Supplementary Information

Theoretical Investigation of Nucleophilic Substitution Reaction of Phenyl Carbonyl Isothiocyantes with Pyridines in Gas and Polar Aprotic Solvent

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Abstract:

The current study focuses on the mutual interaction of substituents in the nucleophile and substrate – cross interaction constant, ρ_{XY}, in the uncatalyzed aminolysis by substituting pyridine with phenyl carbonyl isothiocyanate. A stepwise reaction mechanism considers the Cross-Interaction Constant (CIC) with rate limiting break down of tetrahedral intermediate in gas and solvent phase. The Hammett coefficient with X, ρ_X (−1.93 to −6.54 for the gas phase and 10.5 to 18.9 in the solvent model), with Y, ρ_Y (0.41 – 3.48 for the gas phase and 1.83 ~ −10.70 for solvent model), Brönsted coefficient with X, β_X (0.11 – 1.52 for gas phase and −2.57 – 3.96 for solvent model), cross interaction constant (CIC), ρ_{XY} (0.69 for gas phase and 0.87 for solvent model). NBO analysis, reaction potential, reaction electronic flux (REF), duel descriptor, and the structure-energy relationships were considered to interpret the mechanistic criteria. The mechanism was proposed as a stepwise process with a rate-limiting breakdown of the –NCS leaving group.

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Bond Perturbation (Δd):

As the type of substrate and nucleophile affect the bonding behavior of a specific system, the bond perturbation technique addresses the tuned combined correlation of resonance or field effect of the corresponding substituents into the corresponding TS. In this respect, it is essential to recognize and understand the factors responsible for governing the chemical reactivity of a specific system. In the present work, the bond formation via interaction of substituted pyridine nucleophile and the breaking of the leaving group, isothiocyanate (−NCS), are greatly affected by the Y-substituent of the phenoxy non-leaving group. In the TS series, the relative bond length variations (Δd) for $C_1 – Nu$ (Δd_{C1-Nu}), $C_1{=}O_2$ ($\Delta d_{C=O}$), $C_1 – N_L$ (Δd_{C1-NL}), and $C_1 – O_3$ (Δd_{C1-O3}) are summarized in **Table ST2b** for Y-substituents' variation in the gas phase and in **Table ST3a** for X-substituents' variation in the continuum solvent model. The reported value is generated from the difference in bond order between the substituted and unsubstituted reactant entity (XY = 33). The data for the relevant X and Y substituents' variation for the gas and solvent phases is summarized in **Tables ST2a** and **ST3b**; **Fig. SF1a, b** and **SF4** in SI.

Specifically, the Δd bond length perturbation values, the differences of XY = 31 to 36 and XY = 33 (**Table ST2b**) for the gas phase or XY = 13 to 63 and XY = 33 (**Table ST3a**) for the solution phase are displayed. The data in **Table ST2b** shows a good correlation between the perturbation values Δd (in Å) and the Hammett substituent constants for different Y substituents. Since the intrinsic thermodynamic properties are directly related to the bond perturbations[1], the slope, sign, and magnitude indicate the efficacious group's (substituent) participation in the TS. The specific value of the correlation coefficient r^2 represents in-line electronic transmissions or other detrimental factors involved in the transition state for physical reorganization. Negative slopes indicate direct incremental electronic transmission effects, whereas positive values are for relaxing. In **Table ST2b**, all the bond perturbations, such as for $C_1 – Nu$, $C_1 – O_3$, $C_1 = O_2$, and $C_1 – N_L$ are nicely correlated (r^2 = 0.95 – 0.97) with the variation of phen-ring Y substituent constants ($\delta\sigma_Y$), means direct electronic transmissions are effective. The smaller magnitude of correlation values for $C_1 – O_3$ (0.009) and $C_1 = O_2$ (-0.003) indicate smaller effects or transmission balanced between phen-ring and the carbonyl moiety, and the balance resulted in the relative propagation of pydn-ring and electronic perturbation of the weak leaving group –NCS. On the other hand, the somewhat larger correlation for $C_1 –$ Nu (slope = −0.030, r^2 = 0.945) and $C_1 – N_L$ (slope = 0.055, r^2 = 0.965 respectively (**Table ST2b**, **Figure SF2**) indicates the direct electronic transmission towards reaction center C_1 (negative value) and withdrawal (positive value). Conversely, in the case of the Hammett substituent constants for the nucleophilic variation ($\delta\sigma_X < |0| < \delta\sigma_X$) in the gas phase, a positive magnitude of the slope (0.022) for $C_1 – Nu$ bond perturbation is observed. This indicates the gradual obstruction of mutual charge transmission to the TS by gradual weaker interaction with the reaction center with a fair correlation coefficient, r^2 = 0.949 (**Table ST2a**, Figure SF1a in SI).

For $C_1 – O_3$, and $C_1 = O_2$ and $C_1 – N_L$, poor correlation coefficients with small values were obtained for the slopes (−0.009, r^2 = 0.687; −0.003, r^2 = 0.738; and 0.003, r^2 = 0.015, respectively) for nucleophilic variation in the gas phase. **Table ST2a** and **Figure SF1a** show the detrimental charge and inductive effect to the reaction moiety by the protection to cleavage of the $C_1 – N_L$ bond. Interestingly, the departure of the leaving group strongly depends on the nucleophilic parity and the phen-ring participations. On the same reaction center, later phen-ring perturbation enhanced the $C_1 – N_L$ bond cleavage with the nucleophile's interaction at the carbonyl moiety. Hence, it can be expected that the TS is positioned closer to the product on the reaction coordinate, giving the late TS with a product-like structure in the gas phase.

The negative slope (−0.005, r^2 = 0.958) for the $C_1 – N_u$ restricted bond formation with a gradual lower basicity of nucleophiles in the TS, applying pK_a(X) values, is strong evidence for the steric congestion regarding these nucleophiles. The very small negative value (−0.002, r^2 = 0.069) in the gas phase for the $C_1 – N_L$ bond also indicates a very small transferring effective charge to perturb the leaving group and an ineffective group participation and, hence, restricts departure of the leaving group.

The nature of the changes is somewhat different in the solution model (**Table ST3a**, **Figure SF3a**), producing a gradual longer $C_1 – N_L$ bond lengths in the TS from strongly basic to weakly basic nucleophiles. The slope regarding the Hammett substituent constant is large positive (0.053), which corresponds to a gradual enhancement of bond

breaking. On the other hand, sizeable positive C_1 **–** Nu bond saturation values indicate spontaneous close interaction of nucleophiles. Similarly, a considerable negative value for the slope (−0.011, see **Table ST3a** and **Figure SF3b**) is obtained, applying a Brönsted acid-base coefficient of the substituents in pyridine nucleophiles, where reasonable correlation coefficients between 0.848 and 0.904 were obtained.

A striking observation is the inefficiency of the leaving group (−NCS) in the gas phase unlikely to be the polarized solvent continuum model concerning the nucleophilic variation. The high positive slope (0.053, r^2=0.848) indicates a large extent of C_1 **–** N_L bond cleavage in the solvent model concerning the weakly basic nucleophiles. $C_1 – O_3$ and $C_1 = O_2$ actively enhance the leaving group departure with corresponding slopes **–**0.019 and **–**0.008 with good correlation coefficients. In the solvent phase, the bond perturbation behavior is mainly similar to the gas phase for the Y-substitution variation, except for the poor correlation coefficient (0.358) in the $C_1 – O_3$ bond (**Table ST3b** and **Figure SF4**). This result indicates that the phen-ring loses the electronic communication towards the leaving group via reaction center C_1 with gradual lower basicity, probably due to the solvent polarity effects. In this respect, the retardation of the reaction rate is ascribed to the electrostatic and intramolecular H-bonding effects.

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Pauling's Bond Valence-Bond Length Empirical Correlation:

We intended to find the valence length correlation using Pauling's bond valence-bond length empirical parameters[1] expressed in Eq. (14), where *s* is the bond softness or bond valence or bond order, and R_0 is the standard bond order:

$$s = \exp\left(\frac{R_0 - R}{b}\right) \tag{14}$$

Interestingly, this Pauling's bond softness *s* is a good indicator for destabilizing or stabilizing the reaction center.

It can be noted that the bond length in the TS when XY = 33 considers as R_0 and R are the respective bonds of the TS with X and Y variations. The empirical fitting parameter *b* is often associated with the softness of the bond. In practice, experimental[2] values for b have been reported as 0.25 to 0.55 Å. Due to the limited results, this value is often assumed to be a universal constant of 0.37 Å. Using Eq. (14), the valence length coefficients (*s*) were calculated and are summarized in **Table ST4** and **ST4a** for the gas phase and **Table ST6** and **ST6a** for the solution model. In addition, we considered the $C_1 – O_2$ single bond instead of C=O due to the examination of transition state behavior.

The Pauling's bond valence-bond length, *s*, for a Y-substituent's variation from an electron donor (ED) to electron-withdrawing (EW) substituents change ($\delta\sigma_Y \geq |0| \geq \delta\sigma_Y$) for gas, and the solvent model shows a decreasing C_1 – Nu but increasing $C_1 – N_L$ bond softness. The observation is common for the nucleophilic substitution at the carbonyl moiety: the increasing trend for the $C_1 – O_3$ destabilizes the reaction center, but conversely stabilizes the TS, and the decreasing trend of the $C_1 = O_2$ bond softness stabilizes the reaction center. Weakly basic phen-ring facilitates the $C_1 – N_L$ bond cleavage, where nucleophilic charge transmission pushes forward the departure of the leaving group.

In the case of gas-phase nucleophilic substituent's variation (**Table ST4**) from stronger basic to weaker ($\delta\sigma_X \geq |0| \geq \delta\sigma_X$), the bond softness for C_1 – Nu is gradually increasing, but for $C_1 – N_L$, it increases for 4-MeO pyridine to 3-Cl ($\delta\sigma_X \geq 0$) and gradually decreases for 3-Cl pyridine to 4-CN pyridine, ($\delta\sigma_X \geq 0$). The 3-Cl pyridine acquired the maximum magnitude (1.037). This observation suggested that stronger nucleophiles interacted within the closest proximity in advance by forming a very tight TS. On the other hand, weaker nucleophiles produce a long-distance

weaker interaction where $C_1 - N_L$ leaving group departure was restricted, e.g., $s_{(C1-NL)}$ of 53 and 63 are 0.971 and 0.967, respectively. At this specific point $C_1 - O_3$ and $C_1 = O_2$ moieties play a vital as well as surprising role in TS tightness by employing remarkable shunt effects through the C_1 reaction center during the stronger and weaker nucleophilic attack. The proposed scenario can be adequately rationalized with the interaction of similar bond softness for the overall process with XY = 11, 22, 33, 44, 55, and 66, respectively, in SI (**Table ST4a**). Except for $C_1 = O_2$ and $C_1 - N_L$, where $C_1 = O_2$ and $C_1 - O_3$ apply the shunt effect, the $C_1 - N_L$ bond cleavage is facilitated by the nucleophilic charge transmission.

Conversely, in the solvent model for the nucleophilic (X) substitution variation from stronger to weaker nucleophiles, the bond softness $s_{(C1-Nu)}$ and $s_{(C1-NL)}$ shows the same trend. The respective values display an increasing trend representing a gradual loosening of the TS. This suggests that the TS is destabilized by the shunt effect during the stronger nucleophiles, whereas it is stabilized by the weaker ones. The phenomenon influences the advanced nucleophilic attack with the formation of a very tight TS with the action of stronger nucleophiles. The structural features (see **Table ST5a** and **b** in SI) indicate that two cyclic structures (**Figure 4** in the manuscript) are present, having five- and six-centered H-bonds. These scenarios are also valid for the gas phase model. The respective $C_1 - N_L$ bond lengths gradually decreased to 1.868, 1.844, and 1.842 or 1.808, 1.798, and 1.812Å respectively for 3-Cl, 4-Ac, and 4-CN pyridines in the gas phase and the solvent model respectively. The corresponding H-bonds were bounded in 2.765 Å or less. The observations indicate the electronic shunting effects between the carbonyl bond and the phen-ring environment. The reflection indicates extra stability to the transitional moments during the weaker nucleophilic interaction in the solvent model. The reason is an advanced nucleophilic attack leaving an N^+ nucleophile residue behind as a tetrahedral zwitterion intermediate (**T**$^{\pm}$ in the manuscript). In the solvent model, the behavior is reasonably different mainly due to the solvent polarization, which controls the shunt effect, which is equally reflected in the bond softness for the XY = 11, 22, 33, 44, 55, 66 in the solvent model (see **ST6a** in SI).

References:

1. F. D. Hardcastle. Valence-Length Correlations for Chemical Bonds from Atomic Orbital Exponents. *J. Ark. Acad. Sci.* **2013**, *67* (11), 53–58.
2. F. D. Hardcastle. A General Valence-Length Correlation for Determining Bond Orders: Application to Carbon-Carbon and Carbon-Hydrogen Chemical Bonds. *J. Ark. Acad. Sci*. **2016**, *Vol. 70, Article 17.* (Article 17), 96–101.

NBO Charges:

A summary of the natural bond order charges (NBO charge), natural valence electron population (VPOP), Wiberg bond index (WBI), the bonding coefficients (BC), and the respective dipole moment (DM) of the TS in gas and solvent continuum models is displayed in **Table ST7** (also **ST7a** and **b**).

In the case of VPOP, carbonyl oxygen (O_2), nucleophilic nitrogen (Nu), and phenylic oxygen (O_3) showed the enriched orbitals for the electron-donating substituents (X and Y) for both the gas and the solvent model and gradually decrease with the decreasing donating nature of the substituents. Carbonyl carbon (C_1) reaction center is populated during the strong donor and strong withdrawer nature of the substituents (X, Y) in the gas phase. However, in the solvent model, the orbital population is gradually decreasing with the substituents' decreasing ability to donate. Leaving nitrogen (N_L) shows the increasing population with the variation of the nucleophilic substituents (X) from donating to withdrawing for the solvent model, whereas the population is similar for stronger to the weaker donor for the gas phase; i.e., consistent with the observation of bond softness. We can assume the pictorial representation of the charge density lobes in **Figure 5** (in the manuxcript).

NBO charges on carbonyl oxygen (O_2), nucleophilic nitrogen (Nu), and phen-ring oxygen (O_3), show a gradually decreasing trend from electron-donating to electron-withdrawing series of substituents (X and Y) in the gas and solvent phase, respectively. This trend indicates the intersection route characteristics of the charge mobilization through the system's carbon reaction center (C_1). In the gas phase, the positive charge on the carbon reaction center, C_1, decreases for strong electron donor and withdrawer (X,Y) substituents; alternatively, the accumulation of negative charges increases, whereas in the solvent model, the amount of positive charge gradually increases with the decreasing electron donor power of the substituents. The EW nature of the Y-substituents affects the hybridization nature of the reaction center (C_1) in the solvent phase, tending to go from sp^2 to sp^3 by pushing ability by σ-inductive effects, resulting in a TS destabilization. On the other hand, the electronic charge on the leaving group′s nitrogen (N_L) is mostly stable in the gas phase but is increasing in the solvent model. The positive charge accumulation in the C_1 reaction center and the negative charge centered on the N_L leaving nitrogen have a parallel nature where the strong donor and the weaker donor substituents play roles assertively, which is indicates the rate-determining step change from formation to breakdown of the TS depending on the substituent's variation. Also in the gas phase, the charge flow towards the leaving group's nitrogen (N_L) is obstructed by creating a charge circulatory zone (shunt effect) between the reaction center, carbonyl group (C=O), and phen-ring. In the solvent model, the positive charge in the C_1 reaction center and the negative charge accumulation in the leaving nitrogen N_L gradually increase with the substituents' decreasing donor ability. The process reports the spontaneous charge separation by breaking the TS, probably due to the polarization function by ion-dipole interactions. This observation reflects in the dipole moment (DM) parameter in **Table ST7**, where the DM is higher in magnitude in the solvent model, and the gas phase is rather low and gradually decreases with the substituents' decreasing donor ability.

In the solvent model, the Wiberg bond index (WBI), C_1 – Nu bond is much higher, reflecting the advanced and stronger nucleophilic interactions. C_1 – O_2 WBI increases with decreasing donating ability of the substituents in the gas, and the solvent model is the general observation for the substitution process. That is opening the resonance and charge transfer function between the reaction center and the leaving group of the TS by providing the sp^2 hybridization characteristic of the C_1 reaction center. Moreover, C_1 – Nu and the C_1 – N_L bond index is not consistent with each other. That indicates charge delocalization takes place. In this regard, H-bonds with the phenyl ring (H_{ph}) and the pyridine moiety (H_{nu}) can be considered. Where, control is situated to form and break the TS i.e. substituted phenyl moiety plays the role for mechanistic criteria. C_1 – O_3 WBI is lower for the stronger and the weaker donor in the gas phase. Again, the indexes are gradually rising in the solvent model. The process indicates spontaneity in the solvent model. However, the gas phase represents a competition of opening charge transformation through phen-ring to activate the departure of the leaving group depending on the substituents' variation.

Table ST1. The comparison of mechanistic pathways for the experimental results with the current computational work is based on Hammett and Brönsted reaction parameters.

System	N_u	ρ_X and β_X	ρ_Y or ρ_Z	ρ_{XY}	Mechanism	Ref.
$YC_6H_4NHC(O)CH_2Br$	BnA	0.55 – 1.38 0.71 – 1.70	0.72 – -0.31	0.16 -1.51	Stepwise Concerted	1
$YC_6H_4N(CH_3)C(O)CH_2Br$	BnA	-0.27 – -1.75 0.50 – 3.23 -0.45 – -1.65 0.45 – 1.65	0.10 – 0.71	-0.32, -1.80 -0.22, -1.43	Concerted Concerted	2
$YC_6H_4NRC(O)CH_2Cl$	Pyn	R=H: -1.49 – -1.58 0.30 – 0.32 R=CH3 -1.48 – -1.60 0.30 – 0.32	 0.22 – 0.24 0.23 – 0.40	 -0.06 -0.10	Stepwise: E-Ad Concerted	3
$YC_6H_4NRC(O)CH_2Cl$	BnA	R=H: -0.43 – -0.66 0.50 – 0.87 R=CH3: -0.47 – -0.68 0.61 – 0.87	0.49 – 0.65 0.54 – 0.67	0.21 0.18	Stepwise Stepwise	4
$CH_3C(S)SC_6H_4Z$	Pyn	-1.71 – -1.78 0.37 – 0.39 -4.68 – -5.29 0.83 – 0.94	2.34 – 3.22	-0.15 1.34	Concerted Stepwise	5
$C_4H_3OC(S)SC_6H_4Z$	pyn	-0.70 – -0.77 0.16 – 0.17 -3.68 – -4.09 0.73 – 0.81	0.97 – 1.60	-0.11 0.86	Concerted Stepwise	6
$YC_6H_4O(EtO)P(O)Cl$	pyn	-5.45 – 6.70 0.87 – 1.07	1.79 – -3.82 -1.78 – 3.10	-6.26 -5.47	Concerted Concerted	7
$YC_6H_4OC(O)NCS$	pyn	Gas: -1.93 – -6.54 0.11 – 1.52 Sol: 10.5 – 18.9 -2.57 – -3.96	0.87 – 3.48 1.83 – -10.7	0.69 0.87	Stepwise Stepwise	This Work

References

(1) Keshab Kumar Adhikary; Hai Whang Lee. Nucleophilic Substitution Reactions of N-Methyl α-Bromoacetanilides with Benzylamines in Dimethyl Sulfoxide. *Bull Korean Chem Soc* **2011**, 32 (3), 857–862. https://doi.org/10.5012/bkcs.2011.32.3.857.

(2) Oh, H. K.; Ku, M. H.; Lee, H. W.; Lee, I. Kinetics and Mechanism of the Pyridinolysis of Aryl Furan-2-Carbodithioates in Acetonitrile. *J. Org. Chem.* **2002**, 67 (25), 8995–8998. https://doi.org/10.1021/jo0264269.

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Table ST2a. The correlation of relative bond-length variations (bond perturbation, Δd, in Å) with respect to unsubstituted reactant and nucleophile with the X-variations for the reactions of unsubstituted phenyl carbonyl isothiocyanates with X-pyridines in the gas phase.

BL Diff with 33	in TS for X3	in TS for X3	in TS for X3	in TS for X3
$^{a}\sigma_X$	$\Delta_{C1\text{-}Nu} \times 10^2$	$\Delta_{C1\text{-}O3} \times 10^2$	$\Delta_{C1=O2} \times 10^2$	$\Delta_{C1\text{-}NL} \times 10^2$
-0.27	1.069	-0.549	-0.250	1.552
-0.17	0.490	-0.273	-0.091	0.668
0	0	0	0	0
0.37	-0.691	0.520	0.157	-1.332
0.50	-0.646	0.002	0.078	1.090
0.66	-1.327	0.407	0.090	1.243
Slope	**0.023±0.02**	**0.009±0.001**	**-0.003±001**	**-0.003±0.006**
r^2	0.949	0.687	0.738	0.015
Slope (pK_a)^a	**0.005±0.02**	**-0.002±0.009**	**-0.001±0.003**	**0.002±0.001**
r^2	0.958	0.841	0.784	0.069

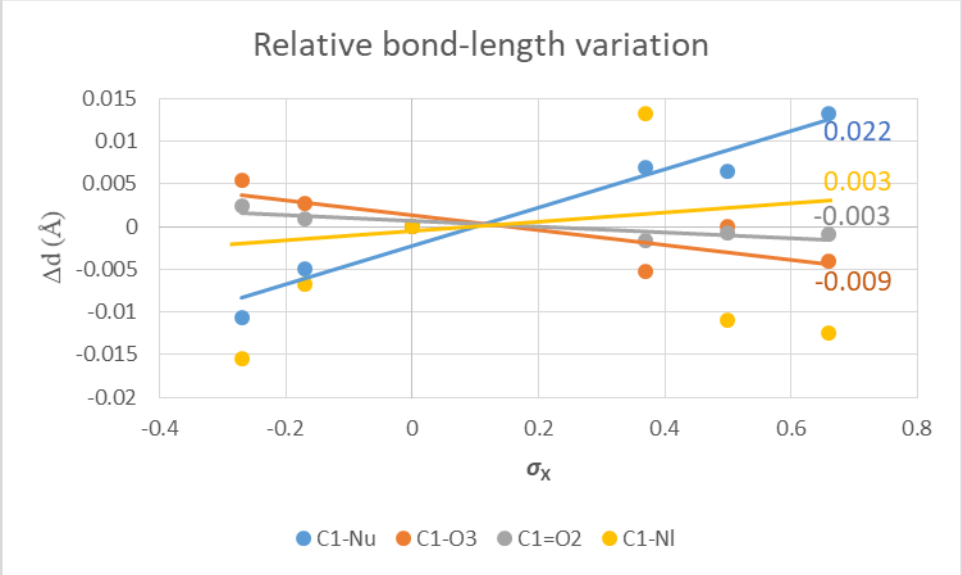


Figure SF1a. Correlation diagram of the relative bond-length variations (Δ_d, in Å) with respect to unsubstituted substrate and nucleophile (XY=33) with the variation of the substituents constants of the nucleophiles for the reactions of phenyl carbonyl isothiocyanate with X-pyridines in gas model (see Table ST2a) where, (●), (●), (●), and (●) represent the $C_1 - N_u$, $C_1 - O_3$, $C_1 = O_2$, and $C_1 - N_L$ with X variations respectively.

Table ST2b: The correlation of relative bond-length variations (bond perturbation, Δ_d, in Å) with respect to unsubstituted reactant and nucleophile with the Y-variations for the reactions of substituted phenyl carbonyl isothiocyanates with pyridine in the gas phase.

