law: $1/\chi = \theta/C - T/C$ From the plot: $y = 1.65765^*x + 5.0814$

 $1/C = -1.65765, C = -0.6033, \theta/C = 5.0814, \theta = -3.065$

Cyclic Voltammetry

All electrochemical measurements were carried out using a conventional three-electrode cell system, with an METROHM PGStat 204 potentiostat/galvanostat apparatus controlled by the software NOVA 2.1.4 in an argon glove box. A glassy carbon disc electrode (d = 3 mm) served as working electrode and a platinum wire was used as pseudo-reference and auxiliary electrode respectively. The performed electrochemical methods were cyclic voltammetry (at various scan rates) and differential pulse voltammetry (DPV) (step: 5 mV; modulation amplitude: 25 mV; modulation time: 0.05 s; interval time: 0.5 s). All voltammograms were referenced against Fc/Fc⁺ = 0 V. The electrochemical measurements were undertaken at room temperature by dissolving ca. 1.0 x 10⁻⁵ mol of analyte in 30 mL acetonitrile containing 0.1 mol l⁻¹ Bu₄NPF₆ electrolyte.

Compounds	<i>Epk</i> (100	Ера (100	<i>E</i> _{1/2} (100	<i>Epk</i> (1000	Ера (1000	<i>E</i> _{1/2} (1000
	mV/s) [V]	mV/s) [V]	mV/s) [V]	mV/s) [V]	mV/s) [V]	mV/s) [V]
	-0.950	-0.908,	-0.929,	-0.898	-0.855,	-0.876,
ECV	(shoulder),	-1.002	-1.036,	(shoulder),	-0.956	-0.957,
5.2	-1.071,	(shoulder),	-1.609	-1.018,	(shoulder),	-1.573
	-1.663	-1.556		-1.622	-1.525	
	-0.893	-0.843,	-0.868,	-0.881	-0.856,	-0.868,
e Cv	(shoulder),	-0.956	-0.984,	(shoulder),	-0.943,	-0.978,
0.2	-1.013,	(shoulder),	-1.555	-1.013,	-1.518	-1.565
	-1.605	-1.505		-1.613		
	-0.895	-0.857,	-0.876,	-0.884	-0.852,	-0.868,
7Cv	(shoulder),	-0.958	-0.989,	(shoulder),	-0.953	-0.987,
1.2	-1.021,	(shoulder),	-1.567	-1.022,	(shoulder),	-1.571
	-1.614	-1.520		-1.621	-1.521	
	-0.613,	-0.553,	-0.583,	-0.588,	-0.538,	-0.563,
5 ^{Et}	-0.722,	-0.682	-0.702	-0.720,	-0.677,	-0.698,
	-0.865			-0.872	-0.798	-0.835
	-0.826	-0.753,	-0.789,	-0.827,	-0-776,	-0.801,
5 Pr	(shoulder),	-0.901	-0.938,	-0.977,	-0.908,	-0.942,
5	-0.976,	(shoulder),	-1.471	-1.562	-1.453	-1.507
	-1.532	-1.411				

Table S15. Summary of the electrochemical data relative to the potential of Fc/Fc+.



Fig. S89 Cyclic voltammograms of 5^{cy} in CH₃CN (0.1 M Bu₄NPF₆) at different scan rates.



Fig. S90 Cyclic voltammogram of 5^{cy} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 100 mV/s.



Fig. S91 Cyclic voltammogram of 5^{cy} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 1000 mV/s.



Fig. S92 Cyclic voltammograms of 5^{cy} in CH₃CN (0.1 M Bu₄NPF₆) at different scan rates.



Fig. S93 Differential pulse voltammograms (DPVs) of 5^{cy} in CH₃CN at scan rate of 10 mV/s with 0.1 M Bu₄NPF₆.



Fig. S94 Cyclic voltammograms of 5^{Cy} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 100 mV/s, considering second and third scans.



Fig. S95 Cyclic voltammograms of 5^{Cy} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 1000 mV/s, considering second and third scans.



Fig. S96 Cyclic voltammogram of 6^{cy} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 100 mV/s.



Fig. S97 Cyclic voltammogram of 6^{cy} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 1000 mV/s.



Fig. S98 Cyclic voltammogram of 7^{cy} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 100 mV/s.



Fig. S99 Cyclic voltammogram of 7^{cy} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 1000 mV/s.



Fig. S100 Cyclic voltammogram of 5^{Et} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 100 mV/s.



Fig. S101 Cyclic voltammogram of 5^{Et} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 1000 mV/s.



Fig. S102 Cyclic voltammogram of 5^{Et} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 100 mV/s, considering only the first reduction.



Fig. S103 Differential pulse voltammograms (DPVs) of 5^{Et} in CH₃CN at scan rate of 10 mV/s with 0.2 M Bu₄NPF₆.



Fig. S104 Cyclic voltammogram of 5^{Pr} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 100 mV/s.



Fig. S105 Cyclic voltammogram of 5^{Pr} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 1000 mV/s.



Fig. S106 Cyclic voltammogram of 5^{Pr} in CH₃CN (0.1 M Bu₄NPF₆) at scan rate of 100 mV/s, considering only the first and second reduction.



Fig. S107 Differential pulse voltammograms (DPVs) of 5^{Pr} in CH₃CN at scan rate of 10 mV/s with 0.1 M Bu₄NPF₆.

Quantum Chemical Calculations

The DFT calculations were performed using Gaussian 16 (Revision C.01) suite^{S10} of electronic structure Programs. The multireference CASSCF calculations were performed using ORCA–4.2.1.^{S11} The geometries of **6**^{Cy} was optimized in the gas phase with ω B97XD, MN12SX, B3LYP-D3, and PBE0 (PBE1PBE) functional and Def2SVP basis-set. To verify the stationary point and to obtain zero-point vibrational energy (ZPVE) corrections, frequency analysis was performed on optimized geometries. The singlet geometries were optimized with spin-unrestricted broken-symmetry (BS) wavefunctions. TD-DFT calculations were performed at MN12SX/Def2SV level on (U)MN12SX/Def2SV optimized geometry. The solvent effect was accounted with polarizable continuum model (PCM) including acetonitrile as the solvent. Multi-reference CASSCF(2,2)/NEVPT2/def2-TZVP provided the adiabatic singlet-triplet energy gap (–0.037 kJmol⁻¹).

DFT ^a	Er ^b / Hartree	$S^2(T)$	$E_{\rm Ps}^{b}$ / Hartree	S ² (BS)	. <i>I</i> ^c (cm ^{−1})	$\Delta F_{et}^{d} / k \text{Imol}^{-1}$
functional		0(1)		0 (00)	U (0111)	
ωB97XD	-3656.452216	2.011	-3656.452196	1.010	4.39	0.105
MN12SX	-3654.542102	2.009	-3654.542118	1.008	-3.51	-0.084
B3LYP-D3	-3657.402097	2.008	-3657.402100	1.008	-0.66	-0.015
PBE0	-3653.797912	2.011	-3653.797924	1.008	-2.63	-0.063
^a Def2SVP ba	^a Def2SVP basis-set. ^b ZPVE corrections are included. ^c The exchange coupling constant $J = (E_{BS} - D_{CS})^{-1}$					
E_T)/(S ² (T)–S ² (BS)). S ² (BS) and S ² (T) are the eigenvalues of the spin operator for broken-symmetry						
singlet and tri	singlet and triplet states, respectively. ^{<i>d</i>} Energy difference between singlet and triplet state $\Delta E_{ST} = 2J$. ^{S12}					

Table S16. Summary of calculated exchange coupling for 6^{Cy}.

Table S17. Summary of TD-DFT calculated key low energy transitions of 6^{Cy}.

Excited singlet state	Wavelength (nm)	Energy (eV)	Major transtions	Contribution	oscillator strength (<i>f</i>)
1	680.48	1.8220	233A -> 234A	0.99993	0.0008
2	542.41	2.2858	233B -> 234B	0.99986	0.0005
3	488.16	2.5398	233A -> 235A	0.99545	0.0304
4	414 31	2 9925	232A -> 234A	0.18233	0.0517
Т	-101	2.0020	233B -> 236B	0.96927	0.0017
	·	HO	MO: 133, LUMO: 134	•	



Fig. S108 TD-DFT calculated electronic absorption spectra of 6^{Cy} . f =oscillator strength



Fig. S109 Spin-density plot of 6^{Cy} (at isovalue of 0.012 and hydrogens are omitted for clarity).



Fig. S110 Spin-density plot of 7^{Cy} (at isovalue of 0.012 and hydrogens are omitted for clarity).



Fig. S111 Spin-density plot of 10^{Et} (at isovalue of 0.012 and hydrogens are omitted for clarity).



Table S18. Selected frontier molecular orbitals of 4^{Cy} , 5^{Cy} , and 7^{Cy} .



Table S19. Selected frontier molecular orbitals of 4^{Et}, 5^{Et}, 8^{Et}, and 9^{Et}.

Compound	НОМО	LUMO
4 ^{Pr}		
5 ^{Pr}		
9 ^{Pr}		

Table S20. Selected frontier molecular orbitals of $4^{\textrm{Pr}},\,5^{\textrm{Pr}},\,\textrm{and}\,9^{\textrm{Pr}}.$

Ca	rtesian Coord	linates		
6 ^{Cy} -	Broken Symmeti	ry Singlet		DFT level: UMN12SX/def2SVP
Ν	-1.652415000	2.551899000	0.527361000	
Ν	-3.982643000	0.380925000	1.223394000	- Thermochemistry -
Ν	-4.449585000	0.727728000	-0.854704000	
Ν	1.820758000	-1.704411000	-1.272195000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Ν	3.912278000	-0.743569000	0.808133000	
Ν	3.065824000	-2.303463000	2.055533000	Zero-point correction= 1.006427
С	-0.596989000	1.626481000	0.130070000	(Hartree/Particle)
C	-0.572143000	0.339516000	0.940552000	Thermal correction to Energy= 1.069835
н	-1.4/4/20000	-0.266286000	0.746973000	Thermal correction to Enthalpy= 1.0/0/80
Н	-0.559531000	0.574807000	2.019809000	I hermal correction to Gibbs Free Energy= 0.910995
	0.658297000	-0.487395000	0.601069000	Sum of electronic and zero-point Energies= -3654.542118
н	0.622038000	-1.413606000	1.195475000	Sum of electronic and thermal Energies = -3654.478709
	1.00000000	0.100767000	0.070904000	Sum of electronic and thermal Enthalpies = -3054.477765
	0.000920000	-0.639171000	-0.004497000	Sum of electronic and thermal Free Energies= -3654.637550
L L	0.003141000	0.430009000	2 704522000	Chargo – 0 Multiplicity – 1
	1 52103000	1 03/050000	-2.794552000	Charge = 0 Multiplicity = 1
C	-0.614390000	1 274593000	-1 353986000	
н	-0.636148000	2 195051000	-1.9665290000	
H	-1 537043000	0 701493000	-1 584803000	
C	-2 973559000	2 438065000	0 171952000	
č	-2.667640000	4.557854000	1.141951000	
Ĥ	-2.896028000	4.433526000	2.216894000	
н	-2.691416000	5.639982000	0.928584000	
С	-1.288716000	3.948135000	0.856112000	
С	-0.568019000	4.631456000	-0.306733000	
Н	0.420360000	4.181749000	-0.477881000	
н	-0.382415000	5.689403000	-0.059047000	
Н	-1.145816000	4.590666000	-1.242935000	
С	-0.384257000	3.986269000	2.085196000	
н	-0.836084000	3.429675000	2.924532000	
н	-0.235277000	5.031872000	2.402649000	
	2 700160000	3.579971000	1.000331000	
	-3.709109000	0.362364000	0.177313000	
ĉ	-3.190010000	-0.502504000	0.45535509000	
c	-3.449414000	0.528419000	2.558141000	
Ĥ	-2.811283000	1.423126000	2.588436000	
Н	-2.852807000	-0.363786000	2.812181000	W
Н	-4.276232000	0.643452000	3.278838000	
С	-4.369116000	1.199057000	-2.214657000	
Н	-3.551148000	1.932647000	-2.283482000	
Н	-5.312036000	1.675858000	-2.531850000	
Н	-4.154384000	0.351789000	-2.88/16/000	
C	-6.0/1095000	-1.102619000	-1.393957000	
н	-0.040894000	-1.874098000	-0.057729000	
н	-0.40200000 -6 702254000	-1.019040000	-2.112193000	
	-5 382864000	-1 622212000	1 800282000	
н	-6.153782000	-2.239717000	1.318884000	
н	-5.830018000	-1.169716000	2.702323000	
н	-4.557432000	-2.283542000	2.113395000	
С	2.524161000	-2.460693000	-0.362654000	
С	2.948081000	-3.808770000	-0.921639000	
С	2.884076000	-3.464536000	-2.416515000	
H	3.870301000	-3.073985000	-2.728984000	
H	2.666204000	-4.341234000	-3.050591000	
C	1.835392000	-2.352154000	-2.612034000	
U U	2.011414000	-4.977167000	-0.581691000	
н	2 1250/20000	-4.100101000	-0.121000000 0.468238000	
н	2.120049000	-5.232102000	-1 208749000	
Ċ	4.369710000	-4.176947000	-0.500728000	
н	4.701773000	-5.095770000	-1.014039000	
н	4.432538000	-4.371460000	0.584732000	
н	5.087967000	-3.373348000	-0.741228000	
С	2.356222000	-1.427125000	-3.720846000	
Н	1.596220000	-0.747192000	-4.130426000	

н	2 711637000	-2 046938000	-4 562434000	
H	3 207923000	-0.823897000	-3 363745000	
	0.458804000	-2 8003/2000	-2 990959000	
ŭ	0.400004000	-2.033342000	-2.990959000	
	0.026426000	-3.526171000	-2.195431000	
н	0.539305000	-3.497808000	-3.913243000	
н	-0.257307000	-2.085207000	-3.195990000	
С	3.148540000	-1.858669000	0.782500000	
С	4.296784000	-0.465211000	2.104999000	
Ĉ	3 773208000	-1 455988000	2 891270000	
č	4 267570000	0.020670000	0.270959000	
	4.307379000	-0.039079000	-0.370636000	
н	5.098183000	-0.661851000	-0.918836000	
Н	4.825257000	0.915840000	-0.079051000	
н	3.516240000	0.182213000	-1.027520000	
С	2.209348000	-3.381928000	2.489017000	
H	2 769932000	-4 327233000	2 598193000	
1	1 202222000	3 518003000	1 756602000	
	1.333223000	-3.310303000	1.750002000	
н	1.765975000	-3.1268/1000	3.463820000	
С	5.130181000	0.706386000	2.455796000	
н	6.142015000	0.636764000	2.019372000	
н	5.240025000	0.784135000	3.546250000	
н	4,681431000	1,639626000	2.077155000	
C	3 854800000	-1 672081000	4 354251000	
Ц	2 976556000	1 5/7977000	4 952224000	
		-1.54/0//000	4.002201000	
H	4.547206000	-0.949821000	4.807340000	
ΙН	4.222396000	-2.684794000	4.598315000	
С	-3.707651000	3.767093000	0.322169000	
С	-5.014951000	3.610598000	1.101280000	
Ĥ	-5 487692000	4 593086000	1 273789000	
ЦЦ	-4 845023000	3 1/2037000	2 086378000	
	-4.043923000	0.00007000	2.080378000	
н	-5.744337000	2.989837000	0.549491000	
С	-4.030902000	4.440011000	-1.019565000	
н	-3.159389000	4.491842000	-1.689805000	
н	-4.394784000	5.470214000	-0.856504000	
н	-4.831958000	3,897420000	-1.550568000	
Ц.	0.354802000	2 148823000	0.327866000	
	0.004002000	2.140023000	1.064194000	
	-0.233769000	-1.430653000	-1.064184000	
S	3.336327000	3.428534000	0.188949000	
0	2.671317000	4.670941000	0.552661000	
0	4.771480000	3.337366000	0.448460000	
0	2.590018000	2.201737000	0.527999000	
Ĉ	3 269354000	3 445233000	-1 662421000	
Ē	2 202757000	1 407880000	2 155802000	
	3.092737000	4.497009000	-2.155892000	
	3.836343000	2.352212000	-2.174187000	
F	2.008873000	3.470465000	-2.099339000	
S	-1.932579000	-3.425016000	0.862818000	
0	-2.290289000	-2.270420000	1.695571000	
0	-2.467885000	-4.702713000	1,289982000	
l õ	-0 542807000	-3 421073000	0 391857000	
	2 260176000	2 00000000	0.001001000	
	-2.003170000	-3.090900000	-0.103333000	
	-2.500397000	-3.908120000	-1.0//15/000	
	-2.679709000	-1.83/245000	-1.142065000	
F	-4.178198000	-3.243626000	-0.517599000	
6 ^{Cy} -	Triplet			DFT level: UMN12SX/def2SVP
Ν	-1.652064000	2.552174000	0.527845000	- Thermochemistry -
Ν	-3,982843000	0.381539000	1.223230000	·
N	-4 449125000	0 728477000	-0 854989000	Temperature 298 150 Kelvin Pressure 1 00000 Atm
N	1 820/04000	_1 70/01/000	-1 272015000	
	1.020404000	-1.704910000	-1.212013000	Zerr asiat correction 1 000 400
IN	3.912310000	-0.743905000	0.808007000	Zero-point correction= 1.006428
N	3.065578000	-2.303482000	2.055614000	(Hartree/Particle)
С	-0.596699000	1.626573000	0.130517000	Thermal correction to Energy= 1.069836
С	-0.572433000	0.339414000	0.940604000	Thermal correction to Enthalpy= 1.070780
н	-1.475028000	-0.266168000	0.746414000	Thermal correction to Gibbs Free Energy= 0.909965
н	-0.560309000	0 574346000	2 019951000	Sum of electronic and zero-point Energies= -3654 542102
	0.658038000	-0 487625000	0 601/20000	Sum of electronic and thermal Energies 2654 /79602
LU LU	0.000020000	1 412020000	1 10570000	Sum of electronic and thermal Enthelpice -5004.470095
	0.021010000	-1.413030000	1.190/00000	Sum of electronic and thermal Enthalpies = -3054.477749
H	1.550114000	0.100441000	0.876557000	Sum of electronic and thermal Free Energies= -3654.638564
С	0.686878000	-0.839226000	-0.884184000	
С	0.603836000	0.436276000	-1.723252000	Charge = 0 Multiplicity = 3
Н	0.539299000	0.196035000	-2.794039000	- , ,
	1.521799000	1 034811000	-1 577563000	

С	-0.613577000	1.275172000	-1.353656000	
н	-0.634645000	2.195821000	-1.965925000	
п С	-2 973182000	2 438590000	0 172197000	
č	-2.666960000	4.558412000	1.142039000	
Н	-2.895307000	4.434256000	2.217010000	(
Н	-2.690579000	5.640515000	0.928529000	
C	-1.288146000	3.948454000	0.856213000	
Ч	-0.567498000	4.631431000	-0.306860000	
н	-0.381535000	5.689355000	-0.059342000	
Н	-1.145519000	4.590690000	-1.242928000	
С	-0.383592000	3.986788000	2.085216000	
Н	-0.835388000	3.430362000	2.924677000	
Н	-0.234549000	5.032446000	2.402453000	<u> </u>
П	-3 708950000	3.580428000	1.868365000	
c	-5 198301000	-0.361621000	-0 455896000	
č	-4.894347000	-0.588270000	0.858376000	10
С	-3.449876000	0.528843000	2.558103000	
Н	-2.811672000	1.423492000	2.588607000	
Н	-2.853409000	-0.363455000	2.812157000	
Н	-4.276828000	0.643875000	3.278647000	
н	-4.308243000 -3 550120000	1.1998/3000	-2.214897000 -2 283390000	
н	-5 311159000	1.933001000	-2.283390000	
н	-4.153052000	0.352672000	-2.887348000	
С	-6.070510000	-1.101818000	-1.394840000	
Н	-6.640409000	-1.873367000	-0.858821000	
Н	-5.481758000	-1.618632000	-2.173586000	
Н	-6.791573000	-0.436272000	-1.899951000	
н	-5.363456000	-1.021432000	1.799009000	
н	-5.830991000	-1.168867000	2.701477000	
Н	-4.558154000	-2.282747000	2.113138000	
С	2.524012000	-2.461082000	-0.362536000	
C	2.947697000	-3.809307000	-0.921321000	
С	2.883160000	-3.465440000	-2.416245000	
н	2 665091000	-4 342283000	-3.050051000	
С	1.834410000	-2.353120000	-2.611675000	
С	2.011178000	-4.977629000	-0.580725000	
Н	0.950433000	-4.733609000	-0.725673000	
н	2.125311000	-5.292381000	0.469206000	
Н	2.272142000	-5.848824000	-1.207737000	
н	4 701346000	-5 096361000	-1 013910000	
н	4.432654000	-4.371512000	0.584718000	
Н	5.087646000	-3.373845000	-0.741799000	
С	2.354760000	-1.428555000	-3.721103000	
н	1.594381000	-0.749207000	-4.130958000	
н	2.710277000	-2.048723000	-4.562388000	
C	0 457742000	-2 900389000	-2 989869000	
Ĥ	0.027490000	-3.528847000	-2.193937000	
Н	0.537811000	-3.499233000	-3.911939000	
Н	-0.258442000	-2.086270000	-3.195032000	
C	3.148477000	-1.858946000	0.782495000	
C	4.∠90709000 3.773043000	-U.400385UUU	2.104844000 2.891244000	
č	4.367883000	-0.040276000	-0.371042000	
Ĥ	5.099042000	-0.662323000	-0.918417000	
Н	4.824993000	0.915560000	-0.079380000	
Н	3.516760000	0.180964000	-1.028200000	
C	2.208836000	-3.381678000	2.489270000	
н	2.769271000	-4.327020000 -3.518788000	∠.598885000 1 756727000	
Н	1.765288000	-3.126220000	3.463889000	
С	5.130332000	0.706138000	2.455493000	
Н	6.142210000	0.636214000	2.019221000	



