Supporting Information for

Uncaging Carbon Disulfide. Delivery Platforms for Potential Pharmacological Applications: A Mechanistic Approach.

Anthony W. DeMartino, Maykon Lima Souza, Peter C. Ford

Contents:

Experimental descriptions of substrate syntheses: Models for acid and buffer catalyzed decay of diisopropyldithiocarbamate (DIDTC-).

Figures

Figure S1. X-ray structure packing diagram (top) and asymmetric unit (bottom) of K[DIDTC] **Figure S2.** X-ray structure packing diagram (top) and asymmetric unit (bottom) of K[ImDTC] **Figure S3.** X-ray structure packing diagram (top) and asymmetric unit (bottom) of K[PyrDTC] **Figure S4.** Optimized geometries of the DTC anions at a PCM/B3LYP/6-31+G(d,p) theory level. **Figure S5.** TD-DFT calculated spectrum for DIDTC⁻ in a PCM model solvent (water) **Figure S6.** TD-DFT calculated spectrum for the ImDTC⁻ in a PCM model solvent (water). **Figure S7.** Plot of log k_{obs} versus pH for decay of K[ImDTC] in aqueous solution **Figure S8.** Plot of k_{obs}^{-1} vs [H⁺]⁻¹ for DIDTC⁻ decay in phosphate buffer. pH 6.5-7.8 at 37 °C **Figure S10.** k_{obs} as a function of phosphate buffer concentration for the decay of K[DIDTC] **Figure S11.** Ionic strength effects on DIDTC⁻ decay. **Figure S12.** Eyring plots (ln(k_{obs}/T) vs. 1/T) for the decay of DIDTC⁻ at pH7.4 and pH 2.0. **Figure S13.** Eyring plot (ln(k_{obs}/T) vs. 1/T) for the decay of ImDTC⁻ at pH7.4 **Figure S14.** Optimized geometries of DTCH species at a PCM/B3LYP/6-31+G(d,p) theory level. **Figure S15.** DFT calculated rotation around the N-CS2 bond of dimethyl DTC⁻

Tables:

- Table S1.
 X-ray structural data for potassium diisopropyldithiocarbamate (K[DIDTC]).
- **Table S2**. X-ray structural data for potassium imidazoledithiocarbamate (K[ImDTC]).
- Table S3. X-ray structural data for potassium pyrroledithiocarbamate (K[PyrDTC])
- **Table S4.** Bond lengths and angles for potassium diisopropyldithiocarbamate (K[DIDTC]).
- Table S5.
 Bond lengths and angles for potassium imidazoledithiocarbamate (K[ImDTC]).
- Table S6. Bond lengths and angles for potassium pyrroledithiocarbamate (K[PyrDTC]).
- **Table S7.** Expt. and calc. key bond lengths and angles of DTC- anions and DTCH conjugate acids
- Table S8.
 Optical spectra of DTC- anions.
- **Table S9.** Calculated E_{rot} values for C-N bonds & GS and TS orbital contributions (aliphatic DTCs)
- Table S10 Calculated E_{rot} values for C-N bonds & GS and TS orbital contributions (aromatic DTCs)
- **Table S11**. DFT calculated Cartesian coordinates (x, y, z) of DTC anions and conjugate acids
- **Table S12.** Graphical representations for calculated HOMO for ground and rotational transitionstates of various DTC and DTCH.

SI References

Experimental descriptions of substrate syntheses:

Note: Carbon disulfide is toxic at high exposures, and long periods of modest exposure have been associated with a number of health conditions. Handle and store CS_2 and CS_2 -generating compounds with care.

Materials and Analytical Instrumentation: Except where noted, starting materials were used without further purification. Diisopropylamine (\geq 99.5%), imidazole (\geq 99%), ammonium pyrrolidinyldithiocarbamate (~99%), pyrrole (98%), calcium hydride, potassium metal and potassium bromide (FT-IR grade) were purchased from Sigma Aldrich. Carbon disulfide (ACS Reagent Grade, \geq 99.9%), morpholine (Alfa Aesar, 99%), potassium hydroxide, and sodium hydroxide were purchased from Fisher Scientific. Pyrrole (98%) was purchased from Sigma and distillated before use under reduced pressure in the presence of calcium hydride (Sigma) as reported in literature.¹ HPLC grade methanol, dichloromethane, acetone, and chloroform were from VWR, acetonitrile was from Fisher Scientific, and absolute ethanol was from Rossville. Nanopure water (\geq 18 megohm) was obtained from a Barnstead Nanopure II system and used in all syntheses. Dry DMF in a Sure-seal bottle was purchased from Sigma-Aldrich.

Electronic absorption spectra were recorded on a Shimadzu UV-2401 PC spectrophotometer. Infrared spectra in KBr pellets were recorded with a Bio-Rad FTS-60 SPC3200 FTIR spectrophotometer, while IR spectra in solutions and solid powders were recorded with a Bruker ALPHA Platinum ATR FTIR with a single reflection diamond. NMR spectra were obtained on a Varian 500 MHz spectrometer in deuterated solvents from Cambridge Isotope Laboratories, Inc. Mass spectrometer y for charged species was conducted on a Waters Micromass QTOF2 mass spectrometer with an electrospray ionization source (ESI, negative mode). Elemental analyses (C,H,N) were conducted at the UCSB MSI Analytical Lab with a thermal conductivity method using a Control Equipment Corporation 440HA Elemental Analyzer.

Syntheses of Dithiocarbamates (DTCs). Sodium and potassium diisopropylammonium disopropyldithiocarbamate: The sodium salt Na[DIDTC] was prepared by a modification of a published procedure.² A round bottom flask was charged with 30 mL of Et₂O and 10 mL of CS₂, cooled to 0 – 5 °C with an ice bath and purged with inert gas. With rapid stirring, finely ground NaOH (1.0 g, 25 mmol) was added to a flask. Sufficient water was added to solubilize the hydroxide $(\sim 2 \text{ mL})$. To this solution, 5 mL diisopropylamine (3.61 g, 35.7 mmol) was added over a two min. period, during which the solution rapidly became light yellow and cloudy. This mixture was stirred for an additional 1 h after which the solid product was collected by filtration and washed with cold Et₂O. The product was recrystallized from a saturated acetonitrile/methanolic solution by slow diffusion of Et₂O and dried *in vacuo*. The typical yield was 75-89%. The compounds were stored in a freezer. Elemental analysis (calculated for C₇H₁₄NS₂Na · 2.5 H₂O): C, 33.8 (34.41); H, 7.46 (7.84); N, 5.61 (5.73). (~2.5 waters were present in the crystal lattice according to thermal gravimetric analysis (TGA), others have reported as high as 5 H₂O's).^{2,3} UV/Vis spectrum λ_{max} 261 (ϵ = 1.15 x $10^4 \text{ M}^{-1} \text{ cm}^{-1}$) and 286 nm ($\varepsilon = 1.1 \text{ x} 10^4 \text{ M}^{-1} \text{ cm}^{-1}$) in pH 7.4 deoxygenated water. Infrared spectrum (ATR, cm⁻¹): 3300 (ν, O-H), 2920, 2968 (ν, C-H), 1615-1700 (δ, O-H), 1470 (ν, C-N), 1356, 1431 (v, CH₃), 1294 (v, N-C), 1137 (ρ , CH₃), 941 (v, C-S). ¹HNMR (CD₃OD): δ 6.25 (broad, singlet, 1H), 3.86 (broad, singlet, 1H), 1.70 (broad, singlet, 6H), 1.21 (broad, singlet, 6H).

The diisopropylammonium salt [${}^{i}Pr_{2}H_{2}N$][DIDTC] was prepared in a similar manner. A round bottom flask in an ice bath (0 – 5 °C) was charged with 30 mL of Et₂O and purged with a gentle flow of argon. To the flask was added 10 mL of CS₂ (166 mmol) and then 5 mL of diisopropylamine (35.7 mmol). The solution was allowed to react for 2 h, producing a pale-yellow precipitate that was collected by filtration and washed with cold Et₂O. The yield was 56%. Crystals suitable for x-ray diffraction studies were obtained by infusion of Et₂O into an carbon disulfide/acetonitrile (1:4) solution of this compound at -20 °C. The volume of the unit cell and the crystallographic parameters were the same as those published previously.⁴ Infrared spectrum (ATR, cm⁻¹): 2970 (ν (C-H), m); 2818 – 2429 (ν (N-H, quartenary amine), w); 1552 (δ (NH₂, quartenary amine), w); 1469 (ν (-N-C=S), m); 1432 (ν (-N=C-S-), m); 1391 and 1362 (ν (-C-CH₃), m); 1282 (ν (N-CS₂), s), 1197 and 1143 ((ν (C-N), s); 1028 (ν (CS₂)_{asym}, s); 944 (ν (CS₂)_{sym}, s); 903 – 786 (ν (C-S), m).⁵⁻⁷ Elemental analysis: C, 55.92 (56.06); H, 11.04 (10.86); N, 10.05 (10.06).

The potassium salt, K[(iPr)₂NCS₂], was prepared from the diisopropylammonium salt [ⁱPr₂H₂N][(iPr)₂NCS₂]. The diisopropylammonium salt (9.0 mmol) was solubilized in a THF solution of potassium tert-butoxide (*t*-butO⁻K⁺) (9.0 mmol) under argon atmosphere (glove box). The solution was stirred for more 30 min and then all the solution was dried under vacuum. The white solid obtained was stirred in Et₂O, filtered and washed with Et₂O. The yield was 61%. Crystals suitable for x-ray diffraction studies were obtained by infusion of Et₂O into an acetonitrile solution of the compound at –20 °C. The crystals were kept in solution until the X-ray analysis. When out of solution the crystals back to the original amorphous solid. Infrared spectrum (ATR, cm⁻¹): 3294 (v(O-H), s); 2972 (v(C-H), m); 1605 (δ (H₂O), m); 1476 (v(-N-C=S), m); 1437 (v(-N=C-S-), m); 1370 and 1358 (v(-C-CH₃), m); 1299 (v(N-CS₂), s), 1196 and 1142 ((v(C-N), s); 1032 (v(CS₂)_{asym}, s); 940 (v(CS₂)_{sym}, s); 907 – 786 (v(C-S), m).⁵⁻⁷ ¹HNMR (CD₃CN): δ 6.48 (*broad*, singlet, 1H), 3.78 (*broad*, singlet, 1H), 1.70 (*broad*, singlet, 6H), 1.11 (*broad*, singlet, 6H). Elemental analysis (calculated for K[(iPr)₂NCS₂]·1/4H₂O): C, 38.32 (38.20); H, 6.22 (6.59); N, 6.29 (6.37).

Ammonium morpholinedithiocarbamate (NH₄[MorDTC]): The procedure was analogous to that used to prepare NH₄[AnDTC]. To an argon-purged flask, 5 mL morpholine (4.97 g, 57.0 mM) was added dropwise to an ice-cold mixture of prepared from 12 mL of 8 M ammonium hydroxide, 4 mL of CS₂ (5.06 g, 67 mM) and 10 mL of diethyl ether with stirring. The solution turned slightly yellow, and a white powder immediately began to precipitate. The vessel was allowed to return to room temperature over the course of 2-6 h. Addition of 5-10 mL of Et₂O precipitated the product further. The solid was collected by filtration, washed with cold ethanol, and dried *in vacuo*. It is sparingly soluble in other than water, including acetonitrile and alcohols. Elemental analysis (calculated for C₅H₁₂N₂S₂): C, 33.82 (33.31); H, 6.56 (6.71); N, 15.38 (15.54). UV/Vis spectrum λ_{max} 263 (ϵ = 1.5 x 10⁴ M⁻¹ cm⁻¹) and 286 nm (ϵ = 1.4 x 10⁴ M⁻¹ cm⁻¹) in pH 7.4 water. ¹HNMR (D₂O): δ 4.28 (m, 4H), 3.64 (m, 4H); ¹³CNMR (D₂O): δ 211.5 (CS₂), 68.7 (-N-CH₂-), 55.1 (-O-CH₂-). These data agree well with those reported elsewhere.^{8,9}

Potassium imidazoledithiocarbamate (K[ImDTC]). Imidazole (7.3 mmol) was dissolved in 1.2 mL of nanopure water containing KOH (7.3 mmol). The water was then removed using a rotary evaporator followed by drying in a vacuum oven at 100 °C for 2 h. The resulting dry pink solid was then rapidly added to a round bottom flask containing 5 mL of dry acetonitrile at -40 °C. Under stirring, CS₂ (0.53 mL, 8.76 mmol) was added dropwise, and the solution color immediately turned orange followed in few minutes by precipitation of a yellow solid. After 30 min reaction, the solution was filtered, and the solid product was washed with chloroform and dried under vacuum overnight. The yield was 53%. Elemental analysis (calculated for C₄H₃N₂S₂K): C: 26.15 (26.35), H: 1.66 (1.66), N: 15.14 (15.37). UV/Vis spectrum λ_{max} 255 (ε = 6.36 x 10³ M⁻¹ cm⁻¹), 280 nm (ε = 9.38 x 10³ M⁻¹ cm⁻¹) and 353 nm (ε = 1.24 x 10⁴ M⁻¹ cm⁻¹) in acetonitrile. Infrared spectrum (ATR, cm⁻¹): 3158 – 3110 (v(C-H), w); 1524 (v(C=N), m); 1464 (v(C=C), m); 1310 (v(C-N), s); 1201 (v(N-CS₂), s); 1070 (δ(C-H), s); 1014 (v(CS₂)_{asym}, s); 830 (v(CS₂)_{sym}, s); 742 (v(C-S), m). ¹HNMR (CD₃CN): δ 6.80 (triplet, 1H), 8.15 (triplet, 1H), 8.74 (*broad*, triplet, 1H). Crystals suitable for X-ray analysis were grown by infusion of diethyl ether in an acetonitrile solution of the compound at -20 °C.

Potassium pyrroledithiocarbamate (K[PyrDTC]). Potassium pyrrolyldithiocarbamate was prepared as described by Bereman.¹⁰ Pyrrole (15.0 mmol), recently distillated, was added to 30 mL of dry THF. Potassium metal (15.0 mmol) was added to the solution and the mixture was allowed to

react for 36 h. The solution was cooled to -78 °C and 1.08 mL (18 mmol) of CS₂ were added dropwise for 30 min. The solution was kept under stirring for 60 minutes, after which, cold hexanes (-20 °C) was added to the solution to precipitate a bright yellow solid in high yield (85%). The compound obtained is highly hygroscopic and air sensitive, and must be handled in a glove box under inert atmosphere and low humidity. Elemental analyses did not give good results probably due exposure to the environment on the analysis. Nevetheless, the compound is stable for days in deoxygenated aqueous solutions. UV/Vis spectrum λ_{max} 297 ($\varepsilon = 1.29 \times 10^4 \text{ M}^{-1} \text{ cm}^{-1}$), 343 nm ($\varepsilon = 6.30 \times 10^3 \text{ M}^{-1} \text{ cm}^{-1}$) in deoxygenated nanopure water; Infrared spectrum (ATR, cm⁻¹): 3371 (v(0-H), s); 3153 – 3096 (v(C-H), w); 1607 ($\delta(\text{H}_2\text{O})$, m); 1447 (v(C=C), m); 1291 (v(C-N), s); 1237 (v(N-CS₂), s); 1072 ($\delta(\text{C-H})$, s); 1001 (v(CS₂)_{asym}, s); 811 (v(CS₂)_{sym}, s); 744 (v(C-S), m).⁵ ¹HNMR (D₂O): δ 6.34 (triplet, 2H), 8.04 (triplet, 2H) Crystals suitable for X-ray analysis were grown by slow evaporation of a saturated water solution of the compound under vacuum.

Models for acid and buffer catalyzed decay of diisopropyldithiocarbamate (DIDTC-).

For simplicity, we will use the following terms:

 $DTC^- = DIDTC^-$ DTCH = DIDTCH $R_2NH = diisopropyl amine$

 $BH = buffer conjugate acid; B^- = buffer conjugate base, [B]_{tot} = total buffer concentration$

Key equilibria:

$$K_{a}$$
DTCH \longrightarrow DTC- + H+ $K_{a} = [DTC-][H+]/[DTCH]$

$$K_{a}^{B}$$
BH \longleftarrow B- + H+ $K_{a}^{B} = [B-][H+]/[BH]$

Note: The pKa's of H2PO4⁻ and MOPS are reported to be 7.165 and 7.044, respectively, at 37 °C.¹¹

Acid (only) catalyzed decay

DTC⁻ + H⁺ $\xleftarrow{K_a^{-1}}$ DTCH DTCH $\xleftarrow{k_1}$ CS₂ + R₂NH

$$d[P]/dt = k_1[DTCH] = k_{obs}[DTC]_{tot}$$

$$[DTC]_{tot} = [DTCH] + [DTC^{-}] = [DTCH] (1 + K_a[H^{+}]^{-1}) = K_a [DTC^{-}] (K_a + [H^{+}])$$
$$[DTCH] = [DTC]_{tot} [H^{+}] / (K_a + [H^{+}])$$

therefore:

$$\frac{d[P]}{dt} = k_1[\text{DTCH}] = \frac{k_1 [\text{H}^+][\text{DTC}]_{\text{tot}}}{K_a + [\text{H}^+]}$$

and:

$$k_{obs} = \frac{k_1 [\mathrm{H}^+]}{K_a + [\mathrm{H}^+]}$$
(eq. A)

From the k_{obs} versus pH curve over the pH range 2.0 to 7.8 (Figure 7 in text), the pK_a is estimated to be 4.6 and k_1 is 0.37 s⁻¹ based on the limiting k_{obs} values at low pH.

for the pH range 6.5-7.8, $K_a >> [H^+]$, thus: $k_{obs} = k_1 K_a^{-1}[H^+]$

Add a buffer catalyzed rate — simple general acid catalysis

DTC⁻ + BH
$$\longrightarrow$$
 CS₂ + R₂NH + B⁻

then

$$\frac{d[P]}{dt} = k_1[\text{DTCH}] + k_{ga}[DTC^-][\text{BH}] = \frac{(k_1[\text{H}^+] + k_{ga}K_a[\text{BH}])[\text{DTC}]_{\text{tot}}}{K_a + [\text{H}^+]}$$

However: for the pH range 6.5-7.8, $K_a >> [H^+]$

thus:
$$k_{obs} = k_1 K_a^{-1}[H^+] + k_{ga}[BH]$$

where
$$[BH] = [B]_{tot}[H+] / ([H^+] + K_a^B)$$
,

giving:

$$k_{obs} = k_1 K_a^{-1}[\mathrm{H}^+] + \frac{k_{ga}[\mathrm{H}^+][\mathrm{B}]_{\mathrm{tot}}}{K_a^B + [\mathrm{H}^+]}$$
 (eq. B)

Thus: a plot of k_{obs} vs [B]_{tot} at constant pH should be linear

intercept = $k_1 K_a^{-1}[H^+]$ and slope = $k_{ga}[H^+]/([H^+] + K_a^B)$

In this context, k_{obs} values for DIDTC⁻ decay in the MOPS buffer at pH 7.4, k_{obs} vs [B]_{tot} gave a linear plot with intercept = 9.1 x 10⁻⁴ s⁻¹ and slope = 0.0123 M⁻¹ s⁻¹

Thus for $[H^+] = 3.98 \times 10^{-8} \text{ M}$ and $K_a^B(\text{MOPS}) = 9.04 \times 10^{-8} \text{ M}$ at 37 °C^{*},

(i) $k_1 K_a^{-1} = 2.29 \text{ x} 10^4 \text{ M}^{-1} \text{ s}^{-1}$

given that a limiting value of 0.37 s⁻¹ was determined for k_1 at low pH this gives an

estimate for $K_a = 1.62 \times 10^{-5}$ M, or pKa (DIDTCH) = 4.79

(ii)
$$k_{ga}[H^+]/([H^+] + K_a^B) = 0.0123 \text{ s}^{-1} \text{ M}^{-1}$$

Therefore, this gives

$$k_{ga} = 0.040 \text{ M}^{-1} \text{ s}^{-1}$$
 for the conjugate acid of MOPS buffer

In contrast, the curvature in the k_{obs} vs. [B]_{tot} plots for phosphate imply a saturation effect at higher buffer concentrations.

Fitting the k_{obs} versus [B]_{tot} data for phosphate buffers at different pH values.

In attempts to fit the phosphate data we have tested two models, with $BH = H_2PO_4^-$ and $B^- = HPO_4^{2-}$ and $[B]_{tot} \sim [BH] + [B^-]$

I. The first is a mechanism where the buffer catalysis step involves proton transfer to the DTC nitrogen within a complex between H_2PO_4 - and DIDTC-.

DTC- + BH
$$\longleftarrow$$
 DTCBH (where DTCBH is a complex between BH and DIDTC-)
DTCBH $\xrightarrow{k_2}$ CS₂ + R₂NH + B-

$$d[P]/dt = k_1 K_a^{-1}[H^+][DTC^-] + k_2[DTCBH] = (k_1 K_a^{-1}[H^+] + k_2 K_B[BH]) [DTC^-]$$

$$[DTC]_{tot} = [DTC^{-}] + [DTCH] + [DTCBH]$$

at near neutral pH:

$$[DTC]_{tot} = [DTC^{-}] + [DTCBH] = [DTC^{-}] + K_B[DTC^{-}] [BH] = [DTC^{-}] (1 + K_B[BH])$$

 $[DTC^{-}] = [DTC]_{tot} / (1 + K_B[BH])$

therefore:

$$\frac{d[P]}{dt} = \frac{(k_1 K_a^{-1} [H^+] + k_2 K_B [BH]) [DTC]_{tot}}{1 + K_B [BH]}$$

and

$$k_{obs} = \frac{k_1 K_a^{-1} [\mathrm{H}^+] + k_2 K_B [\mathrm{BH}]}{1 + K_B [\mathrm{BH}]}$$

However: [BH] is a function of pH

$$\begin{array}{l} K_{a}^{B} \\ BH & \longleftarrow & B^{-} + H^{+} \text{ where } K_{a}^{B} = 6.84 \text{ x } 10^{-8} \text{ M for } H_{2}\text{PO}_{4^{-}} \text{ at } 37 \text{ oC.}^{11} \\ \\ [B]_{\text{tot}} = [BH] + [B^{-}] = [BH] + K_{a}^{B} [BH] [H^{+}]^{-1} = [BH] (1 + K_{a}^{B} [H^{+}]^{-1}) \\ \\ [BH] = [B]_{\text{tot}} / (1 + K_{a}^{B} [H^{+}]^{-1}) = [B]_{\text{tot}} ([H^{+}] / ([H^{+}] + K_{a}^{B})) \end{array}$$

Taking into account the pH dependence of [BH] leads to the following equation

$$k_{obs} = \left(\frac{k_1 K_a^{-1}[\mathrm{H}^+] + \left(\frac{k_2 K_B[\mathrm{H}^+]}{[\mathrm{H}^+] + K_a^B}\right)[\mathrm{B}]_{tot}}{K_a^B + [\mathrm{H}^+] + K_B[\mathrm{H}^+][\mathrm{B}]_{tot}}\right)(K_a^B + [\mathrm{H}^+])$$
(eq. C)

The following constants are known for the above:

 $k_1 = 0.37 \text{ s}^{-1}$ (from limiting rate at low pH) $K_a = 2.5 \times 10^{-5} \text{ M}$ (from k_{obs} vs. pH data, see text Figure 7) $K_a^B = 6.84 \times 10^{-8} \text{ M}^{11}$

[H⁺] (5 sets of k_{obs} data as a function of [B]_{tot} for pH values 6.5, 6.8, 7.0, 7.4 & 7.8) The equation above could be numerically fit to the k_{obs} values at each pH using OriginPro 8.5 (OriginLab software) to determine best values of K_B and k_2 . However, these values (which should have been constants) varied considerably although the product k_2K_B was nearly constant. Nonetheless, we used the K_B and k_2 values obtained from the pH 7.4 data (26 M and 0.27 s⁻¹, which were near the average values from the 5 pH experiments) with eq. C to recalculate the curves for data sets at the 5 pH values. This attempt (as well as those with other K_B and k_2 values) *did not give reasonable fits for the* k_{obs} *vs* $[B]_{tot}$ *plots for all five pH values.*

II. The second prospective mechanism involves proton transfer to the DIDTC- nitrogen from H_2PO_4 but inhibition of DIDTC- decay by formation of a complex with HPO_4^2 -.

In this model the following reactions lead to products:

DTCH $\xrightarrow{k_1}$ CS₂ + R₂NH DTC⁻ + BH $\xrightarrow{k_{ga}}$ CS₂ + R₂NH + B⁻

while one reaction does not

DTC⁻ + B⁻ \longleftrightarrow C \longrightarrow no reaction

This gives

 $d[P]/dt = (k_1 K_a^{-1}[H^+] + k_{ga}[BH]) [DTC^-]$

Although not reactive, the complex C affects the concentrations of the other species

$$[DTC]_{tot} = [DTC^{-}] + [DTCH] + [C] = (1 + K_a^{-1}[H^+] + K_c[B^-])[DTC^{-}]$$
$$= (1 + K_c[B^-])[DTC^{-}] \qquad \text{given that } 1 >> K_a^{-1}[H^+]$$

thus: $[DTC^{-}] = [DTC]_{tot}/(1 + K_c[B^{-}])$

Thereby giving

$$d[P]/dt = (k_1 K_a^{-1}[H^+] + k_{ga}[BH]) [DTC]_{tot}/(1 + K_c[B^-])$$

since: [BH]_{tot} >> [DTC]_{tot}, the formation of C has little effect on [BH] or [B⁻]

Therefore: $[BH] = [B]_{tot}([H^+]/([H^+] + K_a^B))$ and $[B^-] = K_a^B[B]_{tot}/([H^+] + K_a^B)$

Giving:

$$\frac{d[P]}{dt} = (k_1 K_a^{-1} [H^+] + \frac{k_{ga} [H^+] [B]_{tot}}{K_a^B + [H^+]}) (\frac{K_a^B + [H^+]}{K_a^B + [H^+] + K_a^B K_c [B]_{tot}}) [DTC]_{tot}$$

and

$$k_{obs} = (k_1 K_a^{-1} [\mathrm{H}^+] + \frac{k_{ga} [\mathrm{H}^+] [\mathrm{B}]_{tot}}{K_a^B + [\mathrm{H}^+]}) (\frac{K_a^B + [\mathrm{H}^+]}{K_a^B + [\mathrm{H}^+] + K_a^B K_c [\mathrm{B}]_{tot}})$$

given that the following constants are known for the above:

 $k_1 = 0.37 \text{ s}^{-1}$ (from limiting rate at low pH) $K_a = 2.5 \times 10^{-5} \text{ M}$ (from $k_{obs} \text{ vs. pH}$ data, see text) $K_a^B = 6.84 \times 10^{-8} \text{ M}$

[H⁺] (5 sets of k_{obs} data as a function of [B]_{tot} for pH values 6.5, 6.8, 7.0, 7.4 & 7.8)

The equation above could be numerically fit to the k_{obs} values at each pH using OriginPro 8.5 k_{ga} (OriginLab software) to determine best values of K_C and k_{ga} . The calculated values of k_{ga} were remarkably constant, varying by only about $\pm 10\%$. A wider range was seen for the calculated K_C values, although the K_c for the four higher pH values were more tightly grouped with an average variation of $\pm 20\%$. Figure S10 shows the fits of the calculated k_{obs} values to the experimental ones using the average k_{ga} value 0.27 M⁻¹ s⁻¹ and the average K_c value 26 M⁻¹ determined for the four sets of experiments at the higher pH's. The fits of the experimental data to eq. D are reasonable for all 5 pH values.

Notably, the k_{ga} value for the general acid catalysis of DIDTC- decay by H₂PO₄- estimated in this way for the reactions in phosphate buffer is nearly 7 times as large as that determined for the conjugate acid of the MOPS buffer.

Figures



Figure S1. X-ray structure packing diagram (upper) and asymmetric unit (bottom) of potassium diisopropyldithiocarbamate, K[DIDTC]. Thermal ellipsoids are drawn at 50% probability. Water molecules and potassium cation were omitted in the packing representation for clarity (CCDC # 1557062)



Figure S2. X-ray structure packing diagram (upper) and asymmetric unit (bottom) of potassium imidazoledithiocarbamate (K[ImDTC]). Thermal ellipsoids drawn at 50% probability. Potassium cations were omitted in the packing representation for clarity. (CCDC # 1557060)



Figure S3. X-ray structure packing diagram (upper) and asymmetric unit (bottom) of potassium pyrroledithiocarbamate K[PyrDTC] (with 50% thermal ellipsoids). Potassium cations were omitted in the packing representation for clarity. (CCDC# 1557061)



Figure S4. Optimized geometries of various DTCs in a PCM (solvent=water)/B3LYP/6-31+G(d,p) theory level. Abbreviations: DIDTC⁻ = diisopropyldithiocarbamate anion, MorDTC⁻ = morpholine-dithiocarbamate, PDTC⁻ = pyrrolidinedithiocarbamate anion, PyrDTC⁻ = pyrroledithiocarbamate anion, ImDTC⁻ = imidazoledithiocarbamate anion.



Figure S5. DIDTC⁻ TD-DFT-calculated spectrum in an PCM model solvent (water) and M062X/6-31+G(d,p) level of theory for the optimized DIDTC⁻ geometry. The theoretical spectrum was generated from GaussSum 3.0 software with half-widths of 4100 cm⁻¹ (the electronic transitions are identified by their relative oscillator strengths: blue bars). Insert: Calculated MOs involved in electronic transitions.



Figure S6. TD-DFT-calculated spectrum in an PCM model solvent (water) and M062X/6-31+G(d,p) level of theory for the ImDTC⁻ geometry. The theoretical spectrum was generated from GaussSum 3.0 software with half-widths of 4300 cm⁻¹ (the electronic transitions are identified by their relative oscillator strengths: blue bars). Insert: Calculated MOs involved in electronic transitions.



Figure S7. Linear fit of the plot of the $log(k_{obs})$ versus pH for the decay of the ImDTC⁻ anion. $R^2 = 0.999$; Slope = -0.86.



Figure S8. Double reciprocal plot of k_{obs}^{-1} vs [H+]⁻¹ for the decay of DIDTC- in phosphate buffer (50 mM) with ionic strength adjusted to 154 mM with NaCl. pH 6.5-7.8 at 37 °C. According to eq. 2, $k_{obs}^{-1} = K_a/k_1$ [H+] + $1/k_1$ so $k_1 = 1$ /intercept and K_a = slope over internet, from which the values $k_1 = 0.021 \pm 0.002 \text{ s}^{-1}$ and $K_a = 2.02 \times 10^{-7}$ (pK_a =6.69) were derived.