BL Diff with 33	in TS for 3Y	in TS for 3Y	in TS for 3Y	in TS for 3Y
σ_Y	$\Delta_{C1\text{-}Nu} \times 10^2$	$\Delta_{C1\text{-}O3} \times 10^2$	$\Delta_{C1=O2} \times 10^2$	$\Delta_{C1\text{-}NL} \times 10^2$
-0.27	0.681	-0.164	0.111	-1.657
-0.17	0.397	-0.086	0.047	-0.855
0	0	0	0	0
0.12	0.124	0.034	-0.036	-0.168
0.23	-0.772	0.253	-0.025	0.881
0.66	-2.095	0.636	-0.156	3.688
Slope	**-0.030±0.0001**	**-0.009±0.0003**	**0.003±0.0002**	**0.055±0.002**
r^2	0.945	0.965	0.955	0.965

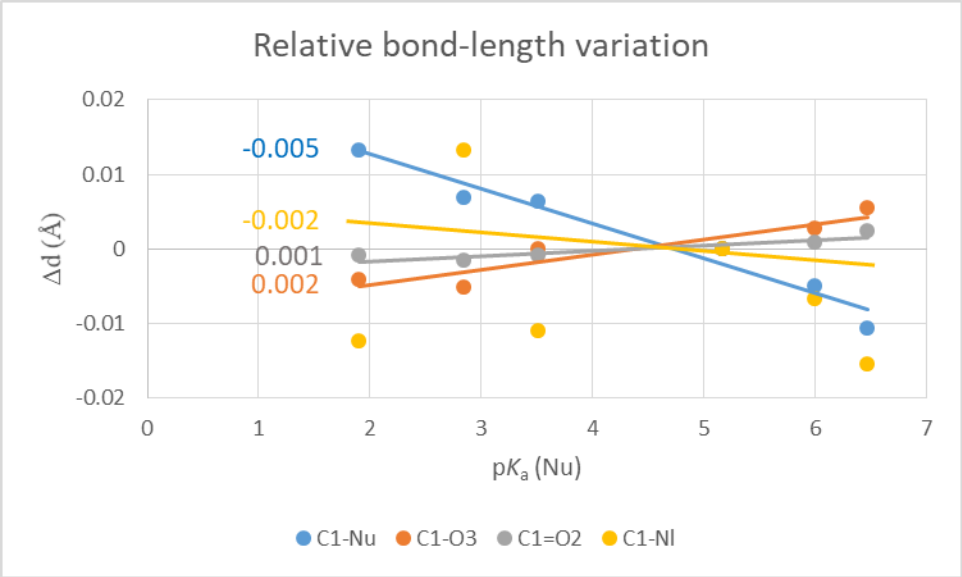


Figure SF1b. Correlation diagram of the relative bond-length variations (Δ_d, in Å) with respect to unsubstituted substrate and nucleophile with the variation of nucleophilic pK_a values (pK_a values are available in Table 7 or Table 8 of the main article) for the reactions of phenyl carbonyl isothiocyanate with X-pyridines in gas-phase model where, (●), (●) (●), (●) represent the $C_1 - N_u$, $C_1 - O_3$, $C_1 = O_2$, and $C_1 - N_L$ with X variations respectively.

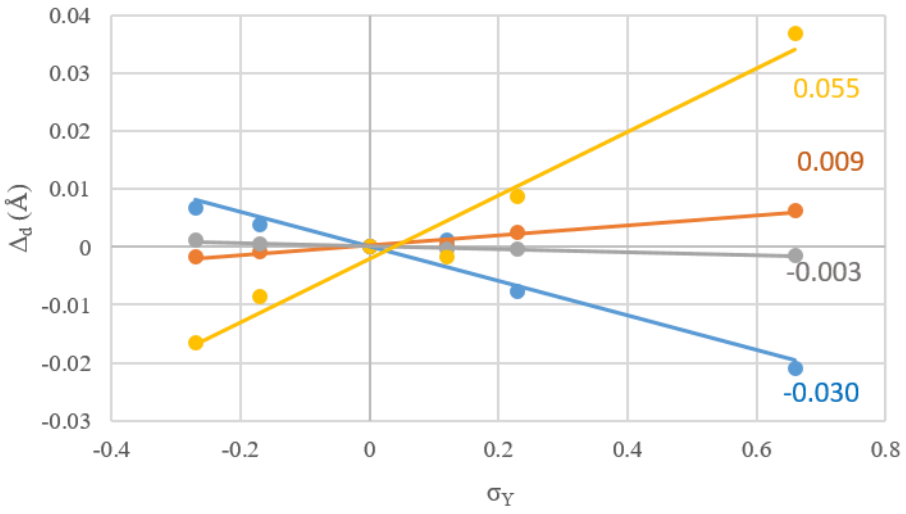


Figure SF2: Correlation diagram of the relative bond-length variations (Δ_d, in Å) with respect to unsubstituted reactant and nucleophile and the variation for Y-substituents constants for the reaction of substituted phenyl carbonyl isothiocyanates with pyridine in the gas phase (see Table ST2b), where (●), (●), (●), and (●) represents the $C_1 - N_u$, $C_1 - O_3$, $C_1 = O_2$, and $C_1 - N_L$ with Y-variation, respectively.

Table ST3a: The correlation of relative bond-length variations (bond perturbation, Δ_d, in Å) with respect to unsubstituted reactant and nucleophile with the nucleophilic variation for the phenyl carbonyl isothiocyanate with X-pyridines in continuum solvent model.

BL Diff with 33	in TS for X3	in TS for X3	in TS for X3	in TS for X3
$^a\sigma_X$	$\Delta_{C1\text{-}Nu} \times 10^2$	$\Delta_{C1\text{-}O3} \times 10^2$	$\Delta_{C1=O2} \times 10^2$	$\Delta_{C1\text{-}NL} \times 10^2$
-0.27	-1.215	1.088	0.451	-3.495
-0.17	-0.546	0.535	0.218	-1.812
0	0	0	0	0
0.37	0.806	-0.638	-0.290	1.772
0.50	0.593	-0.424	-0.149	0.750
0.66	1.167	-0.987	-0.342	2.225
Slope	**0.023±0.003**	**-0.019±0.003**	**-0.008±0.001**	**0.053±0.011**
r^2	0.919	0.908	0.870	0.848
Slope (pK_a)^a	**-0.005±0.022**	**0.004±0.02**	**0.002±0.007**	**-0.011±0.05**
r^2	0.947	0.944	0.924	0.904

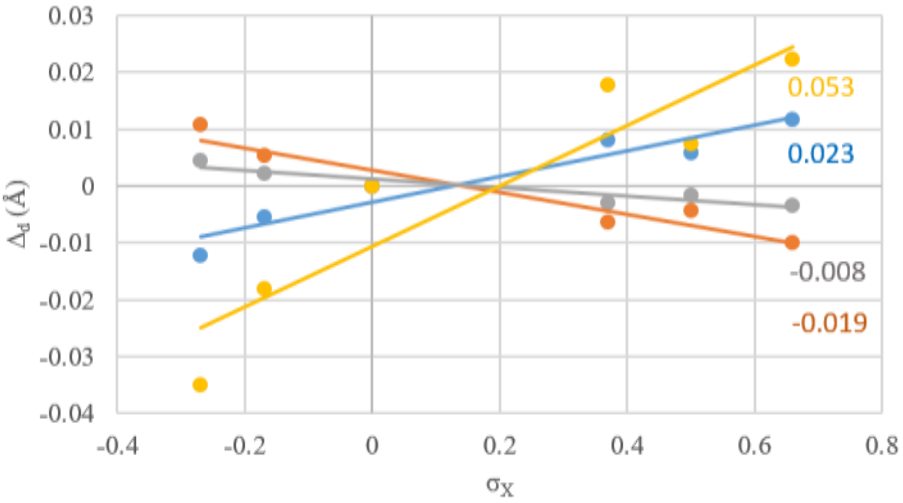


Figure SF3a: Correlation diagram of the relative bond-length variations (Δ_d, in Å) with respect to unsubstituted substrate and nucleophile (XY=33) with the variation of the substituents constants of the nucleophiles for the reactions of phenyl carbonyl isothiocyanate with X-pyridines in continuum solvent model (see Table), where (●), (●), (●), and (●) represent the $C_1 - N_u$, $C_1 - O_3$, $C_1 = O_2$, and $C_1 - N_L$ with X variations, respectively.

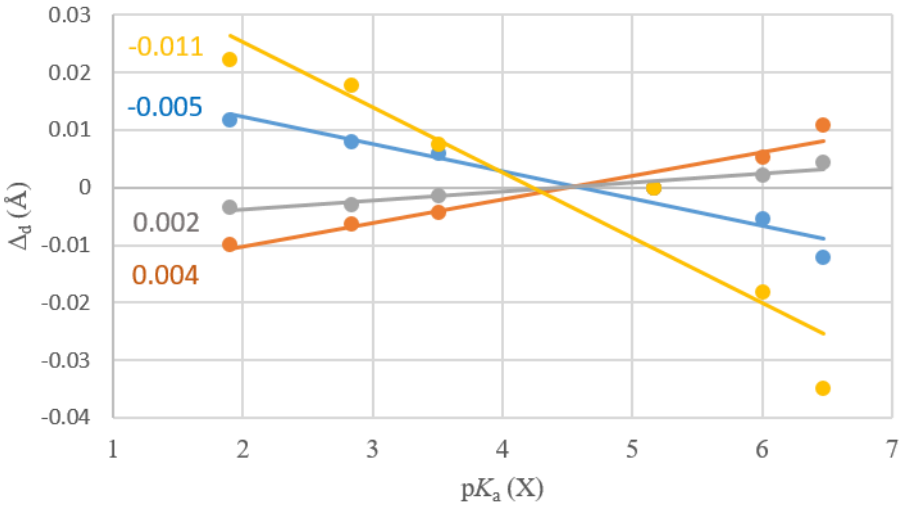


Figure SF3b: Correlation diagram of the relative bond-length variations (Δ_d, in Å) with respect to unsubstituted reactant and nucleophile with the variation of nucleophilic pK_a values (pK_a values are available in Error! Reference source not found. **and** Error! Reference source not found.**) for the reactions of phenyl ca rbonyl isothiocyanate with X-pyridines in continuum solvent model (see Table), where (●), (●) (●), (●), and represent the $C_1 - N_u$, $C_1 - O_3$, $C_1 = O_2$, and $C_1 - N_L$ with X variations, respectively.**

Table ST3b. The correlation of relative bond-length variations (bond perturbation, Δd, in Å) with respect to unsubstituted reactant and nucleophile with the Y-variations for the reactions of substituted phenyl carbonyl isothiocyanates with pyridine in the solvent phase.

BL Diff with 33	in TS for 3Y	in TS for 3Y	in TS for 3Y	in TS for 3Y
σ_Y	$\Delta_{C1\text{-}Nu} \times 10^2$	$\Delta_{C1\text{-}O3} \times 10^2$	$\Delta_{C1=O2} \times 10^2$	$\Delta_{C1\text{-}NL} \times 10^2$
-0.27	0.512	-0.164	0.172	-1.377
-0.17	0.318	-0.090	0.089	-0.821
0	0	0	0	0
0.12	0.042	0.029	-0.032	0.077
0.23	-1.513	1.179	-0.298	3.056
0.66	-1.550	0.560	-0.395	3.845
Slope	**-0.025±0.002**	**0.010±0.002**	**-0.006±0.0002**	**0.060±0.002**
r^2	0.792	0.420	0.902	0.868

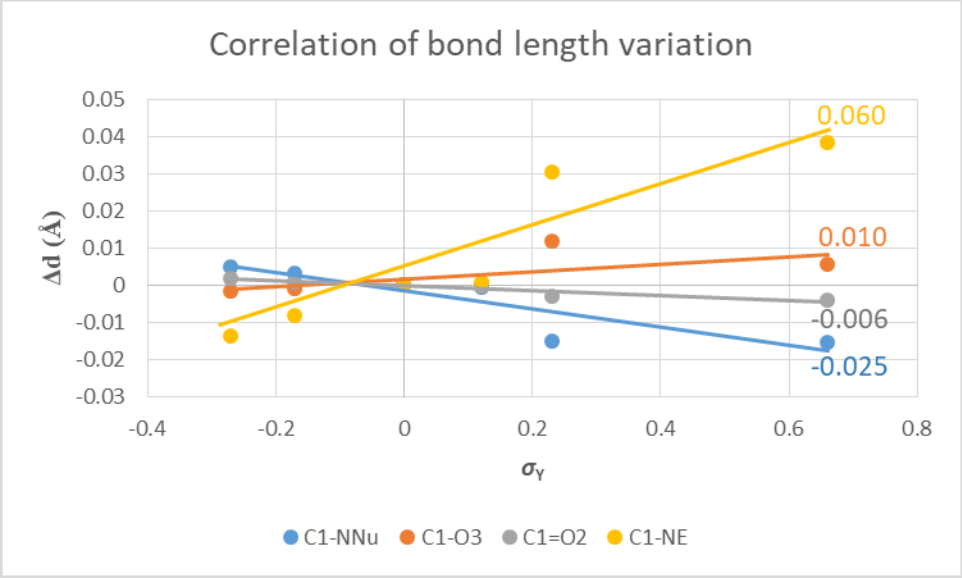


Figure SF4. Correlation diagram of the relative bond-length variations ($\Delta_{d,}$ in Å) with respect to unsubstituted reactant and nucleophile and the variation for Y-substituents constants for the reaction of substituted phenyl carbonyl isothiocyanates with pyridine in the solvent phase (Table ST1b) where, (●), (●), (●), and (●) represents the $C_1 - N_u$, $C_1 - O_3$, $C_1 = O_2$, and $C_1 - N_L$ with Y-variation respectively.

Table ST4. The bond valence length coefficients (*s*) are calculated for some specific system of the nucleophilic substitution reaction between Y-phenyl carbonyl isothiocyanates and X-pyridines in gas phase.

	σ_X	Species	C_1-N_{Nu}	C_1-O_{NL}	C_1=O_2	C_1-N_L	33-X3	dC_1-N_{nu}	dC_1-O_{NL}	dC_1=O_2	dC_1-N_L	V-length	VLC_1-N_{Nu}	VLC_1-O_{NL}	VLC_1=O_2	VLC_1-N_L
	-0.27	tsfD13	1.56199	1.37692	1.20733	1.8391		0.01069	-0.00549	-0.0025	0.01552		0.971521	1.014948	1.00678	0.958922
	-0.17	tsfD23	1.56778	1.37416	1.20574	1.84794		0.0049	-0.00273	-0.00091	0.00668		0.986844	1.007406	1.002462	0.982108
	0	tsfD33	1.57268	1.37143	1.20483	1.85462		0	0	0	0		1	1	1	1
	0.37	tsfD43	1.57959	1.36623	1.20326	1.86794		-0.00691	0.0052	0.00157	-0.01332		1.018851	0.986044	0.995766	1.036656
	0.5	tsfD53	1.57914	1.37145	1.20405	1.84372		-0.00646	-2E-05	0.00078	0.0109		1.017613	1.000054	0.997894	0.97097
	0.66	tsfD63	1.58595	1.36736	1.20393	1.84219		-0.01327	0.00407	0.0009	0.01243		1.036516	0.98906	0.997571	0.966963
	σ_Y	Species	C_1-N_{Nu}	C_1-O_{NL}	C_1=O_2	C_1-N_L	33-3Y	dC_1-N_{nu}	dC_1-O_{NL}	dC_1=O_2	dC_1-N_L	V-length	VLC_1-N_{Nu}	VLC_1-O_{NL}	VLC_1=O_2	VLC_1-N_L
	-0.27	tsfD31	1.57949	1.36979	1.20594	1.83805		-0.00681	0.00164	-0.00111	0.01657		1.018576	0.995577	1.003005	0.956204
	-0.17	tsfD32	1.57665	1.37057	1.2053	1.84607		-0.00397	0.00086	-0.00047	0.00855		1.010787	0.997678	1.001271	0.977157
	0	tsfD33	1.57268	1.37143	1.20483	1.85462		0	0	0	0		1	1	1	1
	0.12	tsfD34	1.57392	1.37177	1.20447	1.85294		-0.00124	-0.00034	0.00036	0.00168		1.003357	1.000919	0.999028	0.99547
	0.23	tsfD35	1.56496	1.37396	1.20458	1.86343		0.00772	-0.00253	0.00025	-0.00881		0.979351	1.006861	0.999325	1.024097
	0.66	tsfD36	1.55173	1.37779	1.20327	1.8915		0.02095	-0.00636	0.00156	-0.03688		0.944952	1.017338	0.995793	1.104813
σ_X	σ_Y	C_1-N_{Nu}	C_1-O_{NL}	C_1=O_2	C_1-N_L		33-XY(X=Y	dC_1-N_{nu}	dC_1-O_{NL}	dC_1=O_2	dC_1-N_L	V-length	VLC_1-N_{Nu}	VLC_1-O_{NL}	VLC_1=O_2	VLC_1-N_L
-0.27	-0.27	tsfD11	1.56858	1.37524	1.20878	1.82143		0.0041	-0.00381	-0.00395	0.03319		0.98898	1.01035	1.010733	0.914203
-0.17	-0.17	tsfD22	1.57135	1.37304	1.20621	1.84114		0.00133	-0.00161	-0.00138	0.01348		0.996412	1.004361	1.003737	0.964223
0	0	tsfD33	1.57268	1.37143	1.20483	1.85462		0	0	0	0		1	1	1	1
0.37	0.12	tsfD44	1.56415	1.37506	1.21223	1.81221		0.00853	-0.00363	-0.0074	0.04241		0.97721	1.009859	1.020201	0.891703
0.5	0.23	tsfD55	1.57065	1.3739	1.20403	1.85229		0.00203	-0.00247	0.0008	0.00233		0.994529	1.006698	0.99784	0.993722
0.66	0.66	tsfD66	1.5631	1.37483	1.20284	1.87178		0.00958	-0.0034	0.00199	-0.01716		0.97444	1.009232	0.994636	1.047471

Table ST4a: The bond valence length coefficients (*s*) are calculated for some specific systems of the nucleophilic substitution reaction between Y-phenyl carbonyl isothiocyanates and X-pyridines in gas phase.

System	*s* C_1-N_u	*s* C_1-O_3	*s* C_1=O_2	*s* C_1-N_L	System	*s* C_1-N_u	*s* C_1-O_3	*s* C_1=O_2	*s* C_1-N_L
31	1.019	0.996	1.003	0.956	13	0.972	1.015	1.007	0.959
32	1.011	0.998	1.001	0.977	23	0.987	1.007	1.003	0.982
33	1.000	1.000	1.000	1.000	33	1.000	1.000	1.000	1.000
34	1.003	1.001	0.999	0.996	43	1.019	0.986	0.996	1.037
35	0.979	1.007	0.999	1.024	53	1.018	1.000	0.998	0.971
36	0.945	1.017	0.996	1.105	63	1.037	0.989	0.998	0.967

Table ST5a. The structural parameters of the respective TSs recorded for the gas phase nucleophilic substitution reactions of Y-phenyl carbonyl Isothiocyano phosphates and X-Pyridines.