н	5 240037000	0 784119000	3 545943000	
Ц	4 681812000	1 630360000	2 076561000	
	2 954620000	1.039309000	4 254252000	
	3.654620000	-1.072013000	4.354253000	
н	2.876399000	-1.547536000	4.852232000	
н	4.547124000	-0.949688000	4.807248000	
н	4.222091000	-2.684649000	4.598413000	
С	-3.707128000	3.767696000	0.322416000	
Č	-5 014344000	3 611320000	1 101708000	
ŭ	5 496097000	4 502040000	1.774259000	
	-3.400907000	4.090049000	1.274236000	
н	-4.845213000	3.142765000	2.086790000	
н	-5.743845000	2.990604000	0.550020000	
С	-4.030534000	4.440594000	-1.019286000	
н	-3.159111000	4.492399000	-1.689650000	
н	-4.394360000	5.470811000	-0.856187000	
н	-4 831689000	3 898026000	-1 550164000	
	0.355147000	2 1/26/1000	0.329795000	
	0.333147000	2.140041000	0.328783000	
н	-0.234046000	-1.430331000	-1.064050000	
S	3.336769000	3.428315000	0.188521000	
0	2.671793000	4.670783000	0.552087000	
0	4.771916000	3.337131000	0.448076000	
0	2 590419000	2 201563000	0.527670000	
č	3 260836000	3 444843000	-1 662856000	
Ĕ	2,0025,0000	4 407044000	-1.002030000	
<u> </u>	3.693366000	4.497241000	-2.156437000	
	3.8364/3000	2.351577000	-2.1/4484000	
F	2.009363000	3.470453000	-2.099783000	
S	-1.933100000	-3.424865000	0.862979000	
0	-2.291044000	-2.270181000	1.695518000	
0	-2 468241000	-4 702576000	1 290301000	
ŏ	-0 5/3395000	-3 /21727000	0.392071000	
	-0.3433330000	2 001056000	0.392071000	
Ē	-2.869610000	-3.091056000	-0.703934000	
F	-2.500993000	-3.908640000	-1.676849000	
F	-2.679849000	-1.837581000	-1.142361000	
F	-4.178676000	-3.243445000	-0.517493000	
6 ^{Cy} -	-Broken Symmeti	ry Singlet		DFT level: UwB97XD/def2SVP
Ν	1.726536000	2.537535000	-0.505644000	- Thermochemistry -
N	4 017361000	0.315122000	-1 172605000	
N	4 437354000	0.646055000	0 919379000	Temperature 208 150 Kelvin Pressure 1 00000 Atm
N	1 972257000	1 626296000	1 296176000	
	-1.073237000	-1.020300000	1.200170000	Zere aciet connection 1 010112
IN	-3.928779000	-0.674621000	-0.832141000	Zero-point correction= 1.010443
N	-3.070236000	-2.249279000	-2.055685000	(Hartree/Particle)
С	0.653768000	1.633258000	-0.100634000	Thermal correction to Energy= 1.073751
С	0.566775000	0.366381000	-0.944199000	Thermal correction to Enthalpy= 1.074695
н	1.451314000	-0.271902000	-0.803084000	Thermal correction to Gibbs Free Energy= 0.914396
н	0.522828000	0.634179000	-2.010649000	Sum of electronic and zero-point Energies= -3656,452196
C	-0.679875000	-0 437783000	-0.587563000	
ŭ	0.667022000	0.407700000		Sum of electronic and thermal Energies = -3656 388888
	-0.007923000	1 252256000	1 188305000	Sum of electronic and thermal Energies= -3656.388888
н	4 500 400000	-1.353356000	-1.188305000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944
	-1.560436000	-1.353356000 0.169657000	-1.188305000 -0.835144000	Sum of electronic and thermal Energies=-3656.388888Sum of electronic and thermal Enthalpies=-3656.387944Sum of electronic and thermal Free Energies=-3656.548243
C	-1.560436000 -0.695383000	-1.353356000 0.169657000 -0.814969000	-1.188305000 -0.835144000 0.895924000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243
C C	-1.560436000 -0.695383000 -0.540320000	-1.353356000 0.169657000 -0.814969000 0.439696000	-1.188305000 -0.835144000 0.895924000 1.762292000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies=-3656.388888 -3656.387944 -3656.548243Charge = 0 Multiplicity = 1
C C H	-1.560436000 -0.695383000 -0.540320000 -0.448226000	-1.353356000 0.169657000 -0.814969000 0.439696000 0.168697000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies=-3656.388888 -3656.387944 -3656.548243Charge = 0 Multiplicity = 1
C C H H	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000	-1.353356000 0.169657000 -0.814969000 0.439696000 0.168697000 1.065263000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000	Sum of electronic and thermal Energies=-3656.388888Sum of electronic and thermal Enthalpies=-3656.387944Sum of electronic and thermal Free Energies=-3656.548243Charge = 0 Multiplicity = 1-3656.548243
C C H H C	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000	-1.353356000 0.169657000 -0.814969000 0.439696000 0.168697000 1.065263000 1.253104000	-1.18305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies=-3656.388888 -3656.387944 -3656.548243Charge = 0 Multiplicity = 1
ССННСН	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000	-1.353356000 0.169657000 -0.814969000 0.439696000 0.168697000 1.065263000 1.253104000 2.160699000	-1.18305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСНИ	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000 1.599701000	-1.353356000 0.169657000 -0.814969000 0.439696000 0.168697000 1.065263000 1.253104000 2.160699000 0.653014000	-1.18305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННС	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000 1.599701000	-1.353356000 0.169657000 -0.814969000 0.439696000 0.168697000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000	-1.18305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 0.155647000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННС	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000	-1.353356000 0.169657000 -0.814969000 0.439696000 0.168697000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННСС	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.78911400	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННССН	-1.560436000 -0.695383000 -0.540320000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННССНН	-1.560436000 -0.695383000 -0.540320000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННССННС	-1.560436000 -0.695383000 -0.540320000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000 1.394000000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000	-1.188305000 -1.188305000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 -0.901784000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
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ССННСННССННССН	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000 1.394000000 0.682978000 -0.319198000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000 4.676533000 4.270541000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 -0.901784000 0.231391000 0.406732000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННССННССНИ	-1.560436000 -0.695383000 -0.540320000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000 1.394000000 0.682978000 -0.319198000 0.544521000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000 4.676533000 4.270541000 5.729075000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 -0.901784000 0.231391000 0.406732000 -0.050930000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННССННССННЫ	-1.560436000 -0.695383000 -0.540320000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000 1.394000000 0.682978000 -0.319198000 0.544521000 1.252678000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000 4.676533000 4.270541000 5.729975000 4.6320472000	-1.18305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 -0.901784000 0.231391000 0.406732000 -0.050930000 1.69890000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
СОТНОННОСТНОСТНЕ	-1.560436000 -0.695383000 -0.540320000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000 1.39400000 0.682978000 -0.319198000 0.544521000 1.252678000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.301297000 4.343038000 5.584131000 3.925834000 4.676533000 4.270541000 5.729975000 4.637947000 2.9072002	-1.188305000 -1.188305000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 -0.901784000 0.231391000 0.406732000 -0.050930000 1.169880000 2.442955000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССТЕСЕЕССЕЕССЕЕСС	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000 1.394000000 0.682978000 -0.319198000 0.544521000 1.252678000 0.497556000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000 4.676533000 4.270541000 5.729975000 4.637947000 3.922607000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 0.231391000 0.406732000 -0.050930000 1.169880000 -2.142385000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ОСТНОТНОСТНОСТНОТ.	$\begin{array}{c} -1.560436000\\ -0.695383000\\ -0.540320000\\ -0.448226000\\ -1.438850000\\ 0.695641000\\ 0.749522000\\ 1.599701000\\ 3.049891000\\ 2.789114000\\ 3.015934000\\ 2.832095000\\ 1.394000000\\ 0.682978000\\ -0.319198000\\ 0.544521000\\ 1.252678000\\ 0.497556000\\ 0.950969000\\ \end{array}$	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000 4.676533000 4.270541000 5.729975000 4.637947000 3.922607000 3.327158000	-1.188305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 -0.901784000 0.231391000 0.406732000 -0.050930000 1.169880000 -2.142385000 -2.950206000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССТНОТНОСТНОСТНОТ	$\begin{array}{c} -1.560436000\\ -0.695383000\\ -0.540320000\\ -0.448226000\\ -1.438850000\\ 0.695641000\\ 0.749522000\\ 1.599701000\\ 3.049891000\\ 2.789114000\\ 3.015934000\\ 2.832095000\\ 1.394000000\\ 0.682978000\\ -0.319198000\\ 0.544521000\\ 1.252678000\\ 0.497556000\\ 0.950969000\\ 0.359933000\\ \end{array}$	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000 4.676533000 4.270541000 5.729975000 3.922607000 3.327158000 4.953232000	-1.18305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 -0.901784000 0.231391000 0.406732000 -0.050930000 1.169880000 -2.142385000 -2.950206000 -2.501627000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННССННССННК	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000 1.394000000 0.682978000 0.544521000 1.252678000 0.497556000 0.950969000 0.359933000 -0.502649000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000 4.676533000 4.676533000 4.676533000 4.676533000 4.67653000 4.67947000 3.922607000 3.922607000 3.327158000 4.953232000 3.528094000	-1.18305000 -0.835144000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 -0.231391000 0.406732000 0.406732000 0.406732000 -2.950206000 -2.950206000 -2.501627000 -1.913007000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННССННССНННСНННС	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000 1.39400000 0.682978000 0.319198000 0.544521000 1.252678000 0.497556000 0.950969000 0.359933000 -0.502649000 3.751840000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000 4.676533000 4.676533000 4.676533000 4.637947000 3.922607000 3.327158000 3.528094000 1.136084000	-1.188305000 -1.188305000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.205051000 -2.271482000 -1.019185000 0.231391000 0.406732000 0.406732000 1.169880000 1.169880000 -2.142385000 -2.501627000 -1.913007000 -0.135754000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
ССННСННССННССННСНННСС	-1.560436000 -0.695383000 -0.540320000 -0.448226000 -1.438850000 0.695641000 0.749522000 1.599701000 3.049891000 2.789114000 3.015934000 2.832095000 1.39400000 0.682978000 0.319198000 0.544521000 1.252678000 0.497556000 0.950969000 0.359933000 -0.502649000 3.751840000 5.150111000	-1.353356000 0.169657000 -0.814969000 0.439696000 1.065263000 1.253104000 2.160699000 0.653014000 2.405864000 4.501297000 4.343038000 5.584131000 3.925834000 4.676533000 4.270541000 5.729975000 4.637947000 3.922607000 3.922607000 3.327158000 4.953232000 3.528094000 1.136084000 -0.479253000	-1.188305000 -1.188305000 0.895924000 1.762292000 2.820568000 1.660411000 1.377846000 1.998860000 1.581687000 -0.155647000 -1.205051000 -2.271482000 -1.019185000 -0.901784000 0.231391000 0.406732000 0.406732000 -1.169880000 2.142385000 -2.142385000 -2.501627000 -1.913007000 -0.135754000 0.543002000	Sum of electronic and thermal Energies= -3656.388888 Sum of electronic and thermal Enthalpies= -3656.387944 Sum of electronic and thermal Free Energies= -3656.548243 Charge = 0 Multiplicity = 1
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ŏ	2 279107000	-2 269411000	-1 682281000	
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	2.230130000	-4.109729000	1.379041000	
	2.342241000	-2.003140000	0.550800000	
CV CV	4.017427000	-3.400309000	0.559609000	DET loval: LlwP07VD/daf2S\/D
N	1 726520000	2 527574000	0 505902000	Thermochamietry
	1.720009000	2.537574000	-0.505602000	- memochemistry -
IN	4.017541000	0.315303000	-1.172531000	
N	4.437265000	0.646236000	0.919505000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	-1.8/31/8000	-1.626496000	1.286177000	
N	-3.928966000	-0.674843000	-0.831979000	∠ero-point correction= 1.010415
N	-3.070210000	-2.249331000	-2.055596000	(Hartree/Particle)
С	0.653786000	1.633230000	-0.100780000	I hermal correction to Energy= 1.073737
С	0.567014000	0.366248000	-0.944159000	Thermal correction to Enthalpy= 1.074681
Н	1.451528000	-0.272001000	-0.802724000	Thermal correction to Gibbs Free Energy= 0.913275
Н	0.523353000	0.633853000	-2.010670000	Sum of electronic and zero-point Energies= -3656.452216
С	-0.679718000	-0.437900000	-0.587711000	Sum of electronic and thermal Energies= -3656.388895
Н	-0.667654000	-1.353483000	-1.188419000	Sum of electronic and thermal Enthalpies= -3656.387950
н	-1.560247000	0.169531000	-0.835446000	Sum of electronic and thermal Free Energies= -3656.549356
С	-0.695396000	-0.814948000	0.895810000	Ű
С	-0.540622000	0.439869000	1.762026000	Charge = 0 Multiplicity = 3
н	-0.448797000	0.169105000	2.820384000	5 1 5
н	-1,439155000	1.065348000	1.659732000	
C	0.695371000	1,253336000	1.377766000	
н	0 748979000	2 161035000	1 998652000	
L H	1 599454000	0.653402000	1.581954000	
	3 0/0885000	2 406013000	-0 155713000	
	2 788025000	2.400013000	1 20/00/000	
L L	2.700923000	4.301499000	2 271452000	
	3.015099000	4.343300000	-2.27 1455000	
	2.031027000	2.025004000	-1.019023000	
	1.393672000	3.925904000	-0.901712000	
C	0.682854000	4.676416000	0.231598000	
H	-0.319229000	4.270236000	0.407061000	17
н	0.544164000	5.729841000	-0.050668000	
н	1.252688000	4.637916000	1.170008000	
C	0.497354000	3.922772000	-2.142263000	
H	0.950695000	3.327340000	-2.950134000	
Н	0.359758000	4.953419000	-2.501449000	
Н	-0.502859000	3.528303000	-1.912845000	
С	3.751900000	1.136271000	-0.135728000	
С	5.150121000	-0.479036000	0.543201000	
С	4.878958000	-0.692123000	-0.779540000	
С	3.498864000	0.466357000	-2.519240000	
Н	2.864308000	1.358197000	-2.550160000	
Н	2.903619000	-0.424065000	-2.762806000	-
н	4.332867000	0.576922000	-3.225891000	
C	4.352990000	1.152121000	2.272942000	
Ι Ĥ	3.578538000	1.927599000	2.301006000	
ЬН	5.312816000	1.581845000	2,591821000	
ЬН	4.075399000	0.335357000	2.952683000	
0	5 972963000	-1 254599000	1 509320000	
н	6 516287000	-2 050473000	0.987088000	
н	5 3/1231000	-1 735026000	2 271804000	
	6 708678000	-0.615780000	2.211004000	
	5 345412000	1 752505000	2.021033000	
	0.040410000 6 061095000	2 412002000	1 207882000	
	0.001200000 5 00000000	-2.412093000	-1.207000000	
	0.039933000	-1.319300000	-2.394003000	
Н	4.400424000	-2.354776000	-2.041072000	
	-2.583846000	-2.38/22/000	0.381927000	
C	-3.026624000	-3.721430000	0.959691000	
C	-2.992805000	-3.352178000	2.454127000	

Н	-3.982214000	-2.964831000	2.743749000	
Н	-2.778903000	-4.216898000	3.099220000	
С	-1.945193000	-2.233008000	2.645988000	
С	-2.063721000	-4.883821000	0.650329000	
н	-1.012035000	-4.593527000	0.755557000	
н	-2.187393000	-5.235488000	-0.383536000	
н	-2.281932000	-5.734199000	1.315997000	
С	-4.441840000	-4.106422000	0.516265000	
Ĥ	-4.772538000	-5.017793000	1.037928000	
H	-4.480439000	-4.314264000	-0.564514000	
H	-5 166634000	-3 306158000	0 732935000	
Ċ	-2 492539000	-1 250449000	3 694336000	
й	-1 753777000	-0 512886000	4 028742000	
ЦЦ	-2 815339000	-1 816173000	4 582415000	
	2.01000000	0.706772000	2 208057000	
	-3.302000000	2 701702000	2.290937000	
ŭ	-0.390003000	-2.191192000	2.095090000	
	-0.1/0/40000	-3.495761000	2.301270000	
	-0.710090000	-3.316290000	4.055109000	
Н	0.151385000	-1.994250000	3.246741000	
C	-3.174535000	-1.794229000	-0.789272000	
С	-4.286479000	-0.399205000	-2.139796000	
С	-3.755950000	-1.397740000	-2.909683000	
С	-4.374923000	0.053424000	0.342406000	
н	-5.133056000	-0.537284000	0.877938000	
н	-4.784228000	1.023272000	0.041554000	
н	-3.521248000	0.235864000	1.000156000	
С	-2.223344000	-3.352930000	-2.468077000	
н	-2.802372000	-4.284277000	-2.552193000	
н	-1.407292000	-3.482161000	-1.740436000	
H	-1 780497000	-3 120896000	-3 444154000	
C	-5 114082000	0 778704000	-2 514819000	
н	-6 146530000	0.776841000	-2 145562000	
L L L	-5 151022000	0.070041000	-3 605085000	
	4 705070000	1 702045000	2 082021000	
	-4.703070000	-1 620/86000	-2.002331000	
Ц	2 822456000	1 512067000	4.300033000	
	-2.822436000	-1.512967000	-4.650149000	
	-4.462373000	-0.000492000	-4.643013000	
	-4.193773000	-2.024591000	-4.022302000	
	5.013173000	3.713393000	-0.330310000	
	5.120000000	3.509660000	-1.123134000	
	5.609929000	4.478632000	-1.322559000	
H	4.956592000	3.012832000	-2.090163000	
H	5.838944000	2.897624000	-0.546112000	
С	4.133496000	4.424235000	0.971773000	
н	3.242362000	4.535744000	1.603374000	
н	4.543569000	5.428889000	0.781227000	
н	4.888692000	3.864923000	1.544902000	
н	-0.284123000	2.180818000	-0.261777000	
Н	0.187423000	-1.457248000	1.046322000	
S	-3.212855000	3.474802000	-0.200845000	
0	-2.596895000	4.737473000	-0.596761000	
0	-4.645997000	3.319124000	-0.479865000	
0	-2.414188000	2.268034000	-0.508931000	
С	-3.161498000	3.539331000	1.659443000	
F	-3.814595000	4.594122000	2.120764000	
F	-3.708633000	2.444912000	2.201629000	
F	-1.900435000	3.606143000	2.102914000	
s	1.829060000	-3.461290000	-0.941671000	
Ō	2.279320000	-2.269312000	-1.682406000	
õ	2.31.3429000	-4.736223000	-1.447215000	
ŏ	0.414667000	-3.413759000	-0.535607000	
č	2 704815000	-3 289811000	0 694919000	
F	2.70-010000	-4 160751000	1 570440000	
F	2.200401000	-2 065007000	1 225499000	
F	4 017624000	-3 486135000	0 559638000	
6Cv	Broken Summet	v Singlet	0.00000000	DET laval: uB3I VP/Def2S\/P
NI	-1 855770000	2 /67217000	0 405070000	- Thermochemistry -
	-1.000770000	2.40/31/000	0.490979000	- memochemistry -
	-4.004004000	0.103000000	1.220210000	Temperature 208 150 Kolvin Proceuro 1 00000 Atm
	1 06020000	1 54207000	1 226700000	1 100000 All.
IN	1.900299000	-1.042976000	-1.200/00000	

Ν	3.948703000	-0.479660000	0.854842000	Zero-point correction
N	3.197610000	-2.131174000	2.069147000	(Hartree/Particle)
C	-0.728180000	1.614327000	0.097366000	Thermal correction
й	-1.441089000	-0.322950000	0.794384000	Thermal correction
н	-0.559285000	0.614540000	2.009606000	Sum of electronic a
С	0.699298000	-0.407961000	0.591501000	Sum of electronic a
н	0.720055000	-1.323598000	1.190516000	Sum of electronic a
Н	1.551166000	0.230955000	0.847849000	Sum of electronic a
C	0.744163000	-0.780920000	-0.897727000	
C	0.532354000	0.469869000	-1.766507000	Charge = 0 Multipli
н	1 399284000	1 136120000	-2.823309000	
C	-0.744932000	1.229308000	-1.386091000	
Ĥ	-0.835894000	2.133522000	-2.008369000	
Н	-1.622053000	0.591523000	-1.591132000	
С	-3.178851000	2.247318000	0.169776000	Q
С	-3.030508000	4.392475000	1.156352000	
н	-3.248629000	4.241637000	2.225753000	
н	-3.136694000	5.467291000	0.948982000	
	-1.600132000	3.890740000	0.861960000	T
н	0.084354000	4.000138000	-0.294204000	
н	-0.853646000	5.724579000	-0.028280000	
H	-1.513386000	4.576606000	-1.225227000	
С	-0.698751000	3.967113000	2.102966000	<pre></pre>
н	-1.115041000	3.362482000	2.924856000	
н	-0.624195000	5.012654000	2.440069000	
Н	0.323839000	3.631118000	1.880469000	
C	-3.808347000	0.943007000	0.174438000	
č	-3.142169000	-0.762362000	-0.463773000	
č	-3.486562000	0.300403000	2.572437000	
Ĥ	-2.912079000	1.231729000	2.596930000	
н	-2.834452000	-0.545769000	2.824673000	
н	-4.323388000	0.361732000	3.283505000	
С	-4.453164000	0.878179000	-2.236992000	
н	-3.716636000	1.687462000	-2.298291000	
н	-5.435645000	1.253039000	-2.559540000	
C	-5.940174000	-1 592207000	-1 407643000	
Ĥ	-6.449495000	-2.399359000	-0.866733000	
н	-5.293544000	-2.065877000	-2.163884000	
н	-6.702535000	-0.993848000	-1.932184000	
С	-5.193641000	-2.050843000	1.794275000	
н	-5.899618000	-2.740048000	1.314314000	
н	-000080708000	-1.004042000	2.707414000	
C.	-4.∠94491000 2 718767000	-2.010007000	-0.381856000	
č	3.222103000	-3.587736000	-0.966958000	
Č	3.182246000	-3.211658000	-2.466222000	
н	4.154767000	-2.778254000	-2.747392000	
н	3.012735000	-4.082715000	-3.116306000	
C	2.080861000	-2.137711000	-2.660374000	
C	2.309286000	-4.801696000	-0.678163000	
п	2 408308000	-4.572661000	-0.831692000	
н	2.603136000	-5.645005000	-1.325156000	
C	4.653201000	-3.916138000	-0.512746000	
H	5.029558000	-4.807421000	-1.039876000	
Н	4.690299000	-4.130887000	0.567018000	
Н	5.343586000	-3.081324000	-0.713659000	
C	2.589886000	-1.112711000	-3.694118000	
H	1.819348000	-0.401577000	-4.015026000	
н	2.931490000 3 <u>4</u> 34572000	-1.040/00000 -0 537115000	-4.392320000 -3.287520000	
C	0.753854000	-2.756652000	-3.131026000	
н	0.370575000	-3.492707000	-2.413503000	
Н	0.907507000	-3.257077000	-4.099258000	
Н	-0.026178000	-1.995096000	-3.273702000	