Figure S9. Temporal spectra of the DIDTC⁻ anion in acidic media. [DIDTC] = 0.1 mM; pH 2.0; μ = 0.154 M (NaCl); T = 37.1 °C.



Figure S10. Fits of k_{obs} values observed at 37 °C for the decay of DIDTC- as a function of the total buffer concentration [B]_{tot} as fit to eq. D for pH's 6.5 and 6.8 (top row), 7.0 and 7.4 (middle) and 7.8 (bottom). Black squares are experimental points; Red dots are theoretical values calculated using $k_1 = 0.37$ s⁻¹, $K_a = 2.5 \times 10^{-5}$ M, $K_a^B = 6.84 \times 10^{-8}$, $k_{ga} = 0.27$ M⁻¹s⁻¹, $K_c = 26$ M⁻¹.

$$k_{obs} = (k_1 K_a^{-1} [\mathrm{H}^+] + \frac{k_{ga} [\mathrm{H}^+] [\mathrm{B}]_{tot}}{K_a^B + [\mathrm{H}^+]}) (\frac{K_a^B + [\mathrm{H}^+]}{K_a^B + [\mathrm{H}^+] + K_a^B K_c [\mathrm{B}]_{tot}})$$
(eq. D)



Figure S11. Ionic strength effects on DIDTC⁻ decay. Conditions: pH 7.4 phosphate buffer (10 mM). m varied from 60 mM to 308 mM.

m (mM)	k_{obs} (s ⁻¹)
60	0.00143
100	0.00152
120	0.00150
154	0.00149
308	0.00153



Figure S12. Eyring plots of k_{obs} values measured at over the temperature range 283.5-320.6 K for the decay of ImDTC⁻. The kinetics experiments were performed by mixing equal volumes of phosphate buffer (pH 7.45, 0.15 M) and K[ImDTC] (0.2 mM) in aq. NaOH (1.5 mM, 3.0 mM and 5.0 mM) in the stopped-flow spectrophotometer. The final pH values for the three solutions were 7.53, 7.55 and 7.59, respectively.



Figure S13. Eyring plot of k_{obs} values measured over the temperature range 286.1 to 322.1 K for the decay of DIDTC in phosphate buffer (pH 7.40, 50 mM, m = 154 mM).



Figure S14. Optimized geometries of the protonated DTCs in a PCM(solvent=water)/B3LYP/6-31+G(d,p) theory level. Abbreviations: DIDTCH = diisopropyldithiocarbamic acid, MorDTCH = N-(morpholine-N-dithiocarbamic acid, PDTCH = pyrrolidinedithiocarbamic acid, PyrDTCH = pyrroledithiocarbamic acid, ImDTCH(SH) = imidazoledithiocarbamic acid, ImDTCH(NH) = N protonated zwiterionic form.



Figure S15. Potential Energy Surface (PES) generated from the CS_2 rotation along the N-C bond on the DIDTC⁻ anion. The transition state (TS_{rot}) correspond to a pyramidal DIDTC⁻ geometry. Calculated at the PCM(water)/B3LYP/6-31+G(d,p) theory level.

Tables:

 Table S1.
 X-ray structural data for potassium diisopropyldithiocarbamate (K[DIDTC).

Formula	C-H-aKNO-S-
	251 14
Temperature	201.44 100 K
	100 N
Wavelength (A)	0.71073
Crystal system	monoclinic
Space group	P 21/m
Unit cell dimensions	a = 5.7640(9) Å; α =90°
	b = 28.756(5) Å; β = 110.631(10
	c = 7.9313(14) Å; γ =90°
Z	4
Calculated density (Mg/cm ³)	1.357
Absorption coefficient (mm ⁻¹)	0.745
Crystal size (mm)	0.200 x 0.100 x 0.100
F(0 0 0)	536.0
Theta range for data collection	1.416 to 26.363
Reflections collected	5442
Independent reflections	2558
Completeness to $\theta = 26.363^{\circ}$	100%
Absorption correction	multi-scan
Max. And min. Transmission	0.745 and 0.639
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	2558/18/153
Goodness-of-fit on F ²	1.039
Final R indices $[I \ge 2\sigma(I)]$	R1=0.0521, wR=0.0992
R indices (all data)	R1=0.0886, wR=0.1115

$C_4H_3KN_2S_2$
182.30
100 K
0.71073
triclinic
P -1
a = 7.425(6) Å; α = 78.314 (12)°
b = 8.392(7) Å; β = 80.939 (15) °
c = 11.614 (9) Å; γ = 89.287 (17)°
4
1.731
1.258
0.250 x 0.200 x 0.100
368.0
1.813 to 24.711
5549
2311
96.9%
multi-scan
0.745 and 0.497
Full-matrix least-squares on F ²
2311/0/151
0.877
R1=0.0521, wR2=0.1103
R1=0.0973, wR2=0.1182

Table S2. X-ray structural data for potassium imidazoledithiocarbamate (K[ImDTC]).

Formula	C ₅ H ₄ KNS ₂
MW (g/mol)	181.31
Temperature	100 K
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	a = 13.41(2) Å; α = 90°
	b = 14.04(2) Å; β = 100.64 °
	c = 8.042 (13) Å; γ = 90°
Z	8
Calculated density (Mg/cm ³)	1.619
Absorption coefficient (mm ⁻¹)	1.179
Crystal size (mm)	0.250 x 0.100 x 0.050
F(0 0 0)	736.0
Theta range for data collection	2.119 to 26.296
Reflections collected	5708
Independent reflections	2936
Completeness to θ = 26.296°	97.6%
Absorption correction	multi-scan
Max. And min. Transmission	0.745 and 0.542
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	2936/0/163
Goodness-of-fit on F ²	0.969
Final R indices [I>2σ(I)]	R1=0.0497, wR2=0.0926
R indices (all data)	R1=0.0983, wR2=0.1100

Table S3. X-ray structural data for potassium pyrroledithiocarbamate (K[PyrDTC])

Atom1	Atom2	Length (Å)
C1	N1	1.344(5)
C1	S1	1.725(3)
C1	S2	1.731(3)
C2	H2	0.999
C2	C3	1.515(5)
C2	C4	1.533(6)
C2	N1	1.486(5)
C3	H3A	0.979
C3	H3B	0.980
C3	H3C	0.979
C4	H4A	0.980
C4	H4B	0.979
C4	H4C	0.980
C5	H5	1.000
C5	C6	1.524(6)
C5	C7	1.525(4)
C5	N1	1.492(4)
C6	H6A	0.980
C6	H6B	0.981
C6	H6C	0.981
C7	H7A	0.980
C7	H7B	0.980
C7	H7C	0.980
H11	01	0.81
H12	01	0.81
H21	02	0.82(5)
H22	02	0.82(4)
H31	03	0.82
H31	03	0.82
H32	03	0.81(4)
K1	01	3.331
K1	02	2.793
K1	S2	3.421
K1	02	2.793
K1	S2	3.421
K1	03	2.841
K1	03	2.841
K1	S2	3.427
К1	S2	3.427
К2	01	2.798
К2	02	2.706
К2	03	3.129

Table S4. Bond lengths and angles for potassium diisopropyldithiocarbamate (K[DIDTC)

К2	03	3.129
К2	02	2.706
К2	03	2.888
К2	03	2.888
К2	S2	3.266
К2	S2	3.266
01	H11	0.81
03	03	1.135(8)
03	K1	2.841
03	К2	2.888
S2	K1	3.427
S2	К2	3.266
H32	03	0.81(4)
03	K1	2.841
03	К2	2.888
C1	N1	1.344(5)
C1	S1	1.725(3)
C1	S2	1.731(3)
C2	H2	0.999
C2	C3	1.515(5)
C2	C4	1.533(6)
C2	N1	1.486(5)
C3	H3A	0.979
C3	НЗВ	0.980
C3	H3C	0.979
C4	H4A	0.980
C4	H4B	0.979
C4	H4C	0.980
C5	H5	1.000
C5	C6	1.524(6)
C5	C7	1.525(4)
C5	N1	1.492(4)
C6	H6A	0.980
C6	H6B	0.981
C6	H6C	0.981
C7	H7A	0.980
C7	H7B	0.980
C7	H7C	0.980
H21	02	0.82(5)
H22	02	0.82(4)
S2	K1	3.427
S2	К2	3.266
K1	S2	3.427
К1	S2	3.427

К2	03	2.888	
K2	03	2.888	
03	03	1.135(8)	
03	03	1.135(8)	
Atom1	Atom2	Atom3	Angle (º)
N1	C1	S1	121.1(3)
N1	C1	S2	121.5(3)
S1	C1	S2	117.3(2)
H2	C2	C3	107.3
H2	C2	C4	107.4
H2	C2	N1	107.4
C3	C2	C4	112.1(3)
C3	C2	N1	111.8(3)
C4	C2	N1	110.6(3)
C2	C3	H3A	109.5
C2	C3	H3B	109.4
C2	C3	H3C	109.5
H3A	C3	H3B	109.5
H3A	C3	H3C	109.4
H3B	C3	H3C	109.5
C2	C4	H4A	109.5
C2	C4	H4B	109.4
C2	C4	H4C	109.5
H4A	C4	H4B	109.4
H4A	C4	H4C	109.5
H4B	C4	H4C	109.5
H5	C5	C6	105.1
H5	C5	C7	105.1
H5	C5	N1	105.1
C6	C5	C7	113.2(3)
C6	C5	N1	113.3(3)
C7	C5	N1	114.0(3)
C5	C6	H6A	109.5
C5	C6	H6B	109.5
C5	C6	H6C	109.4
H6A	C6	H6B	109.4
H6A	C6	H6C	109.5
H6B	C6	H6C	109.5
C5	C7	H7A	109.5
C5	C7	H7B	109.4
C5	C7	H7C	109.5
H7A	C7	H7B	109.5
H7A	C7	H7C	109.5

H7B	C7	H7C	109.5
03	H31	03	87
01	K1	02	63.07
01	K1	S2	59.56
01	K1	02	63.07
01	K1	S2	59.56
01	K1	03	122.0
01	K1	03	122.0
01	K1	S2	139.22
01	K1	S2	139.22
02	K1	S2	81.98
02	K1	02	81.93
02	K1	S2	121.60
02	K1	03	127.4
02	K1	03	150.3
02	K1	S2	76.21
02	K1	S2	115.10
S2	K1	02	121.60
S2	K1	S2	60.79
S2	K1	03	66.0
S2	K1	03	78.2
S2	K1	S2	114.64
S2	K1	S2	158.16
02	K1	S2	81.98
02	K1	03	150.3
02	K1	03	127.4
02	K1	S2	115.10
02	K1	S2	76.21
S2	K1	03	78.2
S2	K1	03	66.0
S2	K1	S2	158.16
S2	K1	S2	114.64
03	K1	03	23.1
03	K1	S2	80.7
03	K1	S2	92.3
03	K1	S2	92.3
03	K1	S2	80.7
S2	K1	S2	60.69
01	K2	02	72.0
01	К2	03	53.5
01	К2	03	53.5
01	К2	02	72.0
01	К2	03	150.6
01	K2	03	150.6

01 K2 S2 128.05 02 K2 03 102.5 02 K2 03 117.5 02 K2 03 80.6 02 K2 03 95.8 02 K2 S2 102.77 02 K2 S2 159.80 03 K2 03 20.9 03 K2 03 146.6 03 K2 03 145.0 03 K2 03 155.0 03 K2 02 102.5 03 K2 02 102.5 03 K2 03 155.0 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 95.8 02 K2 03 95.8 02 K2 S2 102.77 <	0	1	К2	S2	128.05
02 K2 03 102.5 02 K2 03 117.5 02 K2 03 80.6 02 K2 03 95.8 02 K2 S2 102.77 02 K2 S2 159.80 03 K2 03 20.9 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 155.0 03 K2 02 102.5 03 K2 02 102.5 03 K2 02 102.5 03 K2 02 102.5 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 146.6 03 K2 S2 79.3 02 K2 S2 102.77 <	0	1	К2	S2	128.05
02 K2 03 117.5 02 K2 02 85.17 02 K2 03 80.6 02 K2 03 95.8 02 K2 S2 102.77 02 K2 S2 159.80 03 K2 03 20.9 03 K2 03 146.6 03 K2 03 146.6 03 K2 02 102.5 03 K2 02 102.5 03 K2 02 102.5 03 K2 02 102.5 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 146.6 03 K2 S2 79.3 02 K2 S2 102.77 03 K2 S2 102.77	0	2	К2	03	102.5
02 K2 02 85.17 02 K2 03 80.6 02 K2 03 95.8 02 K2 S2 102.77 02 K2 S2 159.80 03 K2 03 20.9 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 155.0 03 K2 02 102.5 03 K2 03 155.0 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 146.6 03 K2 S2 90.4 03 K2 S2 93.8 02 K2 S2 102.77 03 K2 S2 102.77 03 K2 S2 67.7 <t< td=""><td>0</td><td>2</td><td>К2</td><td>03</td><td>117.5</td></t<>	0	2	К2	03	117.5
02 K2 03 80.6 02 K2 03 95.8 02 K2 S2 102.77 02 K2 S2 159.80 03 K2 03 20.9 03 K2 02 117.5 03 K2 03 146.6 03 K2 03 146.6 03 K2 03 155.0 03 K2 S2 90.4 03 K2 02 102.5 03 K2 03 155.0 03 K2 03 146.6 03 K2 03 146.6 03 K2 S2 90.4 03 K2 S2 90.4 03 K2 S2 93 02 K2 S2 102.77 03 K2 S2 102.77 03 K2 S2 67.7	0	2	К2	02	85.17
O2 K2 O3 95.8 O2 K2 S2 102.77 O2 K2 S2 159.80 O3 K2 O3 20.9 O3 K2 O2 117.5 O3 K2 O3 146.6 O3 K2 O3 146.6 O3 K2 O3 155.0 O3 K2 S2 79.3 O3 K2 O2 102.5 O3 K2 O3 155.0 O3 K2 O3 146.6 O3 K2 O3 146.6 O3 K2 S2 79.3 O2 K2 O3 146.6 O3 K2 S2 79.3 O2 K2 S2 79.3 O2 K2 S2 102.77 O3 K2 S2 67.7 O3 K2 S2 67.7	0	2	К2	03	80.6
O2 K2 S2 102.77 O2 K2 S2 159.80 O3 K2 O3 20.9 O3 K2 O2 117.5 O3 K2 O3 146.6 O3 K2 O3 146.6 O3 K2 O3 155.0 O3 K2 S2 79.3 O3 K2 O2 102.5 O3 K2 O3 146.6 O3 K2 S2 79.3 O2 K2 S2 79.3 O2 K2 O3 80.6 O2 K2 S2 102.77 O3 K2 S2 67.7 O3 K2 S2 64.02 <tr< td=""><td>0</td><td>2</td><td>К2</td><td>03</td><td>95.8</td></tr<>	0	2	К2	03	95.8
O2 K2 S2 159.80 O3 K2 O3 20.9 O3 K2 O2 117.5 O3 K2 O3 146.6 O3 K2 O3 146.6 O3 K2 O3 155.0 O3 K2 S2 79.3 O3 K2 O2 102.5 O3 K2 O3 146.6 O3 K2 O3 146.6 O3 K2 O3 146.6 O3 K2 S2 90.4 O3 K2 O3 146.6 O3 K2 S2 90.4 O3 K2 S2 79.3 O2 K2 S2 79.3 O2 K2 O3 80.6 O2 K2 S2 102.77 O3 K2 S2 67.7 O3 K2 S2 67.7	0	2	К2	S2	102.77
03 K2 03 20.9 03 K2 02 117.5 03 K2 03 146.6 03 K2 03 155.0 03 K2 S2 79.3 03 K2 S2 90.4 03 K2 02 102.5 03 K2 03 155.0 03 K2 03 146.6 03 K2 03 146.6 03 K2 S2 90.4 03 K2 S2 90.4 03 K2 S2 90.4 03 K2 S2 79.3 02 K2 S2 79.3 02 K2 S2 102.77 03 K2 S2 102.77 03 K2 S2 67.7 03 K2 S2 67.7 S2 K2 S2 64.02	0	2	К2	S2	159.80
03 K2 02 117.5 03 K2 03 146.6 03 K2 03 155.0 03 K2 S2 79.3 03 K2 S2 90.4 03 K2 02 102.5 03 K2 03 155.0 03 K2 03 146.6 03 K2 03 146.6 03 K2 S2 90.4 03 K2 S2 19.80 02 K2 O3 80.6 02 K2 S2 102.77 03 K2 S2 67.7 03 K2 S2 80.2 03 K2 S2 64.02	0	3	К2	03	20.9
03 K2 03 146.6 03 K2 S2 79.3 03 K2 S2 90.4 03 K2 02 102.5 03 K2 03 155.0 03 K2 03 155.0 03 K2 03 146.6 03 K2 S2 90.4 03 K2 S2 79.3 02 K2 O3 80.6 02 K2 S2 102.77 03 K2 S2 67.7 03 K2 S2 80.2 03 K2 S2 64.02 C1 N1 C2 124.9(3) C2 N1 C5 114.1(3)	0	3	К2	02	117.5
03 K2 03 155.0 03 K2 S2 79.3 03 K2 S2 90.4 03 K2 02 102.5 03 K2 03 155.0 03 K2 03 146.6 03 K2 S2 90.4 03 K2 S2 90.4 03 K2 S2 90.4 03 K2 S2 79.3 02 K2 03 95.8 02 K2 03 80.6 02 K2 S2 102.77 03 K2 S2 102.77 03 K2 S2 67.7 03 K2 S2 80.2 03 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 114.1(3) H11 O1 H12 114 <t< td=""><td>0</td><td>3</td><td>К2</td><td>03</td><td>146.6</td></t<>	0	3	К2	03	146.6
03 K2 S2 79.3 03 K2 O2 102.5 03 K2 O3 155.0 03 K2 O3 146.6 03 K2 S2 90.4 03 K2 O3 146.6 03 K2 S2 90.4 03 K2 S2 90.4 03 K2 S2 90.4 03 K2 S2 79.3 02 K2 O3 95.8 02 K2 O3 80.6 02 K2 S2 102.77 03 K2 S2 67.7 03 K2 S2 80.2 03 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1	0	3	К2	03	155.0
O3 K2 S2 90.4 O3 K2 O2 102.5 O3 K2 O3 155.0 O3 K2 O3 146.6 O3 K2 S2 90.4 O3 K2 S2 90.4 O3 K2 S2 79.3 O2 K2 O3 95.8 O2 K2 O3 80.6 O2 K2 S2 159.80 O2 K2 S2 102.77 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 <tr< td=""><td>0</td><td>3</td><td>К2</td><td>S2</td><td>79.3</td></tr<>	0	3	К2	S2	79.3
O3 K2 O2 102.5 O3 K2 O3 155.0 O3 K2 O3 146.6 O3 K2 S2 90.4 O3 K2 S2 79.3 O2 K2 O3 95.8 O2 K2 O3 80.6 O2 K2 S2 159.80 O2 K2 S2 102.77 O3 K2 S2 102.77 O3 K2 S2 67.7 O3 K2 S2 67.7 O3 K2 S2 64.02 O1 N1 C2 121.0(3) C1 N1 C5 124.9(3) C2 N1 C5 114.1(3) H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1 52	0	3	К2	S2	90.4
O3 K2 O3 155.0 O3 K2 O3 146.6 O3 K2 S2 90.4 O3 K2 S2 79.3 O2 K2 O3 95.8 O2 K2 O3 80.6 O2 K2 S2 159.80 O2 K2 S2 102.77 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 67.7 O3 K2 S2 67.7 O3 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1 52	0	3	К2	02	102.5
O3 K2 O3 146.6 O3 K2 S2 90.4 O3 K2 S2 79.3 O2 K2 O3 95.8 O2 K2 O3 80.6 O2 K2 S2 159.80 O2 K2 S2 102.77 O3 K2 O3 22.7 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 67.7 O3 K2 S2 67.7 O3 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1 52	0	3	К2	03	155.0
O3 K2 S2 90.4 O3 K2 S2 79.3 O2 K2 O3 95.8 O2 K2 O3 80.6 O2 K2 S2 159.80 O2 K2 S2 102.77 O3 K2 O3 22.7 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 67.7 O3 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1 52 H12 O1 K1 52	0	3	К2	03	146.6
O3 K2 S2 79.3 O2 K2 O3 95.8 O2 K2 O3 80.6 O2 K2 S2 159.80 O2 K2 S2 102.77 O3 K2 O3 22.7 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 67.7 S2 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1 52 H12 O1 K2 134	0	3	К2	S2	90.4
O2 K2 O3 95.8 O2 K2 O3 80.6 O2 K2 S2 159.80 O2 K2 S2 102.77 O3 K2 O3 22.7 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 67.7 O3 K2 S2 67.7 O3 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1 52 H12 O1 K1 134 H12 O1 K2 81.9 K1 O1 H11 114 K1 O1 H11	0	3	К2	S2	79.3
O2 K2 O3 80.6 O2 K2 S2 159.80 O2 K2 S2 102.77 O3 K2 O3 22.7 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1 52 H12 O1 K2 134 H12 O1 K1 144 K1 O1 K1 120	0	2	К2	03	95.8
O2 K2 S2 159.80 O2 K2 S2 102.77 O3 K2 O3 22.7 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 67.7 O3 K2 S2 67.7 S2 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 124.9(3) C2 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1 52 H12 O1 K2 81.9 K1 O1 H11 114 K1 O1 K1 120 K2 O1 H11 120 K1 O1 H11	0	2	К2	03	80.6
O2 K2 S2 102.77 O3 K2 O3 22.7 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 124.9(3) C2 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K1 52 H12 O1 K2 81.9 K1 O1 H11 14 K1 O1 H11 120 K2 O1 H11 86	0	2	К2	S2	159.80
O3 K2 O3 22.7 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 124.9(3) C2 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K2 134 H12 O1 K2 81.9 K1 O1 H11 120 K2 O1 H11 86 H21 O2 H22 114(4) <td>0</td> <td>2</td> <td>К2</td> <td>S2</td> <td>102.77</td>	0	2	К2	S2	102.77
O3 K2 S2 67.7 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 67.7 S2 K2 S2 67.7 S2 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 124.9(3) C2 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 120 H12 O1 K1 52 H12 O1 K2 134 H12 O1 K1 14 K1 O1 K1 120 K1 O1 H11 114 K1 O1 H11 120	0	3	К2	03	22.7
O3 K2 S2 80.2 O3 K2 S2 80.2 O3 K2 S2 67.7 S2 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 124.9(3) C2 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 124.9 H11 O1 H12 114 H11 O1 K1 120 H11 O1 K2 86 H11 O1 K1 52 H12 O1 K2 134 H12 O1 K2 81.9 K1 O1 H11 120 K2 O1 H11 86 H21 O2 H22 114(4) <td>0</td> <td>3</td> <td>К2</td> <td>S2</td> <td>67.7</td>	0	3	К2	S2	67.7
O3 K2 S2 80.2 O3 K2 S2 67.7 S2 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 124.9(3) C2 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 124.9 H11 O1 H12 114.1(3) H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 52 H12 O1 K2 134 H12 O1 K1 14.9 K1 O1 K2 81.9 K1 O1 H11 120 K2 O1 H11 86 H21 O2 H22 114(4)	0	3	К2	S2	80.2
O3 K2 S2 67.7 S2 K2 S2 64.02 C1 N1 C2 121.0(3) C1 N1 C5 124.9(3) C2 N1 C5 114.1(3) H11 O1 H12 114 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K1 120 H11 O1 K2 86 H11 O1 K1 52 H12 O1 K1 52 H12 O1 K2 134 H12 O1 K1 14 K1 O1 K2 81.9 K1 O1 H11 120 K2 O1 H11 86 H21 O2 H22 114(4)	0	3	К2	S2	80.2
S2K2S264.02C1N1C2121.0(3)C1N1C5124.9(3)C2N1C5114.1(3)H11O1H12114H11O1K1120H11O1K286H11O1H11118H12O1K152H12O1K2134H12O1H11114K1O1K1120K1O1H11120K2O1H11144K1O1H11120K2O1H1186H21O2H22114(4)	0	3	К2	S2	67.7
C1N1C2121.0(3)C1N1C5124.9(3)C2N1C5114.1(3)H11O1H12114H11O1K1120H11O1K1120H11O1K152H12O1K152H12O1K2134H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	SZ	2	К2	S2	64.02
C1N1C5124.9(3)C2N1C5114.1(3)H11O1H12114H11O1K1120H11O1K286H11O1H11118H12O1K152H12O1K2134H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	C	1	N1	C2	121.0(3)
C2N1C5114.1(3)H11O1H12114H11O1K1120H11O1K1120H11O1K286H11O1H11118H12O1K152H12O1K2134H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	C	1	N1	C5	124.9(3)
H11O1H12114H11O1K1120H11O1K1120H11O1K286H11O1H11118H12O1K152H12O1K2134H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	C	2	N1	C5	114.1(3)
H11O1K1120H11O1K286H11O1H11118H12O1K152H12O1K2134H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	Н	11	01	H12	114
H11O1K286H11O1H11118H12O1K152H12O1K2134H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	Н	11	01	K1	120
H11O1H11118H12O1K152H12O1K2134H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	Н	11	01	К2	86
H12O1K152H12O1K2134H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	Н	11	01	H11	118
H12O1K2134H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	Н	12	01	K1	52
H12O1H11114K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	Н	12	01	К2	134
K1O1K281.9K1O1H11120K2O1H1186H21O2H22114(4)	Н	12	01	H11	114
K1O1H11120K2O1H1186H21O2H22114(4)	K	1	01	К2	81.9
K2 O1 H11 86 H21 O2 H22 114(4)	K	1	01	H11	120
H21 O2 H22 114(4)	K	2	01	H11	86
	Н	21	02	H22	114(4)