Species	DM	C_1	O_2	O_3	N_L	S_L	N_{nu}	N_{nu}-C_1	C_1=O_2	C_1-N_L	C_1-O_3	O_2-H_{nu}	N_L-H_{ph}	<$N_{Nu}C_1O_2$	<$O_2C_1N_L$	<$N_LC_1O_3$	<$O_2C_1O_3$	<$N_{Nu}C_1O_3$	<$N_{Nu}C_1N_L$
tsfD11	7.8294	-0.88714	-0.13312	0.13297	0.185756	-0.34697	0.219018	1.56858	1.20878	1.82143	1.37524	2.23532	2.65881	115.749	111.1321	101.1224	125.7333	102.4159	95.85492
tsfD12	8.6049	-0.90854	-0.13074	0.14344	0.18767	-0.34671	0.21439	1.56583	1.20789	1.83037	1.37606	2.23626	2.65224	115.8876	111.1245	100.9536	125.7545	102.5426	95.64608
tsfD13	8.9841	-0.92223	-0.14535	0.128627	0.135494	-0.34338	0.156616	1.56199	1.20733	1.8391	1.37692	2.23749	2.6461	116.0588	111.066	100.7537	125.7312	102.6771	95.55734
tsfD14	7.7158	-0.83947	-0.14098	0.135559	0.134636	-0.34561	0.221797	1.56233	1.20713	1.8417	1.37616	2.23968	2.68974	116.0185	111.0522	100.7667	125.8722	102.6966	95.35046
tsfD15	10.843	-0.9487	-0.12057	0.150126	0.18012	-0.33645	0.215521	1.55443	1.20693	1.84862	1.37956	2.23938	2.60069	116.4211	110.9741	100.4575	125.4509	102.9459	95.58229
tsfD16	14.0551	-0.8814	-0.10969	0.155716	0.14962	-0.32432	0.209849	1.54116	1.2052	1.88041	1.38327	2.24582	2.60408	117.0546	110.805	99.64665	125.2775	103.469	95.32483
tsfD21	7.0487	-0.9145	-0.13229	0.142757	0.18459	-0.35233	0.20539	1.57476	1.20712	1.82977	1.3726	2.23754	2.65951	115.7629	111.0369	101.024	126.0452	102.4425	95.51014
tsfD22	7.9945	-0.93009	-0.13046	0.152368	0.186733	-0.34988	0.199514	1.57135	1.20621	1.84114	1.37304	2.23881	2.66949	115.9123	110.996	100.797	126.107	102.6068	95.27355
tsfD23	8.3497	-1.04375	-0.13088	0.16812	0.17195	-0.34751	0.188136	1.56778	1.20574	1.84794	1.37416	2.23968	2.64882	116.0747	110.975	100.657	126.0413	102.7305	95.15903
tsfD24	7.2989	-0.8496	-0.14028	0.163808	0.136015	-0.35143	0.205444	1.56947	1.20539	1.84526	1.37464	2.24023	2.61896	116.0998	111.0127	100.8997	126.0467	102.5004	95.08899
tsfD25	10.0097	-1.0014	-0.13271	0.172497	0.180762	-0.34385	0.219125	1.56031	1.20538	1.85658	1.37688	2.24177	2.59833	116.4388	110.8865	100.403	125.7443	102.9756	95.18706
tsfD26	13.0243	-0.92319	-0.10638	0.1651	0.152891	-0.33092	0.199439	1.5469	1.20379	1.88775	1.38058	2.24766	2.60045	117.0657	110.7331	99.62999	125.546	103.5065	94.89665
Species	DM	C_1	O_2	O_3	N_L	S_L	N_{nu}	N_{nu}-C_1	C_1=O_2	C_1-N_L	C_1-O_3	O_2-H_{nu}	N_L-H_{ph}	<$N_{Nu}C_1O_2$	<$O_2C_1N_L$	<$N_LC_1O_3$	<$O_2C_1O_3$	<$N_{Nu}C_1O_3$	<$N_{Nu}C_1N_L$
tsfD31	6.2873	-0.87627	-0.12046	0.125298	0.179121	-0.3429	0.214226	1.57949	1.20594	1.83805	1.36979	2.235	2.6082	115.8087	111.01	101.2478	126.2476	102.5096	94.74575
tsfD32	7.3386	-0.9503	-0.11701	0.138237	0.18804	-0.33967	0.206757	1.57665	1.2053	1.84607	1.37057	2.23622	2.61689	115.9282	111.0106	101.1424	126.2384	102.625	94.54006
tsfD33	7.6399	-1.02478	-0.12006	0.148556	0.160098	-0.33493	0.200588	1.57268	1.20483	1.85462	1.37143	2.23693	2.61583	116.0905	110.9634	100.9517	126.2053	102.7568	94.45685
tsfD34	6.7048	-0.82529	-0.13244	0.135803	0.126466	-0.33398	0.21652	1.57392	1.20447	1.85294	1.37177	2.23792	2.59647	116.0976	111.0188	101.0979	126.2297	102.6342	94.32047
tsfD35	9.1262	-1.02957	-0.11833	0.139927	0.155513	-0.32628	0.197953	1.56496	1.20458	1.86343	1.37396	2.23911	2.59047	116.4285	110.8819	100.6341	125.9461	103.0347	94.48546
tsfD36	12.0081	-0.90735	-0.09682	0.140208	0.140249	-0.31301	0.211016	1.55173	1.20327	1.8915	1.37779	2.24439	2.6007	116.9933	110.7919	99.87475	125.7098	103.6043	94.20521
tsfD41	5.3246	-0.86013	-0.10345	0.122305	0.157418	-0.32282	0.205961	1.58637	1.20431	1.85409	1.36403	2.24422	2.66239	115.6198	110.8783	101.1022	126.8726	102.6288	94.11384
tsfD42	6.3039	-0.92327	-0.10275	0.133294	0.162194	-0.31886	0.198112	1.58334	1.20363	1.86182	1.3651	2.24536	2.67211	115.7365	110.8924	100.9497	126.8755	102.7305	93.9463
tsfD43	6.6181	-0.921	-0.1267	0.118852	0.118846	-0.31414	0.197862	1.57959	1.20326	1.86794	1.36623	2.24734	2.65827	115.907	110.878	100.8083	126.7945	102.8484	93.8463
tsfD44	8.9015	-0.74762	-0.17448	0.130114	0.034371	-0.36872	0.265523	1.56415	1.21223	1.81221	1.37506	2.26289	2.74684	116.2251	110.9892	101.1147	125.1402	102.5872	96.10776
tsfD45	8.138	-1.00359	-0.09425	0.140069	0.152996	-0.30833	0.194048	1.57163	1.20312	1.87503	1.36921	2.2469	2.61876	116.2323	110.8144	100.5304	126.4869	103.0932	93.95883
tsfD46	11.095	-0.89351	-0.08597	0.141827	0.126152	-0.29917	0.200742	1.558	1.20202	1.89989	1.37367	2.24984	2.62238	116.7914	110.7567	99.83145	126.1972	103.5919	93.76893
Species	DM	C_1	O_2	O_3	N_L	S_L	N_{nu}	N_{nu}-C_1	C_1=O_2	C_1-N_L	C_1-O_3	O_2-H_{nu}	N_L-H_{ph}	<$N_{Nu}C_1O_2$	<$O_2C_1N_L$	<$N_LC_1O_3$	<$O_2C_1O_3$	<$N_{Nu}C_1O_3$	<$N_{Nu}C_1N_L$
tsfD51	5.6231	-0.90392	-0.13833	0.124323	0.182275	-0.31848	0.20978	1.58503	1.20535	1.83316	1.36854	2.2399	2.71043	115.5868	111.0934	101.0761	126.5551	102.3702	94.8433
tsfD52	6.8963	-0.96751	-0.13234	0.139653	0.201087	-0.31994	0.205971	1.58291	1.20456	1.83748	1.37009	2.2417	2.66784	115.7512	111.1502	101.1032	126.4801	102.3928	94.57303
tsfD53	7.0444	-0.98228	-0.13331	0.156031	0.180433	-0.31257	0.194252	1.57914	1.20405	1.84372	1.37145	2.24152	2.635	115.9311	111.1157	100.9839	126.3876	102.4735	94.53849
tsfD54	6.4816	-0.86799	-0.13539	0.140953	0.134895	-0.32117	0.198934	1.57927	1.20385	1.84892	1.37022	2.24197	2.70968	115.858	111.063	100.796	126.628	102.4992	94.4949
tsfD55	8.1526	-0.95753	-0.1372	0.136877	0.173096	-0.30426	0.194341	1.57065	1.20403	1.85229	1.3739	2.24409	2.62131	116.265	111.0454	100.6595	126.1159	102.8094	94.51242
tsfD56	10.6841	-0.93359	-0.11145	0.143894	0.165576	-0.29918	0.208868	1.55665	1.20284	1.87798	1.37822	2.24756	2.61698	116.859	110.9448	99.98857	125.8203	103.3501	94.25644
tsfD61	3.4765	-0.89583	-0.11985	0.114435	0.178777	-0.2988	0.216542	1.59201	1.20505	1.83337	1.36436	2.24032	2.73732	115.3003	111.1981	101.459	126.9056	102.4057	93.97093
tsfD62	4.5949	-0.93507	-0.11302	0.133272	0.183404	-0.29973	0.210236	1.5896	1.20428	1.83816	1.36579	2.24153	2.7033	115.442	111.2416	102.4447	126.8627	102.4447	93.78692
tsfD63	4.5674	-1.0492	-0.11148	0.149548	0.170521	-0.29508	0.201645	1.58595	1.20393	1.84219	1.36736	2.24259	2.67405	115.6077	111.2443	101.3145	126.7507	102.5144	93.73114
tsfD64	4.5171	-0.81844	-0.12779	0.128943	0.136791	-0.29771	0.216279	1.58686	1.20375	1.84417	1.36655	2.24461	2.73196	115.534	111.2463	101.2927	126.9226	102.4641	93.63105
tsfD65	5.1997	-1.02628	-0.10378	0.144648	0.178599	-0.28775	0.205206	1.5773	1.20386	1.84963	1.3701	2.24261	2.64503	115.94	111.1769	101.0214	126.4465	102.7959	93.81651
tsfD66	7.607	-0.93472	-0.09359	0.14558	0.157653	-0.27432	0.212519	1.5631	1.20284	1.87178	1.37483	2.24572	2.64314	116.5044	111.1082	100.3638	126.1283	103.2917	93.67726

Table ST5b. The structural parameters of the respective TSs recorded for the solution phase nucleophilic substitution reactions of Y-phenyl carbonyl Isothiocyano phosphates and X-Pyridines

Species	DM	C	O	O_{NL}	N_E	S_E	N_{nu}	N_{nu}-C	C=O	C-N_E	C-O_{NL}	O-H_{nu}	N_E-H_{NL}	<N_{Nu}CO	<OCN_E	<N_ECO_{NL}	<OCO_{NL}	<$N_{Nu}CO_{NL}$	<$N_{Nu}CN_E$
tssfD11	11.5358	-0.81755	-0.2684	0.059801	0.183987	-0.41747	0.350106	1.54837	1.22179	1.74597	1.39111	2.25989	2.91435	115.9115	111.5338	101.582	123.4263	102.3344	98.39906
tssfD12	12.6237	-0.87383	-0.24987	0.100269	0.179525	-0.42197	0.355728	1.54701	1.22135	1.7452	1.39224	2.26017	2.72122	116.0849	111.7226	101.7077	123.2614	102.2563	98.11149
tssfD13	13.1637	-0.99185	-0.24527	0.121725	0.15781	-0.42389	0.358569	1.54341	1.22027	1.75521	1.39298	2.26185	2.70093	116.2989	111.655	101.4893	123.284	102.3771	97.95804
tssfD14	11.8836	-0.91102	-0.24124	0.124014	0.150372	-0.43079	0.395236	1.54164	1.21959	1.75996	1.39308	2.26474	2.6842	116.4436	111.7837	101.4869	123.3121	102.2999	97.63807
tssfD15	18.0663	-1.06337	-0.24011	0.116472	0.170708	-0.43189	0.480928	1.53029	1.21794	1.78451	1.39739	2.26783	2.96603	116.7408	112.1051	100.5183	123.5193	102.6282	97.14271
tssfD16	19.198	-0.82568	-0.2112	0.13888	0.132431	-0.42226	0.375251	1.52604	1.21554	1.80095	1.39796	2.27053	2.66624	117.3474	111.2781	100.2434	123.2269	103.0126	97.60026
tssfD21	11.9696	-1.06669	-0.28591	0.069072	0.194606	-0.4892	0.421086	1.55309	1.21902	1.74665	1.39636	2.26729	2.94166	116.3112	111.0731	101.9107	123.4656	102.3528	97.97216
tssfD22	12.0923	-0.89068	-0.24197	0.104576	0.162488	-0.4274	0.371006	1.5534	1.21889	1.76356	1.38655	2.26248	2.73681	116.1527	111.4955	101.5829	123.7673	102.3912	97.49202
tssfD23	12.5097	-0.9944	-0.23624	0.127168	0.141049	-0.42956	0.371338	1.5501	1.21794	1.77204	1.38745	2.26272	2.7134	116.3291	111.4368	101.3838	123.7785	102.5071	97.37676
tssfD24	11.0565	-0.88773	-0.23654	0.129257	0.134413	-0.42972	0.394926	1.5501	1.21749	1.77313	1.38776	2.26218	2.69079	116.3678	111.4197	101.4684	123.7977	102.3909	97.36677
tssfD25	14.4673	-0.88157	-0.22812	0.121179	0.142552	-0.42635	0.376701	1.54369	1.2167	1.7859	1.38897	2.2661	2.71038	116.696	111.2728	100.9559	123.7106	102.7402	97.35305
tssfD26	17.9763	-0.83996	-0.20424	0.142508	0.119163	-0.4249	0.382885	1.53341	1.21349	1.81589	1.39256	2.27122	2.6744	117.3426	111.0652	100.2143	123.6905	103.1088	97.04724
Species	DM	C	O	O_{NL}	N_E	S_E	N_{nu}	N_{nu}-C	C=O	C-N_E	C-O_{NL}	O-H_{nu}	N_E-H_{NL}	<N_{Nu}CO	<OCN_E	<N_ECO_{NL}	<OCO_{NL}	<$N_{Nu}CO_{NL}$	<$N_{Nu}CN_E$
tssfD31	9.7583	-1.00607	-0.23669	0.097305	0.206694	-0.46416	0.406326	1.56068	1.21748	1.77639	1.38046	2.25447	2.81253	116.0191	111.2789	101.4909	124.2497	102.5275	97.13023
tssfD32	11.2348	-0.86639	-0.23721	0.095776	0.14619	-0.42348	0.356498	1.55874	1.21665	1.78195	1.3812	2.25579	2.7694	116.1666	111.332	101.4216	124.2779	102.4944	96.92211
tssfD33	11.5915	-0.97185	-0.23275	0.115768	0.125146	-0.42385	0.357644	1.55556	1.21576	1.79016	1.3821	2.25644	2.74596	116.3434	111.2823	101.2334	124.2775	102.6125	96.79212
tssfD34	10.208	-0.85564	-0.2317	0.120071	0.11956	-0.42467	0.373202	1.55514	1.21544	1.79093	1.38239	2.25469	2.71191	116.3657	111.2966	101.3077	124.2906	102.5607	96.70028
tssfD35	16.1992	-0.95986	-0.26681	0.074232	0.057122	-0.43674	0.433089	1.54043	1.21278	1.82072	1.39389	2.26538	3.46461	116.9365	110.6666	100.564	124.5262	102.9519	96.63291
tssfD36	16.6354	-0.80641	-0.20056	0.132625	0.109731	-0.41575	0.364769	1.54006	1.21181	1.82861	1.3877	2.2629	2.68527	117.2671	110.8895	100.1859	124.1202	103.1601	96.65299
tssfD41	9.96	-0.9286	-0.25485	0.056971	0.132796	-0.47504	0.427049	1.56691	1.21325	1.79022	1.38239	2.26781	3.04638	116.174	110.6285	101.5219	124.8734	102.5758	96.6507
tssfD42	9.8475	-0.82335	-0.21029	0.113414	0.12172	-0.41781	0.361163	1.56818	1.21356	1.79943	1.37445	2.25918	2.72085	115.9842	111.0325	101.4058	125.0303	102.4616	96.42004
tssfD43	10.4314	-0.84335	-0.22202	0.113914	0.090553	-0.41786	0.366914	1.56362	1.21286	1.80788	1.37572	2.26114	2.692	116.215	111.12	101.2373	124.9509	102.6026	96.09523
tssfD44	8.9031	-0.7731	-0.21967	0.120594	0.093892	-0.41773	0.366366	1.56414	1.21222	1.81239	1.37504	2.2629	2.74966	116.2225	110.9845	101.1065	125.1439	102.5911	96.11628
tssfD45	12.0537	-0.82502	-0.20171	0.121417	0.104461	-0.4129	0.363544	1.55822	1.21181	1.82016	1.37715	2.26274	2.71242	116.491	110.8391	100.7945	124.9317	102.8259	96.30849
tssfD46	15.5001	-0.7582	-0.18289	0.138034	0.086971	-0.40916	0.36266	1.54792	1.2092	1.84717	1.38104	2.26638	2.69599	117.0661	110.6782	100.068	124.8576	103.2222	96.05889
Species	DM	C	O	O_{NL}	N_E	S_E	N_{nu}	N_{nu}-C	C=O	C-N_E	C-O_{NL}	O-H_{nu}	N_E-H_{NL}	<N_{Nu}CO	<OCN_E	<N_ECO_{NL}	<OCO_{NL}	<$N_{Nu}CO_{NL}$	<$N_{Nu}CN_E$
tssfD51	13.0874	-1.03478	-0.27048	0.078425	0.087519	-0.43445	0.491448	1.55228	1.21285	1.81802	1.38627	2.26665	3.41789	116.4267	110.6762	101.1044	125.0341	102.7728	96.15914
tssfD52	10.9413	-0.84539	-0.23376	0.105435	0.138097	-0.41195	0.393435	1.56461	1.21512	1.78995	1.3768	2.25735	2.76916	116.0012	111.1666	101.4978	124.7415	102.5364	96.48051
tssfD53	11.1304	-0.85916	-0.23046	0.113605	0.111824	-0.4117	0.389187	1.56149	1.21427	1.79766	1.37786	2.25924	2.75204	116.1708	111.1047	101.2971	124.7386	102.6704	96.3733
tssfD54	9.8037	-0.80832	-0.21862	0.143742	0.12753	-0.41232	0.398133	1.56237	1.21397	1.79488	1.37861	2.25665	2.69317	116.1881	111.084	101.4337	124.7311	102.4748	96.49202
tssfD55	12.358	-0.84221	-0.22281	0.123073	0.116559	-0.41142	0.395633	1.55435	1.21323	1.81069	1.37953	2.26051	2.73212	116.5469	110.9908	100.8883	124.6316	102.8584	96.36582
tssfD56	15.1073	-0.80353	-0.19882	0.139609	0.105509	-0.40725	0.400924	1.54402	1.21048	1.83795	1.38337	2.26436	2.69938	117.1464	110.8196	100.1784	124.5556	103.2528	96.0848
tssfD61	7.6637	-1.13647	-0.25136	0.085714	0.173873	-0.4538	0.440552	1.57313	1.21335	1.78189	1.38107	2.26426	2.93516	115.9369	110.63	101.9343	124.9742	102.4869	96.46125
tssfD62	7.3592	-0.80746	-0.218	0.105924	0.119401	-0.40583	0.37449	1.57067	1.21302	1.80628	1.37102	2.25635	2.81459	115.8524	110.9713	101.3701	125.3938	102.6071	95.93025
tssfD63	7.5083	-0.95078	-0.20724	0.133931	0.102309	-0.40878	0.371601	1.56723	1.21234	1.81241	1.37223	2.2565	2.76503	116.0339	110.9674	101.2504	125.3357	102.6828	95.79857
tssfD64	3.7627	-0.75056	-0.28503	0.05227	0.289972	-0.30749	0.300671	1.85811	1.21732	1.46311	1.41892	2.31674	3.33966	108.049	119.3407	109.4579	121.9271	94.16927	97.38946
tssfD65	8.2827	-0.81081	-0.20444	0.124169	0.115525	-0.39401	0.361258	1.56284	1.21182	1.81697	1.37486	2.25991	2.75594	116.2786	110.8035	101.0195	125.1556	102.8205	96.04181
tssfD66	11.1222	-0.8002	-0.18129	0.148671	0.104203	-0.38884	0.362273	1.55213	1.2094	1.84153	1.37908	2.264	2.71174	116.877	110.6699	100.4061	125.0228	103.1475	95.79265

Table TS6. The bond valence length coefficients (*s*) are calculated for some specific system of the nucleophilic substitution reaction between Y-phenyl carbonyl isothiocyanates and X-pyridines in solution phase.

	σX	Species	C_1-N_{Nu}	C_1-O_3	C_1=O_2	C_1-N_L	33-X3	dC_1-N_{nu}	dC_1-O_3	dC_1=O_2	dC_1-N_L	V-length	VLC_1-N_{Nu}	VLC_1-O_3	VLC_1=O_2	VLC_1-N_L
	-0.27	tsfD13	1.54341	1.39298	1.22027	1.75521		0.01215	-0.01088	-0.00451	0.03495		0.967695	1.029842	1.012264	0.909865
	-0.17	tsfD23	1.5501	1.38745	1.21794	1.77204		0.00546	-0.00535	-0.00218	0.01812		0.985352	1.014565	1.005909	0.952207
	0	tsfD33	1.55556	1.3821	1.21576	1.79016		0	0	0	0		1	1	1	1
	0.37	tsfD43	1.56362	1.37572	1.21286	1.80788		-0.00806	0.00638	0.0029	-0.01772		1.022023	0.982905	0.992193	1.049057
	0.5	tsfD53	1.56149	1.37786	1.21427	1.79766		-0.00593	0.00424	0.00149	-0.0075		1.016156	0.988606	0.995981	1.020477
	0.66	tsfD63	1.56723	1.37223	1.21234	1.81241		-0.01167	0.00987	0.00342	-0.02225		1.032043	0.973677	0.990799	1.06198
	σY	Species	C_1-N_{Nu}	C_1-O_3	C_1=O_2	C_1-N_L	33-3Y	dC_1-N_{nu}	dC_1-O_3	dC_1=O_2	dC_1-N_L	V-length	VLC_1-N_{Nu}	VLC_1-O_3	VLC_1=O_2	VLC_1-N_L
	-0.27	tsfD31	1.56068	1.38046	1.21748	1.77639		-0.00512	0.00164	-0.00172	0.01377		1.013934	0.995577	1.004659	0.963468
	-0.17	tsfD32	1.55874	1.3812	1.21665	1.78195		-0.00318	0.0009	-0.00089	0.00821		1.008632	0.997571	1.002408	0.978055
	0	tsfD33	1.55556	1.3821	1.21576	1.79016		0	0	0	0		1	1	1	1
	0.12	tsfD34	1.55514	1.38239	1.21544	1.79093		0.00042	-0.00029	0.00032	-0.00077		0.998866	1.000784	0.999136	1.002083
	0.23	tsfD35	1.54043	1.39389	1.21278	1.82072		0.01513	-0.01179	0.00298	-0.03056		0.959933	1.032378	0.991978	1.086101
	0.66	tsfD36	1.54006	1.3877	1.21181	1.82861		0.0155	-0.0056	0.00395	-0.03845		0.958973	1.01525	0.989381	1.10951
σX	σY	Species	C_1-N_{Nu}	C_1-O_3	C_1=O_2	C_1-N_L	33-XY(X=Y	dC_1-N_{nu}	dC_1-O_3	dC_1=O_2	dC_1-N_L	V-length	VLC_1-N_{Nu}	VLC_1-O_3	VLC_1=O_2	VLC_1-N_L
-0.27	-0.27	tssfD11	1.54837	1.39111	1.22179	1.74597		0.00719	-0.00901	-0.00603	0.04419		0.980755	1.02465	1.016431	0.887424
-0.17	-0.17	tssfD22	1.5534	1.38655	1.21889	1.76356		0.00216	-0.00445	-0.00313	0.0266		0.994179	1.0121	1.008495	0.930631
0	0	tssfD33	1.55556	1.3821	1.21576	1.79016		0	0	0	0		1	1	1	1
0.37	0.12	tssfD44	1.56414	1.37504	1.21222	1.81239		-0.00858	0.00706	0.00354	-0.02223		1.02346	0.9811	0.990478	1.061923
0.5	0.23	tssfD55	1.55435	1.37953	1.21323	1.81069		0.00121	0.00257	0.00253	-0.02053		0.996735	0.993078	0.993185	1.057055
0.66	0.66	tssfD66	1.55213	1.37908	1.2094	1.84153		0.00343	0.00302	0.00636	-0.05137		0.990773	0.991871	0.982958	1.148938

Table ST6a: The bond valence length coefficients (*s*) are calculated for some specific systems of the nucleophilic substitution reaction between Y-phenyl carbonyl isothiocyanates and X-pyridines in continuum acetonitrile polarization model.

System	*s* C_1-N_u	*s* C_1-O_3	*s* C_1=O_2	*s* C_1-N_L	System	*s* C_1-N_u	*s* C_1-O_3	*s* C_1=O_2	*s* C_1-N_L
31	1.014	0.996	1.005	0.964	13	0.968	1.030	1.012	0.910
32	1.009	0.998	1.002	0.978	23	0.985	1.015	1.006	0.952
33	1.000	1.000	1.000	1.000	33	1.000	1.000	1.000	1.000
34	0.999	1.001	0.999	1.002	43	1.022	0.983	0.992	1.049
35	0.960	1.032	0.992	1.086	53	1.016	0.989	0.996	1.021
36	0.959	1.015	0.989	1.110	63	1.032	0.974	0.991	1.062

Table ST7. NBO charges, bond-coefficients and dipole moments of the TS for XY = 11, 33 and 66 are summarized of theoretical studies for the nucleophilic substitution reaction between Y-phenyl carbonyl isothiocyanates and X-pyridines in the gas phase and acetonitrile solvent continuum model.

System	Area	Postn	ts11(g)	ts33(g)	ts66(g)	ts11(s)	ts33(s)	ts66(s)
Natl Pop	C_1	Val	2.990	2.988	2.991	2.993	2.988	2.986
	O_2	Val	6.655	6.639	6.628	6.714	6.691	6.663
	N_u	Val	5.362	5.340	5.337	5.371	5.344	5.333
	O_3	Val	6.564	6.562	6.556	6.570	6.562	6.547
	N_L	Val	5.532	5.536	5.534	5.527	5.538	5.547
Charge	C_1	Nat	0.937	0.939	0.935	0.933	0.941	0.942
	O_2	Nat	-0.665	-0.649	-0.637	-0.723	-0.701	-0.673
	N_u	Nat	-0.387	-0.365	-0.361	-0.393	-0.366	-0.356
	O_3	Nat	-0.582	-0.581	-0.574	-0.587	-0.579	-0.566
	N_L	Nat	-0.559	-0.563	-0.560	-0.555	-0.566	-0.574
WBI	C_1-N_u		0.722	0.718	0.728	0.757	0.749	0.751
	C_1-O_2		1.639	1.662	1.674	1.568	1.600	1.635
	C_1-O_3		0.911	0.918	0.908	0.888	0.900	0.901
	C_1-N_L		0.476	0.445	0.429	0.546	0.502	0.456
	C_{ph}-H		0.906	0.905	0.901	0.907	0.908	0.902
	C_{nu}-H		0.894	0.895	0.891	0.898	0.899	0.894
Dipole M			7.829	7.640	7.607	11.536	11.592	11.122

Table ST7a. NBO Calculation data-base for tsfD11, tsfD33 and tsfD66 in the gas phase.