C				
<u> </u>	3.269716000	-1.657851000	0.795874000	
	4 294791000	0 100945000	2 170882000	
U U	4.204701000	-0.190845000	2.170002000	
С	3.824507000	-1.236088000	2.934319000	
C	4 362228000	0 281669000	-0 316984000	
Ň	5.40400000	0.201000000	0.010004000	
н	5.124023000	-0.286387000	-0.873973000	
H	4.754701000	1.255092000	-0.009704000	
ы	3 400111000	0 458000000	0.060088000	
	3.499111000	0.456909000	-0.900900000	
С	2.415541000	-3.289037000	2.480115000	
н	3 047558000	-4 187283000	2 556812000	
	5.047 550000	-4.107203000	2.550012000	
н	1.605085000	-3.462260000	1.757264000	
н	1 964389000	-3 090917000	3 460767000	
	5.04000000	4.045040000	0.100101000	
C	5.016838000	1.045942000	2.562255000	
H	6.047452000	1.048574000	2.169593000	
L L	5 060022000	1 1 2 9 1 7 7 0 0 0	3 655727000	
	5.009922000	1.120477000	3.033727000	
H	4.521618000	1.941307000	2.158627000	
С	3 897546000	-1 464579000	4 405499000	
ŭ	0.001010000	4 400574000	1.100100000	
н	2.901389000	-1.430571000	4.879129000	
Н	4.515974000	-0.690978000	4.878794000	
н	1 312180000	-2 445168000	4 641981000	
	4.342400000	-2.445100000	4.041901000	
C	-4.010940000	3.526226000	0.321030000	
С	-5.322803000	3.278213000	1.086658000	
ŭ	E 9E1077000	4 000 4 00000	1 266006000	
	-5.051077000	4.220430000	1.200000000	
ΙH	-5.135807000	2.804613000	2.062800000	
н	-6 002442000	2 623080000	0 517148000	
	4.0504442000		4.000404000	
C	-4.356441000	4.18/1/5000	-1.032401000	
н	-3.467627000	4.319188000	-1.663533000	
	4 900660000	5 170262000	0.970544000	
п	-4.809009000	5.179505000	-0.870344000	
H	-5.084791000	3.581252000	-1.593042000	
н	0 175840000	2 210363000	0 265564000	
	0.175040000	2.210000000	0.200004000	
н	-0.101511000	-1.466055000	-1.058128000	
S	3.009819000	3.610434000	0.214263000	
õ	2 288002000	1 010000000	0 591420000	
0	2.200092000	4.040023000	0.561450000	
0	4.464234000	3.574861000	0.485107000	
0	2 304758000	2 341729000	0 560543000	
č	2.304730000	2.041720000	0.000040000	
C	2.939674000	3.623938000	-1.668475000	
F	3.525310000	4.708735000	-2.168034000	
-	2 540057000	2 5 4 2 4 9 9 0 0 0	2 101625000	
	3.549957000	2.542166000	-2.191625000	
I F	1.663238000	3.600857000	-2.102395000	
		0 504000000	0.91/201000	
s	-1 621212000	-3 521088000		
S	-1.621212000	-3.521088000	0.314201000	
s O	-1.621212000 -2.094443000	-3.521088000 -2.353556000	1.701773000	
s O O	-1.621212000 -2.094443000 -2.094956000	-3.521088000 -2.353556000 -4.830985000	1.701773000 1.372185000	
S O O O	-1.621212000 -2.094443000 -2.094956000	-3.521088000 -2.353556000 -4.830985000 -3.436525000	1.701773000 1.372185000 0.503804000	
s 0000	-1.621212000 -2.094443000 -2.094956000 -0.197255000	-3.521088000 -2.353556000 -4.830985000 -3.436525000	1.701773000 1.372185000 0.503804000	
S 0 0 0 0 0	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000	1.701773000 1.372185000 0.503804000 -0.738162000	
- S O O O C F	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000	1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000	
SOOOCF	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000	1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000	
SOOOCFF	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000	1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000	
SOOOCFFF	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000	-3.521088000 -2.353556000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000	1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000	
- SOOOCFFF FF	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -2.425469000 -3.817834000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000	1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000	
S 0 0 0 F F F 6 ^{cy} -	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000	1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000	DFT level: uB3LYP/Def2SVP
S O O C F F F 6^{cy}-	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
S O O C F F F 6^{cy} N N	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
SOOCFF F 6 ^{Cy-} N N	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501190000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405302200	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
SOOOCFF FF 6 ^{cy} -	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 -2.467709000 0.104121000 0.405393000	0.514201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
SOOOCFFF 6 ^{Cy} - NNN	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000	0.31420 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
SOOCFFF <mark>6^{cy-1}</mark> NNNN	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088
SOOOCFFF <mark>6</mark> NNNN	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 2.066020000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 2.127272600	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.050024000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Letter (Datial))
. \$0000FFF <mark>6</mark> 7 80000FFFF	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000	0.3142000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle)
. \$0000FFF <mark>6</mark> ZZZZC	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.05956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886
. \$0000FFF <mark>6</mark> ZZZZCC	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000 0.942581000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886 Thermal correction to Energy= 1.064831
. \$0000FFF <mark>6</mark> ZZZZCC:	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 4.441242000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 0.222420002	0.3142000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000 0.942281000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886 Thermal correction to Enthalpy= 1.064831 Thermal correction to Enthalpy= 0.000010
. \$0000 F F F <mark>6</mark> Z Z Z Z Z C C H	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 -0.322120000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000 0.942581000 0.794934000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 0.322120000 0.614799000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000 0.942581000 0.794934000 2.010261000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. \$0000 F F F 6 Z Z Z Z Z C C T T C	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000 0.658885000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.6147999000 -0.408777000	0.31420 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000 0.942581000 0.794934000 2.010261000 0.592325000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886 Thermal correction to Energy= 1.064831 Thermal correction to Gibbs Free Energy= 0.903013 Sum of electronic and thermal Energies= -3657.239200
. \$0000 F F F <mark>6</mark> Z Z Z Z Z C C H H C:	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000 0.698886000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.614799000 -0.408727000 -2.025555 -2.52556 -2.52556 -2.52556 -3.52556 -3.555600 -3.555700 -3.555700 -3.555700 -3.555700 -3.555700 -3.5577000 -3.5577700 -3.5577700 -3.5577700 -3.5577700 -3.5577700 -3.55777700 -3.5577777777777777777777777777777777777	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000 0.942581000 0.794934000 2.010261000 0.592325000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. \$0000 с н н н <mark>6</mark> 2 Z Z Z Z Z C C I I C I	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 0.658886000 0.718377000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 0.348169000 0.614799000 0.614799000 -0.408727000 -1.324625000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000	DFT level: uB3LYP/Def2SVP - Thermochemistry Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886 Thermal correction to Energy= 1.064831 Thermal correction to Gibbs Free Energy= 0.903013 Sum of electronic and zero-point Energies= -3657.402097 Sum of electronic and thermal Energies= -3657.337355
. \$0000 F F F <mark>6</mark> Z Z Z Z Z C C T T C T T	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 1.551477000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -0.322120000 0.614799000 -0.408727000 -1.324625000 0.228958000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000 0.849437000	DFT level: uB3LYP/Def2SVP - Thermochemistry Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886 Thermal correction to Enthalpy= 1.064831 Thermal correction to Gibbs Free Energy= 0.903013 Sum of electronic and zero-point Energies= -3657.02097 Sum of electronic and thermal Enthalpies= -3657.337355 Sum of electronic and thermal Eree Energies= -3657.499172
	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 0.727728000 -0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 1.551477000 0.742652000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.614799000 -0.408727000 -1.324625000 0.228958000 0.78445000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000 0.849437000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. \$0000 с н н н <mark>6</mark> 2 Z Z Z Z Z C C I I C I I C I I C	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 0.698886000 0.718377000 1.551477000 0.743653000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.105912000 -2.034957000 -3.0591471000 -2.034957000 -3.591471000 -2.034957000 -1.04121000 0.405393000 -0.478608000 -2.127375000 1.614594000 0.324120000 0.614799000 0.614799000 -0.408727000 -1.324625000 0.228958000 -0.781459000	0.31420000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000 0.849437000 -0.896965000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. \$0000 F F F <mark>6</mark> Z Z Z Z Z C C H H C H H C C	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 0.3.950632000 0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 1.551477000 1.551477000 0.532419000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.408727000 -1.324625000 0.228958000 -0.781459000 0.469445000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000 0.849437000 -0.896965000 -1.765688000	DFT level: uB3LYP/Def2SVP - Thermochemistry Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886 Thermal correction to Enthalpy= 1.064831 Thermal correction to Gibbs Free Energy= 0.903013 Sum of electronic and zero-point Energies= -3657.402097 Sum of electronic and thermal Energies= -3657.337355 Sum of electronic and thermal Free Energies= -3657.499172 Charge = 0 Multiplicity = 3
. %ОООС	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 1.551477000 0.743653000 0.532419000 0.4570350000 0.4570350000 0.4570350000 0.457035000000000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.305956000 -3.105912000 -2.034957000 -3.591471000 2.034957000 -3.591471000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.614799000 -0.408727000 -1.324625000 0.228958000 -0.781459000 0.469445000 0.469445000 0.194844000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000 0.942581000 0.794934000 2.010261000 0.899325000 1.190995000 0.849437000 -0.896965000 -1.765688000 -2.824736000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. \$0000 с н н н <mark>6</mark> Z Z Z Z Z Z C C I I С I I С C I I C C I I	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 0.559072000 0.698886000 0.718377000 1.551477000 0.743653000 0.532419000 0.457035000 1.20202020	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.305956000 -3.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -0.478608000 -0.478608000 -0.478608000 -0.478608000 0.348169000 0.348	0.31420000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000 0.849437000 -0.896965000 -1.765688000 -2.824736000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886 Thermal correction to Enthalpy= 1.064831 Thermal correction to Gibbs Free Energy= 0.903013 Sum of electronic and zero-point Energies= -3657.402097 Sum of electronic and thermal Energies= -3657.337355 Sum of electronic and thermal Free Energies= -3657.499172 Charge = 0 Multiplicity = 3
. \$0000 F F F <mark>6</mark> Z Z Z Z Z C C H H C H H C C H H	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.004015000 -4.501199000 1.967504000 3.950632000 0.3.950632000 0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 1.551477000 0.532419000 0.457035000 1.399606000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.05956000 -4.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.104121000 0.104121000 0.405393000 -1.543850000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.614799000 -0.408727000 -1.324625000 0.228958000 -0.781459000 0.469445000 0.194844000 1.135254000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000 0.849437000 -0.896965000 -1.765688000 -1.663177000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. %ОООС	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -2.511059000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 1.551477000 0.743653000 0.532419000 0.457035000 1.399606000 -0.744690000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.105912000 -3.03957000 -3.03957000 -3.591471000 -2.034957000 -3.591471000 -2.034957000 -1.04121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.1324625000 0.228958000 -0.781459000 0.469445000 0.194844000 1.135254000 1.229429000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000 0.942581000 0.794934000 2.010261000 0.899325000 1.190995000 0.849437000 -0.896965000 -1.765688000 -2.824736000 -1.663177000 -1.385470000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. %ОООС н н н <mark>6</mark> Z Z Z Z Z Z C C T T C T T C C T T C T T C T	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 0.698886000 0.718377000 1.551477000 0.532419000 0.457035000 1.399606000 -0.744690000 -0.835230000 -0.744690000 -0.835230000 -0.83520000 -0.835230000 -0.835230000 -0.835230000 -0.835230000 -0.835230000 -0.835230000 -0.835230000 -0.835230000 -0.835220000 -0.835230000 -0.835220000 -0.83520000 -0.8	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.4677099000 -1.543850000 -1.543850000 -0.478608000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.614799000 -0.408727000 -1.324625000 0.228958000 -0.781459000 0.469445000 0.194844000 1.135254000 1.229429000 2.133504000 2.133504000	0.31420000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.8995000 1.190995000 0.849437000 -2.824736000 -1.663177000 -1.8547000 -2.07889000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886 Thermal correction to Enthalpy= 1.064831 Thermal correction to Gibbs Free Energy= 0.903013 Sum of electronic and zero-point Energies= -3657.402097 Sum of electronic and thermal Energies= -3657.337355 Sum of electronic and thermal Free Energies= -3657.499172 Charge = 0 Multiplicity = 3
. \$0000 F F F 6 Z Z Z Z Z C C T T C T T C C T T C T	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -2.511059000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 0.19920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 1.551477000 0.532419000 0.532419000 0.457035000 1.399606000 -0.744690000 -0.835230000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.305956000 -3.105912000 -2.034957000 -3.591471000 2.467709000 0.104121000 0.104121000 0.104121000 0.405393000 -1.543850000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.614799000 -0.408727000 -1.324625000 0.228958000 -0.781459000 0.469445000 0.194844000 1.135254000 1.229429000 2.133594000 2.5240000 2.5240000 2.5240000 2.133594000 2.524000 2.5250000 2.524000 2.524000 2.524000 2.524000 2.5240000 2.5254000 2.52554000 2.52554000 2.525555555555555555555555555555555555	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000 0.896965000 -1.765688000 -1.885470000 -2.824736000 -1.385470000 -2.007889000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. %ОООС н н н <mark>6</mark> Z Z Z Z Z C C I I C I I C U I I C I	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -1.996365000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.004015000 -4.501199000 0.3950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 1.551477000 0.743653000 0.532419000 0.457035000 1.399606000 0.744690000 -0.744690000 -0.835230000 -1.622042000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.105912000 -3.05956000 -3.05956000 -3.05956000 -3.0591471000 -2.034957000 -3.591471000 0.104121000 0.405393000 -1.543850000 -0.478608000 -0.478608000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.781459000 0.228958000 -0.781459000 0.469445000 0.194844000 1.135254000 1.229429000 2.133594000 0.591960000	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.097947000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000 0.849437000 -0.896965000 -1.765688000 -2.824736000 -1.385470000 -1.385470000 -1.590602000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. \$0000+++ <mark>6</mark> 222222001101100110110	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 0.532419000 0.532419000 0.457035000 1.399606000 -0.744690000 -0.744690000 -0.835230000 -1.622042000 -3.178467000	-3.521088000 -2.353556000 -4.830985000 -3.436525000 -3.305956000 -4.105912000 -2.034957000 -3.591471000 2.4677099000 -0.405393000 -1.543850000 -0.478608000 -0.478608000 -0.478608000 -0.478608000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322425000 0.228958000 -0.781459000 0.228958000 -0.781459000 0.469445000 0.194844000 1.135254000 1.229429000 2.133594000 0.591960000 2.248061000	0.31420 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.849437000 -889955000 1.190995000 0.849437000 -0.896965000 -1.385470000 -2.824736000 -1.663177000 -1.590602000 0.170558000	DFT level: uB3LYP/Def2SVP - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 1.000088 (Hartree/Particle) Thermal correction to Energy= 1.063886 Thermal correction to Enthalpy= 1.064831 Thermal correction to Gibbs Free Energy= 0.903013 Sum of electronic and zero-point Energies= -3657.402097 Sum of electronic and thermal Energies= -3657.337355 Sum of electronic and thermal Free Energies= -3657.499172 Charge = 0 Multiplicity = 3
. \$0000 F F F <mark>6</mark> Z Z Z Z Z Z C C T T C T T C C T T C T T C T T C T T C T T C T T C T T C C T T C T T C T T C C T T C T	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -2.511059000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.950632000 3.196920000 -0.727728000 -0.585385000 -1.441344000 -0.559072000 0.698886000 0.718377000 1.551477000 0.532419000 0.457035000 1.399606000 -0.744690000 -0.835230000 -1.622042000 -3.178467000 2.02969000	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.305956000 -3.105912000 -2.034957000 -3.591471000 2.034957000 -3.591471000 2.467709000 0.104121000 0.405393000 -1.543850000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.614799000 -0.408727000 -1.324625000 0.228958000 -0.781459000 0.469445000 0.194844000 1.135254000 1.229429000 2.133594000 0.5919600000 2.248061000 4.20225500	0.314201000 1.701773000 1.372185000 0.503804000 -0.738162000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.592325000 1.190995000 0.86965000 -1.765688000 -2.824736000 -1.385470000 -2.007889000 -1.590602000 0.170558000	DFT level: uB3LYP/Def2SVP - Thermochemistry -
. \$000СFFF <mark>6</mark> ZZZZZCCHHCHHCCHHCHHCC	-1.621212000 -2.094443000 -2.094956000 -0.197255000 -2.511059000 -2.511059000 -2.511059000 -2.425469000 -3.817834000 Triplet -1.855311000 -4.004015000 -4.501199000 1.967504000 3.196920000 0.727728000 -0.785385000 -0.743653000 0.743653000 0.532419	-3.521088000 -2.353556000 -4.830985000 -3.305956000 -3.305956000 -3.105912000 -2.034957000 -3.591471000 2.034957000 -3.591471000 0.104121000 0.405393000 -1.543850000 -0.478608000 -2.127375000 1.614594000 0.348169000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.614799000 -0.322120000 0.54385000 0.22858000 -0.781459000 0.469445000 0.194844000 1.135254000 1.229429000 2.133594000 0.591960000 2.248061000 4.393325000	0.31420 1.701773000 1.372185000 0.503804000 -0.738162000 -1.675713000 -1.201915000 -0.621839000 0.496810000 1.226276000 -0.864788000 -1.286195000 0.853634000 2.069934000 0.97947000 0.942581000 0.794934000 2.010261000 0.8995000 1.190995000 0.896965000 -1.765688000 -2.824736000 -1.38547000 -2.007889000 -1.590602000 0.170558000 1.156757000	DFT level: uB3LYP/Def2SVP - Thermochemistry -

Н	-3.135651000	5.468143000	0.949255000	
С	-1.599418000	3.891265000	0.862208000	
С	-0.935460000	4.659993000	-0.294592000	
н	0.084804000	4.307440000	-0.475143000	
Н	-0.853211000	5.724619000	-0.029271000	
н	-1.513112000	4.575850000	-1.225392000	
С	-0.697674000	3.967835000	2.102906000	
н	-1.113923000	3.363663000	2.925162000	
н	-0.622699000	5.013509000	2.439550000	
Н	0.324760000	3.631498000	1.880211000	
С	-3.808191000	0.943933000	0.174879000	
С	-5.142530000	-0.761066000	-0.463675000	
С	-4.819662000	-0.956869000	0.855423000	
С	-3.486021000	0.299889000	2.572672000	- 1
Н	-2.910232000	1.230395000	2.597391000	
Н	-2.835121000	-0.54/251000	2.824807000	
H	-4.322989000	0.362324000	3.283492000	
C	-4.453198000	0.879865000	-2.236501000	
Н	-3./16469000	1.688989000	-2.297597000	
Н	-5.435518000	1.255006000	-2.559245000	
Н	-4.145169000	0.056473000	-2.896689000	
	-5.940600000	-1.590614000	-1.407734000	
	-0.451577000	-2.390055000	-0.806/02000	
H	-5.293/43000	-2.065697000	-2.162918000	
Н	-0.701651000	-0.991707000	-1.933549000	
	-5.192825000	-2.050847000	1.793717000	
	-5.696334000	-2.740301000	1.313420000	
	-3.000034000	-1.000000000	2.700003000	
	2 718050000	-2.013333000	-0.380038000	
č	3 224106000	-3 587044000	-0.300930000	
C C	3 181445000	-3 213113000	-2 464772000	
н	4 152841000	-2 778405000	-2 747880000	
H	3.012492000	-4.085234000	-3.113587000	
С	2.078092000	-2.141169000	-2.658847000	
С	2.314642000	-4.802740000	-0.673151000	
н	1.254195000	-4.576945000	-0.826287000	
н	2.415592000	-5.134015000	0.369754000	
Н	2.610016000	-5.646533000	-1.318854000	
С	4.656551000	-3.911642000	-0.512138000	
H	5.034208000	-4.802956000	-1.038320000	
Н	4.695349000	-4.124603000	0.567951000	
Н	5.344913000	-3.075669000	-0.715193000	
C	2.583436000	-1.11/918000	-3.696144000	
Н	1.810711000	-0.409676000	-4.018254000	
	2.931109000	-1.655792000	-4.593244000	
	3.427303000	-0.539093000	-3.292369000	
L L	0.750725000	-2.702003000	-3.123130000	
	0.309445000	-3.490052000	-2.404041000	
ЦЦ	-0.902803000	-2.203090000	-3 268389000	
C	3 270086000	-1 655961000	0.796083000	
C	4 286843000	-0 188465000	2 169360000	
c	3 824798000	-1 232029000	2 934136000	
č	4 365368000	0.280648000	-0.319138000	
Ĥ	5,130131000	-0.286885000	-0.872628000	
H	4.754504000	1.255881000	-0.013365000	
н	3.503380000	0.453789000	-0.965839000	
С	2.413681000	-3.284022000	2.482102000	
н	3.045510000	-4.182038000	2.563037000	
н	1.605244000	-3.459328000	1.757510000	1
н	1.959818000	-3.083067000	3.460959000	
С	5.021368000	1.047368000	2.559238000	
н	6.052318000	1.046745000	2.167395000	
H	5.073796000	1.131533000	3.652620000	
H	4.528687000	1.943320000	2.153758000	1
C	3.896519000	-1.458509000	4.405685000	1
Н	2.900090000	-1.421698000	4.878558000	1
Н	4.516257000	-0.0054/1000	4.878218000	
	4.339230000	-2.4390/0000	4.043930000	