H21O2K2107H22O2K1111H22O2K2124K1O2K294.48H31O3H32115H31O3K295H31O3K1121H31O3K251H32O3K2118H32O3K2118H32O3K279K2O3K279K2O3K191.4K2O3K2146.6O3O3K2146.6O3O3K2146.6O3O3K2146.6O3O3K2146.6O3O3K2108.5C1S2K1119.7C1S2K1114.64K1S2K279.43H31O3K279.5K1S2K279.43H31O3K295H31O3K251K1S2K279.43H31O3K251K2O3G379.5K2O3K1121H31O3K279.5K2K279.43H31O3K251K2O3K1121H31O3K2146.6O3O3H32115H31O3K2146.6	H21	02	K1	104
H22O2K1111H22O2K2124K1O2K294.48H31O3H32115H31O3K295H31O3K1121H31O3K251H32O3K2118H32O3K2118H32O3K279K2O3K279K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K278.7K1O3K2108.5C1S2K1119.7C1S2K1114.64K1S2K279.43H31O3K295H31O3K279.5K2O3K2145.8K1S2K1114.64K1S2K279.43H31O3K295H31O3K295H31O3K2115H31O3K251K2O3K1121H31O3K2146.6O3O3H32115H31O3K2146.6G3O3K191.4K2O3K191.4K2O3K1121H31O3K279.5K2O3K191.4<	H21	02	К2	107
H22O2K2124K1O2K294.48H31O3H32115H31O3O346H31O3K1121H31O3K251H32O3K2118H32O3O3158(4)H32O3K279K2O3O379.5K2O3K2146.6O3O3K191.4K2O3K2146.6O3O3K178.5O3O3K2188.7K1O3K2108.5C1S2K1103.1C1S2K1114.64K1S2K1114.64K1S2K295H31O3K279.43H31O3K279.43H31O3K251K1S2K279.43H31O3K251K2O3O379.5K2O3O379.5K2O3G379.5K2O3G379.5K2O3K1121H31O3K251K2O3G379.5K2O3G379.5K2O3G379.5K2O3K1121H31O3K251K2O3K114.66 <td>H22</td> <td>02</td> <td>К1</td> <td>111</td>	H22	02	К1	111
K1 O2 K2 94.48 H31 O3 H32 115 H31 O3 C2 95 H31 O3 K1 121 H31 O3 K2 51 H32 O3 K2 118 H32 O3 K2 118 H32 O3 K2 79 K2 O3 K2 79 K2 O3 K2 146.6 O3 O3 K1 91.4 K2 O3 K2 79 K2 O3 K2 146.6 O3 O3 K1 78.5 O3 O3 K1 78.5 O3 O3 K2 108.5 C1 S2 K1 103.1 C1 S2 K1 114.64 K1 S2 K2 79.43 H31 O3 K2 79.43 H31 O3 K2 95 H31 O3 K2 51 </td <td>H22</td> <td>02</td> <td>К2</td> <td>124</td>	H22	02	К2	124
H31 O3 H32 115 H31 O3 K2 95 H31 O3 K1 121 H31 O3 K2 51 H32 O3 K2 118 H32 O3 K2 118 H32 O3 K2 118 H32 O3 K2 79 K2 O3 K2 79 K2 O3 K1 91.4 K2 O3 K1 91.4 K2 O3 K2 146.6 O3 O3 K2 146.6 O3 O3 K2 108.5 C1 S2 K1 119.7 C1 S2 K1 103.1 C1 S2 K1 103.1 C1 S2 K1 114.64 K1 S2 K2 79.43 H31 O3 K2 51 H31 O3 K2 51 H31 O3 K2 51 </td <td>К1</td> <td>02</td> <td>К2</td> <td>94.48</td>	К1	02	К2	94.48
H31 O3 K2 95 H31 O3 K1 121 H31 O3 K2 51 H32 O3 K2 118 H32 O3 K2 118 H32 O3 K2 118 H32 O3 K2 79 K2 O3 K2 79 K2 O3 K1 91.4 K2 O3 K1 91.4 K2 O3 K2 146.6 O3 O3 K2 145.5 O3 O3 K2 108.5 C1 S2 K1 119.7 C1 S2 K1 103.1 C1 S2 K1 103.1 C1 S2 K2 79.43 H31 O3 K2 79.5 K1 S2 K2 79.43 H31 O3 K2 51 H31 O3 K2 51 H31 O3 K2 51 <td>H31</td> <td>03</td> <td>H32</td> <td>115</td>	H31	03	H32	115
H31O3O346H31O3K1121H31O3K251H32O3O3158(4)H32O3K1113H32O3K1113H32O3K279K2O3O379.5K2O3K191.4K2O3K178.5O3O3K178.5O3O3K278.7K1O3K2108.5C1S2K1103.1C1S2K2145.8K1S2K279.43H31O3K295H31O3K295H31O3K251K2O3K1121H31O3K295H31O3K251K2O3K1121H31O3K251K2O3K1121H31O3K251K2O3K191.4K2O3K191.4K2O3K191.4K2O3K278.7H32O3K278.7H32O3K178.5O3O3K278.7H32O3K1113H32O3K278.7H32O3K178.5O3O3K278.7H	H31	03	К2	95
H31O3K1121H31O3K251H32O3O3158(4)H32O3K1113H32O3K279K2O3O379.5K2O3K191.4K2O3K191.4K2O3K2146.6O3O3K278.7K1O3K2108.5C1S2K1119.7C1S2K1103.1C1S2K1114.64K1S2K279.43H31O3K295H31O3K251K2O3K1121H31O3K2146.6K1S2K2145.8K1S2K279.43H31O3K295H31O3K295H31O3K1121H31O3K251K2O3K1121H31O3K251K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K178.5O3O3K278.7H32O3K278.7H32O3K1113H32O3K278.7H32O3K1113H32O3K278.7	H31	03	03	46
H31O3K251H32O3O3158(4)H32O3K1113H32O3K279K2O3O379.5K2O3K2146.6O3O3K178.5O3O3K178.5O3O3K2108.5C1S2K1119.7C1S2K1103.1C1S2K1114.64K1S2K279.43H31O3K279.5K2O3K2145.8K1S2K1114.64K1S2K279.43H31O3K295H31O3K1121H31O3K1121H31O3K251K2O3K191.4K2O3K1121H31O3K251K2O3K251K2O3K1121H31O3K2158(4)O3O3K178.5O3O3K178.5O3O3K279K1O3K279K1O3K279K1O3K279K1O3K2121.5(3)S1C1S2121.5(3)S1C1S2117.3(2)	H31	03	K1	121
H32O3K2118H32O3O3158(4)H32O3K1113H32O3K279K2O3O379.5K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K278.7K1O3K2108.5C1S2K1103.1C1S2K1103.1C1S2K1114.64K1S2K279.43H31O3K295H31O3K251K2O3O379.5K2O3K1121H31O3K1121H31O3K1121H31O3K251K2O3K191.4K2O3K1121H31O3K1121H31O3K251K2O3K191.4K2O3K191.4K2O3K2158(4)O3O3K178.5O3O3K279K1O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	H31	03	К2	51
H32O3O3158(4)H32O3K1113H32O3K279K2O3O379.5K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K2108.5C1S2K1119.7C1S2K1103.1C1S2K1114.64K1S2K2145.8K1S2K2145.8K1S2K1114.64K1S2K279.43H31O3O346H31O3K251H31O3K251K2O3M32115H31O3K251K2O3K191.4K2O3K191.4K2O3K178.5O3O3K278.7H32O3K1113H32O3K278.7H32O3K1113H32O3K279K1O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2121.5(3)	H32	03	К2	118
H32O3K1113H32O3K279K2O3O379.5K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K278.7K1O3K2108.5C1S2K1119.7C1S2K1103.1C1S2K2145.8K1S2K279.43H31O3K295H31O3K251H31O3K251H31O3K1121H31O3K251K2O3K191.4K2O3K1118K2O3K191.4K2O3K251K2O3K1118K2O3K191.4K2O3K278.7K3O3K278.7K3O3K278.7K3O3K278.7K3O3K278.7K32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2121.5(3)S1C1S2121.5(3)	H32	03	03	158(4)
H32O3K279K2O3O379.5K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K278.7K1O3K2108.5C1S2K1119.7C1S2K1103.1C1S2K1114.64K1S2K2145.8K1S2K288.09K1S2K279.43H31O3K295H31O3K295H31O3K1121H31O3K251K2O3K1115H31O3K2118K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K278.7H32O3K1113H32O3K279K1O3K279K1O3K2108.5N1C1S2121.5(3)S1C1S2121.5(3)S1C1S2117.3(2)	H32	03	K1	113
K2 O3 O3 79.5 K2 O3 K1 91.4 K2 O3 K2 146.6 O3 O3 K1 78.5 O3 O3 K2 108.5 C1 S2 K1 119.7 C1 S2 K1 103.1 C1 S2 K1 103.1 C1 S2 K1 114.64 K1 S2 K1 114.64 K1 S2 K2 145.8 K1 S2 K2 145.8 K1 S2 K2 88.09 K1 S2 K2 79.43 H31 O3 K2 95 H31 O3 K1 121 H31 O3 K1 121 H31 O3 K2 51 K2 O3 O3 79.5 K2 O3 K1 91.4 K2 O3 K1 91.4 K2 O3 K1 <	H32	03	К2	79
K2 O3 K1 91.4 K2 O3 K2 146.6 O3 O3 K1 78.5 O3 O3 K2 78.7 K1 O3 K2 108.5 C1 S2 K1 119.7 C1 S2 K1 103.1 C1 S2 K2 145.8 K1 S2 K2 145.4 K1 S2 K2 145.4 K1 S2 K2 145.4 K1 S2 K2 145.4 K1 S2 K2 79.43 H31 O3 K2 95 H31 O3 K2 95 H31 O3 K2 115 H31 O3 K1 121 H31 O3 K2 51 K2 O3 H32 118 K2 O3 K1 91.4 K2 O3 K1 91.4 K2 O3 K1 9	К2	03	03	79.5
K2 O3 K2 146.6 O3 O3 K1 78.5 O3 O3 K2 78.7 K1 O3 K2 108.5 C1 S2 K1 119.7 C1 S2 K1 103.1 C1 S2 K1 103.1 C1 S2 K1 114.64 K1 S2 K2 145.8 K1 S2 K2 145.4 K1 S2 K2 146.4 K1 S2 K2 9.43 H31 O3 K2 95 H31 O3 K2 95 H31 O3 K2 115 H31 O3 K2 51 K2 O3 M32 118 K2 O3 K1 91.4 K2 O3 K1 91.4 K2 O3 K1 91.4 K2 O3 K1 78.5 O3 O3 K1 7	К2	03	K1	91.4
O3 O3 K1 78.5 O3 O3 K2 78.7 K1 O3 K2 108.5 C1 S2 K1 119.7 C1 S2 K1 103.1 C1 S2 K1 103.1 C1 S2 K2 145.8 K1 S2 K1 114.64 K1 S2 K2 88.09 K1 S2 K2 79.43 H31 O3 K2 95 H31 O3 K2 95 H31 O3 K1 121 H31 O3 K2 51 K2 O3 O3 79.5 K2 O3 K1 91.4 K2 O3 K1 78.5 O3 O3 K2 146.6 O3 O3 K1 78.5 O3 O3 K2 78.7	К2	03	K2	146.6
O3 O3 K2 78.7 K1 O3 K2 108.5 C1 S2 K1 119.7 C1 S2 K1 103.1 C1 S2 K1 103.1 C1 S2 K2 145.8 K1 S2 K2 145.4 K1 S2 K2 145.4 K1 S2 K2 88.09 K1 S2 K2 79.43 H31 O3 K2 95 H31 O3 K1 121 H31 O3 K1 121 H31 O3 K2 51 K2 O3 O3 79.5 K2 O3 K1 91.4 K2 O3 K2 146.6 O3 O3 K1 91.4 K2 O3 K1 78.5 O3 O3 K2 78.7	03	03	K1	78.5
K1O3K2108.5C1S2K1119.7C1S2K1103.1C1S2K2145.8K1S2K1114.64K1S2K288.09K1S2K279.43H31O3K295H31O3O346H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K278.7H32O3K1113H32O3K278.7H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	03	03	K2	78.7
C1S2K1119.7C1S2K1103.1C1S2K2145.8K1S2K1114.64K1S2K288.09K1S2K279.43H31O3K295H31O3O346H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K178.5O3O3K1113H32O3K278.7H32O3K279K1O3K279K1O3K2108.5N1C1S2121.1(3)N1C1S2121.5(3)S1C1S2117.3(2)	K1	03	K2	108.5
C1S2K1103.1C1S2K2145.8K1S2K1114.64K1S2K288.09K1S2K279.43H31O3K295H31O3O346H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K191.4K2O3K2146.6O3O3K278.7H32O3K1113H32O3K279K1O3K279K1O3K2108.5N1C1S2121.5(3)S1C1S2117.3(2)	C1	S2	K1	119.7
C1S2K2145.8K1S2K1114.64K1S2K288.09K1S2K279.43H31O3K295H31O3O346H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K191.4K2O3K178.5O3O3K1113H32O3K1113H32O3K279K1O3K279K1O3K2108.5N1C1S2121.5(3)S1C1S2117.3(2)	C1	S2	K1	103.1
K1S2K1114.64K1S2K288.09K1S2K279.43H31O3K295H31O3O346H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K178.5O3O3K1113H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	C1	S2	К2	145.8
K1S2K288.09K1S2K279.43H31O3K295H31O3O346H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K2146.6O3O3K2158(4)O3O3K178.5O3O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	K1	S2	K1	114.64
K1S2K279.43H31O3K295H31O3O346H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K178.5O3O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	K1	S2	K2	88.09
H31O3K295H31O3O346H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K2146.6O3O3H32158(4)O3O3K178.5O3O3K1113H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	K1	S2	К2	79.43
H31O3O346H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K2146.6O3O3K178.5O3O3K178.5O3O3K278.7H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	H31	03	К2	95
H31O3H32115H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K2146.6O3O3H32158(4)O3O3K178.5O3O3K278.7H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	H31	03	03	46
H31O3K1121H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K2146.6O3O3H32158(4)O3O3K178.5O3O3K278.7H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	H31	03	H32	115
H31O3K251K2O3O379.5K2O3H32118K2O3K191.4K2O3K2146.6O3O3H32158(4)O3O3K178.5O3O3K278.7H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2117.3(2)	H31	03	K1	121
K2 O3 O3 79.5 K2 O3 H32 118 K2 O3 K1 91.4 K2 O3 K2 146.6 O3 O3 H32 158(4) O3 O3 K1 78.5 O3 O3 K2 78.7 H32 O3 K1 113 H32 O3 K2 79 K1 O3 K2 108.5 N1 C1 S1 121.1(3) N1 C1 S2 121.5(3) S1 C1 S2 117.3(2)	H31	03	К2	51
K2 O3 H32 118 K2 O3 K1 91.4 K2 O3 K2 146.6 O3 O3 H32 158(4) O3 O3 K1 78.5 O3 O3 K2 78.7 H32 O3 K1 113 H32 O3 K2 79 K1 O3 K2 108.5 N1 C1 S1 121.1(3) N1 C1 S2 121.5(3) S1 C1 S2 117.3(2)	К2	03	03	79.5
K2O3K191.4K2O3K2146.6O3O3H32158(4)O3O3K178.5O3O3K278.7H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2117.3(2)	К2	03	H32	118
K2O3K2146.6O3O3H32158(4)O3O3K178.5O3O3K278.7H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2117.3(2)	К2	03	K1	91.4
O3O3H32158(4)O3O3K178.5O3O3K278.7H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2117.3(2)	К2	03	К2	146.6
O3 O3 K1 78.5 O3 O3 K2 78.7 H32 O3 K1 113 H32 O3 K2 79 K1 O3 K2 108.5 N1 C1 S1 121.1(3) N1 C1 S2 121.5(3) S1 C1 S2 117.3(2)	03	03	H32	158(4)
O3O3K278.7H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2117.3(2)	03	03	K1	78.5
H32O3K1113H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2117.3(2)	03	03	К2	78.7
H32O3K279K1O3K2108.5N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2117.3(2)	H32	03	К1	113
K1O3K2108.5N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2117.3(2)	H32	03	К2	79
N1C1S1121.1(3)N1C1S2121.5(3)S1C1S2117.3(2)	К1	03	К2	108.5
N1C1S2121.5(3)S1C1S2117.3(2)	N1	C1	S1	121.1(3)
<u>S1 C1 S2 117.3(2)</u>	N1	C1	S2	121.5(3)
	S1	C1	S2	117.3(2)

H2	C2	C3	107.3
H2	C2	C4	107.4
H2	C2	N1	107.4
C3	C2	C4	112.1(3)
C3	C2	N1	111.8(3)
C4	C2	N1	110.6(3)
C2	C3	H3A	109.5
C2	C3	H3B	109.4
C2	C3	H3C	109.5
H3A	C3	H3B	109.5
H3A	C3	H3C	109.4
H3B	C3	H3C	109.5
C2	C4	H4A	109.5
C2	C4	H4B	109.4
C2	C4	H4C	109.5
H4A	C4	H4B	109.4
H4A	C4	H4C	109.5
H4B	C4	H4C	109.5
H5	C5	C6	105.1
H5	C5	C7	105.1
H5	C5	N1	105.1
C6	C5	C7	113.2(3)
C6	C5	N1	113.3(3)
C7	C5	N1	114.0(3)
C5	C6	H6A	109.5
C5	C6	H6B	109.5
C5	C6	H6C	109.4
H6A	C6	H6B	109.4
H6A	C6	H6C	109.5
H6B	C6	H6C	109.5
C5	C7	H7A	109.5
C5	C7	H7B	109.4
C5	C7	H7C	109.5
H7A	C7	H7B	109.5
H7A	C7	H7C	109.5
H7B	C7	H7C	109.5
C1	N1	C2	121.0(3)
C1	N1	C5	124.9(3)
C2	N1	C5	114.1(3)
K1	02	K2	94.48
K1	02	H21	104
K1	02	H22	111
К2	02	H21	107
К2	02	H22	124

H21	02	H22	114(4)
K1	S2	C1	119.7
K1	S2	K1	114.64
K1	S2	K2	88.09
C1	S2	K1	103.1
C1	S2	K2	145.8
K1	S2	К2	79.43
03	K1	03	23.1
03	K1	S2	80.7
03	K1	S2	92.3
03	K1	S2	92.3
03	K1	S2	80.7
S2	K1	S2	60.69
S2	K1	S2	60.69
03	K2	03	22.7
S2	К2	S2	64.02
S2	K2	03	67.7
S2	К2	03	80.2
S2	К2	03	80.2
S2	K2	03	67.7
03	K2	03	22.7
K2	03	03	78.7
K1	03	K2	108.5
K1	03	03	78.5
K2	03	03	78.7
К2	03	03	78.7
K1	03	K2	108.5
K1	03	03	78.5
К2	03	03	78.7
К2	S2	K1	79.43
K2	S2	K1	79.43

Atom1	Atom2	length
C1	N1	1 /19(8)
C1	S1	1.413(8)
C1	52	1.005(5)
C2	ы2	0.950
C2	N1	1 354(6)
C2		1.334(0)
C2		1.232(8)
C3		1 252(8)
C3	N2	1.395(8)
C1	NZ HЛ	0.950
C4	N1	1 399(6)
C5	N/	1.355(0)
C5	C2	1.410(7)
C5	53	1.703(5)
C5	54 ЦС	0.051
C6		1 202(7)
C6	N/	1.302(7)
C7		1.338(8)
C7	(1) (2)	1 327(9)
C7	NB	1.327(3)
C7		0.950
C8	N/	1 391(6)
C0 K1	N2	1.331(0)
KI K1		2.831(5)
KI K1	NJ S1	2.814(0)
KI K1	51	3.300(3)
K1	52	3.238(3) 3.594(2)
K1	52	3.267(3)
K1	22	3.620(3)
KI K1	53	3.020(3)
K1 K2	N2	2.343(5)
K2	ND	2.805(5)
KZ K2	NZ C1	2.880(3)
κ <u>z</u>	51	3.310(3)
κ <u>2</u> κ2	32 57	3.230(3) 2.500(2)
κz ν 2	32 52	(כ) כעניכ גרעניכ
κ <u>2</u> κ2	33 C2	3.241(3) 2 516(2)
κz κ2	33 64	3.340(3)
ĸZ	54	3.366(2)

Table S5. Bond lengths and angles for potassium imidazoledithiocarbamate (K[ImDTC]).

N2	K2	2.886(5)
S1	K1	3.306(3)
S1	K2	3.316(3)
S2	K1	3.298(3)
S2	K1	3.594(2)
S2	K2	3.296(3)
S2	K2	3.509(3)
S3	K1	3.267(3)
S3	K1	3.620(3)
S3	K2	3.247(3)
S3	K2	3.546(3)
S4	K1	3.343(3)
S4	K2	3.366(2)
K1	S2	3.594(2)
K1	S2	3.298(3)
K1	S3	3.620(3)
K1	S3	3.267(3)
K2	S1	3.316(3)
K2	S2	3.296(3)
K2	S3	3.546(3)
K2	S2	3.509(3)
K2	S2	3.296(3)
K2	S3	3.247(3)
		_

Atom1	Atom2	Atom3	Angle
N1	C1	S1	118.8(4)
N1	C1	S2	116.2(4)
S1	C1	S2	125.0(3)
H2	C2	N1	123.1
H2	C2	N2	123.1
N1	C2	N2	113.8(5)
H3	C3	C4	124.7
H3	C3	N2	124.6
C4	C3	N2	110.7(5)
C3	C4	H4	127.3
C3	C4	N1	105.4(5)
H4	C4	N1	127.3
N4	C5	S3	116.7(4)
N4	C5	S4	118.1(4)
S3	C5	S4	125.2(3)
H6	C6	N3	123.2

H6	C6	N4	123.3
N3	C6	N4	113.4(5)
H7	C7	C8	124.8
H7	C7	N3	124.7
C8	C7	N3	110.4(5)
C7	C8	H8	126.5
C7	C8	N4	107.0(5)
H8	C8	N4	126.5
N2	K1	N3	136.8(1)
N2	K1	S1	75.9(1)
N2	K1	S2	104.8(1)
N2	K1	S2	155.7(1)
N2	K1	S3	86.4(1)
N2	K1	S3	68.8(1)
N2	K1	S4	76.3(1)
N3	K1	S1	77.2(1)
N3	K1	S2	85.2(1)
N3	K1	S2	67.3(1)
N3	K1	S3	103.9(1)
N3	K1	S3	154.2(1)
N3	K1	S4	76.9(1)
S1	K1	S2	53.80(4)
S1	K1	S2	120.74(5)
S1	K1	S3	153.04(6)
S1	K1	S3	113.35(5)
S1	K1	S4	101.68(5)
S2	K1	S2	76.76(4)
S2	K1	S3	152.60(6)
S2	K1	S3	83.25(4)
S2	K1	S4	152.77(6)
S2	K1	S3	82.98(5)
S2	K1	S3	87.59(4)
S2	K1	S4	113.64(5)
S3	K1	S3	77.61(4)
S3	K1	S4	53.70(4)
S3	K1	S4	121.00(5)
N3	K2	N2	136.3(1)
N3	K2	S1	77.7(1)
N3	K2	S2	86.4(1)
N3	K2	S2	68.1(1)
N3	K2	S3	103.3(1)

N3	К2	S3	154.2(1)
N3	К2	S4	75.9(1)
N2	К2	S1	75.1(1)
N2	К2	S2	103.6(1)
N2	К2	S2	155.5(1)
N2	К2	S3	86.4(1)
N2	К2	S3	69.4(1)
N2	К2	S4	76.5(1)
S1	К2	S2	53.73(4)
S1	K2	S2	120.40(5)
S1	K2	S3	151.94(6)
S1	K2	S3	115.04(5)
S1	K2	S4	100.80(5)
S2	K2	S2	76.24(4)
S2	K2	S3	153.61(6)
S2	K2	S3	84.44(4)
S2	K2	S4	152.12(6)
S2	К2	S3	84.61(5)
S2	К2	S3	86.30(4)
S2	К2	S4	115.27(5)
S3	К2	S3	76.25(4)
S3	К2	S4	53.65(4)
S3	К2	S4	120.26(5)
C1	N1	C2	127.5(5)
C1	N1	C4	126.8(4)
C2	N1	C4	105.7(4)
C2	N2	C3	104.4(5)
C2	N2	K1	113.6(4)
C2	N2	K2	112.6(4)
C3	N2	K1	125.1(4)
C3	N2	K2	119.2(4)
K1	N2	K2	81.0(1)
C6	N3	C7	104.0(5)
C6	N3	K1	116.7(4)
C6	N3	K2	113.3(4)
C7	N3	K1	122.6(4)
C7	N3	K2	118.0(4)
K1	N3	K2	81.7(1)
C5	N4	C6	126.2(5)
C5	N4	C8	128.7(5)
C6	N4	C8	105.1(4)

C1	S1	K1	85.4(2)
C1	S1	К2	85.4(2)
K1	S1	К2	68.20(4)
C1	S2	K1	85.1(2)
C1	S2	K1	128.6(2)
C1	S2	К2	85.4(2)
C1	S2	К2	128.9(2)
K1	S2	K1	103.24(5)
K1	S2	K2	68.54(4)
K1	S2	K2	145.35(6)
K1	S2	K2	145.18(5)
K1	S2	K2	63.00(4)
K2	S2	K2	103.76(5)
C5	S3	K1	85.7(2)
C5	S3	K1	127.2(2)
C5	S3	K2	87.6(2)
C5	S3	K2	129.1(2)
K1	S3	K1	102.39(5)
K1	S3	К2	69.50(4)
K1	S3	К2	145.03(6)
K1	S3	К2	144.47(5)
K1	S3	К2	62.41(4)
К2	S3	К2	103.75(5)
C5	S4	K1	83.8(2)
C5	S4	К2	84.3(2)
K1	S4	К2	67.19(4)
S3	K1	S4	53.70(4)
S1	K1	S2	53.80(4)
S3	K1	S2	87.59(4)
S3	K1	S2	83.25(4)
S2	K1	S2	76.76(4)
S2	K1	S3	87.59(4)
S2	K1	S3	82.98(5)
S3	K1	S3	77.61(4)
S3	K2	S4	53.65(4)
N2	K2	S1	75.1(1)
N2	K2	S2	103.6(1)
N2	K2	S3	69.4(1)
S1	K2	S2	53.73(4)
S1	K2	S3	115.04(5)
S2	K2	S3	84.44(4)

S1	K2	S2	53.73(4)
S3	K2	S2	86.30(4)
S3	K2	S2	84.44(4)
S2	K2	S2	76.24(4)
S2	K2	S3	84.61(5)
K1	S1	K2	68.20(4)
K2	S2	K2	103.76(5)
K1	S2	K1	103.24(5)
K1	S2	K2	68.54(4)
K1	S2	K2	145.18(5)
K1	S2	K2	63.00(4)
K1	S2	K1	103.24(5)
K1	S2	K2	145.18(5)
K2	S2	K1	145.35(6)
K2	S2	K2	103.76(5)
K1	S2	K2	68.54(4)
K1	S3	K2	69.50(4)
K1	S3	K1	102.39(5)
K2	S3	K1	144.47(5)
K1	S3	K1	102.39(5)
K1	S3	K2	62.41(4)
K1	S3	K2	144.47(5)
K1	S3	K2	145.03(6)
K1	S3	K2	69.50(4)
K2	S3	K2	103.75(5)
K1	S4	K2	67.19(4)

Atom1	Atom2	Length (Å)
C1	N1	1.408(6)
C1	S1	1.712(4)
C1	S2	1.685(5)
C2	H2	0.931
C2	C3	1.347(6)
C2	N1	1.413(6)
C3	H3	0.930
C3	C4	1.432(8)
C4	H4	0.930
C4	C5	1.359(7)
C5	H5	0.930
C5	N1	1.415(6)
C6	К2	3.307(6)
C6	N2	1.404(7)
C6	S3	1.712(5)
C6	S4	1.693(5)
C7	H7	0.930
C7	C8	1.354(7)
C7	N2	1.403(6)
C8	H8	0.930
C8	C9	1.424(6)
C9	H9	0.930
C9	C10	1.354(7)
C10	H10	0.930
C10	N2	1.394(6)
K1	S1	3.161(4)
K1	S2	3.350(5)
K1	S2	3.213(4)
K1	S3	3.403(5)
K1	S3	3.240(5)
K1	S4	3.264(4)
K2	S2	3.153(5)
K2	S3	3.499(5)
К2	S4	3.156(3)
K2	S1	3.170(4)
К2	S1	3.220(4)
К2	S3	3.336(5)
S1	К2	3.170(4)
S1	К2	3.220(4)
S2	K1	3.213(4)
S3	K1	3.403(5)
S3	K1	3.240(5)

Table S6. Bond lengths and angles for potassium pyrroledithiocarbamate (K[PyrDTC]).

S3	К2	3.336(5)	
S4	K1	3.264(4)	
K1	S2	3.350(5)	
К2	S3	3.499(5)	
К2	S4	3.156(3)	
К2	S1	3.170(4)	
К2	S3	3.336(5)	
Atom1	Atom2	Atom3	Angle (°)
N1	C1	S1	116.8(3)
N1	C1	S2	119.8(3)
S1	C1	S2	123.4(3)
H2	C2	C3	126.1
H2	C2	N1	126.1
C3	C2	N1	107.8(4)
C2	C3	H3	125.4
C2	C3	C4	109.2(4)
H3	C3	C4	125.4
C3	C4	H4	126.3
C3	C4	C5	107.3(5)
H4	C4	C5	126.3
C4	C5	H5	125.9
C4	C5	N1	108.3(4)
H5	C5	N1	125.8
K2	C6	N2	121.8(3)
К2	C6	S3	81.8(2)
К2	C6	S4	69.9(1)
N2	C6	S3	117.8(3)
N2	C6	S4	118.4(3)
S3	C6	S4	123.7(3)
H7	C7	C8	125.9
H7	C7	N2	125.9
C8	C7	N2	108.1(4)
C7	C8	H8	126.0
C7	C8	C9	108.0(4)
H8	C8	C9	126.0
C8	C9	H9	126.1
C8	C9	C10	107.8(4)
H9	C9	C10	126.0
C9	C10	H10	125.8
C9	C10	N2	108.5(4)
H10	C10	N2	125.8
S1	K1	S2	54.60(4)
S1	K1	S2	81.92(4)
S1	K1	S3	66.27(4)

S1	K1	S3	126.38(5)
S1	К1	S4	174.36(5)
S2	К1	S2	81.11(4)
S2	К1	S3	109.18(4)
S2	К1	S3	88.24(4)
S2	К1	S4	121.45(4)
S2	K1	S3	126.83(5)
S2	К1	S3	133.96(5)
S2	K1	S4	93.62(4)
S3	К1	S3	99.02(4)
S3	К1	S4	119.34(4)
S3	К1	S4	54.99(3)
C6	К2	S2	73.43(8)
C6	К2	S3	28.97(8)
C6	К2	S4	30.25(8)
C6	К2	S1	120.97(9)
C6	К2	S1	151.23(9)
C6	К2	S3	126.50(9)
S2	К2	S3	71.10(4)
S2	К2	S4	99.57(4)
S2	К2	S1	162.04(5)
S2	К2	S1	81.68(4)
S2	К2	S3	89.95(4)
S3	К2	S4	53.33(3)
S3	К2	S1	115.58(4)
S3	К2	S1	148.65(5)
S3	К2	S3	97.58(4)
S4	К2	S1	97.42(4)
S4	К2	S1	150.37(5)
S4	К2	S3	142.71(5)
S1	К2	S1	86.46(4)
S1	К2	S3	72.90(4)
S1	К2	S3	66.46(4)
C1	N1	C2	127.3(4)
C1	N1	C5	125.2(4)
C2	N1	C5	107.4(4)
C6	N2	C7	126.4(4)
C6	N2	C10	126.0(4)
C7	N2	C10	107.6(4)
C1	S1	K1	93.5(2)
C1	S1	K2	96.9(2)
C1	S1	K2	92.4(2)
K1	S1	K2	129.21(5)
K1	S1	K2	103.60(5)

К2	S1	K2	125.33(5)
C1	S2	K1	87.6(2)
C1	S2	K2	123.5(2)
C1	S2	K1	92.0(2)
K1	S2	K2	90.71(4)
K1	S2	K1	98.89(4)
К2	S2	K1	143.69(5)
C6	S3	K2	69.3(2)
C6	S3	K1	111.4(2)
C6	S3	K1	88.7(2)
C6	S3	K2	151.5(2)
К2	S3	K1	171.34(5)
К2	S3	K1	80.78(4)
К2	S3	K2	82.42(4)
K1	S3	K1	107.80(4)
K1	S3	K2	96.18(4)
K1	S3	K2	89.48(4)
C6	S4	K2	79.8(2)
C6	S4	K1	88.3(2)
К2	S4	K1	85.81(4)
S3	K1	S4	54.99(3)
S2	K1	S2	81.11(4)
S3	К2	S3	97.58(4)
S3	К2	S4	142.71(5)
S3	К2	S4	53.33(3)
S1	К2	S1	86.46(4)
S1	K2	S3	66.46(4)
S1	K2	S3	72.90(4)
К2	S1	K2	125.33(5)
К1	S2	K1	98.89(4)
К1	S3	K2	96.18(4)
К1	S3	K2	89.48(4)
К1	S3	K2	80.78(4)
К2	S3	K2	82.42(4)
K1	S4	K2	85.81(4)

DTC anion	N-CS ₂ (Å)	C _(R1) -N-C _(R2) (°)	S-C ₁ -S (°)
ImDTC-	1.418 (1.435; <mark>1.398</mark>)	105.4 (105.8; <mark>105.8</mark>)	125.1 (125.6; <mark>124.3</mark>)
PyrDTC-	1.406 (1.421; <mark>1.384</mark>)	107.5 (107.8; <mark>107.9</mark>)	123.6 (124.2; <mark>123.0</mark>)
PDTC-	1.326 (1.349; <mark>1.331</mark>)	111.0 (111.9; <mark>111.4</mark>)	122.1 (122.3; <mark>121.7</mark>)
MorDTC-	1.341 (1.364; <mark>1.341</mark>)	112.1 (111.4; <mark>112.1</mark>)	119.8 (120.7; <mark>119.9</mark>)
DIDTC-	1.345 (1.362; 1.339)	113.4 (113.5; <mark>114.3</mark>)	118.1 (118.1; <mark>117.5</mark>)
MeDTC-	- (1.358; 1.339)	- (117.4; 118.5)	- (121.9; <mark>121.3</mark>)
DMDTC-	- (1.359; 1.338)	- (113.9; 114.9)	- (120.5; 119.9)

Table S7. Experimental (black) and calculated (blue) important bond and angles of the DTC⁻ anions. The second value in the parentheses (red) is the calculated value for the conjugate acids DTCH.

Table S8. Selected chemical and spectroscopic data relevant to the dithiocarbamato anions.