Gas Phase															
NBO Charge:															
		Natl Pop							Natl CRG						
sys	Orbt	C1	O2	O3	NNu	NL	C-hnl	C-hnu	C1	O2	O3	NNu	NL	Hnl	Hnu
Dts11T	Val	2.98987	6.65526	6.56382	5.36219	5.53178	4.20953	3.84385	0.93686	-0.66481	-0.5819	-0.38661	-0.55893	0.24272	0.25832
Dts33T	Val	2.98771	6.63878	6.56221	5.34006	5.53644	4.22768	3.85977	0.93878	-0.64856	-0.58068	-0.36467	-0.56325	0.24415	0.25954
Dts66T	Val	2.99144	6.62745	6.55561	5.33688	5.53367	4.22385	3.85637	0.9354	-0.63732	-0.57412	-0.36111	-0.56013	0.25164	0.26744

Continued …

WBI						NBO											
C1-O2	C1-Nu	C1-O3	C1-NL	Cnl-H	Cnu-H	C1-O2(BD	C1-O2(BD	Ocu% C	*	Ocu% O2	*	C1-O3(BD	C1-O3(BD	Ocu% C	*	Ocu% O3	*
1.6391	0.7219	0.9109	0.4755	0.9062	0.8942	1.99431	0.02628	0.5832	0.8123	0.8123	-0.5832	1.98719	0.12446	0.5576	0.8301	0.8301	-0.5576
1.6621	0.7177	0.9176	0.4451	0.9052	0.8945	1.99432	0.02648	0.5807	0.8141	0.8141	-0.5807	1.98693	0.12425	0.5577	0.8301	0.8301	-0.5577
						1.97588	0.44298	0.4981	0.8671	0.8671	-0.4981						
1.6744	0.7283	0.9078	0.429	0.9011	0.8911	1.99445	0.02484	0.5814	0.8136	0.8136	-0.5814	1.98697	0.12662	0.557	0.8305	0.8305	-0.557
						1.97722	0.43704	0.504	0.8637	0.8637	-0.504						

Continued …

C1-N26(BI	C1-N26(BI	Ocu% C	*	Ocu% N	*	C6-H10(BI	C6-H10(BI	Ocu% C6	*	Ocu% H10	*	C18-H21(B	C18-H21(B	Ocu% C18	*	Ocu% H21	*
1.97274	0.20333	0.5641	0.8257	0.8257	-0.5641	1.97535	0.01343	0.7887	0.6148	0.6148	-0.7887	1.9768	0.01769	0.7945	0.6073	0.6073	-0.7945
1.96982	0.21475	0.5631	0.8264	0.8264	-0.5631	1.97494	0.01342	0.7888	0.6146	0.6146	-0.7888	1.97744	0.01733	0.7948	0.6068	0.6068	-0.7948
1.97083	0.2084	0.5644	0.8255	0.8255	-0.5644	1.97397	0.0132	0.7911	0.6117	0.6117	-0.7911	1.97662	0.01631	0.7971	0.6039	0.6039	-0.7971

Table ST7b. NBO Calculation data-base for tssfD11, tssfD33 and tssfD66 in the solvent phase.

Solvent Phase															
NBO Charge:															
		Natl Pop							Natl CRG						
sys	Orbt	C1	O2	O3	NNu	NL	C-hnl	C-hnu	C1	O2	O3	NNu	NL	Hnl	Hnu
Dsts11T	Val	2.99314	6.71368	6.56966	0.74303	5.52676	4.23005	3.84864	0.933	-0.72261	-0.58681	-0.39245	-0.55469	0.23917	0.25526
Dsts33T	Val	2.98752	6.69144	6.56146	5.34404	5.53819	4.25161	3.8632	0.94045	-0.70056	-0.57928	-0.36627	-0.56582	0.23803	0.25558
Dsts66T	Val	2.98574	6.66307	6.54734	5.33282	5.54677	4.23821	3.85202	0.94232	-0.67254	-0.56551	-0.35548	-0.57375	0.24984	0.26589

Continued …

WBI						NBO											
C1-O2	C1-Nu	C1-O3	C1-NL	Cnl-H	Cnu-H	C1-O2(BD	C1-O2(BD	Ocu% C	*	Ocu% O2	*	C1-O3(BD	C1-O3(BD	Ocu% C	*	Ocu% O3	*
1.5683	0.7573	0.8877	0.5456	0.9069	0.898	1.99375	0.02828	0.5854	0.8108	0.8108	-0.5854	1.9866	0.13005	0.5579	0.8299	0.8299	-0.5579
1.6002	0.7489	0.9	0.5019	0.9081	0.8985	1.99406	0.02701	0.5838	0.8119	0.8119	-0.5838	1.98747	0.12572	0.5573	0.8303	0.8303	-0.5573
1.6346	0.7511	0.9007	0.4562	0.9018	0.8936	1.99437	0.02586	0.5828	0.8126	0.8126	-0.5828	1.98749	0.12581	0.5562	0.8311	0.8311	-0.5562

Continued …

C1-N26(BI	C1-N26(BI	Ocu% C	*	Ocu% N	*	C6-H10(BI	C6-H10(BI	Ocu% C6	*	Ocu% H10	*	C18-H21(B	C18-H21(B	Ocu% C18	*	Ocu% H21	*
1.97459	0.18184	0.5756	0.8178	0.8178	-0.5756	1.97624	0.01467	0.7879	0.6158	0.6158	-0.7879	1.97742	0.01628	0.7932	0.6089	0.6089	-0.7932
1.97406	0.18713	0.574	0.8189	0.8189	-0.574	1.97633	0.01421	0.7875	0.6163	0.6163	-0.7875	1.97821	0.0162	0.7934	0.6087	0.6087	-0.7934
1.97466	0.18664	0.5726	0.8198	0.8198	-0.5726	1.97435	0.01353	0.7906	0.6123	0.6123	-0.7906	1.97714	0.01523	0.7964	0.6048	0.6048	-0.7964

Table ST8a. Energy profiles for the nucleophilic substitution reaction of Y-phenyl carbonyl isothiocyanate and X-pyridines in the gas phase.

Species	$\Delta Eo^{\ddagger}$ Kcal	$\Delta Et^{\ddagger}$ Kcal	$\Delta H^{\ddagger}$ Kcal	$\Delta G^{\ddagger}$ Kcal	ΔEo° Kcal	ΔEt° Kcal	ΔH° Kcal	ΔG° Kcal
	TS-RC	TS-RC	TS-RC	TS-RC	PC-RC	PC-RC	PC-RC	PC-RC
tsfD11	18.3421	17.48932	17.48869	20.80821	9.525594	9.772205	9.771577	10.48066
tsfD12	18.04027	17.20631	17.20631	20.30181	9.666783	9.933475	9.933475	10.39093
tsfD13	19.68685	19.43773	20.0301	19.03111	11.64783	11.91515	12.50752	11.77459
tsfD14	18.54353	17.76668	17.76668	20.10164	10.46184	10.79316	10.79316	10.08345
tsfD15	17.44665	16.59386	16.59386	19.89958	9.893942	10.13365	10.13365	10.75049
tsfD16	18.9991	18.30822	18.30822	19.36494	12.74346	12.56023	12.56023	14.10202
tsfD21	18.38289	16.92017	16.92017	22.8997	9.838093	9.444018	9.444018	12.9656
tsfD22	18.96522	18.03023	18.03023	22.06763	10.78312	10.96447	10.9651	11.62775
tsfD23	18.62448	17.68384	17.68384	21.59386	10.84713	10.98518	10.98518	12.46799
tsfD24	20.2353	19.37749	19.37812	22.38452	12.44791	12.63302	12.63302	13.17393
tsfD25	18.33583	17.44225	17.44288	20.9789	10.92996	10.55596	10.55596	13.4331
tsfD26	17.29165	16.40121	16.40059	19.44087	11.17908	10.77183	10.77183	14.11645
Species								
tsfD31	20.49007	19.61595	19.61595	22.66062	11.93837	12.13227	12.13227	12.71209
tsfD32	21.36419	20.42606	20.42606	24.06624	13.20343	12.76166	12.76166	16.20982
tsfD33	21.1433	20.24471	20.24408	23.27244	13.35215	12.94803	12.9474	15.87473
tsfD34	21.13515	20.25538	20.25538	23.4676	13.20594	12.82629	12.82629	15.69903
tsfD35	20.71472	19.35678	19.35741	23.95141	13.28751	13.00639	13.00702	14.96798
tsfD36	20.29742	19.39318	19.39318	22.5301	14.06751	13.66841	13.66841	16.59135
tsfD41	23.79704	22.98881	22.98881	25.79566	15.36394	15.63503	15.63503	15.90172
tsfD42	23.59436	22.76165	22.76165	25.89606	15.55659	15.80759	15.80759	16.34223
tsfD43	24.24132	22.8062	22.8062	28.68032	16.48969	16.15774	16.15774	19.29466
tsfD44	10.2579	9.494846	9.494846	11.71811	16.28387	16.0153	16.0153	18.15071
tsfD45	24.13966	23.26805	23.26805	26.79716	16.79906	17.02496	17.02559	17.70392
tsfD46	24.05307	23.28813	23.28813	25.45492	17.85202	17.59976	17.59976	19.78663
Species								
tsfD51	21.93083	19.9548	19.95543	28.76754	12.40712	12.06324	12.06387	16.27509
tsfD52	21.63653	20.80759	20.80821	23.85289	12.51568	12.72526	12.72526	13.80207
tsfD53	22.55646	21.79654	21.79654	23.19212	13.78952	14.06625	14.06625	13.81023
tsfD54	22.11971	21.33407	21.33344	23.92819	13.55734	13.28751	13.28689	15.21459
tsfD55	21.13326	20.2993	20.2993	23.43371	12.78049	12.99384	12.99384	13.79266
tsfD56	20.11544	19.27584	19.27584	22.38138	12.94489	12.59537	12.59537	15.67268
tsfD61	25.83582	24.97739	24.97739	27.86456	15.49509	15.73166	15.73229	15.76555
tsfD62	25.70153	24.79855	24.79917	28.36782	15.75614	15.94439	15.94502	16.74635
tsfD63	25.70906	24.3731	24.3731	29.5011	16.11507	15.87285	15.87285	18.28186
tsfD64	25.42982	24.57202	24.57202	27.80118	15.7919	16.00463	16.004	16.32466
tsfD65	25.36017	24.49483	24.49483	27.50186	16.16402	16.38239	16.38239	16.60578
tsfD66	24.62786	24.33168	24.33231	24.86883	16.58194	16.80533	16.80533	16.9666

Table ST8b. Energy profiles for the nucleophilic substitution reaction of Y-phenyl carbonyl isothiocyanate and X-pyridines in the solution phase.

Species	$\Delta Eo^{\ddagger}$ Kcal	$\Delta Et^{\ddagger}$ Kcal	$\Delta H^{\ddagger}$ Kcal	$\Delta G^{\ddagger}$ Kcal	ΔEo° Kcal	ΔEt° Kcal	ΔH° Kcal	ΔG° Kcal
	TS-RC	TS-RC	TS-RC	TS-RC	PC-RC	PC-RC	PC-RC	PC-RC
tssfD11	0.311245	-0.52774	-0.52774	3.203436	-13.7456	-13.2549	-13.2549	-13.5335
tssfD12	0.35517	-1.03916	-1.03978	4.310363	-13.3578	-12.8734	-12.874	-13.3007
tssfD13	1.194151	1.052333	1.051706	0.244101	-12.1316	-11.5299	-11.5305	-13.6257
tssfD14	0.613704	0.343248	0.343875	1.541791	-12.6619	-11.6064	-11.6064	-14.5683
tssfD15	1.426329	1.277609	1.278237	0.654492	-10.0671	-9.94477	-9.94414	-11.0831
tssfD16	1.158382	0.972012	0.972012	1.578814	-10.0094	-9.4459	-9.4459	-10.6187
tssfD21	0.313755	0.103539	0.103539	-0.06087	-12.5282	-12.035	-12.0344	-12.9311
tssfD22	0.677083	0.424824	0.424824	1.241841	-12.0783	-11.0962	-11.0962	-13.061
tssfD23	0.738579	0.522088	0.522088	0.906751	-11.6598	-11.1559	-11.1559	-12.0319
tssfD24	0.882906	0.623744	0.623117	1.520455	-11.506	-10.4656	-10.4662	-13.4312
tssfD25	0.938127	0.735441	0.734814	1.060491	-10.8314	-10.3677	-10.3683	-10.7517
tssfD26	1.403739	0.68524	0.68524	2.804967	-8.78011	-8.28124	-8.28124	-9.05371
Species								
ttsfD31	13.58935	12.64808	12.64808	15.72978	1.142067	0.903614	0.903614	2.718999
tssfD32	13.16327	12.2722	12.27158	14.70631	1.175953	0.959462	0.958834	3.099269
tssfD33	1.101279	0.870356	0.870356	1.066766	-10.5127	-10.0226	-10.0226	-10.7154
tssfD34	13.23543	11.73945	11.73945	17.89155	1.608934	1.376128	1.376128	3.730544
tssfD35	1.565636	1.406876	1.407504	1.487197	-8.98719	-8.41929	-8.41929	-10.3483
tssfD36	1.858683	1.089356	1.089356	3.729289	-7.70519	-7.20444	-7.20444	-8.06036
tssfD41	17.49496	17.21886	17.21886	16.86118	6.63905	7.015556	7.015556	6.718116
tssfD42	17.42719	16.59825	16.59825	19.60528	6.500371	6.335963	6.335963	8.894947
tssfD43	17.12599	16.27571	16.27571	18.95392	6.229286	6.655365	6.655993	5.771832
tssfD44	17.5847	16.70744	16.70744	20.31248	6.747609	7.115957	7.115957	6.682348
tssfD45	16.7658	15.91929	15.91866	19.6674	6.484683	6.280742	6.280115	9.444645
tssfD46	15.79253	15.52647	15.52584	15.57918	6.883151	7.252127	7.251499	6.922684
Species								
tssfD51	16.30081	16.05608	16.05608	15.6275	4.700673	5.176326	5.176326	3.465107
tssfD52	16.73066	15.99773	15.9971	17.33307	4.922812	5.413524	5.412897	3.483933
tssfD53	16.42004	15.61306	15.61306	16.7112	4.937245	4.811115	4.811743	5.671431
tssfD54	16.83043	16.02471	16.02534	18.49459	5.438625	5.867214	5.867214	4.642315
tssfD55	16.11758	15.92431	15.92431	15.16	5.248489	5.689628	5.689628	4.379389
tssfD56	2.224521	2.040033	2.039406	2.323668	-7.2013	-6.76769	-6.76769	-6.99799
tssfD61	18.48455	17.65561	17.65561	20.29805	6.916409	6.718116	6.718116	9.346754
tssfD62	18.49082	17.63804	17.63866	20.52709	6.932725	7.275345	7.275345	7.1329
tssfD63	18.08106	16.67355	16.67355	21.79529	6.910134	6.701801	6.702429	8.75062
tssfD64	15.65824	14.74396	14.74396	18.19464	7.362569	7.179336	7.179336	8.62449
tssfD65	17.87649	17.03563	17.03563	20.04705	7.216359	7.585334	7.585334	7.025596
tssfD66	17.04504	16.22426	16.22426	18.92694	7.769822	8.160761	8.160761	7.343116

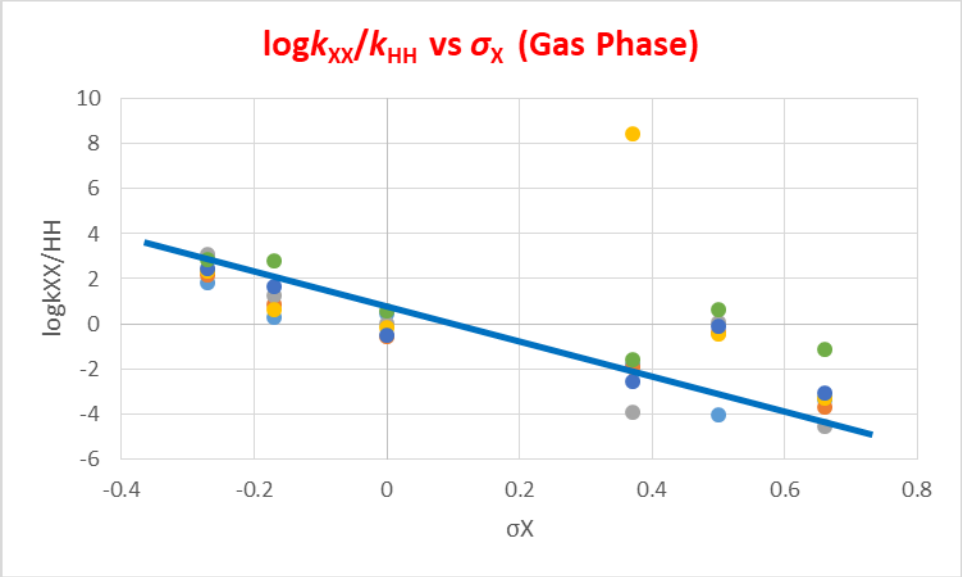


Figure SF5a. Hammett plots for nucleophilic variation in the substitution reaction between Y-phenyl carbonyl isothiocyanate and X-Pyridine in gas phase.

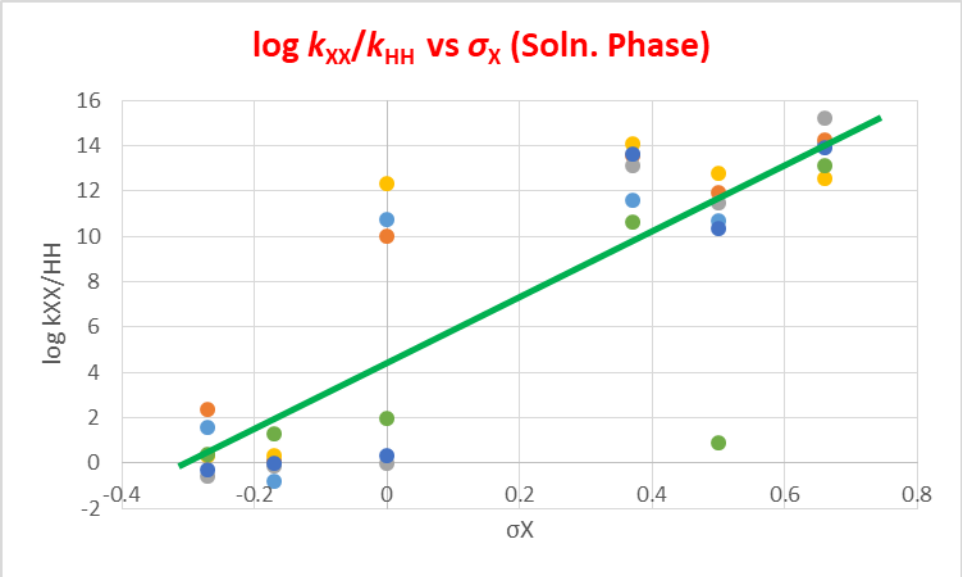


Figure SF6a. Hammett plots for nucleophilic variation in the substitution reaction between Y-phenyl carbonyl isothiocyanate and X-Pyridine in solution phase.

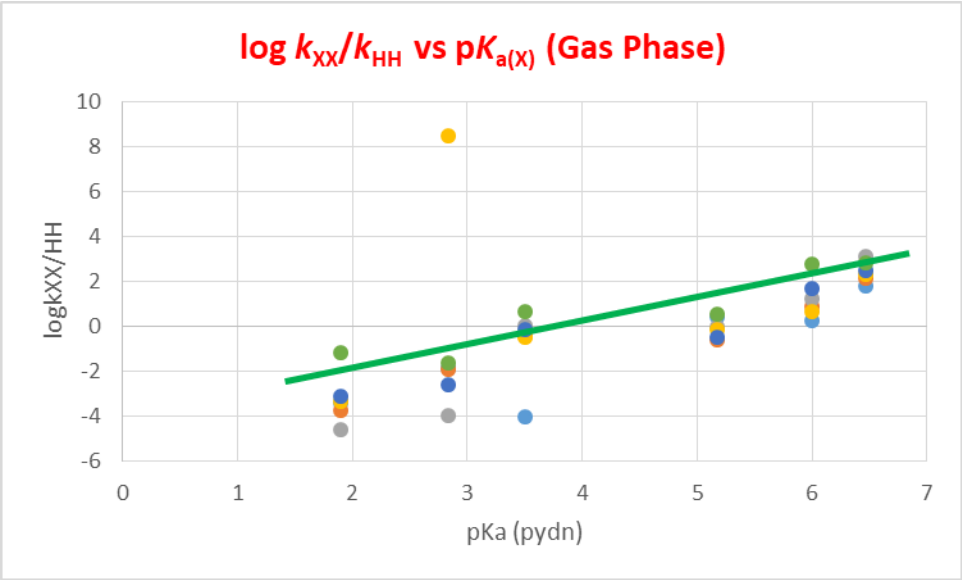


Figure SF5b. Brönsted plots for nucleophilic pK_a variation in the substitution reaction between Y-phenyl carbonyl isothiocyanate and X-Pyridine in gas phase.

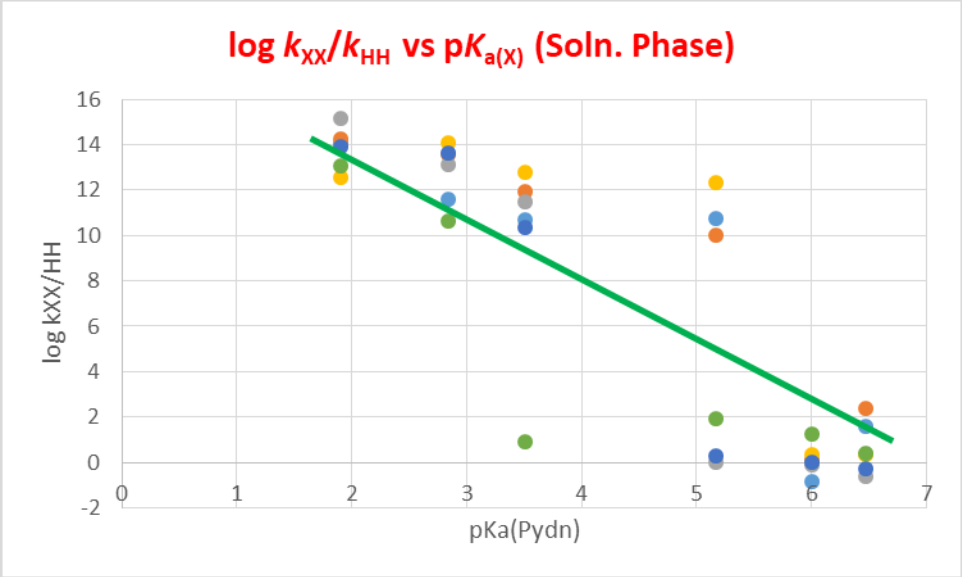


Figure SF6b. Brönsted plots for nucleophilic pK_a variation in the substitution reaction between Y-phenyl carbonyl isothiocyanate and X-Pyridine in gas phase.