	-4.010331000	3.527094000	0.321598000	
С	-5.322153000	3.279204000	1.087452000	
Ĥ	-5 850345000	4 229472000	1 266844000	
L H	-5 135021000	2 805607000	2 063576000	
	-6 001888000	2.000007000	0.518003000	
	4 256004000	4 197026000	1 021020000	
	-4.330004000	4.167930000	-1.031020000	
H	-3.467319000	4.319836000	-1.663178000	
н	-4.809084000	5.180196000	-0.869944000	
н	-5.084536000	3.582060000	-1.592304000	
н	0.176355000	2.210628000	0.265871000	
н	-0.102264000	-1.466283000	-1.057293000	
S	3.010047000	3.608535000	0.212113000	
0	2.288163000	4.837745000	0.580124000	
Ō	4,464870000	3.573981000	0.481035000	
Ō	2 306440000	2 339419000	0 559376000	
č	2 938070000	3 622208000	-1 670527000	
Ē	2.550070000	4 706660000	2 170471000	
	3.524007000	4.700000000	-2.170471000	
12	3.547165000	2.540033000	-2.194236000	
F	1.661233000	3.600050000	-2.103490000	
S	-1.621138000	-3.521669000	0.913752000	
0	-2.092505000	-2.353530000	1.701533000	
0	-2.095190000	-4.831027000	1.372823000	
0	-0.197646000	-3.438299000	0.501588000	
С	-2.512785000	-3.306558000	-0.737655000	
F	-1.999998000	-4.107336000	-1.675456000	
F	-2,426616000	-2.035732000	-1.202082000	
F	-3.819713000	-3.590890000	-0.619811000	
6 ^{Cy}	-Broken Symmet	ry Singlet	0.010011000	DET level: PBE1PBE/def2SVP
Ň	-1 551830000	2 662897000	0.459278000	
N	4.036543000	0.680260000	1 182002000	Thormochomistry
	-4.030343000	0.009200000	0.001001000	
IN	-4.467093000	1.045431000	-0.901094000	
N	1.722622000	-1.759722000	-1.380674000	Temperature 298.150 Keivin. Pressure 1.00000 Atm.
N	3.885562000	-1.068865000	0.776271000	
N	2.902855000	-2.616167000	1.942143000	Zero-point correction= 1.003205
С	-0.558853000	1.667948000	0.054630000	(Hartree/Particle)
С	-0.555990000	0.387788000	0.883223000	Thermal correction to Energy= 1.067975
н	-1.485160000	-0.188609000	0.750391000	Thermal correction to Enthalpy= 1.068919
н	-0.481981000	0.638399000	1.952785000	Thermal correction to Gibbs Free Energy= 0.902876
С	0.633886000	-0.493175000	0.508480000	Sum of electronic and zero-point Energies= -3653.797924
н	0.565787000	4 440070000	4 404 440000	
н		-1.413072000	1.101419000	Sum of electronic and thermal Energies = -3653.733154
	1 557216000	-1.413072000	1.101419000 0.757276000	Sum of electronic and thermal Energies= -3653.733154 Sum of electronic and thermal Enthalpies= -3653.732210
C	1.557216000	-1.413072000 0.050119000 -0.854696000	1.101419000 0.757276000 -0.976125000	Sum of electronic and thermal Energies= -3653.733154 Sum of electronic and thermal Enthalpies= -3653.732210 Sum of electronic and thermal Free Energies= -3653.898254
C	1.557216000 0.618742000 0.559888000	-1.413072000 0.050119000 -0.854696000 0.421550000	1.101419000 0.757276000 -0.976125000 -1 820144000	Sum of electronic and thermal Energies=-3653.733154Sum of electronic and thermal Enthalpies=-3653.732210Sum of electronic and thermal Free Energies=-3653.898254
C C L	1.557216000 0.618742000 0.559888000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000	1.101419000 0.757276000 -0.976125000 -1.820144000 2.885981000	Sum of electronic and thermal Energies= -3653.733154 Sum of electronic and thermal Enthalpies= -3653.732210 Sum of electronic and thermal Free Energies= -3653.898254 Chargo = 0 Multiplicity = 1
C C H	1.557216000 0.618742000 0.559888000 0.461893000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000	Sum of electronic and thermal Energies= -3653.733154 Sum of electronic and thermal Enthalpies= -3653.732210 Sum of electronic and thermal Free Energies= -3653.898254 Charge = 0 Multiplicity = 1 -3653.898254
C C H H C	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000 0.986755000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000	Sum of electronic and thermal Energies= -3653.733154 Sum of electronic and thermal Enthalpies= -3653.732210 Sum of electronic and thermal Free Energies= -3653.898254 Charge = 0 Multiplicity = 1
ССННС	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.696243000 -1.427147000	Sum of electronic and thermal Energies= -3653.733154 Sum of electronic and thermal Enthalpies= -3653.732210 Sum of electronic and thermal Free Energies= -3653.898254 Charge = 0 Multiplicity = 1
ССННСН	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000 0.986735000 1.306666000 2.222394000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000	Sum of electronic and thermal Energies= -3653.733154 Sum of electronic and thermal Enthalpies= -3653.732210 Sum of electronic and thermal Free Energies= -3653.898254 Charge = 0 Multiplicity = 1
ССННСНН	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000 0.986735000 1.306666000 2.222394000 0.773716000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000	Sum of electronic and thermal Energies= -3653.733154 Sum of electronic and thermal Enthalpies= -3653.732210 Sum of electronic and thermal Free Energies= -3653.732210 -3653.898254 Charge = 0 Multiplicity = 1
ССННСННС	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
ССННСННСС	$\begin{array}{c} 1.557216000\\ 0.618742000\\ 0.559888000\\ 0.461893000\\ 1.497562000\\ -0.621247000\\ -0.614156000\\ -1.565407000\\ -2.884468000\\ -2.414393000\end{array}$	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
ССННСННССН	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
ССННСННССНН	$\begin{array}{c} 1.557216000\\ 0.618742000\\ 0.559888000\\ 0.461893000\\ 1.497562000\\ -0.621247000\\ -0.614156000\\ -1.565407000\\ -2.884468000\\ -2.414393000\\ -2.698809000\\ -2.331608000\end{array}$	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 -3653.732210 -3653.898254
ССННСННССННС	1.557216000 0.618742000 0.559888000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -1.082807000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
ССННСННССННСС	1.557216000 0.618742000 0.559888000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -1.082807000 -0.241145000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.680103000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
ССННСННССННССН	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -1.082807000 -0.241145000 0.710603000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.680103000 4.155636000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
ССТНСННССННССНН	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -1.082807000 -0.241145000 0.710603000 0.018083000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.155636000 5.702302000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000 0.089634000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
ССТТСТТССТТССТТТ	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -0.241145000 0.710603000 0.018083000 -0.771203000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.680103000 4.155636000 5.702302000 4.736021000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000 0.089634000 -1.182929000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
ССТТСТТССТТССТТС	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -1.082807000 -0.241145000 0.710603000 0.018083000 -0.771203000 -0.244481000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.680103000 4.155636000 5.702302000 4.736021000 3.917694000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000 0.089634000 -1.182929000 2.144441000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
ССТТСТТССТТССТТТСТ	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -0.241145000 0.710603000 0.018083000 -0.244481000 -0.244481000 -0.788579000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 4.607073000 4.60103000 4.155636000 4.155636000 5.702302000 4.736021000 3.917694000 3.381978000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
соттоттосттостттотт	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.414393000 -2.331608000 -1.082807000 -0.241145000 0.710603000 0.018083000 -0.771203000 -0.244481000 -0.788579000 -0.010009000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 4.607073000 4.607073000 4.601036000 4.155636000 5.702302000 4.736021000 3.917694000 3.381978000 4.930087000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
СОТТОТТООТТООТТТОТТТ	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.414393000 -2.698809000 -2.331608000 -0.241145000 0.710603000 0.018083000 -0.771203000 -0.244481000 -0.788579000 -0.010009000 0.717968000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 4.607073000 4.680103000 4.155636000 5.702302000 4.736021000 3.917694000 3.917694000 3.381978000 4.930087000 3.420082000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.16980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
СОТТОТТООТТООТТТОТТТС	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -2.331608000 -0.241145000 0.710603000 0.018083000 -0.771203000 -0.244481000 -0.788579000 0.717968000 -3720376000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.680103000 4.155636000 5.702302000 4.736021000 3.917694000 3.381978000 4.930087000 3.420082000 1.478553000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000 0.129266000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1 Charge = 0 Multiplicity = 1
соттоттооттоотттотттос	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -2.331608000 -0.241145000 0.710603000 0.711203000 -0.244481000 -0.788579000 -0.244481000 -0.788579000 -0.717968000 -3.720376000 -5.29255000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.155636000 4.155636000 4.736021000 3.917694000 3.381978000 4.930087000 3.420082000 1.478553000 0.002221000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.22254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000 0.129266000 0.49552020	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
соттоттосттостттотттос	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -2.331608000 -0.241145000 0.710603000 0.7170603000 -0.244481000 -0.788579000 -0.244481000 -0.788579000 -0.717968000 -3.720376000 -5.292559000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.010636000 4.010636000 4.55636000 5.702302000 3.917694000 3.917694000 3.917694000 3.917694000 3.917694000 3.917694000 3.917694000 3.9202000 1.478553000 -0.002221000 0.20202000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.22254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000 0.129266000 -0.492593000 0.896775000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
ооттоттосттостттоттсосо	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -2.331608000 -1.082807000 -0.241145000 0.710603000 0.7170603000 -0.244481000 -0.788579000 -0.244481000 -0.788579000 -0.217968000 -3.720376000 -5.292559000 -5.002979000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.177694000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.010636000 4.010636000 4.155636000 5.702302000 4.736021000 3.917694000 3.381978000 3.420082000 1.478553000 -0.002221000 -0.230307000 0.26055000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000 0.129266000 -0.492593000 0.826775000 2.56775000 2.56775000 2	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
ооттоттооттоотттотттоосо:	1.557216000 0.618742000 0.559888000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.884468000 -2.331608000 -2.331608000 -2.331608000 -0.241145000 0.710603000 0.7170603000 -0.771203000 -0.244481000 -0.788579000 -0.717968000 -3.720376000 -5.292559000 -5.002979000 -3.479439000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 4.607073000 4.607073000 4.607073000 4.010636000 4.010636000 4.736021000 3.81978000 3.81978000 3.81978000 3.420082000 1.478553000 -0.002221000 -0.230307000 0.796953000 4.93007	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000 0.129266000 -0.492593000 0.826775000 2.514209000 2.514209000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
соттоттооттоотттотттоооот:	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.414393000 -2.698809000 -2.331608000 -2.331608000 -0.241145000 0.710603000 0.2414481000 -0.771203000 -0.244481000 -0.788579000 -0.240000 0.717968000 -3.720376000 -5.292559000 -5.002979000 -3.479439000 -2.763763000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.010636000 4.010636000 4.010636000 4.010636000 4.736021000 3.917694000 3.917694000 3.917694000 3.917694000 3.420082000 1.478553000 -0.002221000 -0.230307000 0.796953000 1.625478000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.16980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.222254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000 0.129266000 -0.492593000 0.826775000 2.514209000 2.529147000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
соттоттооттоотттотттосоотт:	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -2.331608000 -0.241145000 0.710603000 0.710603000 -0.771203000 -0.771203000 -0.244481000 -0.788579000 -0.244481000 -0.788579000 -3.720376000 -5.292559000 -5.002979000 -3.479439000 -2.763763000 -2.96643000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.607073000 5.816580000 4.680103000 4.680103000 4.680103000 4.55636000 5.702302000 4.736021000 3.917694000 3.917694000 3.381978000 4.930087000 3.420082000 1.478553000 -0.02221000 -0.230307000 0.796953000 1.625478000 -0.144380000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.427147000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.222254000 -0.222254000 -0.222254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000 0.129266000 -0.492593000 0.826775000 2.514209000 2.529147000 2.757318000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
соттоттооттостттотттососттт	1.557216000 0.618742000 0.559888000 0.461893000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -2.331608000 -2.331608000 -0.241145000 0.710603000 0.711203000 -0.244481000 -0.788579000 -0.244481000 -0.788579000 -0.717968000 -3.720376000 -5.002979000 -3.479439000 -2.763763000 -2.966430000 -4.283533000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.421550000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.680103000 4.680103000 4.680103000 4.736621000 3.917694000 3.917694000 3.917694000 3.381978000 4.930087000 3.420082000 1.478553000 0.002221000 0.796953000 1.625478000 -0.144380000 0.988231000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.427147000 -1.3154000 0.113154000 1.116980000 2.173971000 0.930391000 0.869352000 -0.22254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000 0.129266000 -0.492593000 0.826775000 2.529147000 2.529147000 2.757318000 3.239275000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1
соттоттооттоотттотттосооттто	1.557216000 0.618742000 0.559888000 1.497562000 -0.621247000 -0.614156000 -1.565407000 -2.884468000 -2.414393000 -2.698809000 -2.331608000 -2.331608000 -2.331608000 -0.241145000 0.710603000 0.717203000 -0.244481000 -0.788579000 -0.71203000 -3.720376000 -5.292559000 -5.292559000 -5.002979000 -3.479439000 -2.763763000 -2.966430000 -4.283533000 -4.401128000	-1.413072000 0.050119000 -0.854696000 0.421550000 0.986735000 1.306666000 2.222394000 0.773716000 2.662006000 4.735673000 4.607073000 5.816580000 4.010636000 4.010636000 4.155636000 4.736021000 3.917694000 3.81978000 4.930087000 3.420082000 1.478553000 -0.02221000 0.796953000 0.796953000 1.625478000 -0.144380000 0.988231000 1.526097000	1.101419000 0.757276000 -0.976125000 -1.820144000 -2.885981000 -1.696243000 -1.427147000 -2.039821000 -1.427147000 -2.039821000 -1.641136000 0.113154000 1.116980000 2.173971000 0.869352000 -0.22254000 -0.22254000 -0.369924000 0.089634000 -1.182929000 2.144441000 2.938182000 2.506767000 1.955509000 0.129266000 -0.492593000 0.826775000 2.529147000 2.529147000 2.757318000 3.239275000 -2.259283000	Sum of electronic and thermal Energies= Sum of electronic and thermal Enthalpies= Sum of electronic and thermal Free Energies= Charge = 0 Multiplicity = 1

_			
H	-5.301515000	2.091832000	-2.540720000
۱Ŀ	-4.283295000	0.675910000	-2.945297000
	· _6 206132000	-0.716056000	-1 418040000
		1 422 41 4000	0 959364000
	-0.030012000	-1.423414000	-0.838384000
	-5.644185000	-1.300464000	-2.164429000
F	-6.874332000	-0.024763000	-1.954754000
0	-5.547172000	-1.228077000	1.778936000
L F	I -6.333809000	-1 822072000	1 298431000
Li	5 080580000	0 743406000	2 668176000
11	-5.980580000	-0.743490000	2.008170000
	-4.742230000	-1.908028000	2.099062000
0	2.361510000	-2.602257000	-0.490381000
0	2.642463000	-3.972689000	-1.093521000
0	2.649805000	-3.574451000	-2.578614000
ÌÈ	3.675702000	-3,289353000	-2.861041000
11	1 2247602000	1 101612000	2 228205000
12		-4.401013000	-3.230293000
	, 1.729469000	-2.350294000	-2.751851000
(1.550895000	-5.019220000	-0.805464000
H	1 0.537196000	-4.605986000	-0.875429000
۱Ŀ	1 1.648232000	-5.427478000	0.210119000
Ŀ	1 652523000	-5 862787000	-1 507532000
	1 1.052525000	-5.002707000	-1.507552000
C	, 4.001705000	-4.537909000	-0.678257000
ŀ	4.209878000	-5.470754000	-1.225585000
H	4.031312000	-4.778376000	0.395816000
LE	4.818793000	-3.830452000	-0.890046000
Ċ	2 376812000	-1 418880000	-3 786056000
	1 727101000	0.577450000	4.078214000
15	1 1.737101000	-0.577156000	-4.078314000
ŀ	2.597117000	-1.995362000	-4.698758000
۱ŀ	3.325672000	-1.011951000	-3.406911000
0	; 0.328999000	-2.754473000	-3.221796000
۱ŀ	-0.162937000	-3.438566000	-2.517701000
L F	1 0.405941000	-3 259310000	-4 196344000
Ľ	0.206957000	1 00000	2 256964000
	-0.320637000	-1.002303000	-3.330604000
	3.017020000	-2.106427000	0.692154000
0	<i>i</i> 4.314681000	-0.914112000	2.080546000
0	3.703958000	-1.897332000	2.814639000
0	; 4,412347000	-0.323568000	-0.349558000
Ì	4 5 207602000	0.826225000	0.758277000
	1 5.297602000	-0.030223000	-0.756277000
	4.680289000	0.688790000	-0.025613000
F	1 3.641790000	-0.249070000	-1.122223000
0	; 1.959829000	-3.639670000	2.341422000
۱ŀ	2.433555000	-4.632920000	2.362441000
l i	1 100613000	-3 648666000	1 652564000
Ľ	1.100013000	-3.040000000	1.052504000
	1 1.587616000	-3.410246000	3.347766000
0	5.276617000	0.140113000	2.485398000
H	6.280814000	-0.051047000	2.072528000
۱ŀ	5.364037000	0.175006000	3.578610000
l i	4 965865000	1 133653000	2 120457000
	4.905005000	0.00000000	2.120457000
1.	, 3.790576000	-2.206287000	4.263983000
1 6	2.830777000	-2.044457000	4.781713000
۱ŀ	4.535286000	-1.556681000	4.740482000
H	4.092598000	-3.250533000	4.442489000
0	-3 486064000	4 063470000	0 232869000
	1 848070000	4.062250000	0.020845000
1.	, -4.848979000	4.002339000	0.929845000
۱ŀ	-5.2051/3000	5.094075000	1.077740000
۱ŀ	-4.799396000	3.579921000	1.917961000
H	-5.610653000	3.536246000	0.331815000
0	-3.637628000	4.776986000	-1.121381000
ÌÌ	1 -2 715827000	4 737688000	-1 716968000
11	1 2 204712000	5 927620000	0.067024000
!	-3.094/13000	5.03/020000	-0.90/034000
۱ŀ	-4.447015000	4.330791000	-1./18811000
۱ŀ	0.418520000	2.143248000	0.223999000
I F	-0.316331000	-1.421339000	-1.134096000
	3 547412000	3 276736000	0.367229000
) 3 070340000	1 572022000	0 855245000
	· J.079240000	4.07.0032000	0.000240000
	4.896365000	2.855847000	0.786357000
) 2.543154000	2.185527000	0.419856000
0	3.755713000	3.537898000	-1.459378000
F	4 621143000	4 507265000	-1 712520000
Ľ	. 4 40 40 78000	2.400550000	2.052525000
	4.194978000	2.422552000	-2.032535000
- F	2.392138000	3.030104000	-2.031340000