DTC	pK _a	pK _a	λ_1 , nm	λ_2 , nm	λ_3 , nm
	$(CA)^{a}$	(NH)*	$(\epsilon, M^{-1}cm^{-1})$	$(\epsilon, M^{-1}cm^{-1})$	$(\varepsilon, M^{-1}cm^{-1})$
DIDTC	11.07 ^b	36 ^c	261 (1.15 x 10 ⁴)	286 (1.1 x 10 ⁴)	-
MorDTC ⁻	8.5 ^e	-	263 (1.50 x 10 ⁴)	286 (1.40 x 10 ⁴)	-
PDTC ⁻	11.27 ^b	44 ^f	253 (1.40 x 10 ⁴)	277 (1.30 x 10 ⁴)	-
PyrDTC ⁻	-2	$23^{f}(17.5)$	-	297 (1.29 x 10 ⁴)	343 (6.30 x 10 ³)
ImDTC ⁻	7.0 ^g	$18.6^{l}(14.5)^{g}$	255 (6.36 x 10 ³)	280 (9.38 x 10 ³)	353 (1.24 x 10 ⁴)

^aConjugate acid of the amine; water, ^bref.12; ^cref.13; ^d value for diethylamine; ^eref.9; ^fref.14; ^gref.15; *Values measured in DMSO and water in parentheses. IDTC crystalline structure was solved as a potassium complex formed by two asymmetric unity of the dithiocarbamate.

Table S9. Calculated E_{rot} for rotation around DTC C-N bonds and HOMO orbital composition of several deprotonated (DTC⁻) and protonated (DTCH) aliphatic DTCs at the ground state (GS) and rotation transition state (TS_{rot}). DFT calculations at a PCM(water)/B3LYP/6-31+G(d,p) level of theory.

DTC	N* ^a	N-C (Å)	N-C (Å)	HOMO (%)(GS)	HOMO (%) (TS)	E _{rot}
		(GS)	(TS)			(kJ/mol)
DIDTC ⁻	14.68	1 363	1 /31	$CS_{1}(95) N(0)$	CS- (87) N (10)	70.6
DIDIC	14.00	1.505	1.451	$CS_2(95) IV(0)$	$CS_2(87) IV(10)$	70.0
DIDTCH		1.339	1.408	CS ₂ (98) N (0)	CS ₂ (50) N (38)	75.6
MorDTC ⁻	15.62	1.364	1.453	CS ₂ (96) N (0)	CS ₂ (94) N (4)	60.2
MorDTCH		1.341	1.454	CS ₂ (100) N (0)	CS ₂ (82) N (15)	67.8
PDTC ⁻	17.21	1.349	1.444	CS ₂ (95) N (0)	CS ₂ (95) N (3)	83.4
PDTCH		1.331	1.421	CS ₂ (99) N (0)	CS ₂ (83) N (15)	92.4

*Mayr nucleophilicity parameter for the secondary amine (ref.50); ^avalue for diethylamine.

Table S10. Calculated E_{rot} for rotation around DTC C-N bonds and HOMO orbital composition of several deprotonated (DTC⁻) and protonated (DTCH) aromatic DTCs at the ground state (GS) and rotation transition state (TS_{rot}). DFT calculations at a PCM(water)/B3LYP/6-31+G(d,p) level of theory.

DTC	N-C (Å) (GS)	N-C (Å) (TS _{rot})	HOMO (%) (GS)	HOMO (%) (TS _{rot})	E _{rot} (kJ/mol)
PyrDTC ⁻	1.421	1.455	CS ₂ (94); N (0)	CS ₂ (96); N (1)	29.48
PyrDTCH	1.384	1.426	CS ₂ (95); N (0)	CS ₂ (2); N (0)	37.9
ImDTC ⁻	1.435	1.462	CS ₂ (96); N (1)	CS ₂ (97); N (1)	22.3
ImDTCH (SH) ^a	1.398	1.434	CS ₂ (94); N (0)	CS ₂ (8); N (4)	25.6
ImDTCH (NH) ^b	1.483	1.492	CS ₂ (94); N (2)	CS ₂ (98); N (1)	15.4

^a S protonated. ^b N protonated

Table S11. DFT calculated Cartesian coordinates (x, y, z) of anions DTC-, their conjugate acids DTCH and rotational transition states (TS_{rot}). (PCM-model, water) - B3LYP/6-31+G(d,p). The transition state geometries were optimized with the QST3 keyword using three geometries: 1) the DTCs and DTCHs initial geometries (syn), 2) the higher energy geometry (TS guess) taken from the potential energy surface (PES) generated by scanner the dihedral angle (see Figure S14), 3) a lower energy geometry (no imaginary frequency) from the potential energy surface (PES).

$\begin{array}{llllllllllllllllllllllllllllllllllll$
N0.28121800-0.01644900-0.00005200N-0.28129900-0.01630400-0.00007200C0.726810001.414859000.00018300C-0.725979001.415380000.00011600H1.814904001.337029000.00007800H-1.814110001.337944000.00023600C1.41214200-0.99264500-0.00017600C-1.41242800-0.99227100-0.00004400H0.93095700-1.96895700-0.00039200H-0.93131200-1.96863700-0.00038100C2.25607800-0.895467001.27862900C-2.25658900-0.89423300-1.27857400H1.62766100-1.003225002.16844700H-1.62833100-1.00187200-2.16850700H2.99269500-1.706102001.28373600H-2.99344100-1.70466500-1.28378300H2.807438000.047728001.35792800H-2.807612000.04920600-1.35734500C2.25622100-0.89497300-1.27884700C-2.25620000-0.894997001.27882100H2.99284300-1.70560200-1.28417800H-2.99273600-1.705708001.28400200
C0.726810001.414859000.00018300C-0.725979001.415380000.00011600H1.814904001.337029000.00007800H-1.814110001.337944000.00023600C1.41214200-0.99264500-0.00017600C-1.41242800-0.99227100-0.0004400H0.93095700-1.96895700-0.00039200H-0.93131200-1.96863700-0.00038100C2.25607800-0.895467001.27862900C-2.25658900-0.89423300-1.27857400H1.62766100-1.003225002.16844700H-1.62833100-1.00187200-2.16850700H2.99269500-1.706102001.28373600H-2.99344100-1.70466500-1.28378300H2.807438000.047728001.35792800H-2.807612000.04920600-1.35734500C2.25622100-0.89497300-1.27884700C-2.25620000-0.894997001.27882100H2.99284300-1.70560200-1.28417800H-2.99273600-1.705708001.28400200
H1.814904001.337029000.00007800H-1.814110001.337944000.00023600C1.41214200-0.99264500-0.00017600C-1.41242800-0.99227100-0.00004400H0.93095700-1.96895700-0.00039200H-0.93131200-1.96863700-0.00038100C2.25607800-0.895467001.27862900C-2.25658900-0.89423300-1.27857400H1.62766100-1.003225002.16844700H-1.62833100-1.00187200-2.16850700H2.99269500-1.706102001.28373600H-2.99344100-1.70466500-1.28378300H2.807438000.047728001.35792800H-2.807612000.04920600-1.35734500C2.25622100-0.89497300-1.27884700C-2.25620000-0.894997001.27882100H2.99284300-1.70560200-1.28417800H-2.99273600-1.705708001.28400200
C1.41214200-0.99264500-0.00017600C-1.41242800-0.99227100-0.00004400H0.93095700-1.96895700-0.00039200H-0.93131200-1.96863700-0.00038100C2.25607800-0.895467001.27862900C-2.25658900-0.89423300-1.27857400H1.62766100-1.003225002.16844700H-1.62833100-1.00187200-2.16850700H2.99269500-1.706102001.28373600H-2.99344100-1.70466500-1.28378300H2.807438000.047728001.35792800H-2.807612000.04920600-1.35734500C2.25622100-0.89497300-1.27884700C-2.25620000-0.894997001.27882100H2.99284300-1.70560200-1.28417800H-2.99273600-1.705708001.28400200
H0.93095700-1.96895700-0.00039200H-0.93131200-1.96863700-0.00038100C2.25607800-0.895467001.27862900C-2.25658900-0.89423300-1.27857400H1.62766100-1.003225002.16844700H-1.62833100-1.00187200-2.16850700H2.99269500-1.706102001.28373600H-2.99344100-1.70466500-1.28378300H2.807438000.047728001.35792800H-2.807612000.04920600-1.35734500C2.25622100-0.89497300-1.27884700C-2.25620000-0.894997001.27882100H2.99284300-1.70560200-1.28417800H-2.99273600-1.705708001.28400200
C2.25607800-0.895467001.27862900C-2.25658900-0.89423300-1.27857400H1.62766100-1.003225002.16844700H-1.62833100-1.00187200-2.16850700H2.99269500-1.706102001.28373600H-2.99344100-1.70466500-1.28378300H2.807438000.047728001.35792800H-2.807612000.04920600-1.35734500C2.25622100-0.89497300-1.27884700C-2.25620000-0.894997001.27882100H2.99284300-1.70560200-1.28417800H-2.99273600-1.705708001.28400200
H1.62766100-1.003225002.16844700H-1.62833100-1.00187200-2.16850700H2.99269500-1.706102001.28373600H-2.99344100-1.70466500-1.28378300H2.807438000.047728001.35792800H-2.807612000.04920600-1.35734500C2.25622100-0.89497300-1.27884700C-2.25620000-0.894997001.27882100H2.99284300-1.70560200-1.28417800H-2.99273600-1.705708001.28400200
H2.99269500-1.706102001.28373600H-2.99344100-1.70466500-1.28378300H2.807438000.047728001.35792800H-2.807612000.04920600-1.35734500C2.25622100-0.89497300-1.27884700C-2.25620000-0.894997001.27882100H2.99284300-1.70560200-1.28417800H-2.99273600-1.705708001.28400200
H2.807438000.047728001.35792800H-2.807612000.04920600-1.35734500C2.25622100-0.89497300-1.27884700C-2.25620000-0.894997001.27882100H2.99284300-1.70560200-1.28417800H-2.99273600-1.705708001.28400200
C 2.25622100 -0.89497300 -1.27884700 C -2.25620000 -0.89499700 1.27882100 H 2.99284300 -1.70560200 -1.28417800 H -2.99273600 -1.70570800 1.28400200
H 2.99284300 -1.70560200 -1.28417800 H -2.99273600 -1.70570800 1.28400200
H 1.62790400 -1.00239800 -2.16877700 H -1.62759800 -1.00274100 2.16850100
H 2.80758600 0.04825500 -1.35772700 H -2.80758600 0.04816300 1.35817600
C 0.37127500 2.18000000 1.28412200 C -0.37061800 2.18083700 -1.28367400
H 0.67236300 1.61172000 2.16995300 H -0.67200400 1.61280800 -2.16955900
H 0.91932200 3.12933600 1.28999600 H -0.91857400 3.13023100 -1.28916700
H -0.69651700 2.38926200 1.34819200 H 0.69718400 2.38989900 -1.34795700
C 0.37104900 2.18048600 -1.28340400 C -0.37010200 2.18053700 1.28394400
H 0.67197600 1.61254200 -2.16950400 H -0.67160400 1.61254500 2.16980500
H -0.69675400 2.38977600 -1.34720400 H 0.69781000 2.38912700 1.34798200
H 0.91909800 3.12982300 -1.28901800 H -0.91757900 3.13020600 1.28965600
C -1.01408500 -0.44039400 -0.00012500 C 1.01382400 -0.44075800 -0.00039400
S -1.38745100 -2.15628900 -0.00024600 S 2.34016700 0.68622300 0.00004800
S -2.33985800 0.68721200 0.00003000 S 1.38640400 -2.15680700 -0.00019400
Table 11c. DIDTC- (TSrot geometry); Table 11d. DIDTCH (Syn geometry);
E(B3LYP) = -1126.46782243 a.u. $E(B3LYP) = -1126.94931321 a.u.$
N 0.31355500 -0.06182500 -0.28008600 N 0.30455200 -0.00610600 -0.00009700
C 0.85729700 1.30918700 -0.35555500 C 0.88385400 1.38378900 0.00019500
H 1.91121900 1.16563700 -0.61699600 H 1.95847700 1.20240500 0.00016300
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
H 0.58070100 -2.05657100 0.14054700 H 0.77882700 -2.04247000 -0.00057800
C 2.06275300 -1.03905900 1.30155000 C 2.17273400 -1.08569300 1.28114000
H 1.41525500 -0.84779400 2.16098200 H 1.53616000 -1.12542200 2.16960000
H = 2.82222300 - 1.96088100 - 1.48916100 H = 2.82222300 - 1.96630200 - 1.28591700
H = 2.78765100 - 0.22112100 + 1.22110800 + 2.81471600 - 0.20263900 + 1.34971100 + 0.20263900 + 1.34971100 + 0.20263900 + 0.2026900 +
C = 2.14322000 - 1.48265100 - 1.19465000 C = 2.17292800 - 1.08512800 - 1.28160300 C = 2.17292800 - 1.28160300 - 1.28160300 - 1.28160300 - 1.28160300 - 1.28160300 - 1.28160300 - 1.28160300 - 1.2816000 - 1.2816000 - 1.2816000 - 1.2816000 - 1.2816000 - 1.28160000 - 1.28160000 - 1.28160000 - 1.28160000 - 1.281600000 - 1.28160000000 - 1.2816000000000000000000000000000000000000
H = 2.75579200 - 2.36996200 - 0.99713600 $H = 2.82234900 - 1.96578500 - 1.28668700$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$
H = 2.82762000 - 0.65174700 - 1.40039000 H = 2.81499900 - 0.20210100 - 1.34966400
C = 0.82927800 - 2.15315700 - 0.93772000 - C = 0.58093900 - 2.15509300 - 1.28571400 - 0.58093900 - 1.512400 - 0.2507200 - 0.512400 - 0.2507200 - 0.520700 - 0.5207000 - 0.52070000 - 0.52070000000000000000000000000000000000
H $1.264/9/00$ $1.61/26800$ 1.78355000 H 0.82814300 $1.571/2400$ $2.17092/00$
$\begin{array}{cccccccccccccc} H & 1.40/1/300 & 3.0/164000 & 0.7/694900 & H & 1.20495400 & 3.06502000 & 1.29704700 \\ H & 1.20495400 & 1.2970400 & 1.2970400 \\ H & 1.204000 & 1.297000 & 1.2970000 \\ H & 1.20400 & 1.297000 & 1.29700$
Π -0.19150400 2.43694900 1.20873900 Π -0.46487300 2.46088600 1.34556500
L 0.2203/900 2.09910900 -1.50884000 L 0.58088900 2.10556000 -1.28501800
$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
S = -2.11566900 - 0.74661700 - 1.19658000 - S = -1.01000400 - 0.23900100 - 0.00002900 - S = -1.01000400 - 0.23900100 - 0.00002900 - 0.0000002900 - 0.000002900 - 0.000002900 - 0.000002900 - 0.00000000000 - 0.000000000000 - 0.00000000

S -1.57172800 -0.15402200 1.70284400	S -2.26551800 0.88166500 0.00018000 H -2.78898700 -1.73689400 -0.00011300
Table 11e. DIDTCH (Anti geometry);	Table 11f. DIDTCH (TSrot geometry);
E(B3LYP) = -1126.94915774 a.u.	E(B3LYP) = -1126.92052942 a.u.
N 0.32591500 -0.02162600 0.00002600	N 0.33112900 -0.03135300 -0.27222000
C 0.69341100 1.43816700 0.00023800	C 0.87220900 1.35632100 -0.21342200
Н 1.78215700 1.41496300 0.00061300	Н 1.92459100 1.23610200 -0.48609500
C 1.50088000 -0.95600400 0.00018600	C 1.26525100 -1.18606200 -0.10376400
Н 1.06098600 -1.95129900 -0.00009500	Н 0.61559200 -2.06711400 -0.06250300
C 2.33116700 -0.81154700 1.28131800	C 2.09221900 -1.15703700 1.19156800
Н 1.70635100 -0.94304800 2.16976900	Н 1.44858800 -1.05992600 2.06975700
Н 3.10040800 -1.59017500 1.28939600	Н 2.65887400 -2.09013300 1.28310100
H 2.84208700 0.15395600 1.35355800	Н 2.81245100 -0.33197300 1.19071300
C 2.33189300 -0.81116700 -1.28043100	C 2.15740000 -1.33719100 -1.34434300
H 3.10110900 -1.58982200 -1.28829900	H 2.77320800 -2.23809000 -1.24984100
H 1.70758600 -0.94238900 -2.16928000	H $1.55026600 - 1.42502800 - 2.24993100$
H $2.84290100 0.15433300 -1.35209700$	H 2.83632/00 -0.48621200 -1.46454100
L = 0.28953000 - 2.1/391200 - 1.28/60000	L = 0.82409900 - 2.04653500 - 1.16192200
H = 0.59450400 - 1.60794800 - 2.17203900	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$\Pi = 0.00057400 - 5.15050500 - 1.50052500 - 0.000574000000 - 0.00057400000000000000000000000000000000$	$\Pi = 1.30390000 - 2.90377900 - 1.10370000 = 0.20152000 - 2.20770600 - 1.45502000 = 0.20150000 = 0.20150000 = 0.20150000 = 0.20150000 = 0.20150000 = 0.201500000 = 0.20150000000000000000000000000000000000$
C = 0.29033700 - 2.17393900 - 1.28735200	$\begin{array}{c} 11 & -0.20132300 & 2.20773000 & 1.43333000 \\ 0 & 21962400 & 2.24134800 & 1.28538500 \end{array}$
H = 0.59640800 - 1.60827700 - 2.17160400	H = 0.31202900 - 1.78880800 - 2.27693300
H $-0.78105700 - 2.36930900 - 1.35451400$	H = -0.84389000 - 2.40209600 - 1.07767900
H = 0.80687500 - 3.13887600 - 1.30546200	H $0.70561600 = 3.22255600 = 1.07707500$
C = -0.91715700 - 0.52548800 - 0.00021900	C = -0.99235600 - 0.27796200 - 0.13769700
S -2.28042600 0.64879200 -0.00025000	S -2.00003600 -0.55644100 -1.29010600
S -1.31785000 -2.18391800 -0.00049000	S -1.56365500 -0.36500400 1.69213300
Н -3.21443000 -0.31683600 -0.00057200	Н -3.17514900 -0.80817500 -0.67276400
Table 11g. MorDTC ⁻ (Syn geometry):	Table 11h. MorDTC ⁻ (Anti geometry):
F(B3IVP) = -112187417563 211	F(B3LVP) = -112187417600 a u
-1 (1) (1) (1) -1 -1 (2) (1) (1) (1) (2) $($	-1 -1 -1 -1 -1 -1 -1 -1
N = -0.11044100 - 0.00000300 - 0.26479500	N $-0.11033700 -0.00015000 0.26764100$
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400	N -0.11033700 -0.00015000 0.26764100 C -0.90816800 1.21433200 0.49213200
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600	N -0.11033700 -0.00015000 0.26764100 C -0.90816800 1.21433200 0.49213200 C -2.18567800 1.17506100 -0.34282700
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300	N -0.11033700 -0.00015000 0.26764100 C -0.90816800 1.21433200 0.49213200 C -2.18567800 1.17506100 -0.34282700 O -2.95658600 0.00002300 -0.08052700
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300 C -2.18695600 -1.17489700 -0.34264400	N -0.11033700 -0.00015000 0.26764100 C -0.90816800 1.21433200 0.49213200 C -2.18567800 1.17506100 -0.34282700 O -2.95658600 0.00002300 -0.08052700 C -2.18575300 -1.17485100 -0.34388700
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300 C -2.18695600 -1.17489700 -0.34264400 C -0.90763500 -1.21474800 0.48959200	N -0.11033700 -0.00015000 0.26764100 C -0.90816800 1.21433200 0.49213200 C -2.18567800 1.17506100 -0.34282700 O -2.95658600 0.00002300 -0.08052700 C -2.18575300 -1.17485100 -0.34388700 C -0.90801200 -1.21498500 0.49080400
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300 C -2.18695600 -1.17489700 -0.34264400 C -0.90763500 -1.21474800 0.48959200 H -1.16186700 -1.27548500 1.55772500	N -0.11033700 -0.00015000 0.26764100 C -0.90816800 1.21433200 0.49213200 C -2.18567800 1.17506100 -0.34282700 O -2.95658600 0.00002300 -0.08052700 C -2.18575300 -1.17485100 -0.34388700 C -0.90801200 -1.21498500 0.49080400 H -1.16448800 -1.27552900 1.55839400
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300 C -2.18695600 -1.17489700 -0.34264400 C -0.90763500 -1.21474800 0.48959200 H -1.16186700 -1.27548500 1.55772500 H -0.30956300 -2.08460500 0.22403400	N -0.11033700 -0.00015000 0.26764100 C -0.90816800 1.21433200 0.49213200 C -2.18567800 1.17506100 -0.34282700 O -2.95658600 0.00002300 -0.08052700 C -2.18575300 -1.17485100 -0.34388700 C -0.90801200 -1.21498500 0.49080400 H -1.16448800 -1.27552900 1.55839400 H -0.30958400 -2.08501200 0.22658900
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300 C -2.18695600 -1.17489700 -0.34264400 C -0.90763500 -1.21474800 0.48959200 H -1.16186700 -1.27548500 1.55772500 H -0.30956300 -2.08460500 0.22403400 H -0.30964200 2.08459900 0.22427700	N -0.11033700 -0.00015000 0.26764100 C -0.90816800 1.21433200 0.49213200 C -2.18567800 1.17506100 -0.34282700 O -2.95658600 0.00002300 -0.08052700 C -2.18575300 -1.17485100 -0.34388700 C -0.90801200 -1.21498500 0.49080400 H -1.16448800 -1.27552900 1.55839400 H -0.30958400 -2.08501200 0.22658900 H -0.30974300 2.08472300 0.22917900
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-0.309642002.084599000.22427700H-1.161824001.275279001.55790700	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300 C -2.18695600 -1.17489700 -0.34264400 C -0.90763500 -1.21474800 0.48959200 H -1.16186700 -1.27548500 1.55772500 H -0.30956300 -2.08460500 0.22403400 H -0.30964200 2.08459900 0.22427700 H -1.16182400 1.27527900 1.55790700 H -2.82197700 2.02836200 -0.09146200	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300 C -2.18695600 -1.17489700 -0.34264400 C -0.90763500 -1.21474800 0.48959200 H -1.16186700 -1.27548500 1.55772500 H -0.30956300 -2.08460500 0.22403400 H -0.30964200 2.08459900 0.22427700 H -1.16182400 1.27527900 1.55790700 H -1.3863800 1.21944200 -1.41406100	$\begin{array}{c c c c c c c c c c c c c c c c c c c $
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300 C -2.18695600 -1.17489700 -0.34264400 C -0.90763500 -1.21474800 0.48959200 H -1.16186700 -1.27548500 1.55772500 H -0.30956300 -2.08460500 0.22403400 H -0.30964200 2.08459900 0.22427700 H -1.16182400 1.27527900 1.55790700 H -1.3863800 1.21944200 -1.41406100 H -1.93863800 1.21944200 -1.41428000	$\begin{array}{c c c c c c c c c c c c c c c c c c c $
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c c c c c c c c c c c c c c c c c c c $
N -0.11044100 -0.00000300 0.26479500 C -0.90767400 1.21466900 0.48976400 C -2.18702800 1.17491200 -0.34242600 O -2.95740200 -0.00003500 -0.07819300 C -2.18695600 -1.17489700 -0.34264400 C -0.90763500 -1.21474800 0.48959200 H -1.16186700 -1.27548500 1.55772500 H -0.30956300 -2.08460500 0.22403400 H -0.30964200 2.08459900 0.22427700 H -1.16182400 1.27527900 1.55790700 H -1.6182400 1.27527900 1.55790700 H -1.8863800 1.21944200 -1.41406100 H -1.93852900 -1.21918100 -1.41428000 H -2.82187900 -2.02845900 -0.09189300 C 1.23391300 0.00004100 0.03137800 S 2.08211600 1.51281100 -0.11661900	N -0.11033700 -0.00015000 0.26764100 C -0.90816800 1.21433200 0.49213200 C -2.18567800 1.17506100 -0.34282700 O -2.95658600 0.00002300 -0.08052700 C -2.18575300 -1.17485100 -0.34388700 C -0.90801200 -1.21498500 0.49080400 H -1.16448800 -1.27552900 1.55839400 H -0.30958400 -2.08501200 0.22658900 H -0.30974300 2.08472300 0.22917900 H -1.16491800 1.27344900 1.55974500 H -2.82109900 2.02856400 -0.09325600 H -1.93510200 1.21871800 -1.41392400 H -1.93549500 -1.21871800 -1.41508200 H -2.82121300 -2.02844600 -0.09473500 C 1.23356500 0.00005000 0.03200600 S 2.08139100 1.51303100 -0.11779200
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-1.161824001.275279001.55790700H-2.821977002.02836200-0.09146200H-1.938638001.21944200-1.41406100H-1.93852900-1.21918100-1.41428000H-2.82187900-2.02845900-0.09189300C1.233913000.000041000.03137800S2.082116001.51281100-0.11667200S2.08216500-1.51281100-0.11661900Table11i.MorDTC'(TSrot geometry); $E(B3LYP) = -1121.85123666 a H-1.2185123666 a H$	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600H-1.935102001.21871800-1.41392400H-2.82121300-2.02844600-0.09473500C1.233565000.000050000.03200600S2.08179500-1.51274700-0.11693000S2.081391001.51303100-0.11779200Table 11j. MorDTCH (Syn geometry);F(B3LYP) = -112232363538 a u
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-0.309642002.084599000.22427700H-1.161824001.275279001.55790700H-2.821977002.02836200-0.09146200H-1.938638001.21944200-1.41406100H-1.93852900-1.21918100-1.41428000H-2.82187900-2.02845900-0.09189300C1.233913000.000041000.03137800S2.082116001.51281100-0.11677200S2.08216500-1.51281100-0.11661900Table 11i. MorDTC- (TSrot geometry);E(B3LYP) = -1121.85123666 a.u.N-0.13509600-0.288009000.00034500	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600H-1.935102001.21871800-1.41392400H-1.35565000.000050000.03200600S2.08179500-1.51274700-0.11693000S2.081391001.51303100-0.11779200Table 11j. MorDTCH (Syn geometry);E(B3LYP) = -1122.32363538 a.u.N0.143147000.034243000.28162400
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-0.309642002.084599000.22427700H-1.161824001.275279001.55790700H-2.821977002.02836200-0.09146200H-1.938638001.21944200-1.41406100H-1.93852900-1.21918100-1.41428000H-2.82187900-2.02845900-0.09189300C1.233913000.000041000.03137800S2.082116001.51281100-0.11677200S2.08216500-1.51281100-0.11661900Table11i.MorDTC'(TSrot geometry);E(B3LYP) = -1121.85123666 a.u.N-0.13509600-0.28809900N-0.13509600-0.288099000.00034500C-0.823020000.19727700-1.20748500	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600H-1.935102001.21965500-1.41392400H-1.93549500-1.21871800-1.41508200H-2.82121300-2.02844600-0.09473500C1.233565000.000050000.03200600S2.081391001.51303100-0.11779200Table 11j. MorDTCH (Syn geometry);E(B3LYP) = -1122.32363538 a.u.N0.143147000.034243000.28162400C0.91244700-1.207815000.49147900
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-0.309642002.084599000.22427700H-1.161824001.275279001.55790700H-2.821977002.02836200-0.09146200H-1.938638001.21944200-1.41406100H-1.93852900-1.21918100-1.41428000H-2.82187900-2.02845900-0.09189300C1.233913000.000041000.03137800S2.082116001.51281100-0.11677200S2.08216500-1.51281100-0.11661900Table 11i. MorDTC- (TS _{rot} geometry);E(B3LYP) = -1121.85123666 a.u.N-0.13509600-0.288099000.00034500C-0.823020000.19727700-1.20748500C-2.27153900-0.28056700-1.18025200	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600H-1.935102001.21871800-1.41392400H-1.93549500-1.21871800-1.41508200H-2.82121300-2.02844600-0.09473500C1.233565000.000050000.03200600S2.081391001.51303100-0.11779200Table 11j. MorDTCH (Syn geometry);E(B3LYP) = -1122.32363538 a.u.N0.143147000.034243000.28162400C0.91244700-1.207815000.49147900C2.18696400-1.18671900-0.35416400
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-0.309642002.084599000.22427700H-1.161824001.275279001.55790700H-2.821977002.02836200-0.09146200H-1.938638001.21944200-1.41406100H-1.93852900-1.21918100-1.41428000H-2.82187900-2.02845900-0.09189300C1.233913000.000041000.03137800S2.08216500-1.51281100-0.11661900Table11i.MorDTC'(TSrot geometry);E(B3LYP) = -1121.85123666 a.u.N-0.13509600-0.28809900N-0.13509600-0.288099000.00034500C-2.27153900-0.28056700-1.18025200O-2.946455000.16869200-0.00027200	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600H-1.935102001.21871800-1.41392400H-1.35565000.000050000.03200600S2.08179500-1.51274700-0.11693000S2.081391001.51303100-0.11779200Table 11j. MorDTCH (Syn geometry);E(B3LYP) = -1122.32363538 a.u.N0.143147000.034243000.28162400C0.91244700-1.207815000.49147900C2.18696400-1.18671900-0.35416400O2.97490900-0.03158200-0.07858300
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-0.309642002.084599000.22427700H-1.161824001.275279001.55790700H-2.821977002.02836200-0.09146200H-1.938638001.21944200-1.41406100H-1.93852900-1.21918100-1.41428000H-2.82187900-2.02845900-0.09189300C1.233913000.000041000.03137800S2.082116001.51281100-0.11661900Table11i.MorDTC'(TSrot geometry);E(B3LYP) = -1121.85123666 a.u.N-0.13509600-0.28800900N-0.13509600-0.288009000.00034500C-2.27153900-0.28056700-1.18025200O-2.946455000.16869200-0.00027200C-2.27170700-0.278349001.18061200	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600H-1.935102001.21871800-1.41392400H-1.93549500-1.21871800-1.41508200H-2.82121300-2.02844600-0.09473500C1.233565000.000050000.03200600S2.081391001.51303100-0.11779200Table 11j. MorDTCH (Syn geometry);E(B3LYP) = -1122.32363538 a.u.N0.143147000.034243000.28162400C0.91244700-1.207815000.49147900C2.18696400-1.18671900-0.35416400O2.97490900-0.03158200-0.07858300C2.237690001.16080800-0.35236700
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-0.309642002.084599000.22427700H-1.161824001.275279001.55790700H-2.821977002.02836200-0.09146200H-1.938638001.21944200-1.41406100H-1.93852900-1.21918100-1.41428000H-2.82187900-2.02845900-0.09189300C1.233913000.000041000.03137800S2.082116001.51281100-0.11667200S2.08216500-1.51281100-0.11661900Table 11i. MorDTC' (TSrot geometry);E(B3LYP) = -1121.85123666 a.u.N-0.13509600-0.288099000.00034500C-0.823020000.19727700-1.20748500C-2.27153900-0.28056700-1.18025200O-2.946455000.16869200-0.00027200C-2.27170700-0.278349001.8061200C-0.823129000.199451001.20720000	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600H-1.935102001.21965500-1.41392400H-1.93549500-1.21871800-1.41508200H-2.82121300-2.02844600-0.09473500C1.233565000.000050000.03200600S2.081391001.51303100-0.11779200Table 11j. MorDTCH (Syn geometry);E(B3LYP) = -1122.32363538 a.u.N0.143147000.034243000.28162400C0.91244700-1.207815000.49147900C2.18696400-1.18671900-0.35416400O2.97490900-0.03158200-0.07858300C2.237690001.16080800-0.35236700C0.967519001.240258000.49118200
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-0.309642002.084599000.22427700H-1.161824001.275279001.55790700H-2.821977002.02836200-0.09146200H-1.938638001.21944200-1.41406100H-1.93852900-1.21918100-1.41428000H-2.82187900-2.02845900-0.09189300C1.233913000.000041000.03137800S2.082116001.51281100-0.11667200S2.08216500-1.51281100-0.11661900Table 11i. MorDTC' (TSrot geometry);E(B3LYP) = -1121.85123666 a.u.N-0.13509600-0.288099000.00034500C-2.27153900-0.28056700-1.18025200O-2.946455000.16869200-0.0027200C-2.27170700-0.278349001.8061200C-0.823129000.199451001.20720000H-0.795715001.300295001.27196800	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600H-1.935102001.21965500-1.41392400H-1.93549500-1.21871800-1.41508200H-2.82121300-2.02844600-0.09473500C1.233565000.000050000.03200600S2.081391001.51303100-0.11779200Table 11j. MorDTCH (Syn geometry);E(B3LYP) = -1122.32363538 a.u.N0.143147000.034243000.28162400C0.91244700-1.207815000.49147900C2.18696400-1.18671900-0.35416400O2.97490900-0.03158200-0.07858300C2.237690001.16080800-0.35236700C0.967519001.240258000.49118200H1.223498001.294583001.55671400
N-0.11044100-0.000003000.26479500C-0.907674001.214669000.48976400C-2.187028001.17491200-0.34242600O-2.95740200-0.00003500-0.07819300C-2.18695600-1.17489700-0.34264400C-0.90763500-1.214748000.48959200H-1.16186700-1.275485001.55772500H-0.30956300-2.084605000.22403400H-0.309642002.084599000.22427700H-1.161824001.275279001.55790700H-2.821977002.02836200-0.09146200H-1.938638001.21944200-1.41406100H-1.93852900-1.21918100-1.41428000H-2.82187900-2.02845900-0.09189300C1.233913000.000041000.03137800S2.082116001.51281100-0.11677200S2.08216500-1.51281100-0.11661900Table 11i. MorDTC- (TSrot geometry);E(B3LYP) = -1121.85123666 a.u.N-0.13509600-0.288099000.00034500C-2.27153900-0.28056700-1.18025200O-2.946455000.16869200-0.00027200C-2.27170700-0.278349001.8061200C-0.823129000.199451001.20720000H-0.795715001.300295001.27196800H-0.32123400-0.208092002.09119400	N-0.11033700-0.000150000.26764100C-0.908168001.214332000.49213200C-2.185678001.17506100-0.34282700O-2.956586000.00002300-0.08052700C-2.18575300-1.17485100-0.34388700C-0.90801200-1.214985000.49080400H-1.16448800-1.275529001.55839400H-0.30958400-2.085012000.22658900H-0.309743002.084723000.22917900H-1.164918001.273449001.55974500H-2.821099002.02856400-0.09325600H-1.935102001.21871800-1.41392400H-1.93549500-1.21871800-1.41508200H-2.82121300-2.02844600-0.09473500C1.233565000.000050000.03200600S2.081391001.51303100-0.11779200Table 11j. MorDTCH (Syn geometry);E(B3LYP) = -1122.32363538 a.u.N0.143147000.034243000.28162400C0.91244700-1.207815000.49147900C2.18696400-1.18671900-0.35416400O2.97490900-0.03158200-0.07858300C2.237690001.16080800-0.35236700C0.967519001.240258000.49118200H1.223498001.294583001.55671400H0.382276002.118127000.22365000