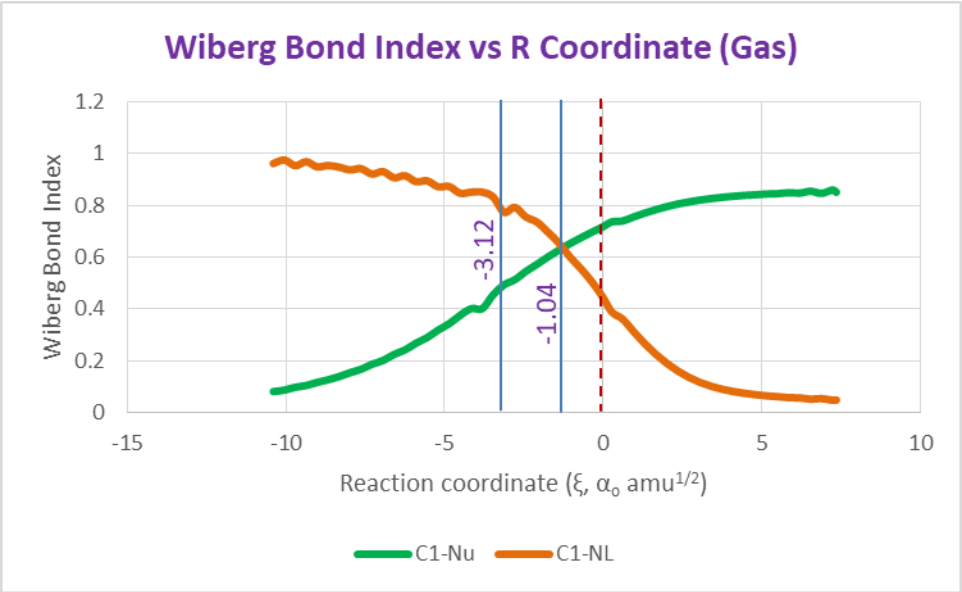


Figure SF7a. The Wiberg bond index crossing point of formation and breaking bond in the gas phase is closer before to the TS.

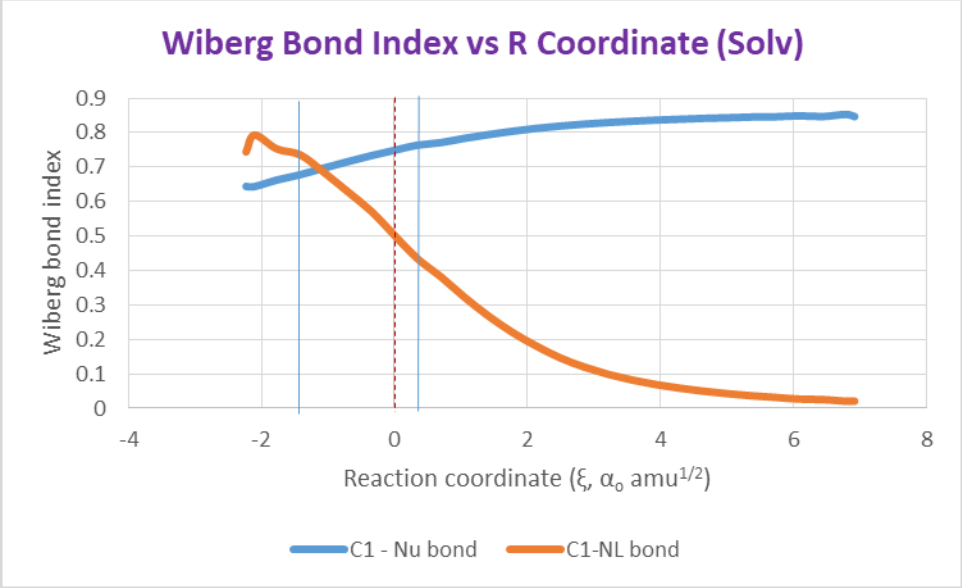


Figure SF7b. The Wiberg bond index crossing point of formation and breaking bond in the solvent model is far before to the TS.

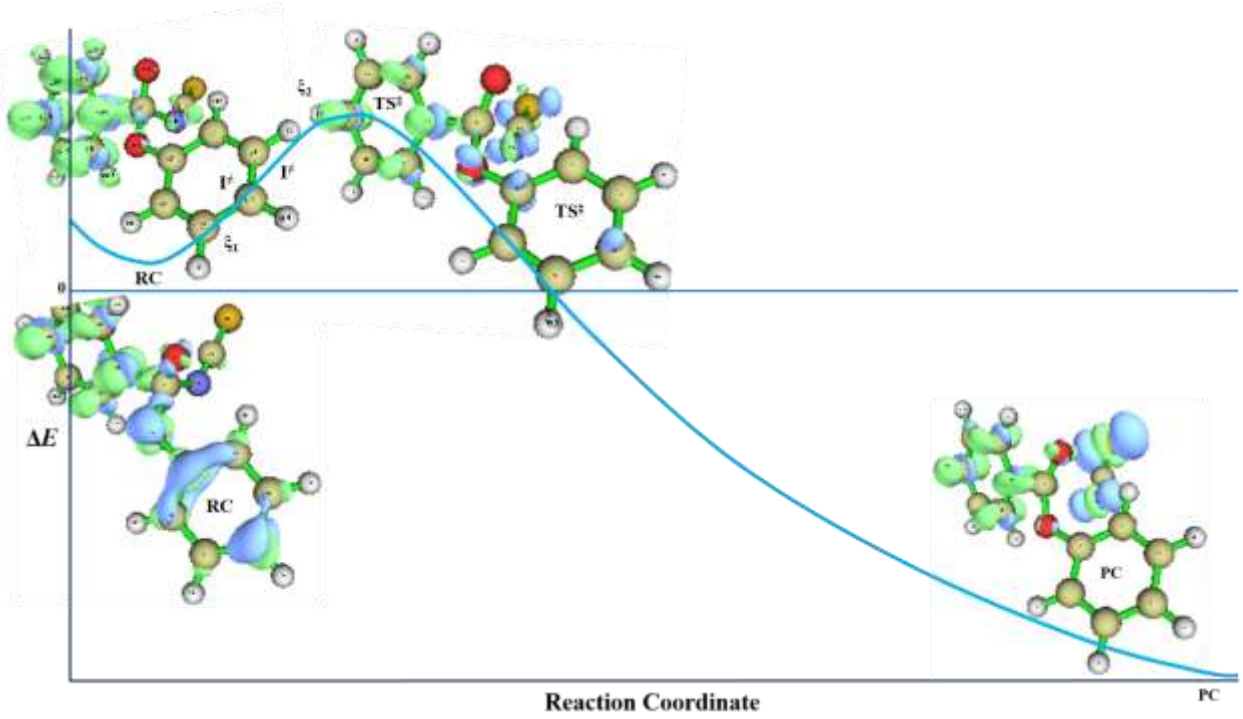
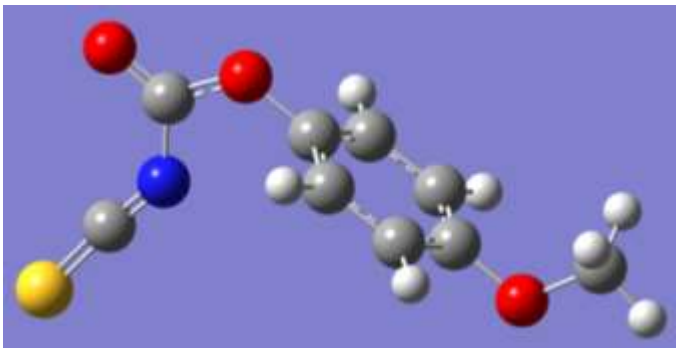


Figure SF8. Dual descriptor densities for RC, ξ_1, I, ξ_2, TS, ξ_3, and PC for the studied substitution process in solvent model.

Carbncs1.



Input orientation:

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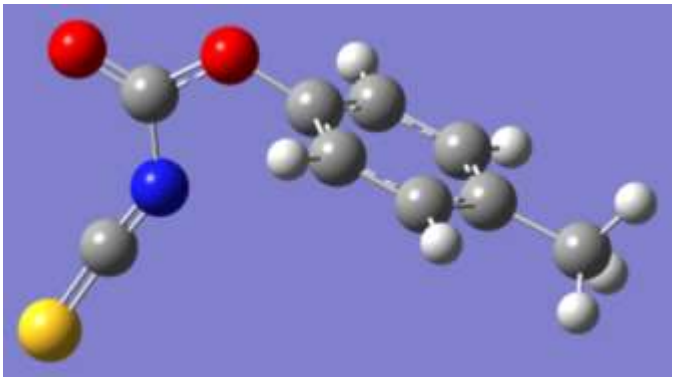
3	8	0	-0.794422	1.895031	0.000090
4	6	0	0.342073	1.060478	0.000061
5	6	0	0.911559	0.700375	-1.214115
6	6	0	0.911479	0.700179	1.214217
7	6	0	2.078399	-0.060381	-1.211055
8	1	0	0.448643	1.006777	-2.144091
9	6	0	2.078321	-0.060575	1.211109
10	1	0	0.448505	1.006433	2.144212
11	6	0	2.658058	-0.441802	0.000016
12	1	0	2.538566	-0.364891	-2.143371
13	1	0	2.538431	-0.365235	2.143405
14	7	0	-2.065832	-0.014029	-0.000064
15	6	0	-2.923039	-0.869375	-0.000103
16	16	0	-3.935719	-2.057604	-0.000161
17	8	0	3.780836	-1.243047	-0.000007
18	6	0	5.030418	-0.532145	-0.000016
19	1	0	5.121817	0.092104	0.894031
20	1	0	5.814386	-1.287820	-0.000034
21	1	0	5.121796	0.092123	-0.894053

Carbncs2.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.579346	1.419590	-0.000783
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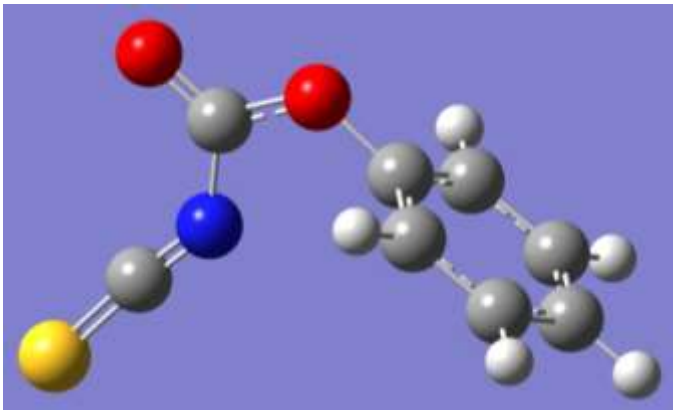
3	8	0	0.319872	1.883860	-0.002692
4	6	0	-0.784836	1.005009	-0.001850
5	6	0	-1.342758	0.624321	1.210193
6	6	0	-1.340833	0.619576	-1.213270
7	6	0	-2.480096	-0.180873	1.200866
8	1	0	-0.894825	0.949385	2.141464
9	6	0	-2.478193	-0.185584	-1.202593
10	1	0	-0.891424	0.940989	-2.145097
11	6	0	-3.066797	-0.597869	-0.000520
12	1	0	-2.916619	-0.487115	2.145314
13	1	0	-2.913216	-0.495523	-2.146526
14	7	0	1.664989	0.025931	0.002009
15	6	0	2.554754	-0.794987	0.004315
16	16	0	3.613393	-1.943122	0.007392
17	6	0	-4.317641	-1.442396	0.000167
18	1	0	-4.367332	-2.078007	0.886666
19	1	0	-5.212357	-0.810634	-0.000938
20	1	0	-4.366748	-2.080322	-0.884694

Carbncs3.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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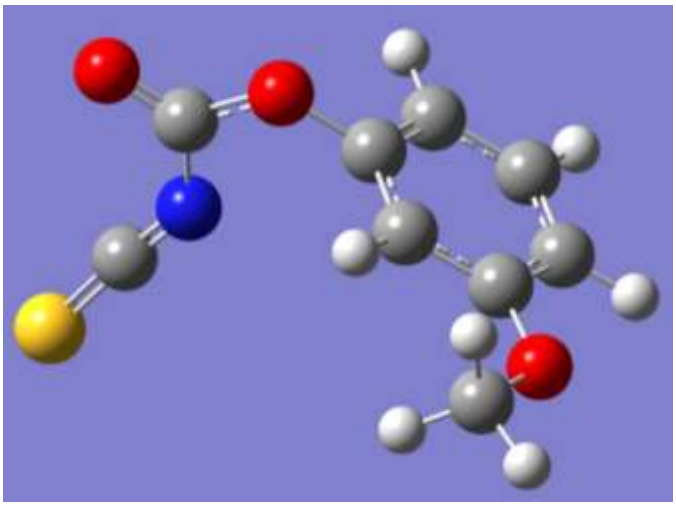
3	8	0	0.365323	1.706363	0.000122
4	6	0	1.306945	0.656203	0.000064
5	6	0	1.789777	0.190544	-1.215798
6	6	0	1.789700	0.190337	1.215878
7	6	0	2.779079	-0.792306	-1.208700
8	1	0	1.400119	0.590881	-2.143740
9	6	0	2.779002	-0.792511	1.208674
10	1	0	1.399985	0.590517	2.143863
11	6	0	3.272158	-1.284930	-0.000039
12	1	0	3.164821	-1.168383	-2.148848
13	1	0	3.164684	-1.168749	2.148783
14	1	0	4.042419	-2.047059	-0.000080
15	7	0	-1.272800	0.101669	-0.000047
16	6	0	-2.288270	-0.558127	-0.000114
17	16	0	-3.523922	-1.512115	-0.000208

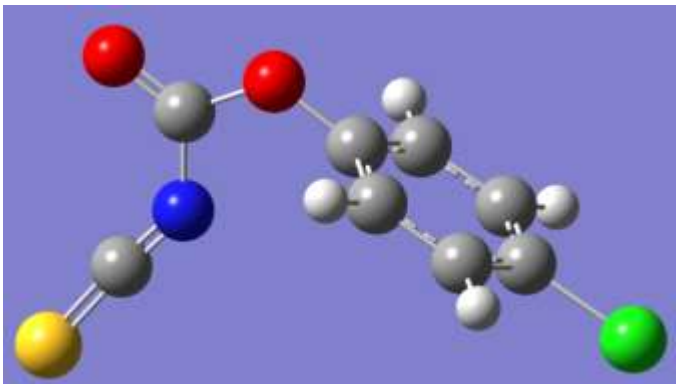
Carbncs4.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.625660	-1.111571	-0.937112
2	8	0	-2.475540	-1.576134	-1.649527
3	8	0	-0.387672	-1.631824	-0.899324
4	6	0	0.608077	-1.094694	-0.056550
5	6	0	0.741944	-1.592836	1.227759
6	6	0	1.471117	-0.148569	-0.599899
7	6	0	1.789040	-1.096868	2.010486
8	1	0	0.055741	-2.341046	1.602626
9	6	0	2.512648	0.332846	0.199305
10	1	0	1.318247	0.186548	-1.615822
11	6	0	2.666017	-0.145260	1.509390
12	1	0	1.919594	-1.463439	3.021680
13	1	0	3.479736	0.238020	2.112870
14	7	0	-1.801152	-0.016229	-0.090728
15	6	0	-2.708568	0.736444	0.185833
16	16	0	-3.798727	1.765482	0.621776
17	8	0	3.420053	1.258388	-0.210890
18	6	0	3.322402	1.775350	-1.542018
19	1	0	4.139169	2.486738	-1.642049
20	1	0	3.438647	0.978773	-2.282140
21	1	0	2.369447	2.289228	-1.695301

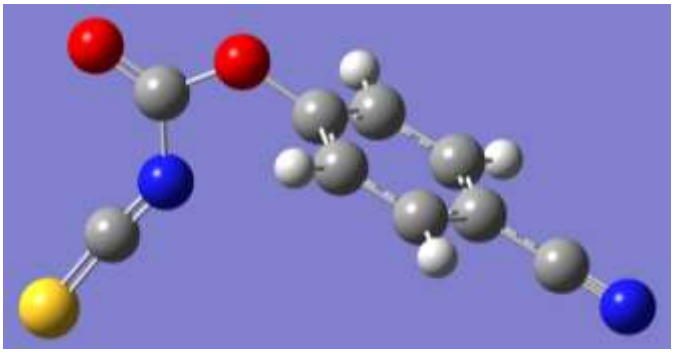
Carbncs5.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.036443	-1.360644	0.000008
2	8	0	3.036550	-2.026272	0.000013
3	8	0	0.819010	-1.935761	0.000017
4	6	0	-0.354152	-1.160378	0.000011
5	6	0	-0.942500	-0.831240	-1.213786
6	6	0	-0.942492	-0.831209	1.213803
7	6	0	-2.148145	-0.133524	-1.215116
8	1	0	-0.469057	-1.116257	-2.144917
9	6	0	-2.148137	-0.133493	1.215123
10	1	0	-0.469043	-1.116202	2.144938
11	6	0	-2.734386	0.208853	0.000001
12	1	0	-2.622677	0.135194	-2.149630
13	1	0	-2.622663	0.135249	2.149633
14	7	0	1.995784	0.032494	-0.000008
15	6	0	2.815264	0.925418	-0.000019
16	16	0	3.773592	2.156324	-0.000035
17	17	0	-4.258928	1.090801	-0.000005

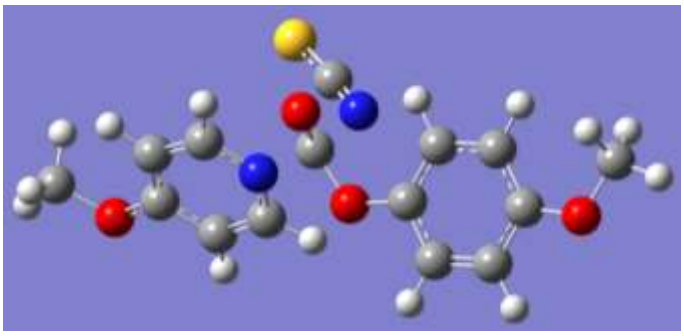
Carbncs6.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.892842	-1.347358	0.030640
2	8	0	-2.882994	-2.025894	0.052126
3	8	0	-0.666077	-1.909820	0.071290
4	6	0	0.496272	-1.127685	0.046714
5	6	0	1.066295	-0.737019	1.252701
6	6	0	1.093334	-0.853570	-1.178164
7	6	0	2.263383	-0.032866	1.232936
8	1	0	0.581261	-0.982834	2.188640
9	6	0	2.290441	-0.149487	-1.199284
10	1	0	0.628922	-1.188298	-2.096827
11	6	0	2.876705	0.264179	0.006460
12	1	0	2.722696	0.282958	2.160559
13	1	0	2.770563	0.076650	-2.142440
14	7	0	-1.862431	0.042903	-0.035663
15	6	0	-2.696083	0.922999	-0.087175
16	16	0	-3.671081	2.136733	-0.156262
17	6	0	4.110319	0.987764	-0.014512
18	7	0	5.107059	1.573124	-0.031492

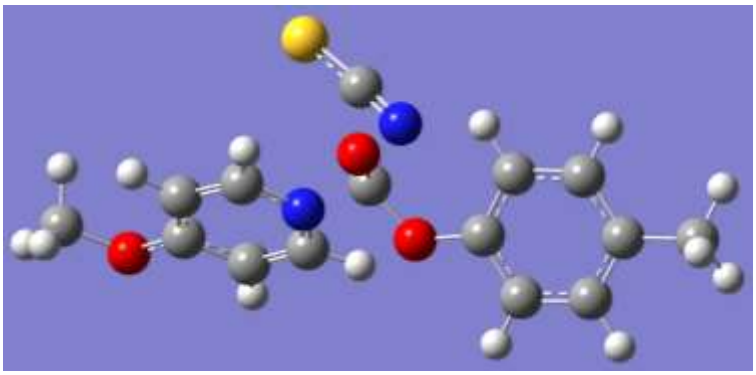
tsfD11.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.070132	0.017509	0.710631
2	8	0	0.099342	0.404256	1.843266
3	8	0	0.723991	-0.885115	0.042862
4	6	0	2.103232	-0.708607	0.018871
5	6	0	2.821650	-1.774927	-0.520919
6	6	0	2.759132	0.431043	0.459468
7	6	0	4.200890	-1.701132	-0.622184
8	1	0	2.288187	-2.655635	-0.856898
9	6	0	4.150522	0.503962	0.355261
10	1	0	2.206031	1.256114	0.879494
11	6	0	4.876446	-0.557284	-0.183888
12	1	0	4.774706	-2.519797	-1.037868
13	1	0	4.646174	1.400016	0.701656
14	7	0	-0.083448	1.409843	-0.463610
15	6	0	-1.040099	2.106471	-0.600157
16	16	0	-2.371776	2.988876	-0.776043
17	6	0	-2.466978	-0.210416	1.271052
18	6	0	-1.823002	-1.037648	-0.823905
19	6	0	-3.793213	-0.502706	1.024344
20	1	0	-2.106063	0.258020	2.177127
21	6	0	-3.119172	-1.351819	-1.134625
22	1	0	-0.991872	-1.189882	-1.494638
23	6	0	-4.137531	-1.081924	-0.202326
24	1	0	-4.529494	-0.253233	1.772613
25	1	0	-3.369242	-1.785209	-2.092684
26	7	0	-1.515316	-0.490354	0.373032
27	8	0	-5.380550	-1.396352	-0.576781
28	6	0	-6.469107	-1.095312	0.305470
29	1	0	-6.523674	-0.020920	0.496589
30	1	0	-7.364074	-1.422638	-0.216999
31	1	0	-6.368201	-1.643980	1.245350
32	8	0	6.236784	-0.576486	-0.323542
33	6	0	6.964764	0.567157	0.095345
34	1	0	8.011382	0.346301	-0.107076
35	1	0	6.665663	1.458446	-0.467163
36	1	0	6.833416	0.753814	1.166919

tsfD12.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.267129	0.039607	0.740573
2	8	0	0.423593	0.397412	1.883587
3	8	0	1.088400	-0.819896	0.047522
4	6	0	2.462006	-0.613336	0.039826
5	6	0	3.206467	-1.648415	-0.517629
6	6	0	3.086502	0.536397	0.510748
7	6	0	4.589061	-1.533165	-0.601975
8	1	0	2.694756	-2.531088	-0.881581
9	6	0	4.473323	0.629647	0.414722
10	1	0	2.508923	1.340827	0.937863
11	6	0	5.249527	-0.392937	-0.134604
12	1	0	5.161755	-2.343846	-1.039924
13	1	0	4.958440	1.529444	0.778082
14	7	0	0.221729	1.471583	-0.398569
15	6	0	-0.754888	2.143383	-0.515303
16	16	0	-2.113783	2.989240	-0.664361
17	6	0	-2.125704	-0.252598	1.276843
18	6	0	-1.449224	-1.011842	-0.833979
19	6	0	-3.443553	-0.565591	1.012130
20	1	0	-1.781709	0.199897	2.197393
21	6	0	-2.736344	-1.343638	-1.162866
22	1	0	-0.610478	-1.129112	-1.502154
23	6	0	-3.766973	-1.119034	-0.231925
24	1	0	-4.190248	-0.350069	1.760554
25	1	0	-2.970462	-1.756223	-2.134043
26	7	0	-1.161521	-0.489884	0.379435
27	8	0	-5.000578	-1.447429	-0.624656
28	6	0	-6.101972	-1.188757	0.255261
29	1	0	-6.176571	-0.120982	0.474523
30	1	0	-6.986493	-1.516984	-0.284146
31	1	0	-6.000015	-1.760829	1.180969
32	6	0	6.752611	-0.284794	-0.194107
33	1	0	7.072467	0.756609	-0.273325
34	1	0	7.213813	-0.702005	0.707712
35	1	0	7.157129	-0.829397	-1.050533