S	-2.188431000	-3.355598000	1.024103000	
0	-2.585567000	-2.110177000	1.714719000	
0	-2.711289000	-4.590184000	1.596089000	
0	-0.774527000	-3.377416000	0.598051000	
С	-3.075773000	-3.224064000	-0.605596000	
F	-2.713993000	-4.200626000	-1.429463000	
F	-2.813863000	-2.059036000	-1.221366000	
F	-4.398558000	-3.290015000	-0.442165000	
6 ^{Cy}	-Triplet			DFT level: PBE1PBE/def2SVP
Ν	-1.551742000	2.662981000	0.459394000	- Thermochemistry -
Ν	-4.036508000	0.689453000	1.183018000	
Ν	-4.487020000	1.045622000	-0.901077000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Ν	1.722576000	-1.759942000	-1.380627000	
Ν	3.885568000	-1.069043000	0.776265000	Zero-point correction= 1.003205
Ν	2.902650000	-2.616166000	1.942188000	(Hartree/Particle)
С	-0.558725000	1.667974000	0.054735000	Thermal correction to Energy= 1.067976
С	-0.556139000	0.387741000	0.883131000	Thermal correction to Enthalpy= 1.068920
Н	-1.485290000	-0.188607000	0.749937000	Thermal correction to Gibbs Free Energy= 0.901835
Н	-0.482457000	0.638170000	1.952763000	Sum of electronic and zero-point Energies= -3653.797912
С	0.633817000	-0.493244000	0.508619000	Sum of electronic and thermal Energies= -3653.733142
н	0.565610000	-1.413103000	1.101581000	Sum of electronic and thermal Enthalpies= -3653.732198
н	1.557103000	0.050069000	0.757550000	Sum of electronic and thermal Free Energies= -3653.899282
С	0.618831000	-0.854723000	-0.975998000	
С	0.560339000	0.421619000	-1.819903000	Charge = 0 Multiplicity = 3
н	0.462587000	0.177967000	-2.885809000	
н	1.498055000	0.986632000	-1.695639000	
С	-0.620741000	1.306942000	-1.427112000	
Н	-0.613231000	2.222758000	-2.039645000	
н	-1.564938000	0.774249000	-1.641545000	
С	-2.884359000	2.662155000	0.113170000	P 🚵 🖉
С	-2.414201000	4.735894000	1.116793000	
н	-2.698625000	4.607408000	2.173796000	
н	-2.331362000	5.816780000	0.930101000	
С	-1.082652000	4.010766000	0.869240000	
С	-0.240986000	4.680060000	-0.222470000	
Н	0.710726000	4.155517000	-0.370114000	
H	0.018314000	5.702277000	0.089297000	
Н	-0.771068000	4.735908000	-1.183135000	
С	-0.244306000	3.917986000	2.144330000	
н	-0.788399000	3.382368000	2.938140000	
н	-0.009829000	4.930425000	2.506523000	
Н	0.718142000	3.420352000	1.955455000	
C	-3.720311000	1.478735000	0.129292000	
C	-5.292512000	-0.002013000	-0.492584000	
C	-5.002955000	-0.230096000	0.826/91000	
	-3.4/9413000	0.797134000	2.514239000	
H	-2.763675000	1.625605000	2.529164000	
н	-2.9004/2000	-0.144232000	2.131309000	
	-4.200000000	0.900401000	3.233234000 -2.250285000	
	-4.400900000	2 120114000	-2.209200000	
	-3.324147000	2.100114000	-2.337099000	
	-0.001071000	2.031000000	-2.04000000	
	-4.203014000	0.070000000	-2.945244000	
Ц	-0.200090000	-0.7 10020000	-1.410037000	
μ	-0.029991000	-1 300233000	-2 164434000	
μ	-6 874286000	-0.024511000	-1 954741000	
	-5 547180000	-1 227844000	1 778958000	
н	-6 333814000	-1 821838000	1 298447000	
н	-5.980598000	-0.743242000	2.668181000	
H	-4.742254000	-1.907804000	2.099108000	
C C	2.361560000	-2.602466000	-0.490393000	
c l	2.642412000	-3.972942000	-1.093464000	
l č	2.649476000	-3.574819000	-2.578580000	
н	3.675321000	-3.289735000	-2.861213000	
H	2.347246000	-4.402023000	-3.238158000	
c	1.729115000	-2.350668000	-2.751753000	
Ċ	1.550931000	-5.019494000	-0.805132000	
Ĥ	0.537204000	-4.606287000	-0.874892000	
H	1.648513000	-5.427730000	0.210437000	

Н	1 652427000	-5 863080000	-1 507195000	
C	4 001740000	-4 538083000	-0.678374000	
й	4 2008/0000	-5 /700000000	-1 225600000	
	4.203040000	4 779404000	0.205720000	
	4.031334000	-4.776401000	0.393729000	
	4.616775000	-3.830634000	-0.890397000	
С	2.376266000	-1.419440000	-3.786254000	
н	1.736367000	-0.577953000	-4.078778000	
н	2.596684000	-1.996166000	-4.698776000	
н	3.325044000	-1.012186000	-3.407253000	
С	0.328532000	-2.754841000	-3.221346000	
Ĥ	-0 163289000	-3 438818000	-2 517058000	
Ц	0.100200000	-3 250708000	-4 195851000	
	0.400240000	1 002720000	2 256296000	
	-0.327301000	-1.002730000	-3.330360000	
	3.017002000	-2.106588000	0.692150000	
С	4.314539000	-0.914165000	2.080565000	
С	3.703681000	-1.897278000	2.814697000	
С	4.412517000	-0.323870000	-0.349569000	
н	5.298072000	-0.836362000	-0.757845000	
н	4,680053000	0.688647000	-0.025786000	
H	3 642198000	-0 249823000	-1 122514000	
	1 050564000	3 630615000	2 241470000	
	1.959504000	-3.039013000	2.341470000	
	2.433299000	-4.632856000	2.362705000	
н	1.100451000	-3.648/12000	1.652489000	
н	1.587198000	-3.410045000	3.347724000	
С	5.276489000	0.140051000	2.485404000	
н	6.280712000	-0.051200000	2.072638000	
н	5.363815000	0.175045000	3.578620000	
н	4 965820000	1 133572000	2 120338000	
C	3 790111000	-2 206072000	4 264087000	
ŭ	2 920255000	2.200072000	4 791690000	
	2.03020000	-2.044139000	4.781080000	
	4.534790000	-1.556443000	4.740602000	
н	4.092065000	-3.250310000	4.442750000	
С	-3.485899000	4.063655000	0.232744000	
С	-4.848809000	4.062648000	0.929732000	
н	-5.204967000	5.094389000	1.077546000	
н	-4.799231000	3.580288000	1.917887000	
н	-5 610507000	3 536512000	0.331752000	
C	-3 637456000	4 777069000	-1 121562000	
ŭ	2 715675000	4.727672000	1 717172000	
	-2.713073000	4.737073000 E 027720000	-1.717175000	
	-3.694473000	5.637736000	-0.967290000	
н	-4.446890000	4.330880000	-1.718932000	
Н	0.418626000	2.143216000	0.224396000	
н	-0.316310000	-1.421223000	-1.134054000	
S	3.547596000	3.276666000	0.367178000	
0	3.079445000	4.572976000	0.855177000	
Ō	4 896550000	2 855764000	0 786289000	
ŏ	2 543331000	2 185466000	0.419846000	
č	2.343331000	2.103400000	1 450427000	
L C	3.133019000	J.JJ// 91000	-1.403407000	
	4.021348000	4.507117000		
	4.195091000	2.422414000	-2.052576000	
ΓF	2.592313000	3.858095000	-2.031392000	
S	-2.188529000	-3.355569000	1.024054000	
0	-2.585592000	-2.110182000	1.714769000	
0	-2.711354000	-4.590184000	1.596007000	
0	-0.774655000	-3.377386000	0.597890000	
Ĉ	-3 075976000	-3 223942000	-0.605578000	
F	-2 714304000	-4 20050000	-1 429497000	
	2.1 14304000	2 050000000	1 224270000	
	-2.014045000	-2.000908000	-1.221332000	
F	-4.398754000	-3.289830000	-0.442063000	
4 ^{≞t}				DFT level: RB3LYP-D3/6-31G(d,p)
Ν	-1.004299000	-1.389584000	-0.811337000	- Thermochemistry -
Ν	-3.079111000	0.612210000	-1.184823000	
Ν	-4.231047000	-0.132486000	0.661333000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
C	-0.173593000	-0.204723000	-0.722646000	
Гй	-0 671452000	0 644822000	-1 205548000	Zero-point correction= 0.847027
	0.071402000	0.221252000	1 275721000	(Hartroo/Darticlo)
	0.751610000	-0.301333000	-1.2/3/21000	Thermal correction to Energy 0.000000
	-2.246013000	-1.4528/5000	-0.125919000	Thermal correction to Energy= 0.890626
C	-2.411226000	-2.854858000	0.450191000	I nermal correction to Enthalpy= 0.891571
С	-3.145274000	-0.431549000	-0.217146000	Thermal correction to Gibbs Free Energy= 0.773371
С	-0.4 <u>3871800</u> 0	-2.724203000	-1.092659000	Sum of electronic and zero-point Energies= -1580.912385

С	-1.569055000	-3.656255000	-0.589910000	
Н	-1.175508000	-4.588444000	-0.172311000	
Н	-2.217580000	-3.923367000	-1.431374000	
С	-3.857577000	-3.372368000	0.438737000	
н	-4.503269000	-2.828760000	1.131668000	
н	-3.883040000	-4.431859000	0.718089000	
Н	-4.291974000	-3.266313000	-0.559771000	
С	0.896626000	-3.000700000	-0.368108000	
Н	1.673349000	-2.286855000	-0.653680000	
Н	1.254721000	-4.002228000	-0.629833000	
Н	0.793171000	-2.952327000	0.716603000	
С	-4.778247000	1.111470000	0.217931000	
С	-2.911836000	0.209630000	-2.581535000	
н	-2.011543000	-0.398210000	-2.673077000	
н	-2.801929000	1.097648000	-3.207660000	
Н	-3.767254000	-0.382374000	-2.942146000	
C	-4.123176000	1.528866000	-0.879381000	
C	-0.212360000	-2.885710000	-2.607831000	
н	-1.140518000	-2.690576000	-3.153230000	
н	0.129537000	-3.897719000	-2.854694000	
Н	0.548115000	-2.180359000	-2.961931000	
	-1.797666000	-3.009992000	1.862200000	
	-0.809764000	-2.546329000	1.910/40000	
н	-1.697646000	-4.069257000	2.128012000	
	-2.417000000	-2.536649000	2.020391000	
	-4.007842000	-0.282555000	2.095295000	
	-3.959771000	-1.333349000	2.371300000	
	-4.042233000	0.100090000	2.045169000	
	-3.070830000	2 738767000	-1 725161000	
й	-4.333023000	3 301332000	-1.822921000	
н	-5.079807000	3 400926000	-1 281522000	
H	-4.670632000	2,490114000	-2,739574000	
C	-5.917466000	1.746067000	0.943416000	
H	-6.713728000	1.014076000	1.123488000	
Н	-6.339817000	2.564455000	0.356685000	
Н	-5.627149000	2.158331000	1.918570000	
Ν	1.004378000	1.389493000	0.811654000	
Ν	3.079228000	-0.612374000	1.184487000	
Ν	4.230955000	0.132709000	-0.661649000	
С	0.173746000	0.204582000	0.722950000	
н	0.671667000	-0.644938000	1.205830000	
Н	-0.751471000	0.381142000	1.276034000	
C	2.246016000	1.452932000	0.126108000	
C	2.411153000	2.855019000	-0.449773000	
C	3.145295000	0.431597000	0.217028000	
	0.436730000	2.72404000	1.093107000	
ц	1.000904000	3.030227000	0.590475000	
н	2 217535000	3 023270000	1 /31038000	
Ċ	3 857485000	3 372585000	-0 438269000	
н	4 503187000	2 829110000	-1 131294000	
H	3.882901000	4,432120000	-0.717460000	
H	4.291905000	3,266395000	0.560215000	
C	-0.896669000	3.000553000	0.368722000	
H	-1.673354000	2.286664000	0.654289000	
н	-1.254783000	4.002047000	0.630547000	
Н	-0.793289000	2.952258000	-0.715998000	
С	4.778184000	-1.111358000	-0.218587000	
С	2.912164000	-0.210078000	2.581308000	1
Н	2.011920000	0.397797000	2.673094000	1
Н	2.802282000	-1.098222000	3.207261000	1
H	3.767670000	0.381792000	2.941932000	1
C	4.123241000	-1.528981000	0.878716000	1
	0.212444000	2.885358000	2.608370000	1
Н	1.140644000	2.690226000	3.153698000	1
H U	-0.129511000	3.89/314000	2.855368000	1
	-0.341902000 1 707564000	2.1/9913000	2.902429000 -1 8617/7000	1
н	0.809665000	2.548686000	-1.916333000	1
•••	2.23000000			



Н	1.697534000	4.069650000	-2.127410000	
н	2.417755000	2.537112000	-2.626213000	
C	4.007569000	0.283101000	-2.095549000	
Ĥ	3,959493000	1.334157000	-2.371517000	
H	4.841874000	-0.155054000	-2.645650000	
H	3 070499000	-0 199555000	-2 417307000	
C	4 333759000	-2 739075000	1 724203000	
н	3 307178000	-3 301630000	1.821955000	
	5.070860000	3 401160000	1.02100000	
	4 670002000	2 400654000	2 728620000	
	4.070902000	-2.490034000	2.730029000	
	5.917502000	-1.743620000	-0.944340000	
	0.713559000	-1.013607000	-1.124352000	
	6.339703000	-2.564346000	-0.357844000	
	5.020002000	-2.157603000	-1.919557000	
5-				DFT level: B3LYP-D3/6-31G(d,p)
94				- Thermochemistry -
sym	metry c1			
N	-1.305337000	-1.388687000	0.173299000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Ν	-3.831434000	0.458703000	1.143553000	
Ν	-3.973877000	0.626760000	-1.029342000	Zero-point correction= 0.851901
С	-0.418659000	-0.278855000	0.592768000	(Hartree/Particle)
Н	0.243609000	-0.671697000	1.365679000	Thermal correction to Energy= 0.895677
н	-1.023792000	0.509706000	1.033517000	Thermal correction to Enthalpy= 0.896621
С	-2.569879000	-1.295368000	-0.142762000	Thermal correction to Gibbs Free Energy= 0.776279
С	-3.356219000	-0.042738000	-0.026604000	Sum of electronic and zero-point Energies= -1579.657223
С	-3.208659000	-2.635769000	-0.450312000	Sum of electronic and thermal Energies= -1579.613447
С	-1.974976000	-3.573002000	-0.498654000	Sum of electronic and thermal Enthalpies= -1579.612502
н	-2.188512000	-4.542530000	-0.045015000	Sum of electronic and thermal Free Energies= -1579.732845
H	-1.695766000	-3.755771000	-1.539981000	g
Ċ	-0.819643000	-2.859148000	0.233822000	Charge = 4 Multiplicity = 1
č	-4 184600000	-2 960245000	0 723456000	
й	-3 696233000	-2 971076000	1 699501000	
ЦЦ	-4 594750000	-3 958366000	0.547090000	
	5 022500000	2 250021000	0.347030000	
	4 012082000	2.239921000	1 767224000	
L L	4.012903000	2.07.5200000	1 720212000	
	-4.077043000	-2.000004000	-1.730212000	
	-4.395969000	-3.069106000	-1.696923000	
Н	-3.395377000	-2.444169000	-2.638678000	
C	-0.699632000	-3.248717000	1.715137000	
н	0.083835000	-2.688231000	2.233997000	
н	-0.427901000	-4.306508000	1.770158000	
н	-1.638570000	-3.124680000	2.257297000	The second secon
С	0.519088000	-3.026745000	-0.484777000	
н	0.470849000	-2.690377000	-1.524603000	
Η	0.760261000	-4.093206000	-0.500957000	
н	1.338988000	-2.522758000	0.038414000	
С	-4.842326000	1.566655000	-0.497380000	
С	-4.762887000	1.450185000	0.879862000	
С	-3.540337000	-0.026642000	2.503512000	
н	-4.433168000	-0.493496000	2.924095000	
н	-3.248588000	0.817079000	3.130354000	
н	-2.734710000	-0.757737000	2.473823000	
С	-3.718064000	0.497496000	-2.474885000	
H	-4.618630000	0.145512000	-2.980050000	
Ь	-2.908952000	-0.210457000	-2.642433000	
ЬH	-3.441573000	1.474044000	-2.875526000	
С	-5.656465000	2.478440000	-1.349369000	
н	-5.026607000	3.135503000	-1.959221000	
ЬН	-6.289449000	3.112585000	-0.728185000	
Гн	-6.310218000	1 914830000	-2 023245000	
C	-5 499432000	2 166507000	1 959396000	
н	-6 103662000	1 474202000	2 556017000	
	-6 176671000	2 904704000	1 529251000	
	-4 818204000	2.004/04000	2 626161000	
N	1 3052/7000	2.033012000	2.000101000	
	2 924 4 40000	0 450703000	1 1/250000	
	3.031440000	-0.430/3/000	1.143309000	
	0.419666000	-0.020/4/000	1.029392000	
	0.410000000	0.210010000	-0.392011000	
	1 022000000	0.071710000	1 022554000	
	1.023000000	-0.309000000	-1.033334000	