Н -0.79576500 1.29801200 -1.27410900	Н 1.16604100 -1.27758600 1.55621900
Н -2.82586300 0.12950500 -2.02862100	Н 2.80062100 -2.05694600 -0.11129900
Н -2.30741500 -1.37968000 -1.22778600	Н 1.92859500 -1.21879300 -1.42287600
Н -2.30762100 -1.37736700 1.23024700	Н 1.98482300 1.20419500 -1.42193200
Н -2.82608800 0.13339500 2.02813300	Н 2.89243700 2.00037300 -0.10898800
C 1.29734600 -0.04143500 0.00010400	C -1.17552500 0.09537900 0.04414200
S 2.28024800 -1.43003300 0.00086900	S -1.99613200 -1.49975200 -0.09429000
S 1.86789100 1.56777600 -0.00097100	S -2.07097000 1.52303600 -0.11967300
	Н -3.20013800 -0.95403600 -0.33390300
Table 11k. MorDTCH (Anti geometry)	Table 111 . MorDTCH (TS _{rot} geometry chair
F(B3LVP) = -1122 32363548 a u	conformation); $F(B3IVP) =$
1(100111) = 1122.020000100.000000000000000000000000	-112229780872 = 11
N 0.14212200 0.02422600 0.28076000	
$\begin{array}{c} N & 0.14312300 & 0.03432000 & 0.20070700 \\ C & 0.01247000 & 1.20756000 & 0.40142200 \\ \end{array}$	$\begin{array}{c} N & -0.13313300 & 0.23339100 & -0.00024100 \\ C & 0.95404000 & 0.22229700 & 1.21904200 \end{array}$
C = 2.19756000 - 1.20730900 - 0.49143200	C = -0.03494000 -0.23230700 -1.21004300
C = 2.18750000 - 1.18078500 - 0.55550800	C = -2.29402300 = 0.27003300 = 1.17921400
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0 -2.90915100 -0.17487700 -0.00001500
C = 2.23001400 - 1.10000000 - 0.33237300	C = -2.293/9100 = 0.20930000 = 1.1/930900
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
C = -1.1/501200 = 0.09555400 = 0.04545400	$\begin{array}{c} 1.24234000 -0.05557800 -0.00002500 \\ 0.00002500 -0.00072100 \\ 0.0007200 \\ 0.000700 \\ 0.000700 \\ 0.000700 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.000000 \\ 0.0000$
5 - 1.99625500 - 1.49986100 - 0.09424400	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
5 - 2.0/129000 - 1.52290000 - 0.11920200	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
Table 11m MorDTCH (TS geometry best	Table 11 DDTC: (Sun geometrul)
Table 11m. MorDTCH (TS _{rot} geometry, boat	Table 11n. PDTC ⁻ (Syn geometry); F(P21 VP)
Table 11m. MorDTCH (TSrot geometry, boat conformation); $E(B3LYP) = -1122.29059003$	Table 11n. PDTC ⁻ (Syn geometry); $E(B3LYP) = -1046.66557228 a.u.$
Table 11m. MorDTCH (TSrot geometry, boat conformation); $E(B3LYP) = -1122.29059003$ a.u.	Table 11n. PDTC ⁻ (Syn geometry); E(B3LYP) = -1046.66557228 a.u.
Table 11m. MorDTCH (TS _{rot} geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u. N -0.01488700 -0.76852000 0.00079400	Table 11n. PDTC ⁻ (Syn geometry); E(B3LYP) = -1046.66557228 a.u. C -2.60982400 0.70285600 0.30864200
n -3.20023000 -0.93418000 -0.33411100 Table 11m. MorDTCH (TS _{rot} geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u. N -0.01488700 -0.76852000 0.00079400 C -0.84235200 -0.79240800 1.22965500	Table 11n. PDTC ⁻ (Syn geometry); E(B3LYP) = -1046.66557228 a.u. C -2.60982400 0.70285600 0.30864200 C -2.60988100 -0.70288800 -0.30851800
H-3.20023000-0.33418000-0.33411100Table 11m.MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 1.22965500 CC-0.84235200-0.792408001.22965500 1.18282400	C -2.60982400 0.70285600 0.30864200 C -2.60982400 0.70285600 0.30864200 C -1.19911400 -0.70288800 -0.30851800 C -1.19911400 -1.21952300 -0.00304100
H-3.20023000-0.33418000-0.33411100Table 11m.MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200	C -2.60982400 0.70285600 0.30864200 C -2.60982400 0.70285600 0.30864200 C -2.60988100 -0.70288800 -0.30851800 C -1.19911400 -1.21952300 -0.00304100 C -1.19909400 1.21945700 0.00294700
H -3.20023000 -0.93418000 -0.33411100 Table 11m. MorDTCH (TS _{rot} geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u. N -0.01488700 -0.76852000 0.00079400 C -0.84235200 -0.79240800 1.22965500 C -2.01041600 0.19295400 1.18282400 O -2.79529000 -0.00735200 -0.00033200 C -2.00989800 0.19093400 -1.18359200	Table 11n. PDTC ⁻ (Syn geometry); E(B3LYP) = -1046.66557228 a.u. C -2.60982400 0.70285600 0.30864200 C -2.60988100 -0.70288800 -0.30851800 C -1.19911400 -1.21952300 -0.00304100 C -1.19909400 1.21945700 0.00294700 H -3.38349500 1.35784200 -0.10126700
H -3.20023000 -0.93418000 -0.33411100 Table 11m. MorDTCH (TS _{rot} geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u. N -0.01488700 -0.76852000 0.00079400 C -0.84235200 -0.79240800 1.22965500 C -2.01041600 0.19295400 1.18282400 O -2.79529000 -0.00735200 -0.00033200 C -0.84185200 -0.79442400 -1.2835400	Table 11n. PDTC(Syn geometry); E(B3LYP) = -1046.66557228 a.u.C-2.609824000.702856000.30864200C-2.60988100-0.70288800-0.30851800C-1.19911400-1.21952300-0.00304100C-1.199094001.219457000.00294700H-3.383495001.35784200-0.10126700H-2.759801000.640027001.39286900
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400C-0.84235200-0.792408001.22965500C-2.010416000.192954001.18282400O-2.79529000-0.00735200-0.00033200C-2.009898000.19093400-1.18359200C-0.84185200-0.79442400-1.22835400H-1.23591100-1.81397500-1.32290900	Table 11n. PDTC(Syn geometry); $E(B3LYP) = -1046.66557228 a.u.$ C-2.60982400C-2.60988100-0.70288800-0.30851800C-1.19911400-1.21952300-0.00304100C-1.199094001.219457000.00294700H-3.383495001.35784200-0.10126700H-2.759801000.640027001.39286900H-2.76002100-0.64005400-1.39272200
H -3.20023000 -0.93418000 -0.33411100 Table 11m. MorDTCH (TS _{rot} geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u. N -0.01488700 -0.76852000 0.00079400 C -0.84235200 -0.79240800 1.22965500 C -2.01041600 0.19295400 1.18282400 O -2.79529000 -0.00735200 -0.00033200 C -2.00989800 0.19093400 -1.18359200 C -0.84185200 -0.79442400 -1.22835400 H -1.23591100 -1.81397500 -1.32290900 H -0.20439100 -0.59866900 -2.09468300	Table 11n. PDTC(Syn geometry); E(B3LYP) = -1046.66557228 a.u.C-2.609824000.702856000.30864200C-2.60988100-0.70288800-0.30851800C-1.19911400-1.21952300-0.00304100C-1.199094001.219457000.00294700H-3.383495001.35784200-0.10126700H-2.759801000.640027001.39286900H-3.38350400-1.357858000.10150600
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 CH-0.20439100-0.59866900-2.09468300 BH-0.20525200-0.595347002.09593400	Table 11n. PDTC(Syn geometry); E(B3LYP) = -1046.66557228 a.u.C-2.609824000.702856000.30864200C-2.60988100-0.70288800-0.30851800C-1.19911400-1.21952300-0.00304100C-1.199094001.219457000.00294700H-3.383495001.35784200-0.10126700H-2.759801000.640027001.39286900H-2.76002100-0.64005400-1.39272200H-3.38350400-1.357858000.10150600H-1.14713100-1.704950000.98005900
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-1.23655400-1.811776001.32559800	a.36070000 b.30002300 b.30002000Table 11n. PDTC ⁻ (Syn geometry); $E(B3LYP) = -1046.66557228 a.u.$ C -2.60982400 0.70285600 0.30864200 C -2.60988100 -0.70288800 -0.30851800 C -1.19911400 -1.21952300 -0.00304100 C -1.19909400 1.21945700 0.00294700 H -3.38349500 1.35784200 -0.10126700 H -2.75980100 0.64002700 1.39286900 H -2.76002100 -0.64005400 -1.39272200 H -3.38350400 -1.35785800 0.10150600 H -0.82281900 -1.93032700 -0.74098300
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.76852000 0.00079400 CC-0.84235200-0.792408001.22965500 CC-2.01041600 0.19295400 1.18282400 OO-2.79529000-0.00735200-0.00033200 CC-0.84185200 0.19093400 -1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400	Table 11n. PDTC(Syn geometry); E(B3LYP) = -1046.66557228 a.u.C-2.609824000.702856000.30864200C-2.60988100-0.70288800-0.30851800C-1.19911400-1.21952300-0.00304100C-1.199094001.219457000.00294700H-3.383495001.35784200-0.10126700H-2.759801000.640027001.39286900H-2.76002100-0.64005400-1.39272200H-3.38350400-1.357858000.10150600H-1.14713100-1.704950000.98005900H-0.82281900-1.93032700-0.74098300H-0.822678001.930280000.74081100
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-0.84185200-0.79442400-1.2835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.650099001.230029001.21593200	Table 11n. PDTC(Syn geometry); E(B3LYP) = -1046.66557228 a.u.C-2.609824000.702856000.30864200C-2.60988100-0.70288800-0.30851800C-1.19911400-1.21952300-0.00304100C-1.199094001.219457000.00294700H-3.383495001.35784200-0.10126700H-2.759801000.640027001.39286900H-2.76002100-0.64005400-1.39272200H-3.38350400-1.357858000.10150600H-1.14713100-1.704950000.98005900H-0.82281900-1.93032700-0.74098300H-0.822678001.930280000.74081100H-1.147243001.70484500-0.98018000
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-0.84185200-0.79442400-1.2835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-1.23655400-1.811776001.32559800 HH-1.23655400-1.811776001.32559800 HH-1.650099001.230029001.21593200 HH-1.649715001.22799100-1.21821500	In 3.36070000^{-} 0.70002300^{-} 0.0002300^{-} Table 11n. PDTC ⁻ (Syn geometry);E(B3LYP) = -1046.66557228 a.u.C-2.60982400 0.70285600 0.30864200 C-2.60988100 -0.70288800 -0.30851800 C-1.19911400 -1.21952300 -0.00304100 C-1.19909400 1.21945700 0.00294700 H-3.38349500 1.35784200 -0.10126700 H-2.75980100 0.64002700 1.39286900 H-2.76002100 -0.64005400 -1.39272200 H-3.38350400 -1.35785800 0.10150600 H-1.14713100 -1.70495000 0.98005900 H -0.82281900 -1.93032700 -0.74098300 H -0.82267800 1.93028000 0.74081100 H -1.14724300 1.70484500 -0.98018000 N -0.36150900 -0.00003800 -0.00008200
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-0.84185200-0.79442400-1.2835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-1.23655400-1.811776001.32559800 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.649715001.22799100-1.21821500 HH-2.678699000.01928000-2.03165600	In 3.36070000^{-} 0.70002300^{-} 0.0002300^{-} Table 11n. PDTC ⁻ (Syn geometry);E(B3LYP) = -1046.66557228 a.u.C-2.60982400 0.70285600 0.30864200 C-2.60988100 -0.70288800 -0.30851800 C-1.19911400 -1.21952300 -0.00304100 C-1.19909400 1.21945700 0.00294700 H-3.38349500 1.35784200 -0.10126700 H-2.75980100 0.64002700 1.39286900 H-2.76002100 -0.64005400 -1.39272200 H-3.38350400 -1.35785800 0.10150600 H-1.14713100 -1.70495000 0.98005900 H -0.82281900 -1.93032700 -0.74098300 H -0.82267800 1.93028000 0.74081100 H -1.14724300 1.70484500 -0.98018000 N -0.36150900 -0.00003800 -0.00008200
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-0.84185200-0.79442400-1.2835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-1.23655400-1.811776001.32559800 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.650099001.230029001.21593200 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300	In 3.36070000^{-} 0.70002300^{-} 0.0002300^{-} Table 11n. PDTC' (Syn geometry);E(B3LYP) = -1046.66557228 a.u.C-2.60982400 0.70285600 0.30864200 C-2.60988100 -0.70288800 -0.30851800 C-1.19911400 -1.21952300 -0.00304100 C-1.19909400 1.21945700 0.00294700 H-3.38349500 1.35784200 -0.10126700 H-2.75980100 0.64002700 1.39286900 H-2.76002100 -0.64005400 -1.39272200 H-3.38350400 -1.35785800 0.10150600 H-0.82281900 -1.93032700 -0.74098300 H-0.82267800 1.93028000 0.74081100 H-1.14724300 1.70484500 -0.98018000 N -0.36150900 -0.00003800 -0.00008200 C 0.98819600 -0.0001400 -0.00012900 S 1.82931800 1.52451900 0.7530900
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-0.09898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.650099001.230029001.21593200 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.879061000.00033300 C	In 3.36070000^{-} 0.70002300^{-} 0.0002300^{-} Table 11n. PDTC' (Syn geometry);E(B3LYP) = -1046.66557228 a.u.C-2.60982400 0.70285600 0.30864200 C-2.60988100 -0.70288800 -0.30851800 C-1.19911400 -1.21952300 -0.00304100 C-1.19909400 1.21945700 0.00294700 H-3.38349500 1.35784200 -0.10126700 H-2.75980100 0.64002700 1.39286900 H-2.76002100 -0.64005400 -1.39272200 H-3.38350400 -1.35785800 0.10150600 H-1.14713100 -1.70495000 0.98005900 H -0.82267800 1.93028000 0.7408300 H -0.82267800 1.93028000 0.74081100 H -1.14724300 1.70484500 -0.98018000 N -0.36150900 -0.00003800 -0.00008200 C 0.98819600 -0.0001400 -0.07530900 S 1.82931800 -1.52459000 -0.07524300
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-0.84185200-0.79442400-1.2835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.650099001.230029001.21593200 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.879061000.00086600H-1.649722001.76635300-0.00086600	In 3.50070000^{-} 0.50022500^{-} 0.00025000^{-} Table 11n. PDTC' (Syn geometry);E(B3LYP) = -1046.66557228 a.u.C-2.60982400 0.70285600 0.30864200 C-2.60988100 -0.70288800 -0.30851800 C-1.19911400 -1.21952300 -0.00304100 C-1.19909400 1.21945700 0.00294700 H-3.38349500 1.35784200 -0.10126700 H-2.75980100 0.64002700 1.39286900 H-2.76002100 -0.64005400 -1.39272200 H-3.38350400 -1.35785800 0.10150600 H-1.14713100 -1.70495000 0.98005900 H -0.82281900 -1.93032700 -0.74098300 H -0.82267800 1.93028000 0.74081100 H -1.14724300 1.70484500 -0.98018000 N -0.36150900 -0.00003800 -0.00008200 C 0.98819600 -0.0001400 -0.07530900 S 1.82931800 -1.52459000 -0.07524300
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-0.20525200-0.595347002.09593400 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.650099001.210029001.21593200 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.879061000.00033300 SS1.082722001.76635300-0.00086600 HHDEDC0.11010700-0.00005500	Table 11n. PDTC(Syn geometry); E(B3LYP) = -1046.66557228 a.u.C-2.609824000.702856000.30864200 C -2.60988100C-2.60988100-0.70288800-0.30851800 C -3.0851800C-1.19911400-1.21952300-0.00304100 C -3.8349500C-1.199094001.219457000.00294700H-3.383495001.35784200-0.10126700H-2.759801000.640027001.39286900H-2.76002100-0.64005400-1.39272200H-3.38350400-1.357858000.10150600H-1.14713100-1.704950000.98005900H-0.82281900-1.93032700-0.74098300H-0.822678001.930280000.74081100H-1.147243001.70484500-0.98018000N-0.36150900-0.00003800-0.00012900S1.82931800-1.524519000.07530900S1.829155001.52459000-0.07524300
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 HH-0.20439100-0.59866900-2.09468300 HH-0.20525200-0.595347002.09593400 HH-1.23655400-1.811776001.32559800 HH-1.650099001.230029001.21893200 HH-1.649715001.22799100-1.21821500 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.87961000.00033300 SS1.082722001.76635300-0.00086600 HH3.472705000.11010700-0.0005500Table 110. PDTC (Anti geometry);	Table 11n. PDTC' (Syn geometry); E(B3LYP) = -1046.66557228 a.u.C-2.609824000.702856000.30864200C-2.60988100-0.70288800-0.30851800C-1.19911400-1.21952300-0.00304100C-1.199114001.219457000.00294700H-3.383495001.35784200-0.10126700H-3.759801000.640027001.39286900H-2.76002100-0.64005400-1.39272200H-3.38350400-1.357858000.10150600H-1.4713100-1.704950000.98005900H-0.82281900-1.93032700-0.74098300H-0.822678001.930280000.74081100H-1.147243001.70484500-0.98018000N-0.36150900-0.00003800-0.00012900S1.82931800-1.524519000.07530900S1.829155001.52459000-0.07524300
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 CH-0.20525200-0.595347002.09593400 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.649715001.22799100-1.21821500 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.879061000.00033300 SS1.082722001.76635300-0.00086600 HH3.472705000.11010700-0.0005500Table 110. PDTC (Anti geometry); E(B3LYP) = -1046.66557228 a.u.	InDistributionDistributionDistributionTable 11n. PDTC' (Syn geometry); $E(B3LYP) = -1046.66557228 a.u.$ C -2.60982400 0.70285600 0.30864200 C -2.60988100 -0.70288800 -0.30851800 C -1.19911400 -1.21952300 -0.00304100 C -1.19911400 -1.21952300 -0.00304100 C -1.19909400 1.21945700 0.00294700 H -3.38349500 1.35784200 -0.10126700 H -2.75980100 0.64002700 1.39286900 H -2.76002100 -0.64005400 -1.39272200 H -3.38350400 -1.35785800 0.10150600 H -1.14713100 -1.70495000 0.98005900 H -0.82267800 1.93028000 0.74081100 H -0.82267800 1.93028000 0.74081100 H -0.36150900 -0.00003800 -0.00008200 C 0.98819600 -0.00001400 -0.00012900 S 1.82931800 -1.524519000 -0.07530900 S 1.82915500 1.52459000 -0.07524300
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 CH-0.20439100-0.59866900-2.09468300 HH-0.20525200-0.595347002.09593400 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.649715001.22799100-1.21821500 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.879061000.00033300 SS1.082722001.76635300-0.00086600 HH3.472705000.11010700-0.0005500Table 110. PDTC (Anti geometry); E(B3LYP) = -1046.66557228 a.u.C-2.60956900-0.703071000.30892100	In 3.50070000^{-} (.50002500^{-} 0.0002500^{-}Table 11n. PDTC' (Syn geometry);E(B3LYP) = -1046.66557228 a.u.C-2.60982400^{-} 0.70285600^{-} 0.30864200^{-}C-2.60988100^{-} 0.70288800^{-} 0.30851800^{-}C-1.19911400^{-} 1.21952300^{-} 0.00304100^{-}C-1.19911400^{-} 1.21952300^{-} 0.00304100^{-}C-1.19909400^{-} 1.21945700^{-} 0.00294700^{-}H-3.38349500^{-} 1.35784200^{-} 0.10126700^{-}H-2.75980100^{-} 0.64002700^{-} 1.39286900^{-}H-2.76002100^{-} 0.64005400^{-} 1.39272200^{-}H-3.38350400^{-} 1.35785800^{-} 0.10150600^{-}H-1.14713100^{-} 1.70495000^{-} 0.98005900^{-}H-0.82281900^{-} 1.93032700^{-} 0.74098300^{-}H-0.82267800^{-} 1.93028000^{-} 0.74081100^{-}H-0.82267800^{-} 1.93028000^{-} 0.74081100^{-}H-1.14724300^{-} 1.70484500^{-} 0.98018000^{-}N-0.36150900^{-} 0.00003800^{-} 0.0008200^{-}C0.98819600^{-} 0.00001400^{-} 0.007530900^{-}S1.82931800^{-} 1.52459000^{-} 0.07524300^{-}Table 11p. PDTC' (TS _{rot} geometry);E(B3LYP) = -1046.63382496^{-} a.u.C-2.60981800^{-} 0.20213300^{-} 0.77851600^{-}
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 CH-0.20439100-0.59866900-2.09468300 HH-0.20525200-0.595347002.09593400 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.649715001.22799100-1.21821500 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.879061000.00033300 SS1.082722001.76635300-0.00086600 HH3.472705000.11010700-0.0005500Table 110. PDTC: (Anti geometry); E(B3LYP) = -1046.66557228 a.u.C-2.60956900-0.703071000.30892100 CC-2.60956900-0.703071000.30892100 C	InDisplay=0.0000Display=0.00012500Display=0.00012500Table 11n. PDTC' (Syn geometry); $E(B3LYP) = -1046.66557228$ a.u.C-2.609824000.702856000.30864200C-2.60988100-0.70288800-0.30851800C-1.19911400-1.21952300-0.00304100C-1.199094001.219457000.00294700H-3.383495001.35784200-0.10126700H-2.759801000.640027001.39286900H-2.76002100-0.64005400-1.39272200H-3.38350400-1.357858000.10150600H-1.14713100-1.704950000.98005900H-0.82281900-1.93032700-0.74098300H-0.822678001.930280000.74081100H-1.147243001.70484500-0.98018000N-0.36150900-0.00003800-0.0008200C0.98819600-0.0001400-0.00012900S1.82931800-1.52459000-0.07524300S1.829155001.52459000-0.07524300E(B3LYP) = -1046.63382496 a.u.C-2.60981800-0.20213300-0.77851600C-2.60981800-0.202133000.77866000
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 CH-0.20439100-0.59866900-2.09468300 HH-0.20525200-0.595347002.09593400 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.649715001.22799100-1.21821500 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.879061000.00033300 SS1.082722001.76635300-0.00086600 HH3.472705000.11010700-0.00005500Table 110. PDTC: (Anti geometry); E(B3LYP) = -1046.66557228 a.u.C-2.60956900-0.703071000.30892100 CC-2.609805000.70268600-0.30817600 CC-2.609805000.70268600-0.00323800	InDistributionDistributionDistributionTable 11n. PDTC' (Syn geometry); $E(B3LYP) = -1046.66557228 a.u.$ C -2.60982400 0.70285600 0.30864200 C -2.60988100 -0.70288800 -0.30851800 C -1.19911400 -1.21952300 -0.00304100 C -1.19909400 1.21945700 0.00294700 H -3.38349500 1.35784200 -0.10126700 H -2.75980100 0.64002700 1.39286900 H -2.76002100 -0.64005400 -1.39272200 H -3.38350400 -1.35785800 0.10150600 H -1.14713100 -1.70495000 0.98005900 H -0.82267800 1.93028000 0.74081100 H -0.82267800 1.93028000 0.74081100 H -0.36150900 -0.00003800 -0.00008200 C 0.98819600 -0.00001400 -0.00012900 S 1.82931800 -1.52451900 0.07530900 S 1.82915500 1.52459000 -0.77851600 C -2.60981800 -0.20213300 -0.778516000 C -2.60982000 -0.20135900 0.77866000 C -1.15382100 0.11576900 1.16759700
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 CH-0.20439100-0.59866900-2.09468300 HH-0.20525200-0.595347002.09593400 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.649715001.22799100-1.21821500 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.879061000.00033300 SS1.082722001.76635300-0.00086600 HH3.472705000.11010700-0.0005500Table 110. PDTC: (Anti geometry); E(B3LYP) = -1046.66557228 a.u.C-2.60986900-0.703071000.30892100 CC-2.609805000.70268600-0.30817600 CC-1.198907001.2192500-0.00323800 CC-1.19895300-1.219656000.0026460	InDistributionDistributionDistributionTable 11n. PDTC' (Syn geometry); $E(B3LYP) = -1046.66557228 a.u.$ C -2.60982400 0.70285600 0.30864200 C -2.60988100 -0.70288800 -0.30851800 C -1.19911400 -1.21952300 -0.00304100 C -1.19909400 1.21945700 0.00294700 H -3.38349500 1.35784200 -0.10126700 H -2.75980100 0.64002700 1.39286900 H -2.76002100 -0.64005400 -1.39272200 H -3.38350400 -1.35785800 0.10150600 H -1.14713100 -1.70495000 0.98005900 H -0.82281900 -1.93032700 -0.74098300 H -0.82267800 1.93028000 0.74081100 H -1.14724300 1.70484500 -0.98018000 N -0.36150900 -0.00003800 -0.00008200 C 0.98819600 -0.00001400 -0.00012900 S 1.82931800 -1.52451900 0.07530900 S 1.82915500 1.52459000 -0.77851600 C -2.60981800 -0.20213300 -0.77851600 C -2.60982000 -0.20135900 0.77866000 C -1.15382100 0.11576900 1.16778100
H-3.20023000-0.33418000-0.33411100Table 11m. MorDTCH (TSrot geometry, boat conformation); E(B3LYP) = -1122.29059003 a.u.N-0.01488700-0.768520000.00079400 CC-0.84235200-0.792408001.22965500 CC-2.010416000.192954001.18282400 OO-2.79529000-0.00735200-0.00033200 CC-2.009898000.19093400-1.18359200 CC-0.84185200-0.79442400-1.22835400 HH-1.23591100-1.81397500-1.32290900 CH-0.20439100-0.59866900-2.09468300 HH-0.20525200-0.595347002.09593400 HH-1.23655400-1.811776001.32559800 HH-2.679513000.022828002.03096400 HH-1.650099001.230029001.21593200 HH-2.678699000.01928000-2.03165600 CC1.098371000.111496000.00025300 SS2.55295500-0.879061000.00033300 SS1.082722001.76635300-0.00086600 HH3.472705000.11010700-0.0005500Table 110. PDTC: (Anti geometry); E(B3LYP) = -1046.66557228 a.u.C-2.60986900-0.703071000.30892100 CC-2.609805000.70268600-0.30817600 CC-1.19897001.2192500-0.00323800 CC-1.19895300-1.219656000.00264600<	InDistributionDistributionDistributionTable 11n. PDTC' (Syn geometry);E(B3LYP) = -1046.66557228 a.u.C-2.609824000.702856000.30864200C-2.60988100-0.70288800-0.30851800C-1.19911400-1.21952300-0.00304100C-1.199094001.219457000.00294700H-3.383495001.35784200-0.10126700H-2.759801000.640027001.39286900H-2.76002100-0.64005400-1.39272200H-3.38350400-1.357858000.10150600H-1.14713100-1.704950000.98005900H-0.82281900-1.93032700-0.74098300H-0.822678001.930280000.74081100H-1.147243001.70484500-0.98018000N-0.36150900-0.0001400-0.00012900S1.82931800-1.524519000.07530900S1.82931800-1.52459000-0.07524300Table 11p. PDTC' (TS _{rot} geometry);E(B3LYP) = -1046.63382496 a.u.C-2.60981800-0.20213300-0.77851600C-1.53821000.115769001.16759700C-1.153821000.115769001.16778100H-2.90801900-1.18226600-1.16232300