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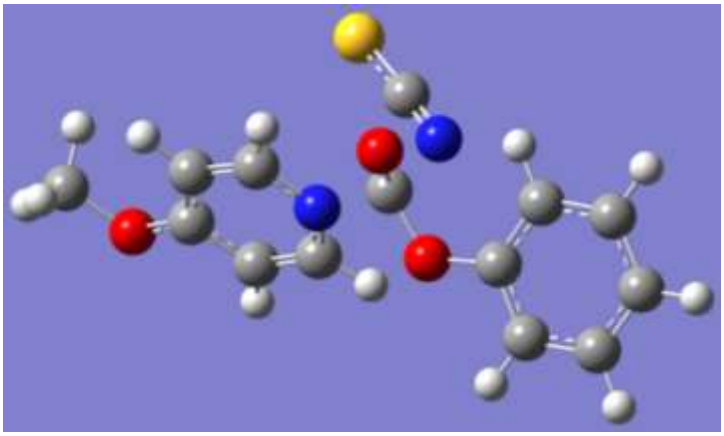
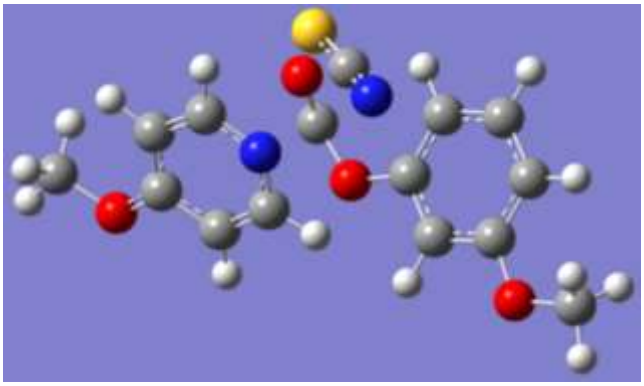
tsfD13.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.641820	0.047523	0.706521
2	8	0	0.812208	0.452928	1.830914
3	8	0	1.452582	-0.845347	0.042177
4	6	0	2.826210	-0.650428	0.011690
5	6	0	3.552627	-1.720606	-0.505240
6	6	0	3.460404	0.515893	0.429191
7	6	0	4.936000	-1.624463	-0.607836
8	1	0	3.025166	-2.613204	-0.818583
9	6	0	4.847671	0.594797	0.318208
10	1	0	2.889356	1.338936	0.828323
11	6	0	5.590770	-0.464614	-0.195982
12	1	0	5.500689	-2.457846	-1.009259
13	1	0	5.347114	1.501180	0.640050
14	1	0	6.668542	-0.388500	-0.274641
15	7	0	0.601783	1.436639	-0.498075
16	6	0	-0.372104	2.109680	-0.629281
17	16	0	-1.729233	2.955919	-0.793364
18	6	0	-1.747572	-0.195080	1.269436
19	6	0	-1.091979	-1.048306	-0.812490
20	6	0	-3.069852	-0.505823	1.025819
21	1	0	-1.393841	0.292028	2.168273
22	6	0	-2.384253	-1.380309	-1.119280
23	1	0	-0.259106	-1.201240	-1.480694
24	6	0	-3.406724	-1.107301	-0.192112
25	1	0	-3.809573	-0.251511	1.768987
26	1	0	-2.628642	-1.830076	-2.071219
27	7	0	-0.791065	-0.479791	0.376999
28	8	0	-4.645604	-1.439513	-0.563326
29	6	0	-5.739072	-1.134025	0.311711
30	1	0	-5.802704	-0.057343	0.486151
31	1	0	-6.629873	-1.476590	-0.208047
32	1	0	-5.636022	-1.667642	1.259954

tsfD14.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.076951	0.358435	0.822780
2	8	0	-0.059114	0.903195	1.899848
3	8	0	0.905514	-0.462302	0.317850
4	6	0	2.229977	-0.050851	0.314488
5	6	0	3.126335	-1.025648	-0.098814
6	6	0	2.654103	1.230206	0.666972
7	6	0	4.487536	-0.726624	-0.167966
8	1	0	2.778481	-2.014405	-0.366909
9	6	0	4.013747	1.505063	0.588650
10	1	0	1.949976	1.980443	0.987030
11	6	0	4.941972	0.548227	0.177380
12	1	0	4.363373	2.495594	0.855233
13	7	0	-0.230377	1.589223	-0.538645
14	6	0	-1.274458	2.110785	-0.774909
15	16	0	-2.719939	2.749221	-1.073855
16	6	0	-2.450452	-0.164911	1.241818
17	6	0	-1.497870	-1.170827	-0.648393
18	6	0	-3.689282	-0.699300	0.952129
19	1	0	-2.250408	0.479746	2.087142
20	6	0	-2.698502	-1.730227	-0.995032
21	1	0	-0.595164	-1.282695	-1.228127
22	6	0	-3.828250	-1.496098	-0.189729
23	1	0	-4.520917	-0.465164	1.598385
24	1	0	-2.790956	-2.331872	-1.888185
25	7	0	-1.386881	-0.415486	0.467819
26	8	0	-4.970826	-2.055246	-0.596909
27	6	0	-6.170714	-1.802259	0.144991
28	1	0	-6.394841	-0.732990	0.159859
29	1	0	-6.955816	-2.336526	-0.383448
30	1	0	-6.083482	-2.186707	1.164413
31	1	0	5.990934	0.803306	0.131911
32	8	0	5.292371	-1.748445	-0.584798
33	6	0	6.688238	-1.504995	-0.675512
34	1	0	7.111619	-1.242759	0.299999
35	1	0	7.131189	-2.436717	-1.022991
36	1	0	6.908347	-0.707707	-1.393502

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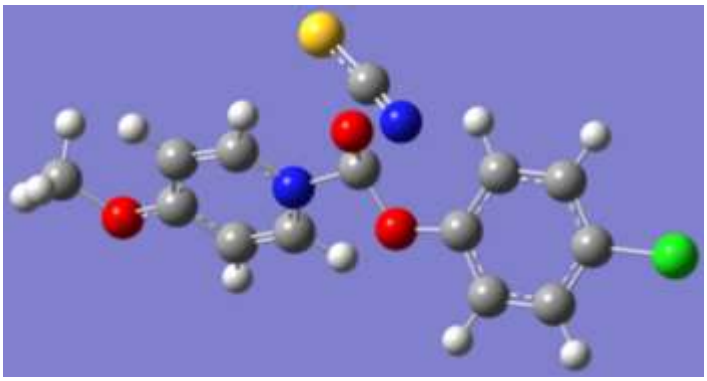
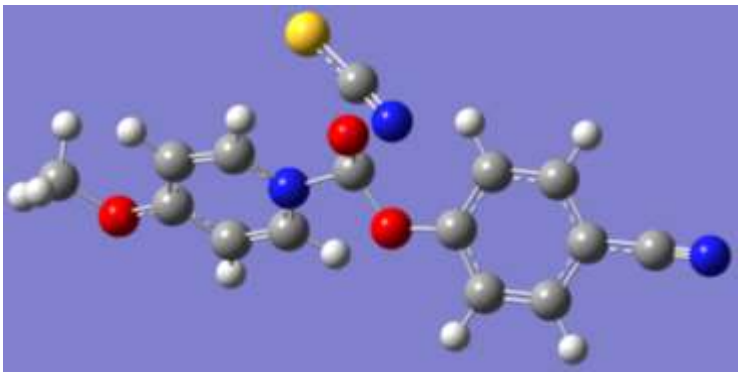
tsfD15.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.076732	0.078595	0.703978
2	8	0	0.089189	0.479720	1.830140
3	8	0	0.761117	-0.786569	0.031160
4	6	0	2.127073	-0.557908	0.027545
5	6	0	2.896939	-1.620079	-0.439075
6	6	0	2.722284	0.636931	0.421786
7	6	0	4.278867	-1.495042	-0.517403
8	1	0	2.407057	-2.538630	-0.736917
9	6	0	4.107335	0.759094	0.342965
10	1	0	2.123435	1.458624	0.780809
11	6	0	4.873801	-0.301498	-0.123440
12	1	0	4.585204	1.681761	0.644514
13	7	0	-0.142174	1.483370	-0.495903
14	6	0	-1.133308	2.134382	-0.611313
15	16	0	-2.512678	2.947181	-0.752248
16	6	0	-2.455036	-0.219621	1.261758
17	6	0	-1.777391	-1.033223	-0.830283
18	6	0	-3.769475	-0.555532	1.011345
19	1	0	-2.114172	0.264189	2.167165
20	6	0	-3.061545	-1.388257	-1.143392
21	1	0	-0.941009	-1.159136	-1.499588
22	6	0	-4.091561	-1.148650	-0.214839
23	1	0	-4.515705	-0.325843	1.755957
24	1	0	-3.294748	-1.830528	-2.101616
25	7	0	-1.490339	-0.473526	0.367636
26	8	0	-5.321762	-1.501339	-0.592987
27	6	0	-6.424318	-1.229376	0.282497
28	1	0	-6.509726	-0.156596	0.470742
29	1	0	-7.306186	-1.582658	-0.245143
30	1	0	-6.313493	-1.773721	1.223667
31	1	0	4.885832	-2.314998	-0.877600
32	17	0	6.622852	-0.134780	-0.216115

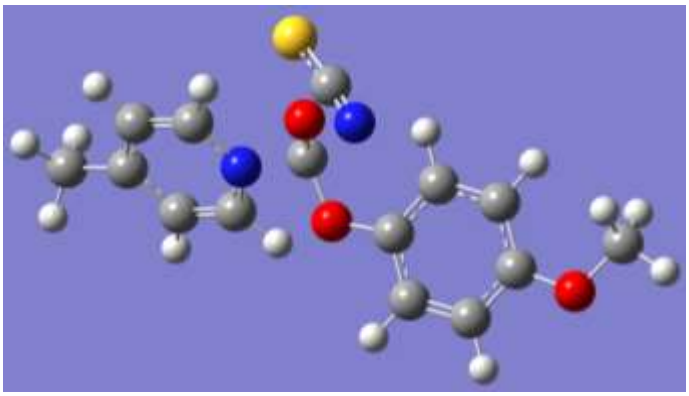
tsfD16.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.056454	0.059840	0.731873
2	8	0	0.222105	0.496082	1.843072
3	8	0	0.902973	-0.823013	0.085806
4	6	0	2.260639	-0.588303	0.065469
5	6	0	3.027526	-1.653519	-0.407131
6	6	0	2.855437	0.611949	0.451226
7	6	0	4.403345	-1.525088	-0.498214
8	1	0	2.532685	-2.571811	-0.696458
9	6	0	4.235119	0.734378	0.357023
10	1	0	2.255197	1.431567	0.811601
11	6	0	5.020146	-0.325537	-0.114869
12	1	0	4.710948	1.661312	0.650392
13	7	0	0.025654	1.450209	-0.533774
14	6	0	-0.963105	2.106085	-0.641862
15	16	0	-2.344412	2.919520	-0.763625
16	6	0	-2.325875	-0.177499	1.259668
17	6	0	-1.624658	-1.064928	-0.796659
18	6	0	-3.639924	-0.502428	0.996326
19	1	0	-1.995430	0.328509	2.156405
20	6	0	-2.908147	-1.409336	-1.120444
21	1	0	-0.780564	-1.221908	-1.449055
22	6	0	-3.950510	-1.127400	-0.216988
23	1	0	-4.395102	-0.237892	1.720039
24	1	0	-3.131959	-1.875590	-2.069475
25	7	0	-1.348132	-0.475032	0.390965
26	8	0	-5.178036	-1.472712	-0.605855
27	6	0	-6.292533	-1.159520	0.241464
28	1	0	-6.365281	-0.080563	0.396142
29	1	0	-7.169566	-1.516055	-0.291838
30	1	0	-6.205763	-1.677645	1.199694
31	1	0	5.005601	-2.347161	-0.862811
32	6	0	6.438578	-0.188597	-0.205046
33	7	0	7.587096	-0.081427	-0.279135

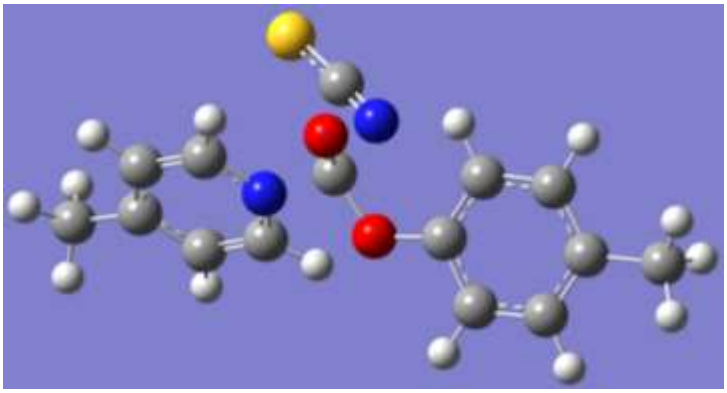
tsfD21.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.369835	-0.013885	0.744378
2	8	0	-0.199709	0.418311	1.858564
3	8	0	0.442976	-0.906763	0.091578
4	6	0	1.816214	-0.685274	0.042463
5	6	0	2.563362	-1.746108	-0.467740
6	6	0	2.437169	0.491906	0.431317
7	6	0	3.937808	-1.629015	-0.591335
8	1	0	2.056375	-2.656460	-0.763211
9	6	0	3.823655	0.608242	0.304796
10	1	0	1.861186	1.313181	0.827390
11	6	0	4.578899	-0.447072	-0.205204
12	1	0	4.534246	-2.442556	-0.984574
13	1	0	4.292386	1.533008	0.610699
14	7	0	-0.454263	1.342728	-0.480584
15	6	0	-1.457030	1.949513	-0.692474
16	16	0	-2.848440	2.705434	-0.969715
17	6	0	-2.753705	-0.304350	1.348995
18	6	0	-2.109576	-1.173956	-0.727619
19	6	0	-4.070363	-0.654082	1.115872
20	1	0	-2.394814	0.202513	2.234758
21	6	0	-3.408536	-1.536909	-1.005629
22	1	0	-1.282073	-1.321911	-1.404043
23	6	0	-4.428603	-1.278609	-0.079450
24	1	0	-4.815552	-0.417896	1.864077
25	1	0	-3.629070	-2.010234	-1.953713
26	7	0	-1.807782	-0.580281	0.442087
27	8	0	5.936751	-0.424765	-0.363524
28	6	0	6.630322	0.757780	0.003209
29	1	0	6.506106	0.979197	1.068949
30	1	0	7.681205	0.565071	-0.205569
31	1	0	6.293587	1.616811	-0.587409
32	6	0	-5.856998	-1.612908	-0.390939
33	1	0	-6.295151	-0.815657	-1.000707
34	1	0	-5.933344	-2.541529	-0.959517
35	1	0	-6.454196	-1.704987	0.516922

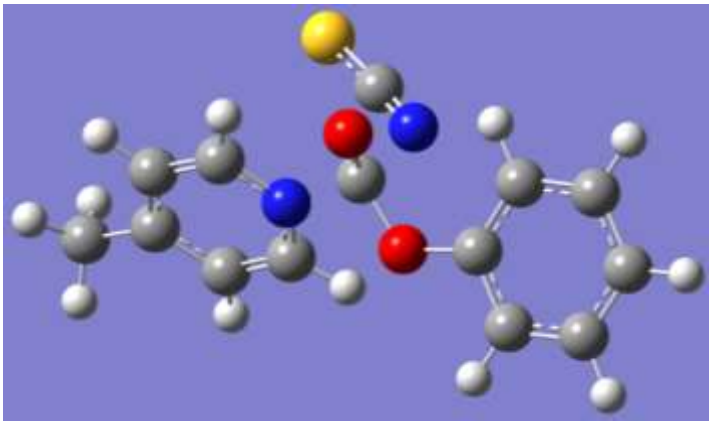
tsfD22.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.032373	0.003359	0.788964
2	8	0	0.113841	0.419444	1.911654
3	8	0	0.818368	-0.843847	0.122837
4	6	0	2.181291	-0.572687	0.082364
5	6	0	2.964202	-1.591724	-0.450667
6	6	0	2.758478	0.617956	0.509493
7	6	0	4.338782	-1.416393	-0.560317
8	1	0	2.489705	-2.512021	-0.768935
9	6	0	4.137971	0.770924	0.388791
10	1	0	2.151845	1.405499	0.927702
11	6	0	4.951788	-0.230388	-0.145379
12	1	0	4.942945	-2.217395	-0.972944
13	1	0	4.587268	1.699746	0.723920
14	7	0	-0.153906	1.388852	-0.417451
15	6	0	-1.177366	1.962978	-0.619838
16	16	0	-2.596290	2.672128	-0.884145
17	6	0	-2.411697	-0.365272	1.356140
18	6	0	-1.713357	-1.185629	-0.723448
19	6	0	-3.713619	-0.751489	1.099854
20	1	0	-2.080925	0.139685	2.253747
21	6	0	-2.996828	-1.583336	-1.024283
22	1	0	-0.872984	-1.298677	-1.390541
23	6	0	-4.036667	-1.369540	-0.108697
24	1	0	-4.475629	-0.548229	1.840726
25	1	0	-3.190060	-2.049415	-1.981862
26	7	0	-1.445219	-0.599972	0.458814
27	6	0	6.438808	-0.028708	-0.295566
28	1	0	6.830264	0.632187	0.481035
29	1	0	6.976912	-0.977558	-0.235370
30	1	0	6.678941	0.424407	-1.263515
31	6	0	-5.450005	-1.741882	-0.444336
32	1	0	-5.903954	-0.948959	-1.048200
33	1	0	-5.491070	-2.663754	-1.027345
34	1	0	-6.055937	-1.865218	0.453989

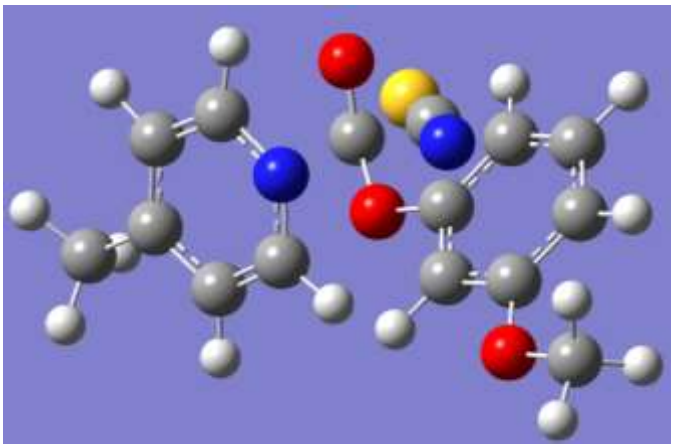
tsfD23.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.350514	0.027223	0.739331
2	8	0	0.517176	0.468117	1.849128
3	8	0	1.194575	-0.829436	0.074494
4	6	0	2.555429	-0.558887	0.011410
5	6	0	3.330007	-1.598785	-0.496655
6	6	0	3.130028	0.650765	0.389201
7	6	0	4.703507	-1.427777	-0.630317
8	1	0	2.847602	-2.526617	-0.778613
9	6	0	4.508249	0.804272	0.247826
10	1	0	2.521360	1.450231	0.780661
11	6	0	5.299533	-0.223682	-0.258283
12	1	0	5.306366	-2.237381	-1.024738
13	1	0	4.962084	1.744418	0.538769
14	1	0	6.369514	-0.089190	-0.361143
15	7	0	0.202887	1.390951	-0.498949
16	6	0	-0.826200	1.962266	-0.679992
17	16	0	-2.253376	2.666220	-0.911357
18	6	0	-2.015970	-0.330175	1.352960
19	6	0	-1.349371	-1.195857	-0.719208
20	6	0	-3.320741	-0.725032	1.126617
21	1	0	-1.672410	0.195786	2.233447
22	6	0	-2.636537	-1.602616	-0.989825
23	1	0	-0.520004	-1.321926	-1.397556
24	6	0	-3.661903	-1.371028	-0.062116
25	1	0	-4.070963	-0.506367	1.875061
26	1	0	-2.844182	-2.090419	-1.933450
27	7	0	-1.063202	-0.583557	0.445601
28	6	0	-5.079406	-1.754450	-0.365869
29	1	0	-5.546133	-0.975436	-0.978062
30	1	0	-5.127250	-2.688218	-0.929078
31	1	0	-5.669606	-1.861031	0.544966

tsfD24.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.364728	0.325949	0.759565
2	8	0	-0.324114	0.872324	1.833249
3	8	0	0.637992	-0.427439	0.196889
4	6	0	1.944344	0.043098	0.195509
5	6	0	2.897613	-0.918963	-0.102181
6	6	0	2.293218	1.371711	0.434797
7	6	0	4.244165	-0.557280	-0.167047
8	1	0	2.606440	-1.945497	-0.280714
9	6	0	3.639302	1.708099	0.364995
10	1	0	1.542446	2.110753	0.662018
11	6	0	4.624630	0.765831	0.068162
12	1	0	3.932455	2.735595	0.545830
13	1	0	5.660731	1.069398	0.025061
14	7	0	-0.686468	1.542417	-0.590133
15	6	0	-1.786741	1.922625	-0.841463
16	16	0	-3.299035	2.363875	-1.163981
17	6	0	-2.657537	-0.397780	1.335174
18	6	0	-1.771514	-1.271981	-0.649467
19	6	0	-3.863856	-1.032351	1.106035
20	1	0	-2.444365	0.239219	2.183042
21	6	0	-2.956275	-1.918283	-0.921556
22	1	0	-0.906905	-1.296935	-1.294443
23	6	0	-4.040998	-1.807846	-0.040167
24	1	0	-4.669179	-0.899431	1.816378
25	1	0	-3.039320	-2.499988	-1.830539
26	7	0	-1.641819	-0.540346	0.473547
27	8	0	5.110136	-1.570507	-0.464194
28	6	0	6.495977	-1.267786	-0.529257
29	1	0	6.867611	-0.893617	0.430674
30	1	0	6.994562	-2.205160	-0.769551
31	1	0	6.707427	-0.532260	-1.312751
32	6	0	-5.357285	-2.455064	-0.352121
33	1	0	-5.920263	-1.822205	-1.046373
34	1	0	-5.219426	-3.426385	-0.830689
35	1	0	-5.962346	-2.586285	0.545641