	2 560002000	1 205291000	0 1 4 2 7 4 1 0 0 0	
~	2.309003000	1.295561000	0.142741000	
C	3.356207000	0.042737000	0.026627000	
С	3.208674000	2.635779000	0.450277000	
С	1.975004000	3.573030000	0.498574000	
й	2 188562000	4 542546000	0.044921000	
	2.100302000	9.342340000	0.044021000	
н	1.695773000	3.755823000	1.539891000	
С	0.819676000	2.859178000	-0.233913000	
С	4.184644000	2.960216000	-0.723478000	
ŭ	3 606208000	2 071022000	1 600534000	
	3.090290000	2.971033000	-1.099554000	
н	4.594805000	3.958335000	-0.547124000	
Н	5.023544000	2.259880000	-0.749372000	
С	4.012972000	2.673291000	1.767214000	
н	4 877021000	2 00557/000	1 738222000	
	4.077021000	2.000074000	1.750222000	
н	4.395972000	3.689189000	1.896891000	
н	3.395346000	2.444221000	2.638650000	
С	0.699705000	3.248716000	-1.715238000	
н	-0.083761000	2 688234000	-2 234104000	
	0.427005000	4 206512000	1 770280000	
	0.427995000	4.300312000	-1.770289000	
н	1.638653000	3.124651000	-2.257375000	
С	-0.519069000	3.026817000	0.484651000	
Н	-0.470862000	2.690471000	1.524486000	
н	-0 760221000	4 003383000	0 500802000	
	4 220007000	7.033203000	0.00002000	
Н	-1.338967000	2.522836000	-0.038549000	
С	4.842275000	-1.566673000	0.497468000	
С	4.762867000	-1.450231000	-0.879778000	
C	3 540381000	0.026585000	-2 503485000	
ц	1 1222200000	0.402420000	2 02/057000	
	4.433220000	0.493420000	-2.924007000	
н	3.248636000	-0.817144000	-3.130316000	
Н	2.734763000	0.757692000	-2.473830000	
С	3 718001000	-0 497443000	2 474928000	
ŭ	4 619567000	0.145469000	2.08000000	
	4.010507000	-0.143400000	2.980099000	
н	2.908902000	0.210533000	2.642445000	
H	3.441481000	-1.473974000	2.875587000	
С	5.656379000	-2.478455000	1.349494000	
н	5 026496000	-3 135491000	1 959350000	
L L	6 280261000	3 112620000	0 728336000	
	0.209301000	-3.112029000	0.728330000	
	1- 111111111111111			
н	0.310131000	-1.914843000	2.023369000	
н С	5.499418000	-1.914843000 -2.166593000	-1.959281000	
н С Н	5.499418000 6.103661000	-1.914843000 -2.166593000 -1.474404000	2.023369000 -1.959281000 -2.555917000	
н С Н Н	5.499418000 6.103661000 6.176646000	-1.914843000 -2.166593000 -1.474404000 -2.904873000	2.023369000 -1.959281000 -2.555917000 -1.529105000	
	5.499418000 6.103661000 6.176646000 4.818293000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000	
	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000	
⊢ C H H B ^{Et}	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000	DFT level: B3LYP-D3/6-31G(d,p)
H C H H 8 ^{Et}	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry -
H C H H 8 ^{Et} N	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry -
H H H 8 ^{Et} N N	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 -0.427869000 -0.535414000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry -
	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 -0.427869000 -0.427869000 -0.535414000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 0.372701000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559994000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
FCHHH 8 ^{Et} NNNCC	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 -0.427869000 -0.535414000 0.559094000 1.396532000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143
ГСННН <mark>8</mark> И И И И И И И И И И И И И И И И И И И	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry -
ГСННН <mark>8</mark> ИNNCCHC	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121
ГСННН <mark>8</mark> ^{EE} NNNCCHCC	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.962881000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.026913000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Enthalpy= 0.897065
Г С Н Н Н <mark>8</mark> Z Z Z C C H C C C	6.310131000 5.499418000 6.10361000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.998512000 2.962881000 0.531776002	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.002402000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 0.226913000 0.226913000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Enthalpy= 0.897065 Thermal correction to Enthalpy= 0.70222
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Г С Н Н Н <mark>8</mark> Z Z Z C C H C C C C	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.9928512000 2.992881000 0.531776000 1.772782000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 -0.334006000 0.230975000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Enthalpy= 0.897065 Thermal correction to Gibbs Free Energy= 0.780293 Sum of electronic and zero-point Energies= -1580.561525
Г С Н Н Н <mark>8</mark> Z Z Z C C H C C C C H	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.962881000 0.531776000 1.772782000 1.570685000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 -0.334006000 0.230975000 1.258051000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Enthalpy= 0.897065 Thermal correction to Gibbs Free Energy= 0.780293 Sum of electronic and zero-point Energies= -1580.561525 Sum of electronic and thermal Energies= -1580.518547
	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.962881000 0.531776000 1.570685000 2.001366000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Enthalpy= 0.897065 Thermal correction to Gibbs Free Energy= 0.780293 Sum of electronic and thermal Energies= -1580.561525 Sum of electronic and thermal Energies= -1580.518547 Sum of electronic and thermal Energies= -1580.517603
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г ∪	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.96281000 0.531776000 1.570685000 2.001366000 3.732484000 3.081251000 4.535264000 4.197253000 3.932991000 4.765150002	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.797863000 3.014272000 2.302104000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.246913000 -0.334006000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 -1.205801000 1.384614000 1.384348000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Enthalpy= 0.897065 Thermal correction to Gibbs Free Energy= 0.780293 Sum of electronic and zero-point Energies= -1580.561525 Sum of electronic and thermal Energies= -1580.518547 Sum of electronic and thermal Energies= -1580.517603 Sum of electronic and thermal Free Energies= -1580.634375 Charge = 2 Multiplicity = 1 1
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гОІТІ <mark></mark> , 	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.992881000 0.531776000 1.772782000 1.570685000 2.001366000 3.732484000 3.081251000 4.535264000 4.197253000 3.932991000 4.765150000 3.432283000 4.366199000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.797863000 3.014272000 2.302104000 2.963014000 4.013769000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 -1.205801000 1.381348000 2.357326000 1.291011000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry -
ΓΟΙΙΙΙ<mark>ω</mark> ΖΖΖΟΟΙΟΟΟΟΙΙΟΙΙΙΟΙΙΙΟ	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.962881000 0.531776000 1.772782000 1.570685000 2.001366000 3.732484000 3.081251000 4.535264000 4.197253000 3.932991000 4.765150000 3.432283000 4.366199000 -0.664099000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.797863000 3.014272000 2.302104000 2.963014000 2.963014000 3.166316000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.246913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 -1.381348000 2.357326000 1.291011000 0.620360000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Enthalpy= 0.897065 Thermal correction to Gibbs Free Energy= 0.780293 Sum of electronic and zero-point Energies= -1580.561525 Sum of electronic and thermal Energies= -1580.518547 Sum of electronic and thermal Energies= -1580.517603 Sum of electronic and thermal Free Energies= -1580.634375 Charge = 2 Multiplicity = 1 -1580.634375
готтт <mark>ж</mark> z z состосоттотттотттот	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.998512000 2.962881000 0.531776085000 1.5770685000 2.001366000 3.732484000 3.081251000 4.535264000 4.197253000 3.932991000 4.765150000 3.432283000 4.366199000 -0.664099000 -0.664099000 -1.571122000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.797863000 3.014272000 2.302104000 2.302104000 2.963014000 4.013769000 3.166316000 3.69895000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -0.389055000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 -1.381481000 1.381484000 1.381348000 2.357326000 1.291011000 0.620360000 0.225576000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Energy= 0.897065 Thermal correction to Gibbs Free Energy= 0.780293 Sum of electronic and zero-point Energies= -1580.561525 Sum of electronic and thermal Energies= -1580.517603 Sum of electronic and thermal Free Energies= -1580.634375 Charge = 2 Multiplicity = 1 1
г ∪	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.992831000 0.531776000 1.772782000 1.570685000 2.001366000 3.732484000 3.081251000 4.535264000 3.932991000 4.765150000 3.432283000 4.366199000 -0.664099000 -1.571122000 -0.871688000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.014272000 2.302104000 2.963014000 4.013769000 3.166316000 2.698995000 4.230453000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 -1.205801000 1.384614000 1.381348000 2.357326000 1.291011000 0.620360000 0.225576000 0.764764000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry -
готтт <mark>ж</mark> z z состосоттотттотттотт	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.992881000 0.531776000 1.772782000 1.570685000 2.001366000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.73248000 4.197253000 3.432283000 4.366199000 -0.664099000 -1.571122000 -0.871688000 0.44864002	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.797863000 3.014272000 2.302104000 2.963014000 2.963014000 2.963014000 2.698995000 4.230453000 2.720453000 2.720453000 2.720453000 2.720453000 2.720453000 2.720453000 2.720453000 2.720453000 2.72000 2.720453000 2.72000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 -1.205801000 1.381348000 2.357326000 1.291011000 0.620360000 0.225576000 0.764764000 1.60282000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry -
ΓΟΙΙΙΙ<mark>ω</mark> ΖΖΖΟΟΙΟΟΟΙΙΟΙΙΙΟΙΙΙΟΙΙΙΟ	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.962881000 0.531776000 1.772782000 1.570685000 2.001366000 3.732484000 3.081251000 4.535264000 4.197253000 3.932991000 4.535264000 4.365150000 3.432283000 4.366199000 -0.664099000 -0.871688000 -0.448661000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.797863000 3.014272000 2.302104000 2.302104000 2.963014000 2.963014000 3.166316000 2.698995000 4.230453000 2.726670000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 -1.205801000 1.384614000 1.381348000 2.357326000 1.291011000 0.620360000 0.225576000 0.764764000 1.600380000 -1.4005000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Enthalpy= 0.897065 Thermal correction to Gibbs Free Energy= 0.780293 Sum of electronic and zero-point Energies= -1580.561525 Sum of electronic and thermal Energies= -1580.518547 Sum of electronic and thermal Energies= -1580.517603 Sum of electronic and thermal Free Energies= -1580.634375 Charge = 2 Multiplicity = 1 -1580.634375
готтт <mark>ж</mark> z z с отооооттотттотттоттто	6.310131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.96281000 0.531776000 1.772782000 1.570685000 2.001366000 3.732484000 3.081251000 4.535264000 4.197253000 3.932991000 4.765150000 3.432283000 4.366199000 -0.664099000 -0.664099000 -0.671688000 -0.871688000 -0.448661000 0.147718000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.797863000 3.014272000 2.302104000 2.963014000 2.963014000 2.963014000 2.698995000 4.230453000 2.726670000 3.456540000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.74533000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 1.381481000 1.3814814000 1.381348000 2.357326000 1.291011000 0.620360000 0.225576000 0.764764000 1.600380000 -1.744685000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry - Temperature 298.150 Kelvin. Pressure 1.00000 Atm. Zero-point correction= 0.853143 (Hartree/Particle) Thermal correction to Energy= 0.896121 Thermal correction to Energy= 0.897065 Thermal correction to Gibbs Free Energy= 0.780293 Sum of electronic and zero-point Energies= -1580.561525 Sum of electronic and thermal Energies= -1580.518547 Sum of electronic and thermal Energies= -1580.517603 Sum of electronic and thermal Free Energies= -1580.634375 Charge = 2 Multiplicity = 1 -1580.634375
τΟ ΙΙΙ Ι <mark>δ</mark> ΖΖΖΟΟΙΟΟΟΟΙΙΟΙΙΟΙΙΙΟΙΙΙΟΙΙΙΟΙ	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.998512000 2.992831000 0.531776000 1.772782000 1.570685000 2.001366000 3.732484000 3.081251000 4.535264000 3.932991000 4.765150000 3.432283000 4.366199000 -0.664099000 -0.571122000 -0.871688000 0.147718000 0.996457000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.014272000 2.302104000 2.963014000 4.013769000 3.166316000 2.698995000 4.230453000 2.726670000 3.456540000 3.395252000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -2.636037000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 -1.295801000 1.384614000 1.381348000 2.357326000 1.291011000 0.620360000 0.225576000 0.764764000 1.600380000 -1.744685000 -2.429698000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry -
τΟ ΙΙΙ Ι <mark>ω</mark> ΖΖΖΟΟΙΟΟΟΟΙΙΟΙΙΙΟΙΙΙΟΙΙΙΟΙΙΙΟΙΙ	6.10131000 5.499418000 6.103661000 6.176646000 4.818293000 0.989861000 3.184872000 3.730042000 0.003938000 2.193404000 1.932387000 2.992881000 0.531776000 1.772782000 1.570685000 2.001366000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.732484000 3.73248000 4.535264000 4.197253000 3.932991000 4.366199000 -0.664099000 -0.571122000 -0.871688000 0.996457000 0.996457000 -0.198389000	-1.914843000 -2.166593000 -1.474404000 -2.904873000 -2.693115000 1.556704000 -0.427869000 -0.535414000 0.559094000 1.396532000 1.305340000 0.164942000 2.750211000 2.993108000 3.736998000 4.056622000 4.638389000 2.813720000 2.669129000 2.070302000 3.797863000 3.014272000 2.302104000 2.963014000 2.963014000 2.963014000 2.698995000 4.230453000 2.726670000 3.456540000 3.395252000 4.493954000	2.023369000 -1.959281000 -2.555917000 -1.529105000 -2.636037000 -1.122136000 0.972761000 -0.377004000 0.410558000 1.479926000 0.074533000 0.226913000 -0.334006000 0.230975000 1.258051000 -0.343219000 -1.103368000 -1.966797000 -1.144280000 -1.205801000 1.381348000 2.357326000 1.291011000 0.620360000 0.225576000 0.764764000 1.600380000 -1.724127000	DFT level: B3LYP-D3/6-31G(d,p) - Thermochemistry -

С	4.393237000	-1.584253000	0.334410000	
C	4.045327000	-1.517710000	-0.985635000	
С	2.589173000	-0.065733000	-2.413898000	
н	1.907541000	0.764586000	-2.265469000	
	2.040203000	-0.926433000	-2.603341000	A 197
	3.362316000	0.212030000	-3.109493000	
н	3 188469000	0.287110000	2.411752000	
ЦЦ	4 892941000	0.494242000	2.730331000	
ГН	3 648868000	-1 205621000	2.055705000	
C	5 288659000	-2 525490000	1 065640000	
н	5,739099000	-3.233055000	0.368986000	
н	4,742969000	-3.103173000	1.819396000	
H	6.101677000	-1.995373000	1.572350000	
C	4.428342000	-2.377087000	-2.141320000	
Ĥ	5.133622000	-3.144932000	-1.822206000	
н	4.905908000	-1.795197000	-2.936078000	
н	3.557131000	-2.882552000	-2.571455000	
н	-0.796955000	0.754530000	-1.082410000	
Ν	-0.989891000	-1.556757000	0.389147000	
Ν	-3.184897000	0.427934000	1.122092000	
Ν	-3.729934000	0.535414000	-0.972842000	
С	-0.003954000	-0.559161000	0.377088000	
С	-2.193418000	-1.396576000	-0.410488000	
н	-1.932370000	-1.305425000	-1.479852000	
С	-2.998498000	-0.164944000	-0.074539000	
С	-2.962929000	-2.750238000	-0.226830000	
С	-0.531833000	-2.993170000	0.334127000	
С	-1.772847000	-3.737047000	-0.230855000	
н	-1.570743000	-4.056695000	-1.257922000	
Н	-2.001457000	-4.638422000	0.343354000	
C	-3.732559000	-2.813721000	1.103437000	
Н	-3.081342000	-2.669134000	1.966878000	
	-4.535328000	-2.070291000	1.144326000	
	-4.197340000	-3.797656000	1.203670000	
	-3.933021000	-3.014306000	-1.304344000	
	-4.705164000	-2.302141000	-1.301290000	
ЦЦ	-4 366227000	-4 013804000	-1 200045000	
C	0 664048000	-3 166416000	-0.620223000	
н	1 571074000	-2 699102000	-0 225437000	
Н	0.871620000	-4.230559000	-0.764606000	
H	0.448627000	-2.726784000	-1.600254000	
C	-0.147798000	-3.456585000	1.744817000	
H	-0.996543000	-3.395272000	2.429821000	
н	0.198291000	-4.494007000	1.724280000	
н	0.664998000	-2.845635000	2.153547000	
С	-4.393135000	1.584299000	-0.334575000	
С	-4.045309000	1.517797000	0.985493000	
С	-2.589287000	0.065850000	2.413910000	
н	-1.907676000	-0.764502000	2.265571000	
н	-2.046373000	0.928553000	2.803339000	
н	-3.382686000	-0.212345000	3.109471000	
С	-3.871246000	0.287073000	-2.411836000	
н	-3.188279000	-0.494332000	-2.730952000	
Н	-4.892734000	-0.026966000	-2.633856000	
Н	-3.648569000	1.205547000	-2.956959000	
C	-5.288476000	2.525540000	-1.065900000	
Н	-5.738928000	3.233155000	-0.369303000	
	-4.742717000	3.10310/000	1 572622000	
	-0.101407000	2 277225000	-1.07200000	
й	-5 133506000	2.377233000	2.14113000 1 821030000	
ЦЦ	-4 9050000	1 795392000	2 935873000	
Н	-3.557159000	2.882687000	2.571285000	
Н	0.796932000	-0.754596000	1.082502000	
9 ^{Et}				DFT level: B3LYP-D3/6-31G(d.p)
С	-0.061582000	0.558740000	-0.376370000	- Thermochemistry -
C	2.265688000	1.419690000	-0.113351000	´
С	3.016297000	0.283245000	-0.241728000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
-				

С	2.692091000	2.815791000	0.321483000
С	1.890267000	3.656608000	-0.718865000
H	1.670610000	4.664523000	-0.352339000
H	2.497498000	3.763683000	-1.624048000
C	0.595602000	2.872023000	-1.054110000
C	4.189829000	3.112686000	0.161133000
H	4.809034000	2.556292000	0.867574000
I H	4.380067000	4.180237000	0.320178000
Н	4.525526000	2.847122000	-0.845750000
	2.219894000	3.158490000	1.753923000
Н	1.177968000	2.864091000	1.900422000
	2.300342000	4.234310000	1.949432000
	2.013214000	2.030020000	2.306/91000
L L	-0.030777000	3.447000000	-0.320736000
L LL	-0.8054928000	2.009299000	-0.524214000
Ц	-0.003420000	3 452605000	0.760/08000
C	0 323536000	2 865128000	-2 569785000
н	1 171662000	2 424346000	-3 102221000
Н	0.165395000	3.881845000	-2.947544000
H	-0.570943000	2.276606000	-2.802171000
C	4.555087000	-1.378785000	0.086214000
č	3.736494000	-1.779503000	-0.905551000
Č	4.088679000	0.136716000	1.974951000
H	3.142581000	-0.235007000	2.400203000
н	4.171829000	1.195745000	2.209830000
н	4.924823000	-0.369301000	2.460420000
С	2.161125000	-0.549443000	-2.415411000
н	1.124777000	-0.227302000	-2.318170000
н	2.181809000	-1.470523000	-2.998727000
н	2.724042000	0.228355000	-2.953921000
С	5.736221000	-2.064103000	0.687263000
н	6.594456000	-1.383113000	0.733150000
н	6.026765000	-2.929671000	0.088032000
н	5.550316000	-2.422556000	1.708337000
С	3.774002000	-3.021611000	-1.730232000
Н	2.801773000	-3.526964000	-1.713985000
H	4.519313000	-3.718143000	-1.341570000
H	4.022392000	-2.821837000	-2.780506000
N	0.939464000	1.507305000	-0.597900000
IN N	4.151595000	-0.085148000	0.532868000
	2.733222000	-0.797824000	-1.101498000
	-0.975162000	0.738041000	-0.928529000
	0.001573000	-0.000099000	0.376439000
	-2.2000/0000	-1.419092000	0.113376000
	-2.602037000	-0.203239000	-0.321446000
c	-1 890212000	-3 656604000	0.321440000
н	-1.670513000	-4.664512000	0.352401000
н	-2.497467000	-3.763698000	1.624086000
C	-0.595584000	-2.871978000	1.054208000
Ċ	-4.189771000	-3.112736000	-0.161114000
н	-4.808979000	-2.556350000	-0.867558000
н	-4.379988000	-4.180291000	-0.320166000
н	-4.525484000	-2.847184000	0.845767000
С	-2.219817000	-3.158516000	-1.753877000
н	-1.177904000	-2.864072000	-1.900378000
н	-2.306215000	-4.234344000	-1.949368000
н	-2.813158000	-2.636694000	-2.508755000
С	0.630845000	-3.447770000	0.320905000
н	1.534961000	-2.869166000	0.524392000
н	0.805528000	-4.477997000	0.648723000
H	0.477936000	-3.452534000	-0.760357000
С	-0.323571000	-2.865069000	2.569892000
H	-1.171733000	-2.424318000	3.102298000
H	-0.165405000	-3.881780000	2.947659000
H	0.570879000	-2.276514000	2.802307000
C	-4.555111000	1.3/8/4/000	-0.086328000
	-3.736556000	1.779498000	0.905454000
C	-4.088636000	-0.136811000	-1.975008000



Н	-3.142486000	0.234815000	-2.400228000	
н	-4.171871000	-1.195840000	-2.209861000	
н	-4.924713000	0.369267000	-2.460527000	
С	-2.161204000	0.549506000	2.415387000	
н	-1.124844000	0.227392000	2.318178000	
н	-2.181929000	1.470599000	2.998681000	
н	-2.724110000	-0.228296000	2.953904000	
С	-5.736238000	2.064032000	-0.687428000	
Ĥ	-6.594457000	1.383022000	-0.733331000	
H	-6.026821000	2.929604000	-0.088222000	
Н	-5.550308000	2,422472000	-1.708502000	
C	-3.774103000	3.021627000	1.730100000	
Ĥ	-2.801882000	3.526996000	1.713859000	
H	-4.519417000	3.718137000	1.341402000	
Н	-4.022513000	2.821880000	2,780374000	
N	-0.939470000	-1.507270000	0.597988000	
N	-4.151591000	0.085101000	-0.532933000	
N	-2,733279000	0.797837000	1.101457000	
H	0.975149000	-0.737993000	0.928628000	
10 ^{Et}	010101100000	0.101000000	0.020020000	DFT level: uB3I YP-D3/6-31G(d p)
N	-0.976684000	-1 557317000	0 1/1555000	- Thermochemietry -
N	-3 794518000	0.633151000	-0 968858000	
N	-3 17200/000	0.000101000	1 107407000	Temperature 298 150 Kelvin Pressure 1 00000 Atm
C	0.017262000	-0.657624000	0.228518000	1011porature 230.100 Newin. 11655016 1.00000 Attil.
Ĭč	-2 208601000	-1 343053000	-0 495007000	Zero-point correction- 0.853167
	2.230001000	-1.343933000	-0.493007000	/Hortroe/Dorticlo)
	-3.035457000	-0.000302000	-0.107093000	Thermal correction to Energy 0 906292
	-3.090942000	2 700027000	-0.230490000	Thermal correction to Enthelpy= 0.090303
	-1.944447000	-3.709927000	-0.210197000	Thermal correction to Cibba Erec Energy 0.097327
	1 71/200000	4.002702000	1 228242000	Sum of electropic and zero point Energies1580 158116
	4 047629000	-4.033307000	1 422215000	Sum of electronic and thermal Energies 1500.150110
	-4.047030000	2.952551000	1 217677000	Sum of electronic and thermal Enthelpice - 1500. 114900
	-4.507744000	-3.937066000	-1.317077000	Sum of electronic and thermal Error Energies - 1560. 113956
	-3.525010000	-2.945141000	-2.393960000	Sum of electronic and thermal Free Energies= -1560.232211
Н	-4.862267000	-2.222773000	-1.467537000	Charge 2 Multiplicity 2
	-3.917748000	-2.675440000	1.045234000	Charge = 3 Multiplicity = 2
Н	-4.705464000	-1.916599000	1.019004000	
Н	-3.315704000	-2.516127000	1.939999000	
Н	-4.410360000	-3.644031000	1.159541000	
	0.573837000	-3.461230000	-0.364768000	
Н	0.653658000	-4.550684000	-0.328513000	
H	1.48/1/6000	-3.055193000	0.081811000	
Н	0.526241000	-3.162145000	-1.416365000	
C	-0.521758000	-3.288387000	1.896602000	1 V V
Н	-1.423372000	-3.065446000	2.467983000	
H	0.305845000	-2.699189000	2.305727000	
H	-0.284568000	-4.343198000	2.056440000	
	-0.696164000	-3.035314000	0.391496000	
	-4.4286/2000	1.6/232/000	-0.289016000	
	-4.030212000	1.585328000	1.019950000	
	-4.018956000	0.399067000	-2.404831000	
	-3.3/3696000	-0.393025000	-2.773688000	
I H	-3.812553000	1.319195000	-2.952/93000	
H	-5.058054000	0.107986000	-2.56/912000	
C	-2.564654000	0.085829000	2.381501000	
Н	-3.350541000	-0.204016000	3.080/1/000	
I H	-2.009320000	0.929370000	2.794977000	
H	-1.893960000	-0.750913000	2.227563000	
C	-5.361524000	2.619580000	-0.964312000	
H	-5.762110000	3.331982000	-0.242868000	
I H	-6.209813000	2.092667000	-1.413401000	
H	-4.863024000	3.190751000	-1./54360000	
C	-4.384581000	2.417962000	2.204649000	
H	-5.078861000	3.207093000	1.915407000	
I H	-3.502926000	2.896612000	2.643947000	
H	-4.869173000	1.821826000	2.984793000	
H	0.913276000	-1.032216000	0.706282000	
H	-2.104252000	-1.2/0204000	-1.5/1568000	
N	0.976730000	1.557338000	-0.141764000	
N	3.794364000	-0.633108000	0.969085000	
	0 170110000	0 40000000	4 407070000	