Π -3.36319000 1.35767600 0.10212100	$\Pi = -2.90790000 - 1.10112000 - 1.10345000$
H = -2.76038800 = 0.63979200 = 1.39230100	H = -3.29/93800 = 0.53943000 = 1.196/2900
H = -0.82318100 = 1.93005500 = -0.74147400	H = -1.01698800 - 1.19976400 - 1.31641600
H = -1.1463/300 -1.7046/200 -0.97984000	H = -0.82103100 - 0.39922100 - 2.07433700
H = -1.14/49900 - 1.70503400 - 0.98052300	H = -1.01690200 = 1.19835500 = 1.31774200
H = -0.82238200 - 1.93044500 - 0.74044200	H -0.82100800 -0.40145400 -2.0/393600
N -0.36141500 -0.00018100 -0.00075800	N -0.38469600 -0.35953500 0.00018700
C 0.98811200 0.00002500 -0.00023900	C 1.02681100 -0.04132400 0.00000100
S 1.82959800 -1.52421000 -0.07509000	S 1.52639200 1.59479700 -0.00038400
<u>S 1.82853700 1.52468300 0.07542200</u>	S 2.08507700 -1.37654400 0.00033900
Table 11q. PDTCH (Syn geometry);	Table 11r. PDTCH (Anti geometry);
E(B3LYP) = -1047.11719676 a.u.	E(B3LYP) = -1047.11719675 a.u.
C 2.62250400 -0.72720000 0.30054900	C -2.65540300 0.68871200 -0.29475800
C 2.65532300 0.68877200 -0.29497900	C -2.62240700 -0.72727800 0.30074400
C 1.25813600 1.23975200 0.00940300	C -1.20217700 -1.21035200 -0.01536700
C 1.20215300 -1.21031300 -0.01506100	C -1.25811600 1.23969500 0.00921800
Н 3.37854600 -1.39220200 -0.12314000	Н -2.81283200 0.64185800 -1.37784200
Н 2.77059800 -0.68862200 1.38507600	Н -3.43986400 1.31574500 0.13531300
Н 2.81237000 0.64182600 -1.37811800	Н -3.37858600 -1.39228300 -0.12268700
Н 3.43993800 1.31584700 0.13475700	Н -2.77016200 -0.68868200 1.38532700
Н 1.20336700 1.71048500 0.99801500	Н -0.81774400 -1.92074800 0.72114300
Н 0.89309900 1.95748800 -0.72751400	Н -1.14005900 -1.66736700 -1.01041700
Н 0.81787100 -1.92040100 0.72183500	Н -1.20309800 1.71066900 0.99769200
Н 1.13970900 -1.66767700 -1.00991500	Н -0.89323300 1.95727000 -0.72794600
N 0.39455400 0.03540000 0.00245600	N -0.39456400 0.03531600 0.00233100
C -0.93510800 0.09368800 0.00535200	C 0.93510600 0.09367600 0.00540200
S -1.73657800 -1.51333100 -0.06661700	S 1.73673300 -1.51326300 -0.06657600
S -1.82938100 1.53157600 0.06564500	S 1.82922400 1.53164600 0.06565400
Н -2.98007400 -1.00466900 -0.03421400	Н 2.98018500 -1.00452600 -0.03358000
	Table Ot Drup DTC (Same as a matura)
Table 95. PDICH (IS geometry): $E(B3LYP) =$	Table 91. PVrD1C ⁻ (SVn geometry):
Table 95. PDTCH (15 geometry); $E(B3LYP) = -1047.08200641 au$	F(B3LVP) = -1044 22918859 a u
Table 95. PDTCH (15 geometry); $E(B3LYP) = -1047.08200641 a.u.$	E(B3LYP) = -1044.22918859 a.u.
Table 95. PDTCH (TS geometry); $E(B3LYP) =$ -1047.08200641 a.u. C -2.63347200 -0.18905900 -0.77838200 C -2.63341100 -0.19057500 0.77838600	Fable 91. PyrD1C (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C 1.33574700 -1.12860000 0.05514000 C 2.64248700 -0.71779200 0.03631300
Table 95. PDTCH (TS geometry); $E(B3LYP) =$ -1047.08200641 a.u. C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -118706700 0.15216400 117662800	Table 91. PyrD1C (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C1.33574700 -1.12860000 0.05514000C2.64248700 -0.71779200 0.03631300C1.33573800 1.12859100 -0.05509300
Table 95. PDTCH (TS geometry); $E(B3LYP) =$ -1047.08200641 a.u. C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C 1.18714500 0.15201000 1.17662800	Table 91. PyrD1C (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 - 1.12860000 0.05514000$ C $2.64248700 - 0.71779200 0.03631300$ C $1.33573800 1.12859100 - 0.05509300$ N $0.51256100 - 0.0001300 - 0.00001100$
Table 95. PDTCH (TS geometry); $E(B3LYP) =$ -1047.08200641 a.u. C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H 2.91344100 1.17354200 1.16296000	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 - 1.12860000 0.05514000$ C $2.64248700 - 0.71779200 0.03631300$ C $1.33573800 1.12859100 - 0.05509300$ N $0.51256100 - 0.00001200 - 0.00001100$ H $0.89498000 - 211149200 - 0.10715400$
Table 95. PDTCH (15 geometry); $E(B3LYP) =$ -1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.16296000H-2.91344100-1.17354200-1.16296000H-2.92260000.540436001.19613500	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 - 1.12860000 0.05514000$ C $2.64248700 - 0.71779200 0.03631300$ C $1.33573800 1.12859100 - 0.05509300$ N $0.51256100 - 0.00001200 - 0.00001100$ H $0.89948000 - 2.11149300 0.10715400$ H $2.5710500 - 1.36704100 0.077184700$
Table 95. PDTCH (15 geometry); $E(B3LYP) =$ -1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.16296000H-2.91344100-1.17354200-1.19613500H-2.912714001.175955001.1611100	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C1.33574700C2.64248700-0.717792000.03631300C1.335738001.12859100-0.05509300N0.51256100-0.00001200-0.00001100H0.89948000-2.111493000.10715400H3.50710500-1.367041000.07194700H0.89452002.111485000.10704200
Table 95. PDTCH (15 geometry); $E(B3LYP) =$ -1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.16296000H-2.91344100-1.17354200-1.16296000H-2.91271400-1.175955001.16101100H-332707000.537754001.1963400	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C1.33574700C2.64248700-0.717792000.03631300C1.335738001.12859100-0.05509300N0.51256100-0.00001200-0.00001100H0.89948000-2.111493000.10715400H3.50710500-1.367041000.07194700H0.899452002.11148500-0.10704200C-0.90933500-0.00001400-0.00001100
Table 95. PDTCH (15 geometry); $E(B3LYP) =$ -1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.17641700H-2.91344100-1.17354200-1.16296000H-3.332609000.54043600-1.19613500H-2.91271400-1.175955001.16101100H-3.332707000.537754001.19762400H-1.063317001.325866001.32454800	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C 1.33574700 C 2.64248700 -0.71779200 0.03631300 C 1.33573800 1.12859100 -0.05509300 N 0.51256100 -0.00001200 -0.00001100 H 0.89948000 -2.11149300 0.10715400 H 3.50710500 -1.36704100 0.07094700 H 0.89945200 2.11148500 -0.00001100 S -1.70891200 -1.50994000 -0.0335800
Table 95. PDTCH (15 geometry); E(B3LYP) = -1047.08200641 a.u.C -2.63347200 C -2.63331100 -0.19057500 0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.32454800 H -0.84269000 0.84269000 2.07706600	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C 1.33574700 C 2.64248700 -0.71779200 0.03631300 C 1.33573800 1.12859100 -0.05509300 N 0.51256100 -0.00001200 -0.00001100 H 0.89948000 -2.11149300 0.10715400 H 3.50710500 -1.36704100 0.07194700 H 0.89945200 2.11148500 -0.10704200 C -0.90933500 -0.0000400 -0.00001100 S -1.70891200 -1.70892500 1.50994000 -0.3535800
Table 95. PDTCH (TS geometry); E(B3LYP) = -1047.08200641 a.u.C -2.63347200 C -2.63331100 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.19762400 H -1.06331700 1.23586600 1.32454800 H -0.84368000 -0.84368000 -132281200	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.0000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$
Table 95. PDTCH (TS geometry); E(B3LYP) = -1047.08200641 a.u.C -2.63347200 C -2.63331100 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.19762400 H -1.06331700 1.23586600 1.32454800 H -0.84368000 -0.36390000 2.07706600 H -1.06320200 1.23779600 -1.32281200	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.0000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1 136697000 -0.07198900$
Table 95. PDTCH (TS geometry); E(B3LYP) = -1047.08200641 a.u.C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.19762400 H -1.06331700 1.23586600 1.32454800 H -0.84368000 -0.36390000 2.07706600 H -1.0632200 1.23779600 -1.32281200 H -0.84389500 -0.36095700 -2.07758400	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C 1.33574700 C 1.33574700 C 2.64248700 0.71779200 0.03631300 C 1.33573800 1.12859100 -0.05509300 N 0.51256100 0.00001200 -0.00001100 H 0.89948000 2.11149300 0.10715400 H 3.50710500 2.11148500 -0.10704200 C -0.90933500 0.0000400 -0.00001100 S -1.70891200 1.50994000 -0.3535800 S -1.70882500 L70774600 -0.03634200 H 3.50710400 1.36697000 -0.07198900
Table 95. PDTCH (TS geometry); E(B3LYP) = -1047.08200641 a.u.C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.19762400 H -1.06331700 1.23586600 1.32454800 H -0.84368000 -0.36390000 2.07706600 H -0.84389500 -0.36095700 -2.07758400 N -0.40520700 -0.30331300 -0.00026600	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.00000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1.36697000 -0.07198900$
Table 95. PDTCH (TS geometry); E(B3LYP) = -1047.08200641 a.u.C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.19762400 H -1.06331700 1.23586600 1.32454800 H -0.84368000 -0.36390000 2.07706600 H -0.84389500 -0.36095700 -2.07758400 N -0.40520700 -0.30331300 -0.00026600 C 0.97038800 0.05202500 -0.0003900 S 191877000 -142498500 -0.00054900	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.00000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1.36697000 -0.07198900$
Table 95. PDTCH (TS geometry); E(B3LYP) = -1047.08200641 a.u.C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.19762400 H -1.06331700 1.23586600 1.32454800 H -0.84368000 -0.36390000 2.07706600 H -0.84389500 -0.36095700 -2.07758400 N -0.40520700 -0.30331300 -0.00026600 C 0.97038800 0.05202500 -0.0003900 S 1.91877000 -1.42498500 -0.00054900	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.00000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1.36697000 -0.07198900$
Table 95. PDTCH (TS geometry); E(B3LYP) = -1047.08200641 a.u.C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.19762400 H -1.06331700 1.23586600 1.32454800 H -0.84368000 -0.36390000 2.07706600 H -1.06320200 1.23779600 -1.32281200 H -0.84389500 -0.30331300 -0.00026600 C 0.97038800 0.05202500 -0.0003900 S 1.91877000 -1.42498500 -0.00054900 S 1.58237200 1.58993300 0.00059800 H 314738000 -0.86431900 -0.00014600	Table 91. PyrD1C* (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C1.33574700C2.64248700-0.717792000.03631300C1.335738001.12859100-0.05509300N0.51256100-0.00001200-0.00001100H0.89948000-2.111493000.10715400H3.50710500-1.367041000.07194700H0.899452002.11148500-0.10704200C-0.90933500-0.0000400-0.00001100S-1.70891200-1.50994000-0.03535800S-1.70882500L708825001.509972000.03535600C2.642486000.71774600-0.07198900
Table 9S. PDTCH (TS geometry); E(B3LYP) = -1047.08200641 a.u. C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.32454800 H -0.84368000 -0.36390000 2.07706600 H -1.06320200 1.23779600 -1.32281200 H -0.84389500 -0.30331300 -0.00026600 C 0.97038800 0.05202500 -0.0003900 S 1.91877000 -1.42498500 -0.00054900 S 1.58237200 1.58993300 0.00059800 H 3.14738000 -0.86431900 -0.0014600	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C1.33574700C1.33574700C2.64248700-0.717792000.03631300C1.335738001.12859100-0.05509300N0.51256100-0.00001200-0.00001100H0.89948000-2.111493000.10715400H3.50710500-1.367041000.07194700H0.899452002.11148500-0.10704200C-0.90933500-0.0000400-0.00001100S-1.70891200-1.708825001.50994000-0.3535600C2.64248600O.71774600-0.03634200H3.507104001.36697000-0.07198900
Table 9S. PDTCH (TS geometry); E(B3LYP) = -1047.08200641 a.u. C -2.63347200 -0.18905900 -0.77838200 C -2.63331100 -0.19057500 0.77828600 C -1.18706700 0.15216400 1.17662800 C -1.18714500 0.15391900 -1.17641700 H -2.91344100 -1.17354200 -1.16296000 H -3.33260900 0.54043600 -1.19613500 H -2.91271400 -1.17595500 1.16101100 H -3.33270700 0.53775400 1.19762400 H -1.06331700 1.23586600 1.32454800 H -0.84368000 -0.36390000 2.07706600 H -1.06320200 1.23779600 -1.32281200 H -0.84389500 -0.30331300 -0.00026600 C 0.97038800 0.05202500 -0.00003900 S 1.91877000 -1.42498500 -0.00054900 S 1.58237200 1.58993300 0.00059800 H 3.14738000 -0.86431900 -0.0014600 Table 11u. PyrDTC	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 - 1.12860000 0.05514000$ C $2.64248700 - 0.71779200 0.03631300$ C $1.33573800 1.12859100 - 0.05509300$ N $0.51256100 - 0.00001200 - 0.00001100$ H $0.89948000 - 2.11149300 0.10715400$ H $3.50710500 - 1.36704100 0.07194700$ H $0.89945200 2.11148500 - 0.10704200$ C $-0.90933500 - 0.0000400 - 0.00001100$ S $-1.70891200 - 1.50994000 - 0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 - 0.03634200$ H $3.50710400 1.36697000 - 0.07198900$ H $3.50710400 1.36697000 - 0.07198900$
Table 95. PDTCH (TS geometry); E(B3LYP) =-1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.17641700H-2.91344100-1.17354200-1.16296000H-3.332609000.54043600-1.19613500H-2.91271400-1.175955001.16101100H-3.332707000.537754001.19762400H-1.063317001.235866001.32454800H-0.84368000-0.363900002.07706600H-1.063202001.23779600-1.32281200H-0.84389500-0.30331300-0.00026600C0.970388000.05202500-0.0003900S1.91877000-1.42498500-0.00054900S1.582372001.589933000.00059800H3.14738000-0.86431900-0.0014600Table 11u. PyrDTC (Anti geometry);E(B3LYP) = -1044.22918841 a.u.C-1.335717001.128801000.05434500	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 - 1.12860000 0.05514000$ C $2.64248700 - 0.71779200 0.03631300$ C $1.33573800 1.12859100 - 0.05509300$ N $0.51256100 - 0.00001200 - 0.00001100$ H $0.89948000 - 2.11149300 0.10715400$ H $3.50710500 - 1.36704100 0.07194700$ H $0.89945200 2.11148500 - 0.10704200$ C $-0.90933500 - 0.0000400 - 0.00001100$ S $-1.70891200 - 1.50994000 - 0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 - 0.03634200$ H $3.50710400 1.36697000 - 0.07198900$ H $3.50710400 1.36697000 - 0.07198900$
Table 95. PDTCH (TS geometry); E(B3LYP) =-1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.17641700H-2.91344100-1.17354200-1.16296000H-3.332609000.54043600-1.19613500H-2.91271400-1.175955001.16101100H-3.332707000.537754001.19762400H-1.063317001.235866001.32454800H-0.84368000-0.363900002.07706600H-1.063202001.23779600-1.32281200H-0.84389500-0.36095700-2.07758400N-0.40520700-0.30331300-0.00026600C0.970388000.05202500-0.0003900S1.91877000-1.42498500-0.00054900S1.582372001.589933000.00059800H3.14738000-0.86431900-0.0014600Table 11u. PyrDTC- (Anti geometry);E(B3LYP) = -1044.22918841 a.u.C-1.335717001.128801000.05434500C-2.642479000.717938000.03627500	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 - 1.12860000 0.05514000$ C $2.64248700 - 0.71779200 0.03631300$ C $1.33573800 1.12859100 - 0.05509300$ N $0.51256100 - 0.00001200 - 0.00001100$ H $0.89948000 - 2.11149300 0.10715400$ H $3.50710500 - 1.36704100 0.07194700$ H $0.89945200 2.11148500 - 0.10704200$ C $-0.90933500 - 0.0000400 - 0.00001100$ S $-1.70891200 - 1.50994000 - 0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 - 0.03634200$ H $3.50710400 1.36697000 - 0.07198900$ H $3.50710400 1.36697000 - 0.07198900$ C $1.30959300 0.00016100 - 1.12394000$ C $2.63109400 0.00011500 - 0.71320900$
Table 95. PDTCH (15 geometry); E(B3LYP) =-1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.17641700H-2.91344100-1.17354200-1.16296000H-3.332609000.54043600-1.19613500H-2.91271400-1.175955001.16101100H-3.332707000.537754001.19762400H-1.063317001.235866001.32454800H-0.84368000-0.363900002.07706600H-1.063202001.23779600-1.32281200H-0.84389500-0.36095700-2.07758400N-0.40520700-0.30331300-0.00026600C0.970388000.05202500-0.0003900S1.91877000-1.42498500-0.00054900S1.582372001.589933000.00059800H3.14738000-0.86431900-0.0014600Table 11u. PyrDTC- (Anti geometry);E(B3LYP) = -1044.22918841 a.u.C-1.335717001.128801000.05434500C-2.642479000.717938000.03627500C-1.33573800-1.12849600-0.05466000	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.0000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1.36697000 -0.07198900$ H $3.50710400 1.36697000 -0.07198900$ C $1.30959300 0.00016100 -1.12394000$ C $2.63109400 0.00011500 -0.71320900$ C $2.63109400 0.00011400 112387700$
Table 95. PDTCH (TS geometry); E(B3LYP) =-1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.17641700H-2.91344100-1.17354200-1.16296000H-3.332609000.54043600-1.19613500H-2.91271400-1.175955001.16101100H-3.332707000.537754001.19762400H-1.063317001.235866001.32454800H-0.84368000-0.363900002.07706600H-1.063202001.23779600-1.32281200H-0.84389500-0.30331300-0.00026600C0.970388000.05202500-0.0003900S1.91877000-1.42498500-0.00054900S1.582372001.589933000.00059800H3.14738000-0.86431900-0.0014600Table 11u. PyrDTC (Anti geometry);E(B3LYP) = -1044.22918841 a.u.C-1.335717001.128801000.05434500C-2.642479000.71793800-0.05466000N-0.512548000.00015300-0.0049900	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.0000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1.36697000 -0.07198900$ H $3.50710400 1.36697000 -0.07198900$ C $1.30959300 0.00016100 -1.12394000$ C $2.63109400 0.00011500 -0.71320900$ C $1.30939900 -0.00011400 1.12387700$ N $0.51152100 0.0002500 -0.00011200$
Table 9S. PDTCH (TS geometry); E(B3LYP) =-1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.17641700H-2.91344100-1.17354200-1.16296000H-3.332609000.54043600-1.19613500H-2.91271400-1.175955001.16101100H-3.332707000.537754001.19762400H-1.063317001.235866001.32454800H-0.84368000-0.363900002.07706600H-1.063202001.23779600-1.32281200H-0.84389500-0.30331300-0.00026600C0.970388000.05202500-0.0003900S1.91877000-1.42498500-0.00054900S1.582372001.589933000.00059800H3.14738000-0.86431900-0.0014600Table 11u. PyrDTC (Anti geometry);E(B3LYP) = -1044.22918841 a.u.C-1.335717001.128801000.05434500C-1.33573800-1.12849600-0.05466000N-0.512548000.00015300-0.00049900H-0.89360002.111736000.10531200	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.00000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1.36697000 -0.07198900$ H $3.50710400 1.36697000 -0.07198900$ C $1.30959300 0.00016100 -1.12394000$ C $2.63109400 0.00011500 -0.71320900$ C $1.30959300 0.00011400 1.12387700$ N $0.51152100 0.0002500 -0.00011200$ H $0.86995300 0.00028600 -2 11052300$
Table 9S. PDTCH (TS geometry); E(B3LYP) =-1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.16296000H-2.91344100-1.17354200-1.16296000H-3.332609000.54043600-1.19613500H-2.91271400-1.175955001.16101100H-3.332707000.537754001.19762400H-1.063317001.235866001.32454800H-0.84368000-0.363900002.07706600H-1.063202001.23779600-1.32281200H-0.84389500-0.36095700-2.07758400N-0.40520700-0.30331300-0.00026600C0.970388000.05202500-0.0003900S1.91877000-1.42498500-0.00054900S1.582372001.589933000.00059800H3.14738000-0.86431900-0.0014600Table 11u. PyrDTC: (Anti geometry);E(B3LYP) = -1044.22918841 a.u.C-1.335717001.128801000.05434500C-1.33573800-1.12849600-0.05466000N-0.512548000.00015300-0.00049900H-0.89360002.111736000.10531200H-3.507074001.367253000.07173100	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.00000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1.36697000 -0.07198900$ H $3.50710400 1.36697000 -0.07198900$ C $1.30959300 0.00016100 -1.12394000$ C $2.63109400 0.00011500 -0.71320900$ C $1.30939900 -0.00011400 1.12387700$ N $0.51152100 0.0002500 -0.00011200$ H $3.49381000 0.00023500 -1 36596600$
Table 95. PDTCH (TS geometry); E(B3LYP) =-1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.17641700H-2.91344100-1.17354200-1.16296000H-3.332609000.54043600-1.19613500H-2.91271400-1.175955001.16101100H-3.332707000.537754001.19762400H-1.063317001.235866001.32454800H-0.84368000-0.363900002.07706600H-1.063202001.23779600-1.32281200H-0.84389500-0.36095700-2.07758400N-0.40520700-0.30331300-0.00026600C0.970388000.05202500-0.0003900S1.91877000-1.42498500-0.00054900S1.582372001.589933000.00059800H3.14738000-0.86431900-0.0014600Table 11u. PyrDTC- (Anti geometry);E(B3LYP) = -1044.22918841 a.u.C-1.335717001.128801000.05434500C-2.642479000.717938000.03627500C-1.33573800-1.12849600-0.05466000N-0.512548000.00015300-0.00049900H-0.899360002.111736000.10531200H-0.89941500-2.1142500-0.10626800 <td>Table 91. PyrDTC (Syn geometry);$E(B3LYP) = -1044.22918859 a.u.C1.33574700 -1.12860000 0.05514000C2.64248700 -0.71779200 0.03631300C1.33573800 1.12859100 -0.05509300N0.51256100 -0.00001200 -0.00001100H0.89948000 -2.11149300 0.10715400H3.50710500 -1.36704100 0.07194700H0.89945200 2.11148500 -0.10704200C-0.90933500 -0.0000400 -0.00001100S-1.70891200 -1.50994000 -0.03535800S-1.70882500 1.50997200 0.03535600C2.64248600 0.71774600 -0.03634200H3.50710400 1.36697000 -0.07198900H3.50710400 1.36697000 -0.07198900C1.30959300 0.00016100 -1.12394000C2.63109400 0.00011500 -0.71320900C1.30939900 -0.00011400 1.12387700N0.51152100 0.0002500 -0.00011200H3.49381000 0.0002500 -1.36596600H0.86955600 -0.00022000 2 11037100$</td>	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.0000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1.36697000 -0.07198900$ H $3.50710400 1.36697000 -0.07198900$ C $1.30959300 0.00016100 -1.12394000$ C $2.63109400 0.00011500 -0.71320900$ C $1.30939900 -0.00011400 1.12387700$ N $0.51152100 0.0002500 -0.00011200$ H $3.49381000 0.0002500 -1.36596600$ H $0.86955600 -0.00022000 2 11037100$
Table 9S. PDTCH (TS geometry); E(B3LYP) =-1047.08200641 a.u.C-2.63347200-0.18905900-0.77838200C-2.63331100-0.190575000.77828600C-1.187067000.152164001.17662800C-1.187145000.15391900-1.17641700H-2.91344100-1.17354200-1.16296000H-3.332609000.54043600-1.19613500H-2.91271400-1.175955001.16101100H-3.332707000.537754001.19762400H-1.063317001.235866001.32454800H-0.84368000-0.363900002.07706600H-1.063202001.23779600-1.32281200H-0.84389500-0.36095700-2.07758400N-0.40520700-0.30331300-0.00026600C0.970388000.05202500-0.0003900S1.91877000-1.42498500-0.00054900S1.582372001.589933000.00059800H3.14738000-0.86431900-0.0014600Table 11u. PyrDTC (Anti geometry);E(B3LYP) = -1044.22918841 a.u.C-1.335717001.128801000.05434500C-2.642479000.717938000.03627500C-1.33573800-1.12849600-0.05466000N-0.512548000.00015300-0.00049900H-0.899360002.111736000.10531200H-0.89941500-2.11142500-0.10626800C<	Table 91. PyrDTC (Syn geometry); $E(B3LYP) = -1044.22918859 a.u.$ C $1.33574700 -1.12860000 0.05514000$ C $2.64248700 -0.71779200 0.03631300$ C $1.33573800 1.12859100 -0.05509300$ N $0.51256100 -0.00001200 -0.00001100$ H $0.89948000 -2.11149300 0.10715400$ H $3.50710500 -1.36704100 0.07194700$ H $0.89945200 2.11148500 -0.10704200$ C $-0.90933500 -0.0000400 -0.00001100$ S $-1.70891200 -1.50994000 -0.03535800$ S $-1.70882500 1.50997200 0.03535600$ C $2.64248600 0.71774600 -0.03634200$ H $3.50710400 1.36697000 -0.07198900$ H $3.50710400 1.36697000 -0.07198900$ C $1.30959300 0.00016100 -1.12394000$ C $2.63109400 0.00011500 -0.71320900$ C $1.30939900 -0.00011400 1.12387700$ N $0.51152100 0.0002500 -0.00011200$ H $3.49381000 0.00023500 -1.36596600$ H $0.86955600 -0.00022000 2.11037100$ C $-0.94437200 0.00000000 -0.00006900$