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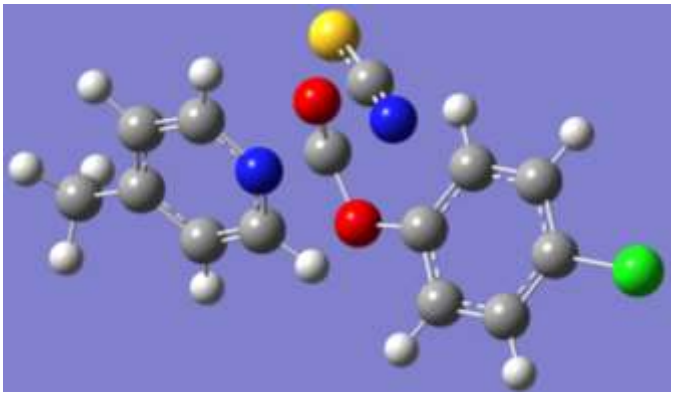
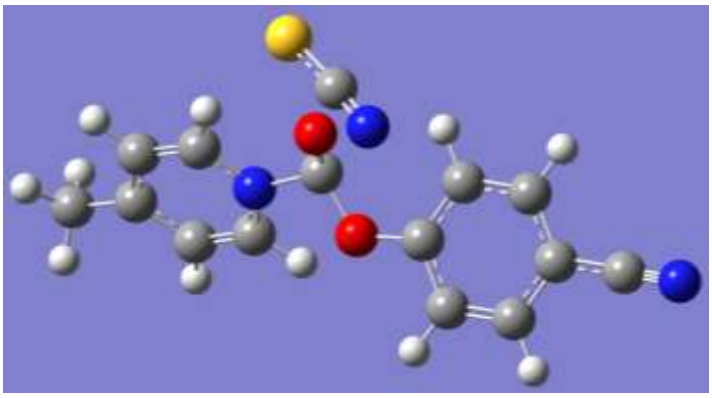
tsfD25.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.353924	0.068160	0.742168
2	8	0	-0.180367	0.499022	1.854448
3	8	0	0.494374	-0.780480	0.066886
4	6	0	1.854145	-0.512945	0.035802
5	6	0	2.647362	-1.566048	-0.410959
6	6	0	2.418507	0.710469	0.384271
7	6	0	4.023661	-1.402998	-0.514909
8	1	0	2.180514	-2.507245	-0.672873
9	6	0	3.797978	0.870486	0.280078
10	1	0	1.800632	1.525220	0.726630
11	6	0	4.588592	-0.181050	-0.166369
12	1	0	4.649344	-2.215418	-0.859739
13	1	0	4.252751	1.815482	0.546045
14	7	0	-0.494700	1.450855	-0.488785
15	6	0	-1.524397	2.028389	-0.647940
16	16	0	-2.952859	2.737905	-0.847688
17	6	0	-2.715425	-0.288326	1.352352
18	6	0	-2.050156	-1.127512	-0.732365
19	6	0	-4.020727	-0.677302	1.120045
20	1	0	-2.371621	0.224826	2.240119
21	6	0	-3.338024	-1.527141	-1.008309
22	1	0	-1.221670	-1.245486	-1.413092
23	6	0	-4.363208	-1.306083	-0.077484
24	1	0	-4.770542	-0.466994	1.871239
25	1	0	-3.546666	-2.000998	-1.958769
26	7	0	-1.762403	-0.532197	0.441642
27	17	0	6.329955	0.033909	-0.291579
28	6	0	-5.781355	-1.681663	-0.386867
29	1	0	-6.244877	-0.894016	-0.990438
30	1	0	-5.831534	-2.608524	-0.961126
31	1	0	-6.372788	-1.796852	0.522072

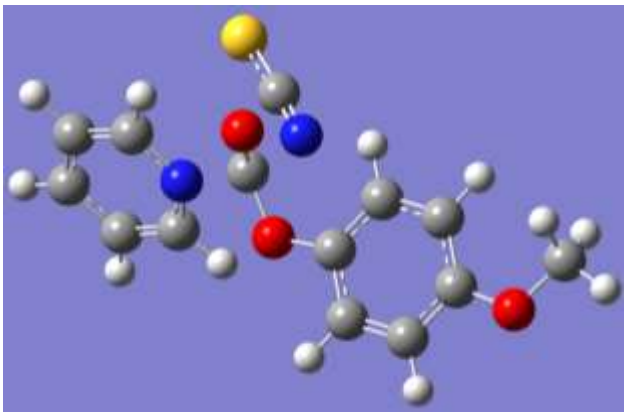
tsfD26.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.237848	-0.039655	0.791729
2	8	0	-0.063680	0.347326	1.918240
3	8	0	0.623764	-0.849387	0.079005
4	6	0	1.972334	-0.562059	0.045404
5	6	0	2.769481	-1.576942	-0.483546
6	6	0	2.527090	0.644256	0.469031
7	6	0	4.137447	-1.391202	-0.593621
8	1	0	2.304725	-2.501736	-0.800665
9	6	0	3.899071	0.824118	0.355765
10	1	0	1.902639	1.425222	0.871758
11	6	0	4.714784	-0.184713	-0.172636
12	1	0	4.763792	-2.173913	-1.001609
13	1	0	4.344595	1.756494	0.677987
14	7	0	-0.363848	1.416395	-0.403115
15	6	0	-1.394918	2.006231	-0.494389
16	16	0	-2.829527	2.724456	-0.597664
17	6	0	-2.599874	-0.396046	1.359250
18	6	0	-1.912112	-1.154445	-0.751168
19	6	0	-3.903473	-0.768428	1.094508
20	1	0	-2.266874	0.077872	2.272232
21	6	0	-3.198204	-1.533891	-1.058327
22	1	0	-1.077163	-1.248411	-1.427270
23	6	0	-4.234236	-1.346066	-0.131491
24	1	0	-4.661376	-0.583227	1.844089
25	1	0	-3.397428	-1.966620	-2.030126
26	7	0	-1.634691	-0.610732	0.451725
27	6	0	6.124984	0.011156	-0.282337
28	7	0	7.266819	0.166134	-0.372545
29	6	0	-5.649951	-1.700602	-0.473243
30	1	0	-5.697286	-2.595008	-1.096913
31	1	0	-6.250062	-1.862038	0.422856
32	1	0	-6.105672	-0.879979	-1.037704

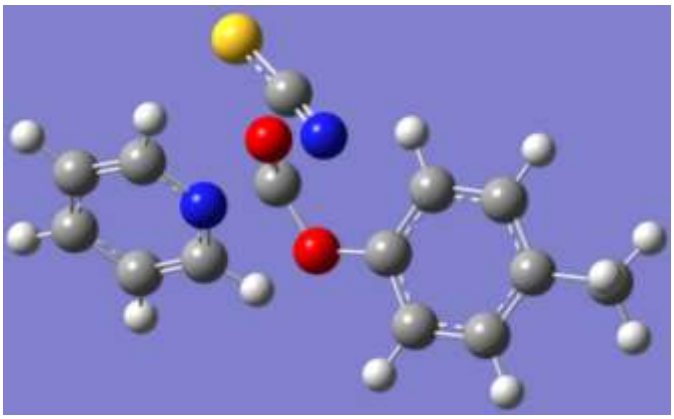
tsfD31.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.693751	-0.137637	0.649700
2	8	0	-0.558709	0.287276	1.770194
3	8	0	0.178144	-0.958017	-0.015966
4	6	0	1.540317	-0.663668	-0.010776
5	6	0	2.370573	-1.707947	-0.413722
6	6	0	2.071030	0.571713	0.326379
7	6	0	3.740575	-1.515356	-0.481619
8	1	0	1.932196	-2.664659	-0.669749
9	6	0	3.453032	0.763274	0.259252
10	1	0	1.428560	1.381125	0.635659
11	6	0	4.292422	-0.274992	-0.143656
12	1	0	4.402021	-2.314586	-0.791260
13	1	0	3.851815	1.732042	0.525339
14	7	0	-0.886395	1.235380	-0.557007
15	6	0	-1.916588	1.825759	-0.657202
16	16	0	-3.344534	2.552298	-0.774238
17	6	0	-3.065202	-0.561393	1.220266
18	6	0	-2.333226	-1.421710	-0.838774
19	6	0	-4.354525	-1.007311	0.980685
20	1	0	-2.748292	-0.016838	2.099533
21	6	0	-3.601649	-1.883387	-1.127075
22	1	0	-1.485901	-1.518752	-1.499510
23	6	0	-4.627456	-1.680258	-0.203364
24	1	0	-5.126700	-0.810679	1.711400
25	1	0	-3.780853	-2.387908	-2.066628
26	1	0	-5.630101	-2.029674	-0.416091
27	7	0	-2.094210	-0.792820	0.326843
28	8	0	5.652580	-0.180944	-0.238528
29	6	0	6.259432	1.060343	0.086522
30	1	0	6.067793	1.337182	1.128992
31	1	0	7.328747	0.917178	-0.058575
32	1	0	5.906941	1.861215	-0.572612

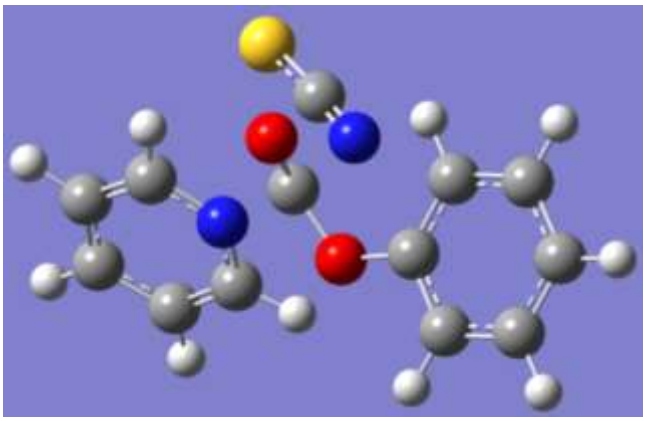
tsfD32.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.340923	-0.054700	0.679400
2	8	0	-0.223177	0.350887	1.808282
3	8	0	0.567889	-0.817841	-0.006257
4	6	0	1.914543	-0.466264	0.004725
5	6	0	2.784547	-1.459152	-0.431537
6	6	0	2.390705	0.785999	0.376529
7	6	0	4.148745	-1.196964	-0.493826
8	1	0	2.385636	-2.424379	-0.718825
9	6	0	3.760956	1.024922	0.306917
10	1	0	1.712870	1.557697	0.706090
11	6	0	4.663079	0.048404	-0.122295
12	1	0	4.822074	-1.975312	-0.836533
13	1	0	4.131805	2.003302	0.593508
14	7	0	-0.598445	1.340515	-0.501710
15	6	0	-1.652826	1.891789	-0.565589
16	16	0	-3.112654	2.559494	-0.631564
17	6	0	-2.692560	-0.584111	1.232819
18	6	0	-1.918372	-1.378987	-0.837567
19	6	0	-3.960980	-1.080622	0.981222
20	1	0	-2.402182	-0.041556	2.122316
21	6	0	-3.165108	-1.889085	-1.137735
22	1	0	-1.065875	-1.429955	-1.496713
23	6	0	-4.201403	-1.745138	-0.214404
24	1	0	-4.743080	-0.928244	1.711916
25	1	0	-3.319919	-2.385481	-2.085911
26	1	0	-5.187589	-2.133448	-0.436417
27	7	0	-1.709384	-0.760123	0.339536
28	6	0	6.146030	0.321033	-0.155105
29	1	0	6.352441	1.363763	-0.407255
30	1	0	6.604226	0.122892	0.819871
31	1	0	6.650556	-0.311026	-0.889318

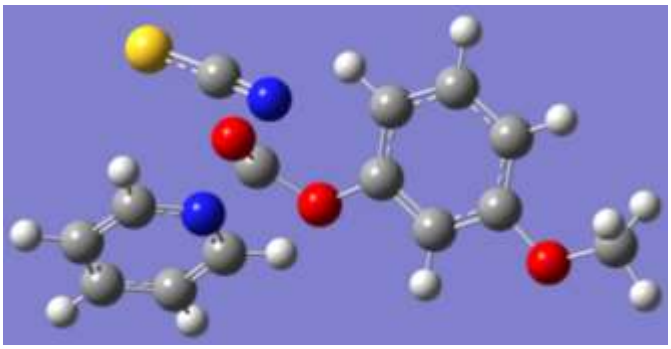
tsfD33.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.031018	-0.060207	0.653937
2	8	0	0.127229	0.393606	1.765884
3	8	0	0.975957	-0.808610	-0.000132
4	6	0	2.304837	-0.399667	-0.004515
5	6	0	3.212358	-1.375221	-0.407768
6	6	0	2.723644	0.884620	0.327872
7	6	0	4.565415	-1.062066	-0.480653
8	1	0	2.848427	-2.364598	-0.656193
9	6	0	4.083547	1.180072	0.250290
10	1	0	2.010919	1.633289	0.635741
11	6	0	5.007294	0.218280	-0.150899
12	1	0	5.273014	-1.821152	-0.792868
13	1	0	4.417444	2.178529	0.507172
14	1	0	6.061216	0.462806	-0.205171
15	7	0	-0.274948	1.283679	-0.587019
16	6	0	-1.351167	1.788888	-0.665562
17	16	0	-2.838676	2.390965	-0.746315
18	6	0	-2.299322	-0.658371	1.214185
19	6	0	-1.479871	-1.498120	-0.821373
20	6	0	-3.544957	-1.214844	0.974610
21	1	0	-2.037430	-0.071913	2.084346
22	6	0	-2.702996	-2.068822	-1.108337
23	1	0	-0.622037	-1.539023	-1.474147
24	6	0	-3.750404	-1.932790	-0.196268
25	1	0	-4.337486	-1.066483	1.694792
26	1	0	-2.831449	-2.605830	-2.038126
27	1	0	-4.718643	-2.368694	-0.408672
28	7	0	-1.303282	-0.828515	0.333526

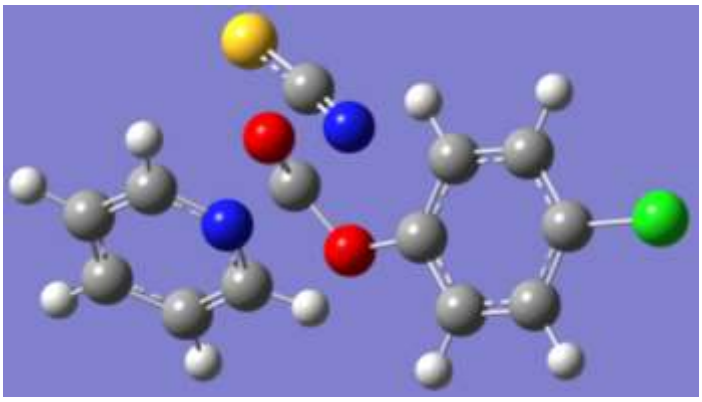
tsfD34.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.675955	0.144325	0.727482
2	8	0	-0.654994	0.612960	1.836852
3	8	0	0.366625	-0.480323	0.091404
4	6	0	1.638221	0.080168	0.135022
5	6	0	2.664132	-0.800763	-0.169051
6	6	0	1.882080	1.422672	0.420020
7	6	0	3.981788	-0.339767	-0.191982
8	1	0	2.453467	-1.840192	-0.382497
9	6	0	3.200924	1.858372	0.392893
10	1	0	1.072946	2.096943	0.649406
11	6	0	4.258614	0.999499	0.091560
12	1	0	3.414064	2.898212	0.611057
13	1	0	5.270371	1.378524	0.081596
14	7	0	-1.142513	1.426012	-0.526710
15	6	0	-2.271966	1.794111	-0.618226
16	16	0	-3.820494	2.211374	-0.718035
17	6	0	-2.914015	-0.756077	1.264464
18	6	0	-1.966297	-1.486379	-0.757599
19	6	0	-4.072450	-1.472571	1.012623
20	1	0	-2.742078	-0.137703	2.134981
21	6	0	-3.099875	-2.214490	-1.056257
22	1	0	-1.102250	-1.416198	-1.399783
23	6	0	-4.167281	-2.214519	-0.157516
24	1	0	-4.886062	-1.428605	1.723173
25	1	0	-3.144438	-2.767485	-1.984487
26	1	0	-5.066897	-2.775083	-0.379061
27	7	0	-1.894274	-0.795260	0.395688
28	8	0	4.925349	-1.277626	-0.498112
29	6	0	6.287578	-0.876359	-0.512155
30	1	0	6.603430	-0.506328	0.469070
31	1	0	6.858217	-1.768657	-0.763302
32	1	0	6.468601	-0.104473	-1.267799

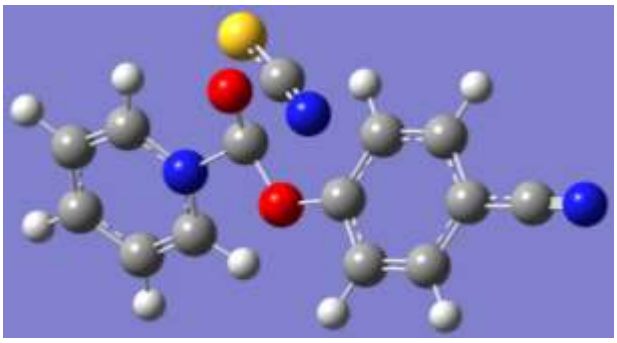
tsfD35.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.697916	-0.105151	0.652549
2	8	0	-0.579234	0.341647	1.764892
3	8	0	0.220942	-0.886979	-0.004878
4	6	0	1.561393	-0.528968	0.007338
5	6	0	2.440990	-1.539225	-0.369740
6	6	0	2.025213	0.742450	0.330139
7	6	0	3.805969	-1.283961	-0.427647
8	1	0	2.050558	-2.519423	-0.612900
9	6	0	3.393594	0.994607	0.273332
10	1	0	1.339190	1.523730	0.616688
11	6	0	4.271526	-0.014414	-0.103061
12	1	0	4.499198	-2.062154	-0.717719
13	1	0	3.771686	1.977639	0.520806
14	7	0	-0.937897	1.262284	-0.590393
15	6	0	-1.991823	1.814926	-0.655395
16	16	0	-3.452620	2.480255	-0.714768
17	6	0	-3.049894	-0.593815	1.201892
18	6	0	-2.259473	-1.464925	-0.833247
19	6	0	-4.318327	-1.091586	0.953854
20	1	0	-2.766523	-0.022944	2.075506
21	6	0	-3.506078	-1.977006	-1.127741
22	1	0	-1.401990	-1.542578	-1.482901
23	6	0	-4.550781	-1.795751	-0.220170
24	1	0	-5.106663	-0.908855	1.670688
25	1	0	-3.654521	-2.504394	-2.060032
26	1	0	-5.536939	-2.185974	-0.438696
27	7	0	-2.057507	-0.807773	0.325542
28	17	0	5.997560	0.316034	-0.168880

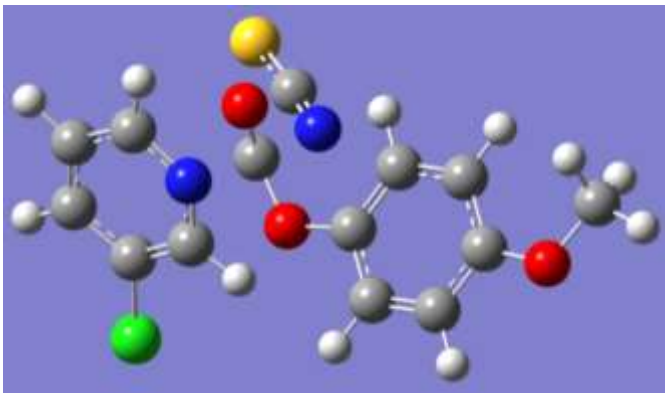
tsfD36.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.569654	-0.115673	0.689545
2	8	0	-0.462448	0.361996	1.788725
3	8	0	0.363252	-0.914748	0.065465
4	6	0	1.693118	-0.544752	0.055738
5	6	0	2.571914	-1.546633	-0.354334
6	6	0	2.153369	0.726817	0.391817
7	6	0	3.929043	-1.281505	-0.432138
8	1	0	2.179000	-2.523560	-0.605367
9	6	0	3.514993	0.985995	0.311834
10	1	0	1.465942	1.496935	0.702576
11	6	0	4.412457	-0.008523	-0.097664
12	1	0	4.619012	-2.053261	-0.747862
13	1	0	3.888127	1.969489	0.566980
14	7	0	-0.761005	1.239742	-0.615831
15	6	0	-1.804808	1.812320	-0.670687
16	16	0	-3.256856	2.498662	-0.705901
17	6	0	-2.937556	-0.531202	1.182737
18	6	0	-2.102936	-1.486451	-0.798635
19	6	0	-4.207394	-1.012133	0.910607
20	1	0	-2.671583	0.061406	2.046877
21	6	0	-3.350026	-1.982283	-1.114155
22	1	0	-1.229342	-1.602058	-1.420046
23	6	0	-4.418462	-1.750368	-0.245830
24	1	0	-5.013165	-0.788649	1.595714
25	1	0	-3.480811	-2.537187	-2.032982
26	1	0	-5.405263	-2.128193	-0.482219
27	7	0	-1.921292	-0.796092	0.346055
28	6	0	5.811105	0.269297	-0.174556
29	7	0	6.943742	0.490462	-0.237980

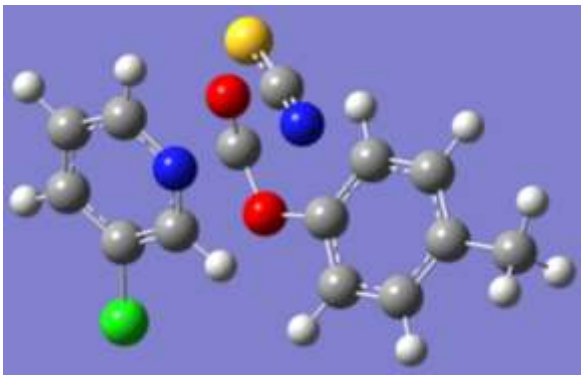
tsfD41.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.199051	0.439423	0.853625
2	8	0	0.063910	1.201504	1.748297
3	8	0	0.519626	-0.655877	0.473641
4	6	0	1.897211	-0.549533	0.279343
5	6	0	2.563502	-1.764278	0.130643
6	6	0	2.585457	0.650706	0.201817
7	6	0	3.929320	-1.778475	-0.097869
8	1	0	2.003176	-2.688747	0.196277
9	6	0	3.963253	0.633787	-0.028443
10	1	0	2.069225	1.590976	0.315185
11	6	0	4.640348	-0.576033	-0.178898
12	1	0	4.465797	-2.711460	-0.215264
13	1	0	4.486728	1.577561	-0.087072
14	7	0	-0.354177	1.341611	-0.758716
15	6	0	-1.317123	2.007808	-0.978115
16	16	0	-2.665534	2.848504	-1.217712
17	6	0	-2.565668	0.579845	1.580840
18	6	0	-2.072249	-1.075167	-0.014425
19	6	0	-3.912740	0.255319	1.541017
20	1	0	-2.131024	1.362047	2.187649
21	6	0	-3.406736	-1.426025	-0.084248
22	1	0	-1.295366	-1.533784	-0.605400
23	6	0	-4.346859	-0.762113	0.705031
24	1	0	-4.610823	0.810642	2.151748
25	1	0	-5.392685	-1.032700	0.645047
26	7	0	-1.691201	-0.098501	0.827059
27	8	0	5.982451	-0.691257	-0.405072
28	6	0	6.747746	0.500324	-0.504805
29	1	0	6.706227	1.079904	0.423907
30	1	0	7.772781	0.182428	-0.686716
31	1	0	6.407126	1.124372	-1.338213
32	17	0	-3.895020	-2.698050	-1.163602

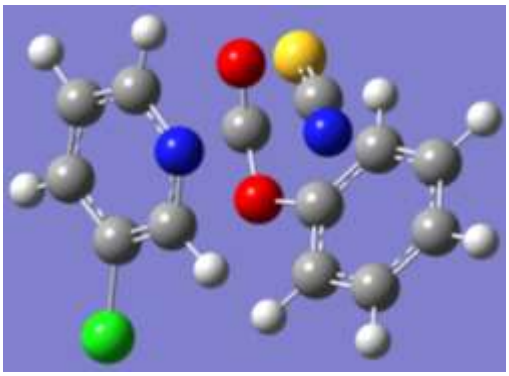
tsfD42.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.100672	0.628866	0.652459
2	8	0	0.322322	1.623691	1.292713
3	8	0	0.883852	-0.486500	0.574404
4	6	0	2.250626	-0.363652	0.331217
5	6	0	2.983838	-1.531015	0.514959
6	6	0	2.866813	0.808838	-0.087315
7	6	0	4.352680	-1.524158	0.274824
8	1	0	2.477611	-2.428834	0.847953
9	6	0	4.240508	0.791097	-0.321665
10	1	0	2.296244	1.713566	-0.226468
11	6	0	5.006716	-0.363346	-0.150198
12	1	0	4.920392	-2.436405	0.424033
13	1	0	4.722491	1.706862	-0.646571
14	7	0	-0.117096	1.035025	-1.151419
15	6	0	-1.119985	1.561925	-1.519536
16	16	0	-2.519892	2.229491	-1.941340
17	6	0	-2.266578	0.836062	1.353413
18	6	0	-1.678740	-1.170409	0.277503
19	6	0	-3.591844	0.437338	1.431952
20	1	0	-1.878636	1.780676	1.708399
21	6	0	-2.989989	-1.601427	0.334072
22	1	0	-0.877374	-1.731731	-0.176001
23	6	0	-3.966331	-0.796933	0.923584
24	1	0	-4.320307	1.101713	1.875350
25	1	0	-4.994244	-1.132309	0.961782
26	7	0	-1.354480	0.023509	0.804295
27	6	0	6.486705	-0.368503	-0.439679
28	1	0	7.023494	-1.031606	0.243024
29	1	0	6.686611	-0.715884	-1.459027
30	1	0	6.912887	0.632358	-0.344400
31	17	0	-3.404006	-3.150802	-0.336233