С	-0.017183000	0.657622000	-0.228751000	
Č	2,298645000	1.344049000	0.494845000	
č	3 035497000	0.086548000	0 107746000	
č	3 006063000	2 681751000	0.256108000	
č	1 044440000	2.001731000	0.230190000	
	1.944449000	3.709973000	0.217931000	
н	2.223839000	4.602821000	-0.345592000	
н	1.714345000	4.033419000	1.237992000	
С	4.047713000	2.952631000	1.432979000	
н	4.507734000	3.937230000	1.317363000	
н	3.525766000	2.945120000	2.395681000	
н	4 862401000	2 222934000	1 467090000	
	3 917720000	2.675451000	-1 0/5558000	
ŭ	4 705207000	2.07.3431000	1.0403030000	
	4.705397000	1.916569000	-1.019343000	
н	3.315648000	2.516161000	-1.940307000	
н	4.410380000	3.644016000	-1.159889000	
С	-0.573827000	3.461215000	0.364613000	
н	-0.653725000	4.550661000	0.328274000	
н	-1.487170000	3.055080000	-0.081870000	
н	-0.526138000	3,162221000	1,416229000	
C	0.521673000	3 288387000	-1 896804000	
ы	1 422244000	3.065421000	2 468230000	
	1.423244000	3.003421000	-2.408239000	
	-0.305968000	2.699207000	-2.305874000	
Н	0.284502000	4.343204000	-2.056632000	
С	0.696159000	3.035325000	-0.391702000	
С	4.428470000	-1.672434000	0.289432000	
С	4.030182000	-1.585525000	-1.019595000	
С	4.018994000	-0.398539000	2.404947000	
Ĥ	3,372189000	0.392184000	2,774082000	
H	3 814624000	-1 319073000	2 952960000	
L L L	5.057564000	0 105278000	2.562653000	
	2.037.304000	-0.105370000	2.307033000	
	2.364996000	-0.065954000	-2.381482000	
н	3.351007000	0.203696000	-3.080641000	
н	2.009576000	-0.929453000	-2.794930000	
н	1.894420000	0.750910000	-2.227710000	
С	5.361195000	-2.619695000	0.964901000	
Н	5.762320000	-3.331762000	0.243424000	
н	6.209117000	-2.092723000	1,414604000	
н	4 862426000	-3 191267000	1 754493000	
C	4 384558000	-2 418350000	-2 204157000	
й	5.078773000	-3 207/85000	-1 91/771000	
	2 502002000	2 907010000	2 642424000	
	3.302692000	-2.097010000	-2.043424000	
	4.669219000	-1.622356000	-2.964366000	
н	-0.913212000	1.032224000	-0.706486000	
H	2.104280000	1.270470000	1.571413000	
5 ^{Pr}				DFT level: B3LYP-D3/6-31G(d,p)
Ν	-2.098433000	1.441876000	0.036807000	- Thermochemistry -
Ν	-4.350425000	-1.228972000	0.648853000	
Ν	-4.423010000	-0.410365000	-1.372662000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	2 098341000	-1 441814000	0.036850000	
N	4,423117000	0.410245000	-1.372625000	Zero-point correction= 0.881479
N	4 350485000	1 228070000	0 648832000	(Hartree/Particle)
Ċ	-3 311523000	1 065/26000	0.320636000	Thermal correction to Energy 0 026440
Ĭč	2 01766 4000	0.2101040000	0.120177000	Thormal correction to Entrology- 0.320443
	-3.91/004000	1 065 400000	-0.129177000	Thermal correction to Cibbo Free Freeway 0.004240
C	3.311432000	-1.065409000	0.329675000	Inermal correction to Globs Free Energy= 0.804319
C	3.917595000	0.210225000	-0.1291/9000	Sum of electronic and zero-point Energies= -1618.9/9/4/
С	-1.082915000	0.652702000	-0.706267000	Sum of electronic and thermal Energies= -1618.934777
Н	-0.627056000	1.341421000	-1.421342000	Sum of electronic and thermal Enthalpies= -1618.933833
н	-1.603137000	-0.119705000	-1.276735000	Sum of electronic and thermal Free Energies= -1619.056907
С	-0.000049000	0.000039000	0.191793000	-
Н	-0.469281000	-0.743756000	0.836311000	Charge = 4 Multiplicity = 1
н	0.469171000	0.743838000	0.836314000	
С	1.082824000	-0.652653000	-0.706243000	
н	0 626960000	-1 341385000	-1 421299000	
	1 603040000	0 110725000	-1 27673/000	
	1.000049000	0.113130000	1 022624000	
	-4.120912000	2.13900/000	1.023024000	
C	-3.052956000	3.21/206000	1.308333000	
H	-3.441469000	4.225757000	1.156159000	
H	-2.731168000	3.145902000	2.350959000	
С	-1.857288000	2.936966000	0.375148000	
С	-4.820642000	1.661309000	2.317832000	

Н	-5.572610000	0.893845000	2.119976000	A a a
н	-5.341246000	2.516614000	2.756984000	
н	-4.106707000	1.297556000	3.060533000	
С	-5.231236000	2.616098000	0.030842000	
н	-4.828143000	2.991562000	-0.911295000	
н	-5.777677000	3.434923000	0.506321000	
Н	-5.950241000	1.819708000	-0.178758000	
C	-0.515918000	3.148773000	1.074467000	
Н	0.332286000	2.970484000	0.406362000	
н	-0.423710000	2.537336000	1.976304000	
H	-0.464598000	4.196583000	1.383223000	0 000
C	-1.914884000	3.723784000	-0.944105000	
Н	-1.828372000	4.788341000	-0.709865000	
Н	-2.858117000	3.581844000	-1.474486000	
Н	-1.089133000	3.476344000	-1.617052000	
	-5.132626000	-2.091389000	-0.104573000	
	-5.188889000	-1.566254000	-1.382255000	
	-3.967296000	-1.46/51/000	2.051920000	
	-3.200983000	-0.743612000	2.386376000	
	-3.34/46/000	-2.463212000	2.120039000	
П	-4.8///02000	-1.440114000	2.680287000	
	-5.741563000	-3.325506000	0.466966000	
	-0.397230000	-3.091007000	1.312127000	
	-4.978795000	-4.031201000	0.813842000	
П	-6.342409000	-3.834620000	-0.286959000	
	-5.907682000	-2.040916000	-2.598618000	
	-0.430401000	-2.957123000	-2.379332000	
	-0.210441000	-2.255211000	-3.420534000	
	-0.032000000	-1.296200000	-2.940310000	
L L	-4.300213000	1 272667000	-2.000201000	
	5 271 451000	0.028722000	-2.323302000	
	3 06220/000	0.920723000	2 207292000	
	4 128823000	-2 139788000	1 023677000	
č	3 052846000	-3 217085000	1 308446000	
й	2 731054000	-3 145717000	2 351070000	
ЦЦ	2.731034000	-4 225651000	1 156333000	
C	1 857194000	-2 936873000	0 375237000	
č	4 820602000	-1 661208000	2 317856000	
н	5 572625000	-0.893814000	2 119938000	
H	5 341147000	-2 516531000	2 757042000	
Н	4.106699000	-1.297359000	3.060539000	
C	5.231089000	-2.616050000	0.030863000	
H	4.827962000	-2.991565000	-0.911239000	
н	5.777561000	-3.434856000	0.506342000	
н	5.950080000	-1.819670000	-0.178823000	
С	0.515817000	-3.148667000	1.074568000	
н	0.423584000	-2.537148000	1.976349000	
н	0.464540000	-4.196449000	1.383423000	
н	-0.332390000	-2.970470000	0.406439000	
С	1.914791000	-3.723774000	-0.943973000	
н	1.828242000	-4.788311000	-0.709666000	
H	2.858041000	-3.581900000	-1.474337000	
H	1.089060000	-3.476346000	-1.616947000	
С	5.189107000	1.566054000	-1.382241000	
C	5.132833000	2.091261000	-0.104587000	
C	4.300040000	-0.483592000	-2.536319000	
H	5.2/1461000	-0.927808000	-2.761302000	
	3.900782000	0.094292000	-3.396922000	
НС	3.583485000	-1.2/433/000	-2.322929000	
	5.907990000	2.040364000	-2.390000000	
	0.21001000	2.234/50000	-3.420001000	
	0.032997000	1.231131000	-2.340302000 -2.370/21000	
	5 7/182/000	2.300/32000	-2.31 342 1000 0 166801000	
н	5.141024000 6 343238000	3.323379000	-0.286870000	
	6 396920000	3.034003000	1 312494000	
н	4 979058000	4 031410000	0.813101000	
C	3,987397000	1.487588000	2.051900000	
Н	3.266801000	0.743922000	2.386287000	

Н	3.547928000	2.483432000	2.126833000	
H	4.877752000	1.439852000	2.680310000	
4 ^{Pr}				DFT level: B3LYP-D3/6-31G(d,p)
N	-1.679272000	-1.860231000	-0.749600000	—
N	-3.968/08000	0.5//222000	0.976837000	- i nermochemistry -
N	-3.720428000	0.140973000	-1.262557000	
N	1.678920000	1.859859000	-0.749364000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
IN N	3.720838000	-0.140510000	-1.262453000	Zero point correction 0.976005
	0.861327000	-0.576656000	1 530711000	(Hartroo/Particlo)
н	-0.001327000	-0.343820000	-1.559711000	Thermal correction to Energy 0 920843
Гн	-0 235177000	-1 543968000	-2 210305000	Thermal correction to Entralpy= 0.320043
Ċ	-0.000083000	-0.000263000	-0.700069000	Thermal correction to Gibbs Free Energy= 0.800320
H	-0.658804000	0.578951000	-0.048685000	Sum of electronic and zero-point Energies= -1620.198427
н	0.658529000	-0.579455000	-0.048538000	Sum of electronic and thermal Energies= -1620.153679
С	0.861273000	0.945303000	-1.539593000	Sum of electronic and thermal Enthalpies= -1620.152735
Н	1.513238000	0.339422000	-2.184564000	Sum of electronic and thermal Free Energies= -1620.274202
н	0.235213000	1.543330000	-2.210381000	
С	-2.506248000	-1.341883000	0.288380000	Charge = 0 Multiplicity = 1
С	-2.399855000	-2.247012000	1.510675000	
C	-2.033698000	-3.586904000	0.803423000	
	-1.491497000	-4.270702000	1.404333000	
	-2.900949000 -1 217062000	-4.00/913000	-0.204900000	79 11
C C	-3 723891000	-2 425710000	2 270825000	
НЙ	-4.056320000	-1.506064000	2.756292000	
H H	-3.616356000	-3.193714000	3.045434000	
H	-4.517798000	-2.734484000	1.584230000	
С	-1.275453000	-1.831922000	2.491565000	
н	-0.358267000	-1.571640000	1.960145000	
н	-1.049195000	-2.646249000	3.190648000	
н	-1.558936000	-0.959877000	3.083726000	
С	0.302301000	-3.355770000	-0.203345000	
I H	0.891342000	-3.013665000	-1.059179000	
Н	0.560159000	-4.405156000	-0.026084000	
H	0.618789000	-2.783401000	0.669125000	
L L	-1.363946000	-4.137019000	-1.039990000	
I H	-2.033009000	-5 203014000	-1 420929000	
н	-1 038027000	-3 867435000	-2 544794000	
c	-3.362440000	-0.309873000	0.039795000	
Č	-4.547024000	1.286644000	-1.095178000	
С	-4.666293000	1.563242000	0.215131000	
С	-3.184743000	1.023978000	2.121825000	
H	-2.148716000	1.258899000	1.833946000	
H	-3.153453000	0.262813000	2.900633000	
H	-3.642155000	1.911936000	2.559775000	
	-4.152142000	-0.879458000	-2.219016000	
	-3.308994000	-1.032400000	-2.31384/000	
Ιμ	-4.322092000	-0.410799000	-3.194313000	
	-5.126293000	1.979667000	-2.281832000	
НЙ	-5.866424000	1.363426000	-2.808357000	
H H	-4.338937000	2.226316000	-3.004622000	
н	-5.618097000	2.909666000	-1.989637000	
С	-5.395329000	2.677642000	0.888331000	
Н	-4.722362000	3.427162000	1.325156000	
H	-6.024081000	2.292183000	1.699657000	
H	-6.043108000	3.197286000	0.179238000	
C	2.506017000	1.341677000	0.288588000	
	2.399082000	2.246563000	1.511018000	
	2.032725000	3.506463000	0.803890000	
	1.430210000 2 959906000	4.210023000 4087755000	0.505620000	
	1.216413000	3.234788000	-0.462398000	
č	1.274473000	1.831014000	2.491473000	
H H	0.357504000	1.570732000	1.959695000	
н	1.047877000	2.645116000	3.190704000	
Н	1.557883000	0.958841000	3.083482000	
C C	3 722846000	2 425512000	2 271573000	

н	4 055389000	1 505889000	2 757023000	
	2 61 4006000	2 102207000	2.757025000	
	3.014000000	3.193307000	3.040236000	
н	4.516871000	2.734567000	1.585241000	
С	-0.303032000	3.355021000	-0.203436000	
Н	-0.891805000	3.012817000	-1.059412000	
н	-0.561107000	4.404364000	-0.026241000	
н	-0.619652000	2 782607000	0.668955000	
	1 592/12000	4 157200000	1 620590000	
C.	1.363412000	4.157506000	-1.039360000	
н	2.654588000	4.090202000	-1.851138000	
н	1.335656000	5.202648000	-1.420463000	
Н	1.037721000	3.867129000	-2.544516000	
С	3.362609000	0.310025000	0.039947000	
Ĉ	4 547974000	-1 285806000	-1 095167000	
č	4 667270000	1 562479000	0.215107000	
	4.007370000	-1.302476000	0.213107000	
C	4.152116000	0.880215000	-2.218789000	
н	3.368593000	1.632824000	-2.313666000	
н	4.322425000	0.419718000	-3.194295000	
н	5.075784000	1.381640000	-1.891148000	
С	3 185233000	-1 024520000	2 121528000	
й	2 1/0020000	-1 261800000	1 832083000	
	2.149920000	-1.201009000	1.852985000	
н	3.151785000	-0.262912000	2.899769000	
н	3.644170000	-1.911213000	2.560458000	
С	5.127575000	-1.978449000	-2.281882000	
н	5.619872000	-2.908210000	-1.989761000	
н	5.867379000	-1.361789000	-2.808373000	
ЦЦ	1 340333000	-2 225/51000	-3 004676000	
	4.340332000	-2.223431000	-3.004070000	
C	5.396978000	-2.676565000	0.888203000	
н	6.044835000	-3.195975000	0.179012000	
н	4.724395000	-3.426337000	1.325185000	
Н	6.025722000	-2.290818000	1.699404000	
5 ^{Cy}				DFT level: B3LYP-D3/6-31G(d.p)
N	4 162827000	-1 175064000	-1 097708000	- Thermochemistry -
N	4.102027000	1 170670000	1 091927000	- memochemistry -
IN	4.170729000	-1.170670000	1.081827000	
N	2.445347000	1.606685000	-0.041158000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
С	3.860903000	-0.432480000	-0.008543000	
С	4.664992000	-2.407166000	0.681295000	Zero-point correction= 0.947173
С	4.660371000	-2.409638000	-0.697664000	(Hartree/Particle)
Ĉ	4 031559000	-0 773469000	-2 507135000	Thermal correction to Energy 0 994121
ŭ	3 557324000	0.204220000	2.568607000	Thermal correction to Enthalpu- 0.005065
	2.404.474.000	0.204230000	-2.300007000	Thermal correction to Enthalpy 0.995005
	3.421471000	-1.507676000	-3.035087000	Thermal correction to Gibbs Free Energy= 0.000995
н	5.019367000	-0.727881000	-2.968203000	Sum of electronic and zero-point Energies= -1/35.686114
С	4.018938000	-0.783019000	2.493284000	Sum of electronic and thermal Energies= -1735.639167
н	3.581727000	0.210501000	2.557368000	Sum of electronic and thermal Enthalpies= -1735.638222
н	4.995322000	-0.779967000	2.980098000	Sum of electronic and thermal Free Energies = -1735.764293
н	3 370656000	-1 502783000	2 995600000	
C	5 102203000	-3 445213000	1 657773000	Charge – 4 Multiplicity – 1
ŭ	5.102203000	4 227044000	1.122597000	onarge = + Manipheny = 1
	5.442967000	-4.337644000	1.132567000	
н	4.289085000	-3.742662000	2.328163000	
н	5.934369000	-3.087135000	2.273311000	
С	5.093378000	-3.449545000	-1.674053000	
Н	5.445175000	-4.337797000	-1.148695000	
н	5.916537000	-3.089143000	-2.300171000	
н	4 274681000	3 754866000	-2 334097000	
	2 611269000	1 027110000	0.021724000	
	3.011200000	1.037110000	-0.031724000	
C	4.774684000	2.018386000	-0.036779000	
С	2.553891000	3.156385000	-0.055876000	
С	5.833389000	1.673597000	-1.106626000	
н	6.308627000	0.707071000	-0.917596000	
н	6.617966000	2,433866000	-1.068341000	V V-Can K
н	5 418451000	1 686686000	-2 116996000	
	5 460054000	2 00521 4000	1 35810/000	1 7
L C	5.400954000	2.000014000	1.000104000	
	5.94/248000	1.048387000	1.500489000	
н	4.773508000	2.244460000	2.1/2770000	
н	6.242288000	2.769943000	1.350056000	<u>ب</u>
С	1.690785000	3.734223000	-1.180464000	
Н	0.617387000	3.653379000	-0.988202000	A / V
н	1,925689000	3,280403000	-2.147328000	e 🏹
	1 0171/0000	1 801620000	-1 25699/000	[
	1.317143000	-+.001020000	1 222564000	
	2 1 1 3 3450000	3.000486000	1.322304000	
	2.1100-10000	0.00-00-00	0 40050 407 -	

Н	1.065116000	3.436077000	1.536363000	
н	2.213595000	4.754079000	1.335394000	
С	1.072499000	1.004142000	0.007486000	
н	0.422964000	1.877541000	0.077678000	
С	0.797139000	0.140338000	1.250407000	
н	1.045132000	0.692150000	2.161452000	
н	1.413893000	-0.764516000	1.229338000	
C	0.696282000	0.259116000	-1.286833000	
Ĥ	1.316346000	-0.638569000	-1.393121000	
H	0.878662000	0.892396000	-2 159217000	
C	4 057742000	3 358144000	-0 334689000	
н	4 461311000	4 173078000	0.268810000	
н	4 205954000	3 628621000	-1 383260000	
N	-1 162723000	1 175003000	1.003200000	
N	4.170620000	1.17060000	1.097075000	
N	-4.170039000	1.170090000	-1.001039000	
	2 960941000	-1.0007070000	0.041140000	
č	-3.000041000	0.432400000	0.000012000	
	-4.004772000	2.407239000	-0.061330000	
	-4.660138000	2.409718000	0.697630000	
C	-4.031484000	0.773481000	2.507098000	
н	-3.557346000	-0.204267000	2.568559000	
н	-3.421314000	1.507827000	3.035044000	
н	-5.019291000	0.727991000	2.968177000	
С	-4.018929000	0.783000000	-2.493313000	
н	-3.581792000	-0.210552000	-2.557393000	
н	-4.995329000	0.780012000	-2.980097000	
н	-3.370611000	1.502708000	-2.995663000	
С	-5.101894000	3.445323000	-1.657808000	
н	-5.442572000	4.337994000	-1.132622000	
н	-4.288759000	3.742683000	-2.328216000	
н	-5.934110000	3.087326000	-2.273326000	
С	-5.093027000	3.449675000	1.674018000	
н	-5.444751000	4.337956000	1.148658000	
н	-5.916206000	3.089356000	2.300156000	
н	-4.274286000	3.754927000	2.334041000	
С	-3.611314000	-1.037125000	0.031706000	
Ċ	-4.774797000	-2.018312000	0.036801000	
č	-2.554068000	-3.156463000	0.055917000	
č	-5 833448000	-1 673440000	1 106673000	
н	-6.308648000	-0 706899000	0.917629000	
н	-6 618064000	-2 433673000	1 068446000	
н	-5.418470000	-1 686511000	2 117028000	
C	-5.461105000	-2.005183000	-1 358064000	
ц	-5.401103000	-1 0/8232000	-1.550004000	
	4 772602000	-1.040232000	2 172756000	
	-4.773093000	-2.244333000	-2.172730000	
	-0.242470000	-2.769760000	-1.330011000	
	-1.091046000	-3.734331000	1.160000000	
н	-0.617636000	-3.653585000	0.988328000	
	-1.925947000	-3.280456000	2.147394000	
Н	-1.91/502000	-4.801706000	1.257008000	
C	-2.113502000	-3.665643000	-1.322488000	
н	-2.735223000	-3.265427000	-2.126548000	
Н	-1.065248000	-3.436309000	-1.536249000	
н	-2.213822000	-4.754230000	-1.335282000	
С	-1.072557000	-1.004284000	-0.007501000	
H	-0.423043000	-1.877697000	-0.077692000	
С	-0.797192000	-0.140481000	-1.250422000	
H	-1.045186000	-0.692292000	-2.161468000	
Н	-1.413946000	0.764373000	-1.229353000	
С	-0.696336000	-0.259259000	1.286817000	
Н	-1.316399000	0.638427000	1.393108000	
Н	-0.878717000	-0.892538000	2.159201000	
С	-4.057940000	-3.358120000	0.334696000	
Н	-4.461556000	-4.173029000	-0.268807000	
Н	-4.206178000	-3.628590000	1.383265000	
8 ^{Pr}				DFT level: B3LYP-D3/6-31G(d,p)
N	-1.303067000	1.563301000	0.160270000	- Thermochemistry -
N	-2.264608000	-1.040640000	-0.997586000	
N	-4.158952000	-0.861254000	0.210598000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N	1.997106000	-1.589210000	1.252189000	
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	Ν	3.210563000	1.022888000	0.977935000
	Ν	3.221920000	0.900915000	-1.315621000
	С	-0.253050000	0.916829000	0.779618000
	C	-2.652610000	1.110628000	0.169952000
	C	-3.548538000	2.320969000	0.394323000
	C	-2.696354000	3.399036000	-0.343537000
	н	-2.973102000	3.395757000	-1.403234000
	Н	-2.885416000	4.407036000	0.039490000
	C	-1.204025000	3.001702000	-0.203264000
		-4.926161000	2.227969000	-0.277840000
	н	-4.821248000	1.944846000	-1.329598000
		-5.434903000	3.197402000	-0.220071000
		-5.575363000	1.490323000	0.197039000
	Ц	-3.707110000	2.000023000	2.00/202000
		-4.142225000	2 672170000	2.004207000
	н	-2.741502000	1 979110000	2.399233000
	C	-4.301380000	3 8/17/3000	0.875550000
	ц	-0.431003000	3 698809000	1 859270000
	Ц	-0.943072000	3.098809000 4.902441000	0.614422000
	н	0.571008000	3 503677000	0.014422000
		0.371000000	3.150704000	1 533202000
	й	0.447320000	2 856176000	-1.333233000
	н	-0.463778000	1 202353000	-1 871/05000
	н	-0.403770000	2 537001000	-7.308061000
	C	-3.005370000	-0 161306000	-2.300301000
	č	-3.000075000	-0.101390000	-0.190273000
	č	-4.120061000	-2.240770000	-0.302530000
	č	-4.120001000	-0.504355000	-2 032640000
	ц	-1.400327000	0.287356000	-2.032040000
	н	-1.107474000	-1 200112000	-2.334070000
	н	-0.500328000	-0.085751000	-1 584249000
	C	-2 507327000	-3 358487000	-1 994330000
	й	-3 156549000	-4 230524000	-1 895606000
	H	-1.494301000	-3.659616000	-1.703384000
	н	-2.472879000	-3.090896000	-3.058279000
	C	-5 211643000	-3 140626000	-0 172636000
	н	-5.113985000	-3.979636000	-0.864882000
	н	-6.193208000	-2.680440000	-0.336509000
	H	-5.213932000	-3.557460000	0.843196000
	С	-4.648771000	-0.688831000	1.573290000
	H	-5.089170000	-1.619510000	1.934706000
	Н	-5.414260000	0.088654000	1.641876000
	Н	-3.814071000	-0.405728000	2.227812000
	С	-0.209742000	-0.321656000	1.318860000
	С	1.041477000	-0.773473000	2.024180000
	Н	1.568794000	0.115013000	2.388760000
	Н	0.786125000	-1.358926000	2.913479000
	С	2.517563000	-1.130917000	0.010613000
	С	2.684320000	-2.320951000	-0.935829000
	С	2.758138000	-3.480821000	0.099001000
	Н	2.425656000	-4.434914000	-0.322124000
	Н	3.800874000	-3.607922000	0.409586000
	С	1.920064000	-3.060093000	1.324449000
	С	1.479276000	-2.544618000	-1.878717000
	Н	0.540373000	-2.450226000	-1.333587000
	Н	1.522008000	-3.543694000	-2.329934000
	Н	1.454935000	-1.817745000	-2.691583000
ļ	C	3.994312000	-2.28/503000	-1./41211000
ļ	H	4.02/166000	-1.46/210000	-2.460583000
ļ	H	4.123180000	-3.224689000	-2.295219000
ļ	H	4.848926000	-2.161702000	-1.069/86000
ļ	C	2.567691000	-3.564881000	2.62/440000
	н	3.593530000	-3.1936//000	2.708973000
ļ	н	2.588975000	-4.660/66000	2.656992000
ļ	Н	2.009670000	-3.220589000	3.504798000
ļ	C	0.4/1541000	-3.599140000	1.256583000
ļ	H	-0.094345000	-3.318565000	2.150082000
ļ	н	0.478145000	-4.693196000	1.201018000
	н	-0.069392000	-3.207994000	0.394494000