S 1.70920500 1.52203900 -1.52203900 -0.0000000 C -2.64245600 -0.716400 -0.0352100 -0.000013400 1.36630100 Table 11x PyrDTCH (Antigeometry); E[B3LYP] = -1044.66900297 a.u. E[B3LYP] = -1044.66900297 a.u. C 1.3665300 -1.12504400 0.05550800 C 2.68291000 0.6956290 -0.02614600 C 2.64559200 0.74448300 0.0330800 C 2.86291000 0.6956290 -0.03536600 C 0.43964200 0.1474700 0.0537600 1.12566100 0.0537600 H 0.89739400 -2.14215300 0.10174700 0.0537600 0.0237600 0.0237600 H 0.3867400 0.0337600 C 0.48973900 0.938400 0.0042700 H 0.38671700 0.037600 1.4248400 0.0378600 1.4248400 0.0433900 C 0.4887400 0.037854700 0.03786700 1.428700 0.0378600 H 0.386714600 1.4448400 0.03786100 1.4287900<	4 50000500 4 50005000 0.00440000	4 (0510000 1 5000000 0 0000000
$ \begin{array}{c} c & -2.64249600 & -0.71766400 & -0.03552100 \\ H & -3.602900 & -1.3669200 & -0.0761700 \\ H & -3.602900 & -1.3669200 & -0.761700 \\ H & -3.602900 & -0.7646900285 a.u. \\ \hline Table 11x. PyrDTCH (Syn geometry); \\ E(B3LYP) = -1044.66900285 a.u. \\ E(B3LYP) = -1044.66900285 a.u. \\ C & 1.33665300 & -1.12502400 & 0.0350800 \\ C & 2.64559200 & -0.74448300 & 0.03103800 \\ C & 2.64559200 & -0.74448300 & 0.03103800 \\ C & 2.64559200 & -0.74448300 & 0.03103800 \\ C & 1.336900 & -1.02502300 & -0.05569700 \\ N & 0.53965200 & 0.03501500 & 0.00490100 \\ N & 0.53965200 & 0.03501500 & 0.00490100 \\ N & 0.53965200 & 0.03501500 & 0.00490100 \\ H & 0.9868800 & 2.1477700 & -0.0057600 \\ H & 0.8968800 & 2.14714100 & -0.09559000 \\ H & 0.8973900 & -2.1077900 & 0.11660300 \\ C & -0.8433900 & 0.09854700 & 0.00426100 \\ C & -0.8433900 & 0.09854700 & 0.00426100 \\ C & -0.8433900 & 0.09854700 & 0.00426100 \\ C & 2.6451200 & 1.52276400 & 0.0330400 \\ S & -1.62992700 & 1.52266400 & 0.0330400 \\ S & -1.6992700 & 1.5227000 & 0.01589300 \\ H & -3.8692700 & 0.99831800 & 0.01589300 \\ H & -2.86992700 & 0.99831800 & 0.01589300 \\ H & -2.86992700 & 0.99831800 & 0.01589300 \\ H & -2.86992700 & 0.99831800 & 0.01589300 \\ L & -2.86992700 & 0.03667800 & -0.0000800 \\ C & 1.34442200 & 0.02560300 & 1.13224200 \\ C & 1.36419700 & 0.03667800 & -0.0000800 \\ S & -1.7000 & 0.3667800 & -0.0000800 \\ R & 0.90116400 & 0.0367800 & 0.71442600 \\ C & 2.6542130 & 0.0367800 & 0.71442600 \\ C & 2.6542130 & 0.0367800 & -0.0000800 \\ S & -1.56286800 & -1.52153900 & 0.007960 & 0.0007300 & 0.00080300 \\ S & -1.56286800 & -1.5642500 & 0.757800 \\ C & -2.858920 & 0.077660 & 0.00004200 \\ S & -1.5628600 & -0.5581000 \\ S & -1.56286800 & -1.5642700 & 0.05381000 \\ C & -2.859200 & 0.0757600 & 0.0074900 \\ H & 0.90114900 & 0.0367800 & 0.07477300 \\ C & -2.369200 & 0.0776780 & 0.00021600 \\ S & -1.56286800 & -1.5642700 & 0.0758200 \\ C & -2.5642030 & 0.07448260 & 0.777300 \\ S & -1.56286800 & -1.5647800 \\ N & 0.52095700 & 0.00338000 \\ C & -1.3612100 & 0.04975500 \\ C & -1.36127300 & 0.1564900 \\ H & -9.95168400 & -$	5 1.70920500 1.50985300 -0.03443800	5 -1.68519200 -1.52203900 -0.00008000
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	C -2.64249600 -0.71766400 -0.03552100	C 2.63097700 -0.00009700 0.71339300
	Н -3.50709900 -1.36698700 -0.07061700	Н 3.49358000 -0.00013400 1.36630100
$ \begin{array}{l l l l l l l l l l l l l l l l l l l $	Table 11y PurDTCH (Sun geometry)	Table 117 PurDTCH (Anti geometry):
	Table IIX. Tyrd fell (Syn geometry),	Table 112. Tyrb fell (And geometry),
$ \begin{array}{c} C & 1.33665300 & -1.12502400 & 0.05350800 & C & 1.39676800 & 1.14764700 & -0.05025300 \\ C & 1.3565100 & 1.14772400 & -0.04800300 & C & 1.33665900 & -1.12506100 & 0.05569700 \\ N & 0.53965200 & 0.03501500 & 0.00490100 & N & 0.53864200 & 0.03618600 \\ L & 0.98739400 & -2.10791700 & 0.11166800 & H & 0.98651900 & 2.14215300 & -0.10017200 \\ H & 0.9868800 & 2.1421400 & -0.09559000 & H & 0.89736900 & -2.1077870 & 0.11660300 \\ C & -0.84333000 & 0.09854700 & 0.00426100 & C & -0.84339900 & 0.09848400 & 0.00462700 \\ S & -1.62362200 & 1.4987400 & -0.03302400 & S & -1.63998700 & 1.52270400 & 0.03159400 \\ C & 2.6831000 & 0.05956100 & 0.03475600 & 2.04552600 & 0.74445400 & 0.03319400 \\ H & 3.56735200 & 1.31659300 & 0.05969300 & H & 2.87004500 & -0.9887550 & 0.06401700 \\ H & -2.86992700 & -0.99831800 & 0.01599300 & H & 2.87004500 & -0.99837500 & 0.0164800 \\ Table 11aa. PyrDTCH (TS_{ret} geometry); \\ E(B3LYP) = -1044.65456892 a.u. \\ C & 1.34145200 & 0.0366200 & 1.13224200 & C & 1.3660300 & 1.11404900 & 0.08205700 \\ C & 2.6542130 & 0.00366200 & 0.71442600 & C & 2.6388400 & 0.62114600 & 0.04601708 \\ H & 0.90116400 & 0.03766100 & 2.11801500 & H & 0.9737520 & 2.11326700 & 0.089205700 \\ C & 0.0549100 & 0.03667800 & -0.0000800 & N & 0.5205500 & 0.0070400 & 0.0315500 \\ H & 0.90116400 & 0.03766100 & 2.11801500 & H & 0.97375200 & 2.10563900 & -0.05881000 \\ S & -1.6280800 & -1.5153900 & 0.0002100 & C & -0.91478900 & 0.00730700 & 0.0089300 \\ S & -1.6280800 & 0.52112100 & 0.0047100 & T.36454900 \\ C & -2.63893600 & 0.51130500 & 0.0047100 & C & 2.62673700 & -0.0034400 & 1.1344200 \\ C & -2.63893600 & 0.71443200 & 0.03746000 & C & -1.34202100 & -0.0032400 & 1.1344200 \\ C & -2.63893600 & 0.71443200 & C & 1.36901700 & L51978500 & -0.048805200 \\ S & -1.65901700 & 1.51673500 & -0.00777300 & C & 2.62673700 & -0.0034400 & 1.10941000 \\ N & -0.52098700 & 0.0069500 & 0.0319900 & N & 5.1893000 & 0.00730700 & 0.00833000 \\ C & -2.62893000 & 0.62121200 & 0.00777300 & S & -1.63901700 & 0.15244000 \\ H & -3.5666700 & 1.07484 a.u. \\ C & 1.33661100 & 1.11$	E(B3LYP) = -1044.66900285 a.u.	E(B3LYP) = -1044.66900297 a.u.
	C 1.33665300 -1.12502400 0.05350800	C 1.39676800 1.14764700 -0.05025300
$ \begin{array}{c} c & 1.37691500 & 1.14772400 & 0.04800300 \\ c & 1.33665900 & 1.12506100 & 0.03509700 \\ N & 0.53965200 & 0.03501500 & 0.0490100 \\ H & 0.8739400 & 2.10791700 & 0.1168000 \\ H & 0.8739400 & 2.10791700 & 0.1168000 \\ H & 0.9861800 & 2.14211300 & 0.00537600 \\ H & 0.89739400 & 2.10791700 & 0.1168000 \\ C & -0.84334000 & 0.09854700 & 0.00426100 \\ C & -0.8430000 & 0.09854700 & 0.00426100 \\ C & 2.6810000 & 0.69569100 & -0.03275600 \\ C & 2.6810000 & 0.69569100 & -0.03475600 \\ C & 2.6810000 & 0.69569100 & -0.03475600 \\ C & 2.6810000 & 0.69569100 & -0.03475600 \\ C & 2.6810000 & 0.06569100 & -0.03475600 \\ C & 2.6452200 & -0.74445400 & 0.03234900 \\ H & 3.49444600 & -1.41305800 & 0.04046100 \\ H & -2.80992700 & -0.99831800 & 0.01589300 \\ H & -2.87094500 & -0.99837800 & 0.148600 \\ C & 1.34143500 & 0.02560300 & 1.13224200 \\ C & 2.6421300 & 0.00366700 & -1.1422400 \\ C & 2.6389400 & 0.672405800 & 0.13224200 \\ C & 1.34143300 & 0.02460600 & -1.13224500 \\ C & 1.34143300 & 0.02460600 & -1.13224500 \\ C & 1.34143300 & 0.03667800 & -0.00000800 \\ N & 0.52095600 & 0.0700400 & 0.00315500 \\ H & 0.90112400 & 0.03667800 & -0.00000800 \\ N & 0.52095600 & 0.0700400 & 0.00315500 \\ H & 0.90112400 & 0.03667800 & -0.00000800 \\ S & -1.71000900 & 1.51673500 & -0.0002400 \\ S & -1.5628600 & -1.52153900 & 0.0002100 \\ C & -2.63893500 & 0.0397660 & 0.0002100 \\ C & -2.63893500 & 0.03667800 & -0.0024600 \\ S & -1.69520300 & -1.50474500 & 0.0482000 \\ C & -2.6389360 & 0.62112100 & 0.00032500 \\ C & -2.6389360 & 0.62112100 & 0.00032100 \\ C & -2.6389360 & 0.62112100 & 0.00047100 \\ H & -3.51816400 & -0.01497070 & -1.34564000 \\ H & -3.51816400 & -0.01497700 \\ C & -2.6389360 & 0.62112100 & 0.00777300 \\ C & -2.6389360 & 0.62112100 & 0.00778700 \\ C & -2.6389360 & 0.62112100 & 0.00778700 \\ C & -2.6389360 & 0.62112100 & 0.00778700 \\ C & -2.6389360 & 0.62114200 & 0.05758600 \\ N & -0.52987700 & -0.05758700 \\ C & -2.6389360 & 0.00319900 \\ N $	C = 2.64559200 -0.74448300 -0.03103800	C = 2.68291000 - 0.69562900 - 0.03618600
$ \begin{array}{llllllllllllllllllllllllllllllllllll$	L 1.39691500 1.14//2400 -0.04800300	L 1.33665900 -1.12506100 0.05569/00
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	N 0.53965200 0.03501500 0.00490100	N 0.53964200 0.03490100 0.00537600
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н 0.89739400 -2.10791700 0.11168000	Н 0.98651900 2.14215300 -0.10017200
H 0.98688800 2.14241400 0.09559000 H 0.89736900 2.10778700 0.11660300 C -0.8433000 0.09854700 0.00426100 C -0.84339900 0.0048400 0.00462700 S -1.6236200 1.5226400 0.0330400 S -1.62374700 0.30378500 C 2.64932000 0.6956910 0.3032400 S -1.62374700 0.03475600 H 3.56735200 1.31659300 -0.0669300 H 3.49444600 -0.4135800 0.0648000 H 3.26992700 -0.99837800 0.01589300 H -2.87045500 0.99837500 0.01648600 C 1.34143200 0.02560300 1.13224200 C 1.3660300 1.1414900 0.08205700 C 1.34143300 0.0248060 -1.13224500 C 2.58384000 0.0709600 0.0001600 N 5.2955600 0.0709600 0.00315500 C 1.34143200 0.03667800 -2.18019100 H 0.95155500 2.09445200 0.1	Н 349442100 -141325700 006148300	Н 3.56716900 1.31642100 -0.07259100
11 0.0303000 2.1421400 0.009854700 0.00426100 12 0.03854700 0.0032500 1.62373700 0.03159400 12 0.03654700 0.0032400 S -1.62373700 0.03159400 13 0.0565200 1.3226400 0.0330400 S -1.62377500 0.03159400 14 -2.86992700 0.099831800 0.01589300 H -3.4944400 0.03234900 14 -2.86992700 0.099831800 0.01589300 H -2.87004500 -0.99837500 0.06401700 15 0.1521700 0.03264900 1.13224200 C 1.36603000 0.21798825 a.u. 15 0.03586200 0.71442600 C 2.6384400 0.6214600 0.04608900 134143200 0.03667800 -0.0000800 N 0.52095600 0.0070400 0.0319500 14 0.90112800 0.03667800 -0.0000800 N 0.52095600 0.0070400 0.0319500 14 0.9112800 0.03667800 0.00042100 <td< td=""><td>H = 0.08688800 2.14241400 0.00550000</td><td>H = 0.80736000 - 2.10778700 - 0.11660300</td></td<>	H = 0.08688800 2.14241400 0.00550000	H = 0.80736000 - 2.10778700 - 0.11660300
$ \begin{array}{c} c & -0.84333900 & 0.078597400 & 0.003602000 \\ s & -1.62366200 & -1.49887400 & 0.003602000 \\ s & -1.6236200 & -1.498877500 & -0.03780500 \\ c & 2.68310000 & 0.069569100 & -0.03475600 \\ c & 2.68310000 & 0.069569100 & -0.03475600 \\ c & 2.68310000 & 0.069569100 & -0.03475600 \\ c & 2.6892700 & -0.99831800 & 0.0159300 \\ d & -2.87004500 & -0.74445400 & 0.03234900 \\ c & 2.86992700 & -0.99831800 & 0.0159300 \\ d & -2.87004500 & -0.97445400 & 0.002324900 \\ c & 1.34145200 & 0.02560300 & 1.13224200 \\ c & 2.65421300 & 0.00386200 & -7.142600 \\ c & 2.65421300 & 0.00386200 & -7.142600 \\ c & 2.65421300 & 0.00386200 & -7.142600 \\ c & 1.34143300 & 0.02480600 & -1.13224500 \\ c & 1.35197500 & -1.09658900 & -0.07965200 \\ h & 0.90116400 & 0.03766100 & -7.1442600 \\ c & 1.35197500 & -1.09658900 & -0.07965200 \\ h & 0.90116400 & 0.03620100 & -1.13224500 \\ c & -0.88855000 & 0.0970600 & 0.00004200 \\ c & -0.91478900 & 0.03620100 & -1.1324500 \\ c & -0.88855000 & 0.09707600 & 0.00004200 \\ s & -1.5248600 & -1.52153900 & 0.00024100 \\ s & -1.5268600 & -1.52153900 & 0.00024100 \\ c & -2.65420300 & 0.033600 & -0.71443200 \\ c & -2.65420300 & 0.033600 & -0.71443200 \\ c & -2.65151000 & -1.6011300 & 0.00047100 \\ c & -2.63893600 & 0.62112100 & 0.00034700 \\ c & -2.63893600 & 0.62112100 & 0.00034700 \\ c & -2.63893600 & 0.62112100 & 0.00034700 \\ c & -2.63893600 & 0.62112100 & 0.0033500 \\ c & -3.36611100 & 1.1412600 & 0.08033500 \\ c & -2.63893600 & 0.62112100 & 0.0497500 \\ c & -2.63893600 & 0.62112100 & 0.0477500 \\ c & -2.63893600 & 0.62112100 & 0.04705700 \\ d & -0.94326300 & 0.00071900 & 0.152447500 & 0.0034600 \\ d & -2.86151000 & -1.14324200 & 0.073736700 \\ c & -2.63893600 & 0.62112100 & 0.06833500 \\ c & -2.63893600 & 0.62112100 & 0.06833500 \\ c & -2.63893600 & 0.62112100 & 0.06833500 \\ c & -0.94326300 & 0.00071900 & 0.0558600 \\ x & -0.52098700 & 0.007316600 \\ x & -0.52098700 & 0.007316600 \\ x & -0.52098700 & 0.007316600 \\ x & -2.63893600 & 0.6211200 & 0.015584400 \\ x & -2.86151000 & 1.14324200 & 0.1760100 \\ c & -2.63893600 & 0.07316600 \\ c & -2.638$		
S -1.6236200 -1.49887400 -0.0320200 S -1.62374700 -1.49877500 -0.033159400 C 2.66310000 0.69569100 -0.03034000 S -1.6989700 -1.52270400 0.03159400 H 3.56735200 1.3159300 0.06969300 H 3.49444600 -1.4305800 0.06401700 H -2.86992700 -0.99831800 0.01589300 H -2.87004500 -0.99837500 0.03284900 Table 11aa. PyrDTCH (TS _{ref} geometry); E(B3LYP) = -1060.27988825 a.u. E(B3LYP) = -1060.27988825 a.u. E(B3LYP) = -1060.027988825 a.u. E(B3LYP) = -1060.27988825 a.u. C 1.3445200 0.02560300 C 2.63884000 0.6219500 1.1404900 0.04809900 C 3.5651100 0.03667800 -0.0000800 N 0.52095600 0.0070400 0.00319500 H 0.90112800 0.03667800 -0.36456400 H 0.95156500 2.04428700 0.15848100 H 0.9112800 0.03234000 C -1.6420300 0.00873600	L -0.84343000 0.09854700 0.00426100	L -0.84339900 0.09848400 0.00462700
S -1.6993400 1.5226400 0.03315400 C 2.6831000 0.69556100 0.03475600 C 2.64552600 0.74445400 0.03234900 H 3.56735200 1.31659300 -0.06969300 H 3.49444600 -1.41305800 0.06401700 H -2.86992700 -0.99831800 0.01589300 H -2.87004500 -0.99837500 0.01648600 Table 11a. PyrDTCH (TSrm geometry); E(B3LYP) = -1064.65456892 L. E(B3LYP) = -1064.65456892 -0.01064800 0.62114000 0.04608900 C 1.34143200 0.02560300 1.13224500 C 2.63884000 0.0215800 -0.07965200 H 0.90116400 0.0362100 2.11801500 H 0.52095600 0.0070600 2.11801500 H 0.90118400 0.0362100 2.11801500 H 3.5669400 1.15745700 0.0882100 S -1.56286800 0.970760 0.11801500 H 3.5673600 0.0578100 S -1.56286800 0.970760 0.11	S -1.62368200 -1.49887400 -0.03620200	S -1.62374700 -1.49877500 -0.03780500
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S -1.69923400 1.52266400 0.03030400	S -1.69898700 1.52270400 0.03159400
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C 2.68310000 0.69569100 -0.03475600	C 2.64552600 -0.74445400 0.03234900
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н 3.56735200 1.31659300 -0.06969300	H $3.49444600 - 1.41305800 - 0.06401700$
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		
Table 11aa. PyrDTCH (TSrot geometry); E(B3LYP) = -1044.65456892 a.u.Table 11bb. ImDTC (Syn geometry); E(B3LYP) = -1060.27988825 a.u.C1.341452000.025603001.13224200C1.36603001.114049000.08205700C2.654213000.003862000.71442600C2.638840000.621146000.04608900C1.341433000.03667800-0.0008000N0.520956000.00704000.00315500N0.538911000.03667800-0.000800N0.520956000.00704000.00315500H0.901128000.0362100-2.11801500H0.973752002.113267000.15766500C-0.888550000.097076000.00004200N2.62235400-0.76546600-0.5786500S-1.52153000.00021000C-0.914789000.007307000.0008300S-1.710099001.51673500-0.0024600S-1.689017001.51978500-0.0482200KS-1.68917001.51673500-0.00447500C2.62673700-0.00324001.1344200C-1.36611100-0.1140700-0.0777300C1.330570000.00034600-1.0946300C-1.68920300-0.097317000.000324001.118442000.62086300C-2.63936000.621121000.04497500C2.62673700-0.000324001.11344200C-1.366111000.11497000.05758600C1.330570000.00324001.11344200C-1.3	П -2.80992700 -0.99851800 0.01589500	П -2.87004500 -0.99857500 0.01648600
E(B3LYP) = -1044.65456892 a.u.E(B3LYP) = 1060.27988825 a.u.C1.341432000.003602001.13224200C1.366030001.114049000.08205700C2.654213000.003862000.71442600C2.638840000.621146000.04608900C1.341433000.02480600-1.13224500C1.35197500-1.09658900-0.07965200N0.538911000.03667800-0.00000800N0.520956000.00704000.00319500H0.901164000.037661002.11801500H0.97372002.113267000.15848100H3.5181700-0.010634001.36454900H3.566694001.174287000.08973600C-0.888550000.097076000.00004200N2.62235400-0.75446200-0.15706500S-1.56286800-1.521539000.00024600S-1.69520300-1.504745000.04820000C2.654230300.00338600-0.7143200S-1.689017001.51978500-0.04805200H-2.86151000-1.16113000.00047100Table 11dd. ImDTC' (TS geometry);E(B3LYP) = -1060.27139834 a.u.E(B3LYP) = -1060.27139834 a.u.C-1.366111001.114126000.08735000N0.518930000.000346001.134202100N-0.520987000.06995000.0319900N0.518930000.0000234001.1342200R-0.973878002.113507000.15524400H0.932585000.0000348001.1342202100	Table 11aa. PyrDTCH (TS _{rot} geometrv):	Table 11bb. ImDTC ⁻ (Syn geometry):
$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	F(B3LVP) = -1044.65456892.311	F(B3IVP) = -1060.27988825.311
C 1.34143200 0.02580300 1.13224200 C 1.36003000 1.11404900 0.08205700 C 2.65421300 0.02480600 -1.13224500 C 1.35197500 -1.09658900 -0.07965200 N 0.53391100 0.03667800 -0.0000800 N 0.52095600 0.00704400 0.0319500 H 0.90116400 0.03667800 -1.0000800 N 0.52095600 0.00707400 0.008973600 H 0.90112800 0.03620100 -2.11801900 H 0.95156500 -2.09445200 -0.15706500 C -0.88855000 0.09077000 0.00004200 N 2.62235400 -0.76546600 0.0088300 S -1.56286800 -1.5173500 -0.00024600 S -1.68910700 -1.50745500 0.0083300 C -2.65420300 -0.0144700 -1.36456400 N 2.6273700 -0.0083240 1.11344200 C -1.36611100 1.1142600 0.08033500 C 1.3402100 -0.0034400 1.1344200 C -1.36611100 1.1142600 0.08033500 C 1.3402100 <td>$\frac{1}{2} = \frac{1}{2} = \frac{1}$</td> <td>$\frac{1}{2} \frac{1}{2} \frac{1}$</td>	$\frac{1}{2} = \frac{1}{2} = \frac{1}$	$\frac{1}{2} \frac{1}{2} \frac{1}$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	L 1.34145200 0.02560300 1.13224200	L 1.36603000 1.11404900 0.08205700
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C 2.65421300 0.00386200 0.71442600	C 2.63884000 0.62114600 0.04608900
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $	C 1.34143300 0.02480600 -1.13224500	C 1.35197500 -1.09658900 -0.07965200
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	N 0.53891100 0.03667800 -0.00000800	N 0.52095600 0.00700400 0.00319500
H3.51818700-0.010634001.34654900H3.566694001.174287000.08973600H0.901128000.03620100-2.11801900H0.95156500-2.09445200-0.15706500C-0.88855000.097076000.00004200N2.62235400-0.7546600-0.05881000S-1.56286800-1.521539000.00021000C-0.914789000.007307000.00080300S-1.710009001.51673500-0.00024600S-1.69520300-1.504745000.004820000C2.65420300-0.0318600-0.71443200S-1.689017001.51978500-0.04805200H3.51816400-0.01140700-1.36456400H-2.86151000-1.16113000.00047100Table 11cc. ImDTC' (Anti geometry);E(B3LYP) = -1060.27988826 a.u.E(B3LYP) = -1060.27988826 a.u.E(B3LYP) = -1060.27139834 a.u.C-1.366111001.114126000.08033500C1.34202100-0.00344001.1044200C-2.638936000.62112100.04497500C2.26273700-0.00191000.62086300C-1.35192300-1.09674900-0.07777300C1.330570000.000491000.00412700H-0.973878002.113507000.1524400H0.932585000.00034600-1.1802210H-0.95168400-2.09848100-0.15342400H0.932585000.00066800-2.9883300N-2.62235200-0.76563700-0.0578600N2.61762000.0022300-0.	Н 0.90116400 0.03766100 2.11801500	H $0.97375200 2.11326700 0.15848100$
$\begin{array}{c c c c c c c c c c c c c c c c c c c $		$\begin{array}{cccccccccccccccccccccccccccccccccccc$
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	П 5.51616/00 -0.01065400 1.56454900	П 5.56669400 1.1/426/00 0.069/5600
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	H 0.90112800 0.03620100 -2.11801900	H 0.95156500 -2.09445200 -0.15706500
$ \begin{array}{c} \mathrm{S} & -1.5286800 & -1.52153900 & 0.00021000 \\ \mathrm{S} & -1.71000900 & 1.51673500 & -0.00024600 \\ \mathrm{S} & -1.69520300 & -1.50474500 & 0.04820000 \\ \mathrm{C} & 2.65420300 & -0.038600 & -0.71443200 \\ \mathrm{H} & -2.86151000 & -1.16011300 & 0.00047100 \\ \end{array} \\ \hline \mathbf{Table 11cc. ImDTC} (Anti geometry); \\ \mathbf{E}(B3LYP) = -1060.27988826 a.u. \\ \mathrm{C} & -1.36611100 & 1.1142600 & 0.08033500 \\ \mathrm{C} & -2.63893600 & 0.62112100 & 0.04497500 \\ \mathrm{C} & -2.63893600 & 0.62112100 & 0.04497500 \\ \mathrm{C} & -1.36611100 & 1.1142600 & 0.08033500 \\ \mathrm{C} & -1.35192300 & -1.09674900 & -0.0777300 \\ \mathrm{C} & -1.33057000 & 0.00034600 & -1.09400100 \\ \mathrm{N} & -0.52098700 & 0.0699500 & 0.00319900 \\ \mathrm{H} & -3.56686700 & 1.17424200 & 0.08748000 \\ \mathrm{H} & -0.97387800 & 2.11350700 & 0.15524400 \\ \mathrm{H} & -0.95168400 & -2.09484100 & -0.15324400 \\ \mathrm{H} & -0.95168400 & -2.09484100 & -0.05758600 \\ \mathrm{C} & 0.00032600 & 1.18072100 \\ \mathrm{H} & -0.95168400 & 0.00730000 & 0.0081500 \\ \mathrm{C} & 0.94326300 & 0.0001000 & 0.0066500 \\ \mathrm{C} & 0.94326300 & -1.09674900 & 0.00759800 \\ \mathrm{N} & -2.62235200 & -0.76563700 & -0.04702200 \\ \mathrm{S} & 1.68890100 & 1.51987400 & -0.04702200 \\ \mathrm{S} & 1.68890100 & 1.51987400 & -0.04702200 \\ \mathrm{S} & 1.69536300 & -1.50469900 & 0.04710200 \\ \mathrm{S} & 1.69536300 & -1.5242400 & 0.11760100 \\ \mathrm{C} & -1.30734800 & -1.14324200 & 0.11760100 \\ \mathrm{C} & -1.36611100 & 1.11412600 & 0.08033500 \\ \mathrm{C} & -2.5989700 & -0.0208400 & 0.00364000 \\ \mathrm{N} & -0.48987700 & -0.0208400 & 0.00364000 \\ \mathrm{N} & -0.48987700 & -0.2008400 & 0.00364000 \\ \mathrm{N} & -0.52098700 & 0.0695900 & 0.0319900 \\ \mathrm{H} & -0.88897700 & -0.212897400 & -0.221682600 \\ \mathrm{H} & -0.92387800 & 2.11350700 & 0.15244000 \\ \mathrm{H} & -0.92844800 & 2.07692400 & 0.21682600 \\ \mathrm{H} & -0.9238700 & -2.09844100 & -0.15342400 \\ \mathrm{H} & -0.92844800 & 2.07692400 & 0.21682600 \\ \mathrm{H} & -0.9238700 & -0.050758600 \\ \mathrm{H} & -0.9238700 & -0.050758600 \\ \mathrm{H} & -0.9238700 & 0.05758600 \\ \mathrm{H} & -0.9238700 & 0.0575860$	C -0.88855000 0.09707600 0.00004200	N 2.62235400 -0.76546600 -0.05881000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	S -1.56286800 -1.52153900 0.00021000	C -0.91478900 0.00730700 0.00080300
C 2.65420300 0.00338600 -0.71443200 S -1.68901700 1.51978500 -0.04805200 H 3.51816400 -0.01140700 -1.36456400 H -2.86151000 -1.16011300 0.00047100 Table 11cc. ImDTC: (Anti geometry); E(B3LYP) = -1060.27988826 a.u. E(B3LYP) = -1060.27139834 a.u. C C -1.36611100 1.11412600 0.08033500 C 2.62673700 -0.00019100 0.62086300 C -1.35192300 -1.09674900 -0.07777300 C 1.33057000 0.00034600 -1.09400100 N -0.52098700 0.00699500 0.00319900 N 0.51893000 0.0001000 0.0012700 H -0.97387800 2.11350700 0.15524400 H 0.94370700 -0.00034900 1.18072100 H -0.95168400 -2.09484100 -0.15342400 H 0.93258500 0.0066800 -2.09883300 N -2.62235200 -0.76563700 -0.05758600 N 2.61176200 0.00022300 -75932800 C -1.30734800 -1.51987400 -0.04702200 S -1.67123000 -1.	S -1.71000900 1.51673500 -0.00024600	S -1.69520300 -1.50474500 0.04820000
H 2.51816400 -0.01140700 -1.36456400 H -2.86151000 -1.16011300 0.00047100 Table 11cc. ImDTC ⁻ (Anti geometry); E(B3LYP) = -1060.27139834 a.u. E(B3LYP) = -1060.27139834 a.u. C -1.36611100 1.11412600 0.08033500 C 1.3202100 -0.00032400 1.11344200 C -2.63893600 0.62112100 0.04497500 C 2.62673700 -0.00034600 -1.09400100 N -0.52098700 0.00699500 0.00319900 N 0.51893000 0.0001000 0.00412700 H -0.97387800 2.11350700 0.15524400 H 0.94370700 -0.00070500 2.11802200 H -0.97387800 2.11350700 0.05758600 N 2.61176200 0.0002300 -2.0983300 N -2.62235200 -0.76563700 -0.05758600 N 2.61176200 0.0002300 -7.5932800 C 0.94189800 0.0730000 0.004710200 S -1.67122000 -1.52463700 0.0066800 S 1.68890100 1.51987400 -0.04702200 S -1.67122000 -1.5246	C = 2.65420300 - 0.00338600 - 0.71443200	S _168901700 151978500 _004805200
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	$\begin{array}{c} C \\ 1 \\ 2 \\ 5 \\ 1 \\ 1 \\ 2 \\ 5 \\ 1 \\ 2 \\ 5 \\ 1 \\ 2 \\ 5 \\ 1 \\ 2 \\ 5 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1$	5 -1.00701700 1.51770500 -0.04003200
H-2.86151000-1.160113000.0004/100Table 11cc.ImDTC· (Anti geometry); E(B3LYP) = -1060.27988826 a.u.Table 11dd.ImDTC· (TS geometry); E(B3LYP) = -1060.27139834 a.u.C-1.366111001.114126000.08033500C2.62673700-0.00034001.11344200C-2.638936000.621121000.04497500C2.62673700-0.000191000.62086300C-1.35192300-1.09674900-0.07777300C1.330570000.00034600-1.0940100N-0.520987000.006995000.00319900N0.518930000.00010000.00412700H-0.973878002.113507000.15524400H0.94370700-0.00075002.11630200H-0.95168400-2.09484100-0.15342400H0.932585000.00066800-2.09883300N-2.62235200-0.7563700-0.05758600N2.611762000.00022300-0.75932800C0.914898000.007300000.0081500C-0.94326300-0.00010000.00665800S1.688901001.51987400-0.04702200S-1.671233001.524626000.00662200Table 11ee.ImDTCH (NH) (Syn geometry);E(B3LYP) = -1060.73176784 a.u.E(B3LYP) = -1060.73176784 a.u.E(B3LYP) = -1060.73176756 a.u.C-1.307348001.143242000.11760100C-1.366111001.14126000.08033500C-2.59692700-0.713434000.07326800C-2.6238936000.621121000.04497500 <t< td=""><td>H 3.51816400 -0.01140/00 -1.36456400</td><td></td></t<>	H 3.51816400 -0.01140/00 -1.36456400	
Table 11cc. ImDTC: (Anti geometry); E(B3LYP) = -1060.27988826 a.u.Table 11dd. ImDTC: (TS geometry); E(B3LYP) = -1060.27139834 a.u.C-1.366111001.114126000.08033500C1.34202100-0.000324001.11344200C-2.638936000.621121000.04497500C2.62673700-0.000191000.62086300C-1.35192300-1.09674900-0.0777300C1.330570000.00010000.00412700N-0.520987000.006995000.0319900N0.518930000.00010000.00412700H-0.973878002.113507000.15524400H0.94370700-0.000705002.11630200H-3.566867001.174242000.08748000H3.55171500-0.000349001.18072100H-0.95168400-2.09484100-0.15342400H0.932585000.00066800-2.09883300N-2.62235200-0.075663700-0.05758600N2.611762000.00022300-0.75932800C0.914898000.007300000.00410200S-1.671230001.524626000.00665800S1.69536300-1.594699000.04710200S-1.67122000-1.524637000.00626200Table 11ee. ImDTCH (NH) (Syn geometry); E(B3LYP) = -1060.73176784 a.u.E(B3LYP) = -1060.73176756 a.u.C-1.30734800-1.432242000.11760100C-1.366111001.114126000.08033500C-2.59692700-0.713434000.02364000N-0.520897000.0777300N	H -2.86151000 -1.16011300 0.0004/100	
E(B3LYP) = -1060.27988826 a.u.E(B3LYP) = -1060.27139834 a.u.C-1.366111001.114126000.08033500C1.34202100-0.000324001.11344200C-2.638936000.621121000.04497500C2.62673700-0.000191000.62086300C-1.35192300-1.09674900-0.07777300C1.330570000.00034600-1.09400100N-0.520987000.006995000.00319900N0.518930000.00010000.00412700H-0.973878002.113507000.15524400H0.94370700-0.000705002.11630200H-0.95168400-2.09484100-0.15342400H0.932585000.00066800-2.09883300N-2.62235200-0.76563700-0.05758600N2.611762000.00022300-0.75932800C0.914898000.007300000.0081500C-0.94326300-0.00010000.00661200S1.688901001.51987400-0.04702200S-1.67123001.524637000.00626200S1.69536300-1.504699000.04710200S-1.6712300-1.524637000.00626200C-1.30734800-1.143242000.11760100C-1.366111001.114126000.08033500C-2.59692700-0.713434000.07326800C-2.638936000.621121000.04497500C-1.278096001.06406400-0.11032900C-1.35192300-1.09674900-0.0777300N-0.48897700 <t< td=""><td>Table 11cc. ImDTC⁻ (Anti geometry);</td><td>Table 11dd. ImDTC (TS geometry);</td></t<>	Table 11cc. ImDTC ⁻ (Anti geometry);	Table 11dd. ImDTC (TS geometry);
LicbertInconstructInconstructC-1.366111001.114126000.08033500C1.34202100-0.000324001.11344200C-2.638936000.621121000.04497500C2.62673700-0.000191000.62086300C-1.35192300-1.09674900-0.07777300C1.330570000.00034600-1.09400100N-0.520987000.006995000.00319900N0.518930000.000010000.00412700H-0.973878002.113507000.15524400H0.94370700-0.000705002.11630200H-0.95168400-2.09484100-0.15342400H0.932585000.0006800-2.09883300N-2.62235200-0.76563700-0.05758600N2.611762000.00022300-0.75932800C0.914898000.007300000.0081500C-0.94326300-0.00010000.00661200S1.688901001.51987400-0.04702200S-1.671233001.524626000.00665800S1.69536300-1.504699000.04710200S-1.67122000-1.524637000.00626200Table 11ee.ImDTCH (NH) (Syn geometry);E(B3LYP) = -1060.73176756 a.u.E(B3LYP) = -1060.73176756 a.u.E(B3LYP) = -1064000-0.07777300C-1.30734800-1.43242000.01726800C-1.35192300-1.0967900-0.07777300N-0.48987700-0.20084000.0364000N-0.520987000.06955000.0319900H-0.88897700-0	$E(B3LYP) = -1060.27988826.3 \mu$	$E(B3LYP) = -106027139834a\mu$
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\frac{1}{2} \frac{1}{2} \frac{1}$	$\frac{1}{24202100} = 0.00022400 = 1.11244200$
C -2.63893600 0.62112100 0.04497500 C 2.62673700 -0.00019100 0.6208300 C -1.35192300 -1.09674900 -0.07777300 C 1.33057000 0.00034600 -1.09400100 N -0.52098700 0.00699500 0.00319900 N 0.51893000 0.0001000 0.00412700 H -0.97387800 2.11350700 0.15524400 H 0.94370700 -0.00070500 2.11630200 H -0.95168400 -2.09484100 -0.15342400 H 0.93258500 0.00066800 -2.09883300 N -2.62235200 -0.76563700 -0.05758600 N 2.61176200 0.00022300 -0.75932800 C 0.91489800 0.00730000 0.0081500 C -0.94326300 -0.0001000 0.00661200 S 1.68890100 1.51987400 -0.04702200 S -1.67123300 1.52462600 0.00665800 S 1.69536300 -1.50469900 0.04710200 S -1.67122000 -1.52463700 0.0022300 C -1.30734800 -1.14324200 0.11760100 C -1.36611100 1.11412600 0.8033500 C -2.59692700 -0.71343400 0.0334600 0.0334600 N -0.5208700 0.00699500 0.00777300 N -0.44987700 -0.2208400 0.0364000 N -0.5208700 0.0669500 0.00319900 H -0.88897700 -2.12897400 0.22122200 H -0.97387800 2.11350700		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C -2.63893600 0.62112100 0.04497500	C 2.62673700 -0.00019100 0.62086300
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C -1.35192300 -1.09674900 -0.07777300	C 1.33057000 0.00034600 -1.09400100
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	N -0.52098700 0.00699500 0.00319900	N 0.51893000 0.00001000 0.00412700
H -3.56686700 1.17424200 0.08748000 H 3.55171500 -0.00034900 1.18072100 H -0.95168400 -2.09484100 -0.15342400 H 0.93258500 0.00066800 -2.09883300 N -2.62235200 -0.76563700 -0.05758600 N 2.61176200 0.00022300 -0.75932800 C 0.91489800 0.00730000 0.00081500 C -0.94326300 -0.00001000 0.00661200 S 1.68890100 1.51987400 -0.04702200 S -1.67123300 1.52462600 0.00626200 S 1.69536300 -1.50469900 0.04710200 S -1.67122000 -1.52463700 0.00626200 Table 11ee.ImDTCH (NH) (Syn geometry); $E(B3LYP) = -1060.73176784$ a.u. $E(B3LYP) = -1060.73176756$ a.u. $E(B3LYP) = -1060.73176756$ a.u.C -1.30734800 -1.14324200 0.11760100 C -1.36611100 1.11412600 0.08033500 C -2.59692700 -0.71343400 0.07326800 C -2.63893600 0.62112100 0.04497500 C -1.27809600 1.06406400 -0.11032900 C -1.35192300 -1.09674900 -0.07777300 N -0.48987700 -0.22084400 0.0364000 N -0.52098700 0.0699500 0.0319900 H -0.92844800 2.07692400 -2.1682600 H -0.97187800 2.11350700 0.15524400 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 <td< td=""><td>Н -0.97387800 2.11350700 0.15524400</td><td>Н 0.94370700 -0.00070500 2.11630200</td></td<>	Н -0.97387800 2.11350700 0.15524400	Н 0.94370700 -0.00070500 2.11630200
H -0.95168400 -2.09484100 -0.15342400 H 0.93258500 0.00066800 -2.09883300 N -2.62235200 -0.7563700 -0.05758600 N 2.61176200 0.00022300 -0.75932800 C 0.91489800 0.00730000 0.00081500 C -0.94326300 -0.0001000 0.00661200 S 1.68890100 1.51987400 -0.04702200 S -1.67123300 1.52462600 0.00665800 S 1.69536300 -1.50469900 0.04710200 S -1.67122000 -1.52463700 0.00626200 Table 11ee. ImDTCH (NH) (Syn geometry); E(B3LYP) = -1060.73176784 a.u.C -1.30734800 -1.14324200 0.11760100 C -1.36611100 1.11412600 0.08033500 C -2.59692700 -0.71343400 0.07326800 C -2.63893600 0.62112100 0.04497500 C -1.27809600 1.06406400 -0.11032900 C -1.35192300 -1.09674900 -0.07777300 N -0.48987700 -0.2008400 0.0364000 N -0.52098700 0.00699500 0.00319900 H -0.88897700 -1.25225300 0.13255100 H -3.56686700 1.17424200 0.08748000 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.5758600 N -2.54619400 0.6235500 -0.07095100 N -2.62235200 -0.76563700 -0.05758600	Н -3 56686700 1 17424200 0 08748000	Н 3 55171500 -0 00034900 1 18072100
N-2.62235200-0.76563700-0.05758600N2.611762000.00022300-2.09883300C0.914898000.007300000.00081500C-0.94326300-0.00010000.00661200S1.688901001.51987400-0.04702200S-1.671233001.524626000.00665800S1.69536300-1.504699000.04710200S-1.67122000-1.524637000.00626200Table 11ee. ImDTCH (NH) (Syn geometry);E(B3LYP) = -1060.73176784 a.u.E(B3LYP) = -1060.73176756 a.u.C-1.30734800-1.143242000.11760100C-1.366111001.114126000.08033500C-2.59692700-0.713434000.07326800C-2.638936000.621121000.04497500C-1.278096001.06406400-0.11032900C-1.35192300-1.09674900-0.07777300N-0.48987700-0.020084000.00364000N-0.520987000.006995000.00319900H-0.88897700-2.128974000.22122200H-0.973878002.113507000.15524400H-3.52817500-1.252253000.13255100H-3.566867001.174242000.08748000H-0.928448002.07692400-0.21682600H-0.95168400-2.09484100-0.15342400N-2.546194000.66235500-0.07095100N-2.62235200-0.75663700-0.5786600		
N -2.62235200 -0.76563700 -0.05758600 N 2.61176200 0.00022300 -0.75932800 C 0.91489800 0.00730000 0.0081500 C -0.94326300 -0.00001000 0.00661200 S 1.68890100 1.51987400 -0.04702200 S -1.67123300 1.52462600 0.00626200 S 1.69536300 -1.50469900 0.04710200 S -1.67122000 -1.52463700 0.00626200 Table 11ee. ImDTCH (NH) (Syn geometry);E(B3LYP) = -1060.73176784 a.u.E(B3LYP) = -1060.73176756 a.u.C -1.30734800 -1.14324200 0.11760100 C -1.36611100 1.11412600 0.08033500 C -2.59692700 -0.71343400 0.07326800 C -2.63893600 0.62112100 0.04497500 C -1.27809600 1.06406400 -0.11032900 C -1.35192300 -1.09674900 -0.07777300 N -0.48987700 -2.12897400 0.22122200 H -0.97387800 2.11350700 0.15524400 H -3.52817500 -1.25225300 0.13255100 H -3.56686700 1.17424200 0.08748000 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.75653700 -0.05758600	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
C 0.91489800 0.00730000 0.0081500 C -0.94326300 -0.00001000 0.00661200 S 1.68890100 1.51987400 -0.04702200 S -1.67123300 1.52462600 0.00665800 S 1.69536300 -1.50469900 0.04710200 S -1.67122000 -1.52463700 0.00626200 Table 11ee. ImDTCH (NH) (Syn geometry);E(B3LYP) = -1060.73176784 a.u.E(B3LYP) = -1060.73176756 a.u.C -1.30734800 -1.14324200 0.11760100 C -1.36611100 1.11412600 0.08033500 C -2.59692700 -0.71343400 0.07326800 C -2.63893600 0.62112100 0.04497500 C -1.27809600 1.06406400 -0.11032900 C -1.35192300 -1.09674900 -0.07777300 N -0.48987700 -0.2008400 0.02122200 H -0.97387800 2.11350700 0.15524400 H -3.52817500 -1.25225300 0.13255100 H -3.56686700 1.17424200 0.08748000 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.76563700 -0.05758600	N -2.62235200 -0.76563700 -0.05758600	N 2.611/6200 0.00022300 -0.75932800
S 1.68890100 1.51987400 -0.04702200 S -1.67123300 1.52462600 0.00665800 S 1.69536300 -1.50469900 0.04710200 S -1.67122000 -1.52463700 0.00626200 Table 11ee.ImDTCH (NH) (Syn geometry); E(B3LYP) = -1060.73176784 a.u.Table 11ff.ImDTCH (NH) (Anti geometry); E(B3LYP) = -1060.73176784 a.u.C -1.30734800 -1.14324200 0.11760100 C -1.36611100 1.11412600 0.08033500 C -2.59692700 -0.71343400 0.07326800 C -2.63893600 0.62112100 0.04497500 C -1.27809600 1.06406400 -0.11032900 C -1.35192300 -1.09674900 -0.07777300 N -0.48987700 -0.2008400 0.00364000 N -0.52098700 0.00699500 0.00319900 H -0.88897700 -2.12897400 0.22122200 H -0.97387800 2.11350700 0.15524400 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.75653700 -0.05758600	C 0.91489800 0.00730000 0.00081500	C -0.94326300 -0.00001000 0.00661200
S $1.69536300 -1.50469900 0.04710200$ S $-1.67122000 -1.52463700 0.00626200$ Table 11ee.ImDTCH (NH) (Syn geometry); E(B3LYP) = -1060.73176784 a.u.Table 11ff. ImDTCH (NH) (Anti geometry); E(B3LYP) = -1060.73176784 a.u.C $-1.30734800 -1.14324200 0.11760100$ CC $-1.36611100 1.11412600 0.08033500$ CC $-1.27809600 1.06406400 -0.11032900$ CC $-1.35192300 -1.09674900 -0.07777300$ NN $-0.48987700 -0.02008400 0.00364000$ HN $-0.52098700 0.0699500 0.00319900$ HH $-0.88897700 -2.12897400 0.22122200$ HH $-0.97387800 2.11350700 0.15524400$ HH $-0.92844800 2.07692400 -0.21682600$ HH $-0.95168400 -2.09484100 -0.15342400$ HN $-2.54619400 0.66235500 -0.07095100$ H $-2.62235200 -0.76563700 -0.05758600$	S 1.68890100 1.51987400 -0.04702200	S -1.67123300 1.52462600 0.00665800
Table 11ee. ImDTCH (NH) (Syn geometry); $E(B3LYP) = -1060.73176784 a.u.$ Table 11ff. ImDTCH (NH) (Anti geometry); $E(B3LYP) = -1060.73176784 a.u.$ C $-1.30734800 - 1.14324200 0.11760100$ CC $-1.36611100 1.11412600 0.08033500$ CC $-2.59692700 - 0.71343400 0.07326800$ CC $-2.63893600 0.62112100 0.04497500$ CC $-1.27809600 1.06406400 - 0.11032900$ CC $-1.35192300 - 1.09674900 - 0.07777300$ NN $-0.48987700 - 0.02008400 0.00364000$ HN $-0.52098700 0.00699500 0.00319900$ HH $-3.52817500 - 1.25225300 0.13255100$ HH $-3.56686700 1.17424200 0.08748000$ HH $-0.92844800 2.07692400 - 0.21682600$ HH $-0.95168400 - 2.09484100 - 0.15342400$ NN $-2.54619400 0.66235500 - 0.07095100$ N $-2.62235200 - 0.76563700 - 0.05758600$	S 1.69536300 -1.50469900 0.04710200	S -1.67122000 -1.52463700 0.00626200
Table 11ee. ImDTCH (NH) (Syn geometry); $E(B3LYP) = -1060.73176784 a.u.$ Table 11ff. ImDTCH (NH) (Anti geometry); $E(B3LYP) = -1060.73176784 a.u.$ C $-1.30734800 - 1.14324200 0.11760100$ CC $-1.36611100 1.11412600 0.08033500$ CC $-2.59692700 - 0.71343400 0.07326800$ CC $-2.63893600 0.62112100 0.04497500$ CC $-1.27809600 1.06406400 - 0.11032900$ NC $-1.35192300 - 1.09674900 - 0.07777300$ NN $-0.48987700 - 0.2008400 0.00364000$ HN $-0.52098700 0.00699500 0.00319900$ HH $-0.38897700 - 2.12897400 0.22122200$ HH $-0.97387800 2.11350700 0.15524400$ HH $-0.92844800 2.07692400 - 0.21682600$ HH $-0.95168400 - 2.09484100 - 0.15342400$ NN $-2.54619400 0.66235500 - 0.07095100$ N $-2.62235200 - 0.76563700 - 0.05758600$		
E(B3LYP) = -1060.73176784 a.u.E(B3LYP) = -1060.73176756 a.u.C -1.30734800 -1.14324200 0.11760100 C -1.36611100 1.11412600 0.08033500 C -2.59692700 -0.71343400 0.07326800 C -2.63893600 0.62112100 0.04497500 C -1.27809600 1.06406400 -0.11032900 C -1.35192300 -1.09674900 -0.07777300 N -0.48987700 -0.2008400 0.00364000 N -0.52098700 0.00699500 0.00319900 H -0.88897700 -2.12897400 0.22122200 H -0.97387800 2.11350700 0.15524400 H -3.52817500 -1.25225300 0.13255100 H -3.56686700 1.17424200 0.08748000 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.75653700 -0.0578600	Table 11ee ImDT(H (NH) (Syn geometry)	Table 11ff ImDTCH (NH) (Anti geometry):
E(B3LYP) = -1060.73176784 a.u.E(B3LYP) = -1060.73176756 a.u.C -1.30734800 -1.14324200 0.11760100 C -1.36611100 1.11412600 0.08033500 C -2.59692700 -0.71343400 0.07326800 C -2.63893600 0.62112100 0.04497500 C -1.27809600 1.06406400 -0.11032900 C -1.35192300 -1.09674900 -0.07777300 N -0.48987700 -0.2008400 0.00364000 N -0.52098700 0.00699500 0.00319900 H -0.88897700 -2.12897400 0.22122200 H -0.97387800 2.11350700 0.15524400 H -3.52817500 -1.25225300 0.13255100 H -3.56686700 1.17424200 0.08748000 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.75653700 -0.0578600	$\mathbf{F}(\mathbf{P}) = \mathbf{F}(\mathbf{P}) + F$	$\mathbf{F}(\mathbf{P}) = \mathbf{F}(\mathbf{P}) + F$
C-1.30734800-1.143242000.11760100C-1.366111001.114126000.08033500C-2.59692700-0.713434000.07326800C-2.638936000.621121000.04497500C-1.278096001.06406400-0.11032900C-1.35192300-1.09674900-0.07777300N-0.48987700-0.020084000.00364000N-0.520987000.006995000.00319900H-0.88897700-2.128974000.22122200H-0.973878002.113507000.15524400H-3.52817500-1.252253000.13255100H-3.566867001.174242000.08748000H-0.928448002.07692400-0.21682600H-0.95168400-2.09484100-0.15342400N-2.546194000.66235500-0.07095100N-2.62235200-0.76563700-0.05758600	E(B3LYP) = -1060.73176784 a.u.	E(B3LYP) = -1060.73176756 a.u.
C-2.59692700-0.713434000.07326800C-2.638936000.621121000.04497500C-1.278096001.06406400-0.11032900C-1.35192300-1.09674900-0.07777300N-0.48987700-0.020084000.00364000N-0.520987000.006995000.00319900H-0.88897700-2.128974000.22122200H-0.973878002.113507000.15524400H-3.52817500-1.252253000.13255100H-3.566867001.174242000.08748000H-0.928448002.07692400-0.21682600H-0.95168400-2.09484100-0.15342400N-2.546194000.66235500-0.07095100N-2.62235200-0.76563700-0.05758600	C -1.30734800 -1.14324200 0.11760100	C -1.36611100 1.11412600 0.08033500
C-1.278096001.06406400-0.11032900C-1.35192300-1.09674900-0.07777300N-0.48987700-0.020084000.00364000N-0.520987000.006995000.00319900H-0.88897700-2.128974000.22122200H-0.973878002.113507000.15524400H-3.52817500-1.252253000.13255100H-3.566867001.174242000.08748000H-0.928448002.07692400-0.21682600H-0.95168400-2.09484100-0.15342400N-2.546194000.66235500-0.07095100N-2.62235200-0.76563700-0.05758600	C -2.59692700 -0.71343400 0.07326800	C -2.63893600 0.62112100 0.04497500
N -0.48987700 -0.02008400 0.00364000 N -0.52098700 0.00699500 0.00319900 H -0.88897700 -2.12897400 0.22122200 H -0.97387800 2.11350700 0.15524400 H -3.52817500 -1.25225300 0.13255100 H -3.56686700 1.17424200 0.08748000 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.76563700 -0.05758600	C -1.27809600 1.06406400 -0.11032900	C -1.35192300 -1.09674900 -0.07777300
H -0.88897700 -2.12897400 0.22122200 H -0.97387800 2.11350700 0.15524400 H -3.52817500 -1.25225300 0.13255100 H -3.56686700 1.17424200 0.08748000 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.76563700 -0.05758600	N -0.48987700 -0.02008400 0.00364000	N -0.52098700 0.00699500 0.00319900
H -0.00007/00 -2.12007400 0.22122200 H -0.97387800 2.11350700 0.15524400 H -3.52817500 -1.25225300 0.13255100 H -3.56686700 1.17424200 0.08748000 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.76563700 -0.05758600	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	
H -3.52817500 -1.25225300 0.13255100 H -3.56686700 1.17424200 0.08748000 H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.76563700 -0.05758600		n -0.9/30/800 2.11350/00 0.15524400
H -0.92844800 2.07692400 -0.21682600 H -0.95168400 -2.09484100 -0.15342400 N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.76563700 -0.05758600	н -3.52817500 -1.25225300 0.13255100	
N -2.54619400 0.66235500 -0.07095100 N -2.62235200 -0.76563700 -0.05758600		H -3.56686700 1.17424200 0.08748000
	Н -0.92844800 2.07692400 -0.21682600	H-3.566867001.174242000.08748000H-0.95168400-2.09484100-0.15342400
C 0.99331500 -0.00074100 0.00095600 C 0.91489800 0.00730000 0.00081500	H -0.92844800 2.07692400 -0.21682600 N -2.54619400 0.66235500 -0.07095100	H-3.566867001.174242000.08748000H-0.95168400-2.09484100-0.15342400N-2.62235200-0.76563700-0.05758600