Zero-point co	rection-	0 8525	57
(Hortroo/Dortio		0.0020	51
		0.0	00770
Thermal corre	ction to Energy=	0.0	90773
Thermal corre	ction to Enthalpy	/= _ 0.8	897717
Thermal corre	ction to Gibbs Fr	ee Energy=	0.780048
Sum of electro	onic and zero-poi	int Energies=	-1619.004322
Sum of electro	onic and thermal	Energies=	-1618.960106
Sum of electro	onic and thermal	Enthalpies=	-1618.959161
Sum of electro	onic and thermal	Free Energies=	-1619.076831
Charge - 0 M	Aultiplicity – 1		
onarge = 0 w	iuniplicity = 1		
T \			
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С	2.980602000	0.146171000	-0.124870000	
C	3.505742000	2.306578000	0.440410000	
C	3.478992000	2.242384000	-0.903115000	
	4.095861000	0.515406000	2.030582000	
	3.717029000	-0.447364000	2.370107000	
	4.104031000	0.277106000	2.071104000	
	3 776623000	3 457571000	1.000024000	
н	3 857161000	4 391027000	0 788505000	
Ιü	4 705413000	3 331974000	1 920618000	
Н.	2.963204000	3.568789000	2.077232000	
C	3.692260000	3.328923000	-1.904154000	
н	4.073820000	4.228257000	-1.416644000	
Н	2.771581000	3.608800000	-2.432516000	
н	4.422970000	3.019902000	-2.660891000	
С	2.369172000	0.696684000	-2.476381000	
н	1.311640000	0.629926000	-2.188182000	
Н	2.636993000	-0.215426000	-3.007937000	
H	2.494432000	1.522283000	-3.177656000	
Н	0.655138000	1.510154000	0.818904000	
н	-1.050152000	-1.001083000	1.259700000	
7 ^{су}				υς ι ιενεί. αρομτη-μογο-οτο(α,ρ)
N	2.416888000	1.610291000	0.058159000	- Thermochemistry -
N	4.043281000	-1.168123000	1.134996000	
N	4.054660000	-1.301359000	-1.032877000	Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
N N	-2.416822000	-1.610281000	0.058031000	Zero point correction 0.045521
	-4.043307000	1.100112000	1.134903000	Zero-point correction= 0.945551
	1 063846000	1.301326000	-1.032910000	Thermal correction to Energy 0 902650
н	0 395042000	1.886008000	0.056644000	Thermal correction to Enthalpy- 0.992039
C	0.740615000	0.212940000	1.328143000	Thermal correction to Gibbs Free Energy= 0.866116
Ĥ	0.957815000	0.809100000	2.219491000	Sum of electronic and zero-point Energies= -1736.133514
H	1.374669000	-0.680041000	1.367798000	Sum of electronic and thermal Energies = -1736.086385
С	-0.740564000	-0.212996000	1.328134000	Sum of electronic and thermal Enthalpies= -1736.085441
н	-0.957752000	-0.809226000	2.219440000	Sum of electronic and thermal Free Energies= -1736.212929
н	-1.374622000	0.679981000	1.367864000	
С	-1.063777000	-1.022139000	0.058102000	Charge = 3 Multiplicity = 2
Н	-0.394975000	-1.885975000	0.056543000	
С	-0.741510000	-0.209125000	-1.208563000	
H	-1.3/04//000	0.68/615000	-1.243556000	
H	-0.964176000	-0.800547000	-2.101924000	
	0.741567000	0.209237000	-1.20600000	
	0.964233000	-0.067494000	-1.243030000	
C	3 601442000	0.000730000	-0.067614000	
č	4.766554000	1.965063000	-0.198694000	
Č	4.090868000	3.296372000	0.219280000	
H	4.457923000	4.140970000	-0.366843000	
Н	4.320917000	3.505995000	1.267678000	
С	2.564629000	3.122075000	0.054792000	a de la constante de
С	3.814804000	-0.459985000	0.001636000	
С	4.426625000	-2.465862000	0.818463000	
C	4.433681000	-2.550635000	-0.553559000	
C	5.295677000	2.0121/8000	-1.654567000	
Н	5.770887000	1.068/10000	-1.935583000	
	0.001204000 4 510478000	2.193319000	-1.730093000	
	5 939857000	2.241028000	-2.37 9400000	
н	5 636756000	1 585148000	1 783399000	
НН	6.729717000	2.351319000	0.631966000	
H	6.376083000	0.632348000	0.474148000	
С	2.037805000	3.677494000	-1.277781000	
Н	2.173440000	4.761913000	-1.294157000	<u>k</u>
Н	0.968840000	3.480807000	-1.406961000	
Н	2.573972000	3.257721000	-2.131569000	
С	1.809865000	3.736411000	1.240598000	
H	2.058519000	4.799579000	1.298822000	
H	2.106860000	3.271406000	2.184942000	
	0 700000000	3 667571000	1 134903000	

H 329728000 -0.678048000 2.98522000 H 3.29435000 -1.6603000 3.08424000 H 3.818622000 -0.378686000 2.480390000 H 3.618622000 -0.378686000 2.480390000 H 3.540106000 -0.68634000 2.55722000 H 3.62344000 -3.68317000 -2.850722000 H 5.621058000 -3.449677000 2.466440000 H 5.6312000 -4.68317000 -2.466440000 H 5.6317000 -3.68311000 -1.46113000 H 5.6317000 -3.98724000 -2.10958600 C -4.76745900 -3.98724000 -3.9872400 C -3.843177000 -9.9934300 -0.0774000 C -3.681377000 -3.987248000 -0.6774400 C -3.8477000 -4.5858000 -0.67364900 C -3.8477000 -5.677380000 -5.67738000 C -3.8477000 -5.67728000 -5.77748000 C -3.84777000	С	3 977342000	-0 647893000	2 504513000	
H 3294354000 -1.28033000 3.085424000 H 361862000 0.378648000 -2.485122000 H 3.5401000 0.286493000 -2.485122000 H 3.23348000 -1.68106100 -2.930017000 H 3.23348000 -1.68106100 -2.930017000 C 4.78537800 3.47385000 2.46542000 H 5.62126800 -3.48847000 2.46544900 H 5.62126800 -3.48847000 -4.424841000 -4.40774000 H 5.62126800 -3.48817700 -2.102721000 -4.424841000 -1.00774000 C -4.090754000 -3.98417700 -2.102721000 -1.00774000 -3.89414700 -0.21895000 H -4.32964000 -4.42774000 -2.187574000 -3.681477200 -0.53821000 -4.4277400 -2.187574000 C -2.5641700 -2.187574000 -3.681477200 -0.53821000 -3.681477200 -2.56451300 -7.3784000 -3.681379000 -3.681477200 -2.56451300 -7.3784000 -2.876451700 -2.585378000 -5.53821000 -2.5744200 -3.774448000 -7.37744	й	4 970780000	-0.676045000	2.004010000	
H 3619802000 -0.387989000 2.489380000 H 3.54900000 -0.387989000 2.48938000 H 3.5440100000 -0.387982000 2.489382000 H 3.22556000 -3.65382700 2.56732000 H 3.832565600 -3.65382700 2.54133000 H 5.6212000 -3.65382700 2.54133000 H 5.6512000 -3.65382700 2.54133000 H 5.6512000 -3.6339700 -0.85114000 H 5.6512000 -3.6339700 -0.06774000 C -4.66748000 -0.19856400 -0.19856400 C -4.66774000 -2.19678000 -0.07381900 C -4.32089000 -0.07381900 -0.07381900 C -4.43773000 -2.4658200 0.0118000 C -4.32089000 -0.53434900 -0.53434900 C -4.32089000 -0.53434900 -0.7341900 C -4.32778000 -2.45853900 -0.7381900 -3.593738000 -5.2345900		2 204254000	1 260202000	2.955225000	
cl 361802000 0.048838000 -2.56726000 H 3.223543000 -1.6891061000 -2.56726000 H 3.82356000 -3.683572000 -3.473690000 -1.8683572000 H 4.88945900 -1.6891061000 -2.56732000 -5.41438000 H 6.521068000 -3.149687000 2.466443000 -1.689106100 -4.6237400 G 4.773416000 -4.683410000 -1.46161300 -4.60774000 -2.81774700 C -4.93776000 -3.934173000 -0.63774000 -2.918528000 -0.6377400 C -4.93776000 -3.81452000 -0.936754000 -2.93674000 -2.93674000 C -4.93776000 -3.81452000 -0.836774000 -2.93674000 -2.93674000 C -4.83773000 -2.45852000 0.53631000 -4.432773000 -2.658451700 C -4.83773000 -2.6584517000 -2.379428000 -4.73248000 -4.73248000 H -6.729532000 -2.537428000 -1.837747000 -2.7379427000 -2.379428000		3.294334000	-1.200303000	3.093424000	
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H 3.840106000 0.02844000 -2.567725000 H 4.88949000 -1.06861000 -2.900372000 H 4.88949000 -1.06861000 -2.900372000 H 3.827568000 -3.633827000 2.841439000 H 5.0512000 -4.6314000 -4.0272800 H 5.0512000 -4.63149000 -4.0272800 H 5.0512000 -3.68311000 -1.46113900 H 5.0512000 -3.83449000 -0.0273700 H -3.0271000 -3.93274000 -0.129556000 C -4.76849000 -3.56632000 -0.07574000 C -2.56451700 -3.129758000 -0.3757000 C -4.30764000 -3.28644000 -0.129758000 C -4.3677000 -3.56327000 0.07351900 C -4.3677000 -3.56327000 0.7381900 C -4.329698000 -1.56349000 -7.3781900 C -4.329982000 -1.56349000 -7.381900 C -3.29738000	С	3.918492000	-0.986939000	-2.459122000	
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H 4.88949500 1.066801000 2.295372000 H 3.925656000 3.653827000 2.541438000 H 5.62168000 3.653827000 2.644449000 H 5.6216800 3.63827000 2.644449000 H 5.6216800 3.638327000 2.64444900 H 5.6216200 3.63837000 2.60444900 H 3.63147000 3.4844900 0.881149000 H 3.630137700 0.99334900 -0.967574000 C -4.7649000 3.92644000 0.19856000 H -4.32708000 4.46873000 0.45989000 C -3.6380300 2.26057000 0.55821000 C -4.8287300 -4.5394000 -353821000 C -5.29883000 -2.5647400 -337347000 H -5.2764700 -3.7384000 -1.32247200 C -4.2267300 -1.7674900 2.37473000 H -5.29883000 -1.32474000 2.37474000 2.37474000 C -2.3754100 -3.26474000 2.37473000 H -2.267373000	н	3.223543000	-1.691061000	-2.920001000	
C - 768375000 - 3473680000 - 1863352000 H - 534756000 - 367375000 - 2466449000 H - 5621056000 - 3683110000 - 1461613000 C - 4773916000 - 3683110000 - 1461613000 H - 5562125000 - 3683110000 - 1461613000 H - 5562125000 - 368317000 - 2103566000 C - 476494000 - 386317000 - 2103566000 C - 4.360754000 - 338447000 - 2103566000 C - 4.360754000 - 3384753000 - 2103568000 C - 4.380754000 - 3384753000 - 2103568000 C - 4.38075000 - 538467000 - 55381000 C - 4.38075000 - 53845000 - 538467000 C - 4.38173000 - 637473000 - 73819900 C - 4.3835000 - 338177000 - 106389000 C - 538463000 - 738477200 - 458394000 C - 538463000 - 73817200 - 548394000 C - 4.38739400 - 73787200 - 568983000 - 138247200	н	4,889495000	-1.066801000	-2.950372000	
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1 3.23050000 3.43632/000 2.49443000 1 6.6210500 3.496443000 1.400728000 1 5.6210600 3.49843000 1.400728000 1 5.621000 3.42840100 1.400728000 1 3.62051000 3.433445000 2.19956000 1 3.8207000 3.39342000 0.067574000 2 3.901377000 3.9033000 0.279366000 1 4.4577600 3.20644000 0.19656000 1 4.320803000 3.50382000 0.27386000 2 3.56657000 0.53381000 0.73381000 1 4.32080300 2.45657600 0.53381000 1 4.3273700 2.4682000 1.63834000 1 4.5771300 2.46554000 1.73712000 1 4.51075100 2.240754000 2.379428000 1 4.57713000 3.2746000 1.34773000 1 3.2746000 1.34773000 1 2.26374000 3.27467000 2 3.27467000 1.28447000 1 3.27467000 <t< td=""><td>L C</td><td>4.700375000</td><td>-3.473090000</td><td>1.003332000</td><td></td></t<>	L C	4.700375000	-3.473090000	1.003332000	
H 5.62108000 3.14987000 2.486449000 C 4.77391000 3.08311000 1.401613000 K 5.0314000 3.08311000 1.401613000 K 5.0314000 3.08317000 3.08317000 K 3.0317000 3.938147000 2.01217000 K 3.03177000 3.938147000 2.01375000 K 3.03000 0.067574000 3.2017000 K 4.32080000 3.05382000 1.67574000 C 4.32773000 3.4803000 0.067574000 C 3.8147000 3.2256000 0.538000 C 3.312205000 0.54601000 5.3386300 C 4.3380300 2.05745000 0.53391000 C 4.53834000 1.73638000 2.31742000 C 4.53834000 4.74888000 1.7363800 C 2.20544000 3.27482000 1.34773000 H -2.0584000 2.273921000 1.47712000 H -2.0584000 3.27752000 2.	н	3.925656000	-3.653827000	2.541438000	
H 5.031140000 - 4.424801000 1 4.00728000 H 5.025128000 - 4.66339000 0 0.881149000 H 5.2052100 - 3.46339000 - 2.102721000 C - 3.0017700 - 0.9802400 - 0.198566000 C - 4.097700 - 0.9802400 - 0.198566000 C - 4.097700 - 0.9802400 - 0.19856000 H - 4.45778000 - 3.25625000 - 0.19856000 C - 4.45773000 - 0.459899000 - 0.357385000 C - 4.43307300 - 2.45989900 - 0.01618000 C - 4.43307300 - 2.45989900 - 0.55362100 C - 4.43380300 - 2.5557600 - 0.55362100 C - 4.43380300 - 2.5557600 - 0.55362100 H - 6.7573900 - 2.45943000 - 0.5352100 H - 6.7573900 - 2.45943000 - 0.5352100 H - 6.7579400 - 0.52362100 - 0.5352100 H - 6.7579400 - 0.52362100 - 0.5352100 H - 6.7579300 - 2.45943000 - 1.735633000 H - 6.7773900 - 2.45943000 - 1.735633000 H - 6.7773900 - 2.45943000 - 1.735742000 H - 6.7773000 - 2.26974400 H - 2.56344000 - 3.27428000 - 1.739712000 H - 2.5534000 - 3.277428000 - 2.137748000 H - 2.26374000 - 3.27745000 - 2.13774000 H - 2.26374000 - 3.27745000 - 2.13774000 H - 2.57373800 - 4.7073000 - 1.4778000 H - 2.57373800 - 4.7078000 - 1.4778000 H - 3.5072400 - 3.25722300 - 1.13971200 C - 3.397447000 - 3.27457000 - 2.739428000 H - 2.553738000 - 4.7078000 - 1.47780000 H - 2.557378000 - 3.27782300 - 1.139712000 C - 3.397447000 - 5.77845000 - 2.49786000 H - 3.50747000 - 3.77845000 - 2.49786000 H - 3.257723000 - 1.47780000 - 1.47780000 H - 3.25722300 - 1.407981000 - 2.49955000 H - 3.32625000 - 3.49977000 - 4.47679000 - 4.47780000 C - 4.7677100 - 3.48977000 - 2.49375000 - 2.493156000 H - 3.322625000 - 1.46083000 - 1.46783000 C - 4.7740400 - 5.7784000 - 2.24278000 H - 3.322623001 - 1.60624000 - 0.25845000 - 2.49352000 C - 4.77404000 - 5.7718000 - 3.797800 - 2.4927800 H - 3.32263000 - 1.60631000 - 2.44278000 C - 4.77494000 - 0.58711800 - 0.342718000 H - 3.224278000 - 0.28813000 - 0.487118000 H - 3.224278000 - 0.28813000 - 0.487118000 H - 3.32242000 - 0.28813000 - 0.487118000 H - 3.32242000 - 0.28813000 - 0.487118000 H - 3.32242000 - 0.28814000 - 0.284467500 H - 3.32242000 - 0.28817000 - 3.24768400	Н	5.621086000	-3.149687000	2.466449000	
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H 4.934824000 -0.063161000 -2.745843000 Sum of electronic and zero-point Energies= -1736.873522 C 4.481013000 -0.837755000 2.332563000 Sum of electronic and thermal Energies= -1736.826489 H 3.529354000 -0.302921000 2.421690000 Sum of electronic and thermal Energies= -1736.82545	н	3.734193000	-1.288972000	-3.242066000	Thermal correction to Gibbs Free Energy= 0.862187
C 4.481013000 -0.837755000 2.332563000 Sum of electronic and thermal Energies= -1736.826489 H 3.529354000 -0.302921000 2.421690000 Sum of electronic and thermal Entralbies= -1736.82545	н	4.934824000	-0.063161000	-2.745843000	Sum of electronic and zero-point Energies= -1736.873522
H 3.529354000 -0.302921000 2.421690000 Sum of electronic and thermal Enthalpies= -1736.825545	С	4.481013000	-0.837755000	2.332563000	Sum of electronic and thermal Energies= -1736.826489
	LЦ	3,529354000	-0.302921000	2.421690000	Sum of electronic and thermal Enthalpies= -1736.825545

Н	5.239972000	-0.273145000	2.884880000	Sum of electronic and thermal Free Energies=	-1736.951554
н	4.380444000	-1.819853000	2.803302000	5	
С	5.975571000	-3.209263000	1.142267000	Charge = 0 Multiplicity = 1	
н	6.305204000	-4.030253000	0.501806000	5 1 5	
H	5 417155000	-3 651905000	1 977267000	~	
н	6 867048000	-2 732837000	1 567624000		
	4 920120000	2.752057000	1.025072000		
	4.629129000	-3.300211000	-1.923972000		
н	5.353416000	-4.225623000	-1.515740000		
н	5.385454000	-3.022205000	-2.809643000		
н	3.844733000	-3.697454000	-2.273045000		
С	3.518704000	0.990636000	0.129160000		
С	4.234377000	2.173836000	0.787703000		
С	2.615788000	2.925758000	-0.976442000		
С	5.753737000	1.995163000	0.950277000		
H	6.012883000	1,290565000	1,742649000		
H	6 215715000	2 956695000	1 202870000		
н	6 202/71000	1 630520000	0.021468000		
	3 640160000	2 626004000	2 120056000	17	
ŭ	2 882167000	2.020004000	2.139930000	//	
	3.003107000	1.909025000	2.929541000	Q.	
н	2.553714000	2.709976000	2.099587000		
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н	2.863700000	4.186606000	-2.754436000	1 23	
С	1.528492000	3.858119000	-0.394855000		
Ĥ	1.479558000	3.809953000	0.693592000		
н	0.533709000	3 638421000	-0 792120000		
H	1 764527000	4 891258000	-0.669425000		
	1.704527000	0.048015000	0.000420000		
ŭ	0.409749000	1 610227000	-0.493780000		
	0.406746000	1.019227000	-1.054769000		
C .	0.590269000	0.926125000	0.970810000		
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С	0.861898000	-0.448783000	-1.103468000		
Н	1.528136000	-1.162708000	-0.608507000		
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С	3.984744000	3.237500000	-0.322782000		
н	4.030251000	4.261769000	0.063335000		
н	4,775105000	3.138603000	-1.075068000		
N	-3 969217000	1 105044000	1 169439000		
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N	-2 /38170000	-1 470150000	0.601001000		
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č	-4.002330000 F 172057000	0.230010000	0.049070000		
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Ц	-4.023211000	1 225202000	1 51652000000		
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Н	-4.030178000	-4.261771000	-0.063572000
Н	-4.775016000	-3.138723000	1.074947000

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