S 1.70537200 1.52534300 0.07022600	S 1.68890100 1.51987400 -0.04702200		
S 1.73688900 -1.50752800 -0.07094900	S 1.69536300 -1.50469900 0.04710200		
Н -3.34375000 1.28348500 -0.14318200			
Table 11gg. ImDTCH (NH) (TS geometry);	Table 11hh. ImDTCH (SH) (Syn geometry);		
E(B3LYP) = -1060.72592113 a.u.	E(B3LYP) = -1060.71477842 a.u.		
C 1.28104600 -0.00033000 1.13962300	C 1.42522200 1.12158000 0.14698100		
C 2.57747500 -0.00024900 0.71342600	C 2.67793500 0.59352700 0.08582100		
C 1.26038300 0.00070000 -1.07553300	C 1.35743300 -1.08876600 -0.15134500		
N 0.48080500 0.00032600 0.00778500	N 0.54853300 0.03987200 -0.00078100		
Н 0.86002700 -0.00059700 2.13146000	Н 1.06031400 2.12450600 0.28855200		
Н 3.50507600 -0.00027100 1.26157700	Н 3.62104800 1.11371600 0.16872900		
Н 0.92215800 0.00116900 -2.09913700	Н 0.94868800 -2.07540300 -0.31194800		
N 2.53493200 0.00045500 -0.66588300	N 2.62509200 -0.78669000 -0.10623500		
C -1.01209400 -0.00003100 -0.00335800	C -0.84848000 0.10497700 -0.00778600		
S -1.69958800 1.53105900 -0.00117400	S -1.61441400 -1.48914400 0.09723900		
S -1.69882400 -1.53145500 -0.00174700	S -1.67657100 1.53221400 -0.08366100		
Н 3.33630900 0.00002800 -1.28541400	Н -2.86231500 -1.01213500 -0.05550100		
Table 11ii. ImDTCH (SH) (Anti geometry);	Table 11jj. ImDTCH (SH) (TSrot geometry);		
E(B3LYP) = -1060.71497685 a.u.	E(B3LYP) = -1060.70500598 a.u.		
C 1.36775300 1.10682100 0.13866200	C -1.37453100 0.03247900 -1.12062200		
C 2.64637100 0.64556500 0.07128800	C -2.65203000 0.00663400 -0.62227900		
C 1.41303600 -1.10884200 -0.12611900	C -1.36480100 0.01075500 1.10288600		
N 0.54713100 -0.02474600 0.01504000	N -0.54723200 0.03341700 -0.00449300		
Н 0.97340600 2.09916900 0.28407300	Н -0.97614100 0.05242400 -2.12300200		
Н 3.56059100 1.21718300 0.13841400	Н -3.57758000 -0.00298200 -1.18005500		
Н 1.03715000 -2.11182500 -0.25338600	Н -0.96474000 0.01149300 2.10675200		
N 2.66297600 -0.73783900 -0.09909900	N -2.63516600 -0.00662900 0.75970400		
C -0.84938400 -0.09164100 0.01065100	C 0.88581000 0.09648900 -0.00705800		
S -1.60659100 1.50483400 -0.08435100	S 1.55739200 -1.52092900 -0.01189600		
S -1.68383800 -1.51783500 0.07473200	S 1.69102200 1.52257800 -0.00031800		
Н -2.86168200 1.03016500 0.00631600	Н 2.85393600 -1.15298200 -0.01231100		

Table S12. Graphical representation of the HOMOs calculated for ground and transition states of various DTC and DTCH. The transition state was generated in each case by rotating the CS_2 group around the N-C bond. The surface contours were generated using Gaussview 5.0 and the composition analysis were performed using the GaussSum software.¹⁶



Ground State (GS)	Transition State (TS)
НОМО	НОМО
PyrDTC ⁻	PyrDTC ⁻
$N = 0\%$ and $CS_2 = 94\%$	$N = 1\%$ and $CS_2 = 96\%$
PyrDTCH	PyrDTCH
$N = 0\%$ and $CS_2 = 95\%$	$N = 0\%$ and $CS_2 = 2\%$
ImDIC	ImDTC
$N = 0\%$ and $CS_2 = 96\%$	$N = 1\%$ and $CS_2 = 97\%$
ImDTCH (NH)	ImDTCH (NH)
$N = 0\%$ and $CS_2 = 94\%$	$N = 1\%$ and $CS_2 = 98\%$
ImDTCH (SH)	ImDTCH (SH)
	N= 49/ m ² C2 = 99/
$N = 0\%$ and $CS_2 = 94\%$	$N = 470$ and $CS_2 = 870$

Table 4. Calculated activation energies for rotation E_{rot} around the DTC C-N bond, the bond lengths and the HOMO orbital compositions of several deprotonated DTCs (DTC-) and protonated DTCs (DTCH) at the ground state (GS) and rotation transition state (TS_{rot}). Calculated in a PCM/B3LYP/6-31+G(d,p) level of theory.

DTC	N-C (Å) (GS)	N-C (Å) (TS _{rot})	HOMO (%) (GS)	HOMO (%) (TS _{rot})	E _{rot} (kJ/mol)
PyrDTC ⁻	1.421	1.455	CS ₂ (94); N (0)	CS ₂ (96); N (1)	29.48
PyrDTCH	1.384	1.426	CS ₂ (95); N (0)	CS ₂ (2); N (0)	37.9
ImDTC ⁻	1.435	1.462	CS ₂ (96); N (1)	CS ₂ (97); N (1)	22.3
ImDTCH (SH)ª	1.398	1.434	CS ₂ (94); N (0)	CS ₂ (8); N (4)	25.6
ImDTCH (NH) ^b	1.483	1.492	CS ₂ (94); N (2)	CS ₂ (98); N (1)	15.4

^a S protonated. ^b N protonated

SI References

- (1) *Purification of Laboratory Chemicals*, 6e ed.; Armarego, W. L. F., Chai, C. L. Eds.; Elsevier Inc.: Burlington, MA, 2009.
- (2) Angeloski, A.; Hook, J. M.; Bhadbhade, M.; Baker, A. T.; McDonagh, A. M. Intramolecular H···S Interactions in Metal Di(isopropyl)dithiocarbamate Complexes. *CrystEngComm* **2016**, *18*, 7070–7077.
- (3) Uhlin, A.; Åkerström, S. The Association of Alkali Metal N,N-Dialkyldithiocarbamates in Solution. *Acta Chem. Scand.* **1971**, *25*, 393–410.
- (4) Wahlberg, A. The Structure of Diisopropylammonium Diisopropyldithiocarbamate. *Acta Crystallogr. Sec. B* **1978**, *34*, 3479–3481.
- (5) Infrared and Raman Characteristic group frequencies, 3rd ed.; George Socrates. John Wiley & Sons, LTD. West Sussex, UK, 2001.
- (6) Reiss, G.J.; Meyer, M.K. Diisopropylammonium methanesulfonate. *Acta Crystallographica Sec.E.* **2011**, E67, o2169,
- (7) Howie, R.A.; Lima, G.M.; Menezes, D.C.; Wardell, J.L.; Wardell, S.M.S.V.; Young, D.J.; Tiekink, E.R.T. The influence of cation upon the supramolecular aggregation patterns of dithiocarbamate anions functionalised with hydrogen bonding capacity—the prevalence of charge-assisted O–H/S interactions. *CrystEngComm*, **2008**, *10*, 1626–1637,
- (8) Mafud, A. C.; Sanches, E. A.; Gambardella, M. T. Morpholin-4-Ium Morpholine-4-Carbodithioate. *Acta Crystallogr. Sect. E* **2011**, *67*, o2008.
- (9) Humeres, E.; Sun Lee, B.; Debacher, N. A. Mechanisms of Acid Decomposition of Dithio-carbamates.
 5. Piperidyl Dithiocarbamate and Analogues. J. Org. Chem. 2008, 73, 7189–7196.
- (10) Bereman, R. D.; Baird, D. M.; Vance, C. T.; Hutchinson, J.; Zubieta, J. Coordination Chemistry of New Sulfur-Containing Ligands. 25. Reduction and Deoxygenation of MoO³⁺(aq) by Pyrrole-N-Carbodithioate (L) to Yield Eight-Coordinate MoL₄: Crystal and Molecular Structure of Tetrakis(pyrrole-N-Carbodithioato)molybdenum-Hemi(methylene chloride). *Inorg. Chem.* 1983, 22, 2316–2318.

- (11) Goldberg, R. N.; Kishore, N.; Lennen, R. N. Thermodynamic Quantities for the Ionization Reactions of Buffers. J. Phys. Chem. Ref. Data, **2002**, *31*, 232-370
- (12) H. K. Hall, Jr. Correlation of the Base Strengths of Amines. J. Am. Chem. Soc., 1957, 79, 5441–5444
- (13) Bruckner R. Organic Mechanisms Reactions, Stereochemistry and Synthesis. Springer-Verlag Berlin Heidelberg 2010.
- (14) Bordwell, F. G.; Drucker, G. E.;. Fried, H. E..Acidities of carbon and nitrogen acids: the aromaticity of the cyclopentadienyl anion. *J. Org. Chem.* **1981**, 46, 632 635.
- (15) Walba, H.; Isensee, R. W. Acidity Constants of Some Arylimidazoles and Their Cations. J. Org. Chem., **1961**, 26, 2789 2791
- (16) O'Boyle, N. M.; Tenderholt, A. L.; Langner, K. M. J. Comput. Chem. 2008, 29, 839.