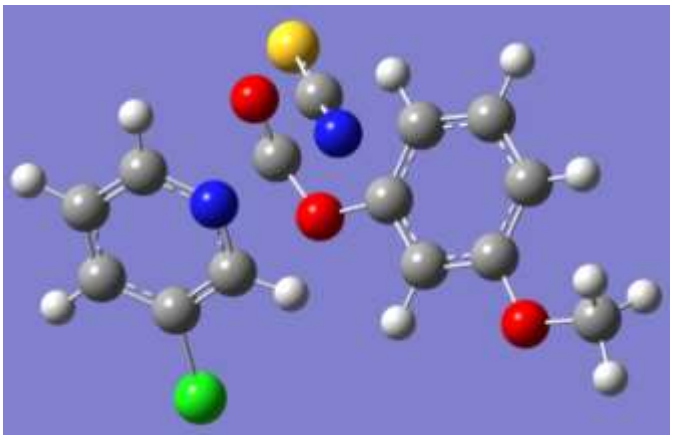
tsfD43.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.505088	0.463902	0.798782
2	8	0	0.795422	1.228236	1.681588
3	8	0	1.221992	-0.625124	0.390547
4	6	0	2.589045	-0.513409	0.151662
5	6	0	3.249141	-1.727589	-0.012501
6	6	0	3.263426	0.698402	0.049048
7	6	0	4.612958	-1.731410	-0.284477
8	1	0	2.689361	-2.650520	0.075518
9	6	0	4.630264	0.674937	-0.223782
10	1	0	2.739915	1.632871	0.175218
11	6	0	5.309956	-0.528805	-0.390785
12	1	0	5.129092	-2.675674	-0.411763
13	1	0	5.163204	1.614797	-0.306770
14	1	0	6.372378	-0.530780	-0.602119
15	7	0	0.289615	1.368741	-0.821110
16	6	0	-0.679433	2.041173	-0.987699
17	16	0	-2.035865	2.888019	-1.149046
18	6	0	-1.836006	0.600459	1.589192
19	6	0	-1.378030	-1.062354	-0.009942
20	6	0	-3.181538	0.267234	1.589414
21	1	0	-1.390114	1.388407	2.179905
22	6	0	-2.711595	-1.420947	-0.039561
23	1	0	-0.616080	-1.520085	-0.620474
24	6	0	-3.633023	-0.757918	0.772665
25	1	0	-3.865136	0.822509	2.216301
26	1	0	-4.678424	-1.035172	0.744213
27	7	0	-0.978441	-0.078284	0.815446
28	17	0	-3.222593	-2.701586	-1.097641

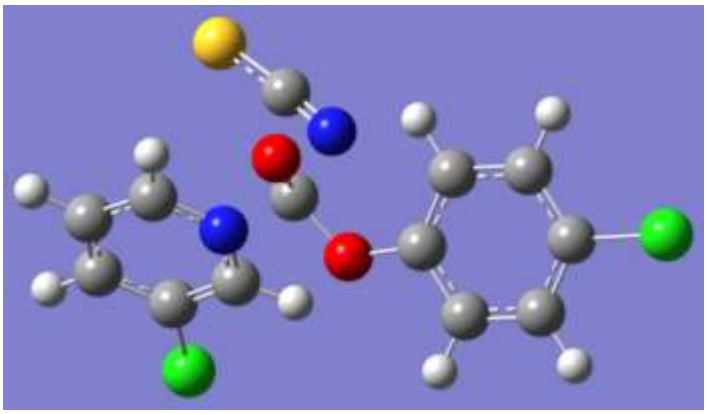
tsfD44.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.338054	-0.883856	0.747606
2	8	0	0.279012	-1.820605	1.514750
3	8	0	-0.635761	0.074430	0.592163
4	6	0	-1.951253	-0.282719	0.335596
5	6	0	-2.818431	0.796429	0.233028
6	6	0	-2.396071	-1.595472	0.173358
7	6	0	-4.170572	0.572819	-0.037327
8	1	0	-2.449759	1.806188	0.358320
9	6	0	-3.746414	-1.793758	-0.099755
10	1	0	-1.718754	-2.429386	0.259064
11	6	0	-4.644318	-0.732342	-0.206847
12	1	0	-4.111610	-2.805537	-0.230641
13	1	0	-5.685384	-0.929496	-0.417116
14	7	0	0.541715	-1.455182	-0.960085
15	6	0	1.450933	-2.095422	-1.381799
16	16	0	2.679619	-2.953860	-1.969498
17	6	0	2.636654	-0.488574	1.581357
18	6	0	1.784965	1.064565	0.028406
19	6	0	3.845974	0.182636	1.630217
20	1	0	2.408636	-1.382686	2.142125
21	6	0	2.977993	1.760765	0.052083
22	1	0	0.939803	1.345481	-0.579157
23	6	0	4.027681	1.323274	0.859349
24	1	0	4.635638	-0.189544	2.266984
25	1	0	4.963801	1.864866	0.877310
26	7	0	1.649380	-0.032578	0.795801
27	8	0	-4.946391	1.689976	-0.118180
28	6	0	-6.339870	1.526300	-0.390533
29	1	0	-6.827415	0.940821	0.393805
30	1	0	-6.757370	2.530510	-0.408661
31	1	0	-6.497310	1.046476	-1.360365
32	17	0	3.148703	3.178180	-0.937880

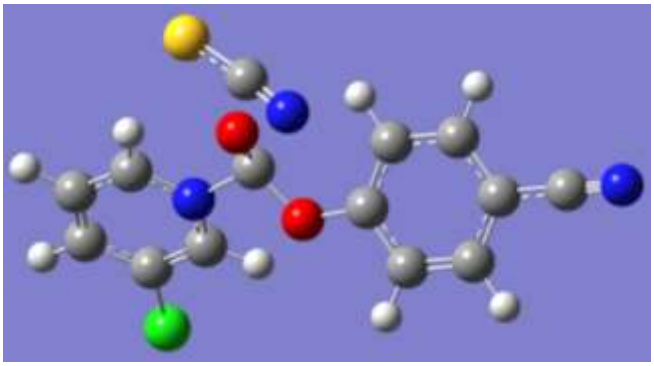
tsfD45.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.224992	0.507134	0.823866
2	8	0	0.025541	1.287417	1.704717
3	8	0	0.541842	-0.559863	0.438871
4	6	0	1.908981	-0.395894	0.253532
5	6	0	2.633167	-1.580678	0.167274
6	6	0	2.533977	0.840015	0.126045
7	6	0	4.005433	-1.538332	-0.049170
8	1	0	2.118351	-2.527445	0.271567
9	6	0	3.909426	0.879026	-0.088909
10	1	0	1.966811	1.755223	0.188270
11	6	0	4.633467	-0.303783	-0.174361
12	1	0	4.579785	-2.452584	-0.117154
13	1	0	4.412598	1.831356	-0.191171
14	7	0	-0.424886	1.394764	-0.815614
15	6	0	-1.416171	2.027284	-1.008148
16	16	0	-2.801792	2.817068	-1.202023
17	6	0	-2.579658	0.574330	1.561425
18	6	0	-2.033460	-1.075723	-0.024541
19	6	0	-3.913291	0.197902	1.532234
20	1	0	-2.172946	1.377374	2.159831
21	6	0	-3.353849	-1.476213	-0.083203
22	1	0	-1.244687	-1.509020	-0.618365
23	6	0	-4.313624	-0.841990	0.707736
24	1	0	-4.627878	0.732183	2.142562
25	1	0	-5.348812	-1.152311	0.656634
26	7	0	-1.683320	-0.078584	0.808655
27	17	0	6.369529	-0.241206	-0.444125
28	17	0	-3.800368	-2.772625	-1.150249

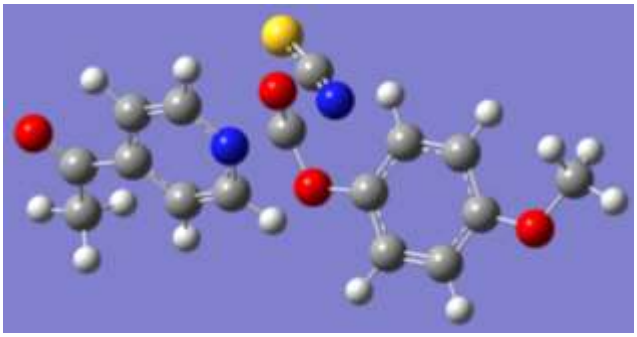
tsfD46.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.101061	0.504054	0.843218
2	8	0	0.149907	1.296729	1.711282
3	8	0	0.671337	-0.571965	0.479138
4	6	0	2.030746	-0.413430	0.284601
5	6	0	2.744705	-1.605802	0.178141
6	6	0	2.663114	0.822299	0.170135
7	6	0	4.111384	-1.569762	-0.044508
8	1	0	2.219525	-2.547530	0.273245
9	6	0	4.033380	0.851274	-0.052654
10	1	0	2.100566	1.738740	0.247829
11	6	0	4.768017	-0.336402	-0.160691
12	1	0	4.675371	-2.489724	-0.127350
13	1	0	4.540169	1.803080	-0.146183
14	7	0	-0.258320	1.374275	-0.838319
15	6	0	-1.237199	2.026906	-1.027563
16	16	0	-2.609864	2.842233	-1.207977
17	6	0	-2.459915	0.619654	1.524899
18	6	0	-1.898843	-1.064817	-0.022115
19	6	0	-3.796529	0.256705	1.472649
20	1	0	-2.058665	1.427656	2.119773
21	6	0	-3.221828	-1.450320	-0.102806
22	1	0	-1.103988	-1.516908	-0.592865
23	6	0	-4.191028	-0.792408	0.657750
24	1	0	-4.517574	0.809927	2.057929
25	1	0	-5.228341	-1.092189	0.589831
26	7	0	-1.553644	-0.057941	0.803934
27	6	0	6.177396	-0.294109	-0.387736
28	7	0	7.318040	-0.263507	-0.571063
29	17	0	-3.660567	-2.757823	-1.158296

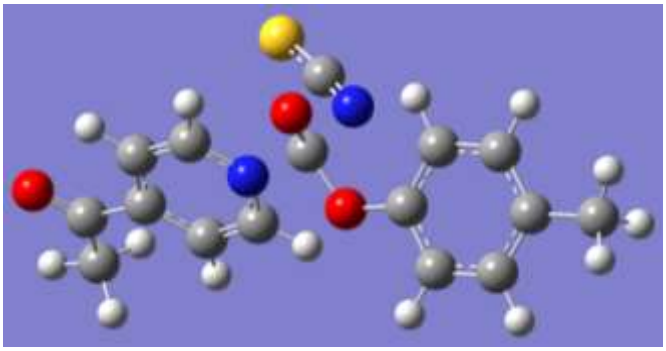
tsfD51.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.198293	0.179415	0.812366
2	8	0	0.412600	0.673318	1.890787
3	8	0	0.924141	-0.813166	0.211685
4	6	0	2.308703	-0.694442	0.104567
5	6	0	2.953702	-1.818479	-0.409022
6	6	0	3.028893	0.440047	0.444719
7	6	0	4.327244	-1.807632	-0.584086
8	1	0	2.369811	-2.693731	-0.666077
9	6	0	4.414445	0.449159	0.265561
10	1	0	2.531451	1.309838	0.843828
11	6	0	5.069105	-0.669824	-0.247819
12	1	0	4.846210	-2.671083	-0.980625
13	1	0	4.961505	1.341685	0.534463
14	7	0	0.185339	1.453243	-0.505839
15	6	0	-0.783370	2.099508	-0.756665
16	16	0	-2.138659	2.901697	-1.075519
17	6	0	-2.204752	0.155613	1.436445
18	6	0	-1.648940	-0.953134	-0.554933
19	6	0	-3.549049	-0.095266	1.234837
20	1	0	-1.794390	0.706892	2.271857
21	6	0	-2.979727	-1.217815	-0.809576
22	1	0	-0.840008	-1.234091	-1.211315
23	6	0	-3.954986	-0.793398	0.098916
24	1	0	-4.286581	0.257057	1.942392
25	1	0	-3.238113	-1.747371	-1.715366
26	7	0	-1.294134	-0.290489	0.559051
27	8	0	6.416678	-0.753830	-0.455956
28	6	0	7.213360	0.376841	-0.136337
29	1	0	7.146516	0.623316	0.928965
30	1	0	8.237374	0.098885	-0.379271
31	1	0	6.922746	1.250188	-0.730346
32	6	0	-5.433244	-1.035940	-0.109245
33	8	0	-6.210407	-0.747823	0.774040
34	6	0	-5.885511	-1.623158	-1.422941
35	1	0	-5.556567	-0.997491	-2.257812
36	1	0	-5.456970	-2.619497	-1.568163
37	1	0	-6.971100	-1.694776	-1.424105

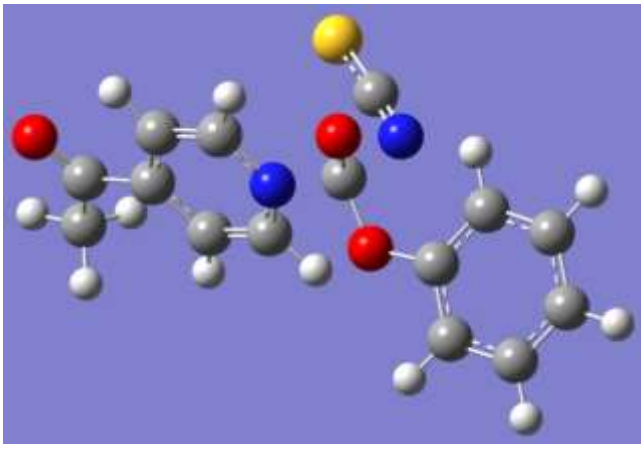
tsfD52.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.532043	0.373557	0.672216
2	8	0	0.738423	1.053033	1.645190
3	8	0	1.279025	-0.695245	0.251708
4	6	0	2.663242	-0.581404	0.155049
5	6	0	3.334785	-1.781297	-0.057794
6	6	0	3.357290	0.619461	0.233835
7	6	0	4.717299	-1.777738	-0.195842
8	1	0	2.769057	-2.703725	-0.107088
9	6	0	4.743835	0.597916	0.092047
10	1	0	2.835922	1.548307	0.403588
11	6	0	5.448377	-0.587189	-0.126054
12	1	0	5.235047	-2.717384	-0.356926
13	1	0	5.285540	1.535461	0.155734
14	7	0	0.487750	1.396497	-0.853549
15	6	0	-0.490663	1.989778	-1.185179
16	16	0	-1.859058	2.723164	-1.598463
17	6	0	-1.868884	0.414039	1.296205
18	6	0	-1.289205	-1.017043	-0.470685
19	6	0	-3.207767	0.104698	1.145388
20	1	0	-1.470808	1.111653	2.020793
21	6	0	-2.614131	-1.348071	-0.671457
22	1	0	-0.474240	-1.393667	-1.069100
23	6	0	-3.598697	-0.789920	0.150950
24	1	0	-3.952656	0.561259	1.782093
25	1	0	-2.861047	-2.033971	-1.469111
26	7	0	-0.948693	-0.161438	0.508506
27	6	0	6.945661	-0.585745	-0.305614
28	1	0	7.394847	0.313185	0.121328
29	1	0	7.405095	-1.453903	0.173581
30	1	0	7.214885	-0.617066	-1.366815
31	6	0	-5.071567	-1.094784	-0.007245
32	8	0	-5.854988	-0.672096	0.814178
33	6	0	-5.511032	-1.912116	-1.196400
34	1	0	-5.192872	-1.437182	-2.129064
35	1	0	-5.063824	-2.910364	-1.164911
36	1	0	-6.595086	-2.003111	-1.182731

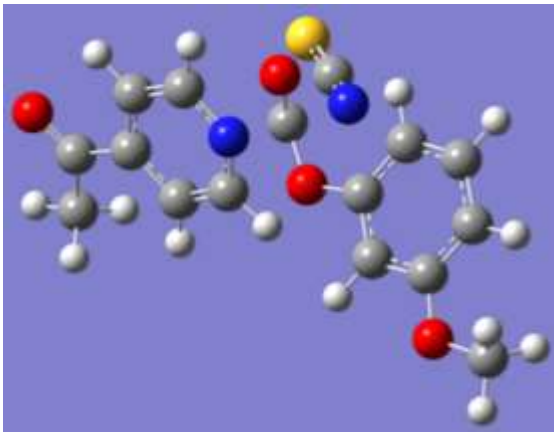
tsfD53.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.919345	0.170071	0.754793
2	8	0	1.166831	0.638321	1.836106
3	8	0	1.635161	-0.803841	0.106746
4	6	0	3.019946	-0.705758	0.018129
5	6	0	3.659056	-1.870040	-0.398856
6	6	0	3.735600	0.456646	0.285590
7	6	0	5.041281	-1.873365	-0.552107
8	1	0	3.068104	-2.756294	-0.594655
9	6	0	5.120355	0.434361	0.127517
10	1	0	3.229329	1.353459	0.605981
11	6	0	5.778598	-0.719957	-0.288835
12	1	0	5.540331	-2.779446	-0.875053
13	1	0	5.684977	1.336086	0.333478
14	1	0	6.855488	-0.722038	-0.406037
15	7	0	0.859710	1.481996	-0.539270
16	6	0	-0.118495	2.136464	-0.724147
17	16	0	-1.487120	2.946442	-0.952071
18	6	0	-1.459575	0.115802	1.447098
19	6	0	-0.956313	-0.925128	-0.595301
20	6	0	-2.807702	-0.137651	1.276567
21	1	0	-1.028721	0.642893	2.287697
22	6	0	-2.292336	-1.189762	-0.818990
23	1	0	-0.165852	-1.179815	-1.284038
24	6	0	-3.242941	-0.801387	0.131102
25	1	0	-3.525950	0.186854	2.016531
26	1	0	-2.574513	-1.691139	-1.733678
27	7	0	-0.572488	-0.295952	0.529117
28	6	0	-4.725332	-1.047360	-0.041475
29	6	0	-5.211519	-1.602060	-1.357160
30	1	0	-6.296052	-1.683226	-1.328604
31	1	0	-4.912603	-0.950543	-2.183526
32	1	0	-4.779224	-2.590048	-1.542571
33	8	0	-5.478175	-0.788081	0.871220

tsfD54.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.315004	1.371933	-1.829067
2	8	0	-1.101317	-0.258131	-0.407921
3	6	0	-2.454889	0.041521	-0.304065
4	6	0	-3.254572	-1.049423	0.000361
5	6	0	-2.986007	1.320407	-0.462541
6	6	0	-4.630390	-0.872194	0.154633
7	1	0	-2.822609	-2.034396	0.117169
8	6	0	-4.358060	1.472499	-0.303395
9	1	0	-2.353517	2.160308	-0.698695
10	6	0	-5.192673	0.397500	0.002293
11	1	0	-4.792195	2.458499	-0.419817
12	1	0	-6.254818	0.559542	0.116376
13	7	0	-0.056123	1.737192	0.674379
14	6	0	0.989785	2.195843	1.012091
15	16	0	2.442903	2.739156	1.433014
16	6	0	2.181288	0.412669	-1.416879
17	6	0	1.388030	-0.906150	0.354771
18	6	0	3.464256	-0.069675	-1.238868
19	1	0	1.891719	1.147811	-2.155488
20	6	0	2.653435	-1.408568	0.581230
21	1	0	0.521099	-1.162985	0.943263
22	6	0	3.716340	-0.997774	-0.230399
23	1	0	4.273607	0.277002	-1.866114
24	1	0	2.793462	-2.111100	1.390347
25	7	0	1.179166	-0.027373	-0.641161
26	8	0	-5.336868	-2.000969	0.453461
27	6	0	-6.742755	-1.886097	0.620823
28	1	0	-7.225027	-1.530124	-0.295690
29	1	0	-7.098002	-2.889072	0.850273
30	1	0	-6.991828	-1.213696	1.448578
31	6	0	5.131950	-1.497262	-0.046827
32	6	0	5.436421	-2.366784	1.147382
33	1	0	6.497640	-2.606428	1.150036
34	1	0	5.172863	-1.851927	2.075883
35	1	0	4.855975	-3.293570	1.107514
36	8	0	5.979338	-1.183864	-0.853651
37	6	0	-0.213039	0.690680	-0.841771

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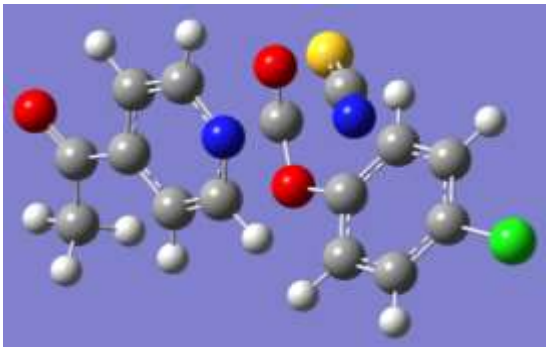
tsfD55.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.190785	0.255692	0.779393
2	8	0	0.410145	0.768344	1.846515
3	8	0	0.957867	-0.708229	0.171087
4	6	0	2.333558	-0.543852	0.088921
5	6	0	3.036087	-1.682356	-0.294745
6	6	0	2.991838	0.657598	0.331242
7	6	0	4.416918	-1.627626	-0.442184
8	1	0	2.496930	-2.604186	-0.473344
9	6	0	4.375745	0.708837	0.183769
10	1	0	2.443629	1.538170	0.626254
11	6	0	5.076772	-0.427492	-0.200363
12	1	0	4.973557	-2.506634	-0.738714
13	1	0	4.903644	1.635204	0.367421
14	7	0	0.108705	1.527173	-0.565068
15	6	0	-0.884215	2.160644	-0.746725
16	16	0	-2.272310	2.938806	-0.962951
17	6	0	-2.192127	0.158389	1.427243
18	6	0	-1.613534	-0.953773	-0.558177
19	6	0	-3.527464	-0.146343	1.241330
20	1	0	-1.796617	0.734456	2.252712
21	6	0	-2.935329	-1.270096	-0.795803
22	1	0	-0.801923	-1.211810	-1.220277
23	6	0	-3.917570	-0.872864	0.118234
24	1	0	-4.270751	0.186800	1.952138
25	1	0	-3.182130	-1.819794	-1.692810
26	7	0	-1.272478	-0.265304	0.546256
27	17	0	6.823718	-0.349731	-0.382695
28	6	0	-5.387997	-1.174369	-0.071022
29	6	0	-5.831016	-1.796448	-1.371446
30	1	0	-5.532915	-1.172040	-2.218757
31	1	0	-5.368512	-2.779032	-1.506344
32	1	0	-6.913264	-1.907026	-1.360860
33	8	0	-6.165261	-0.903608	0.817376

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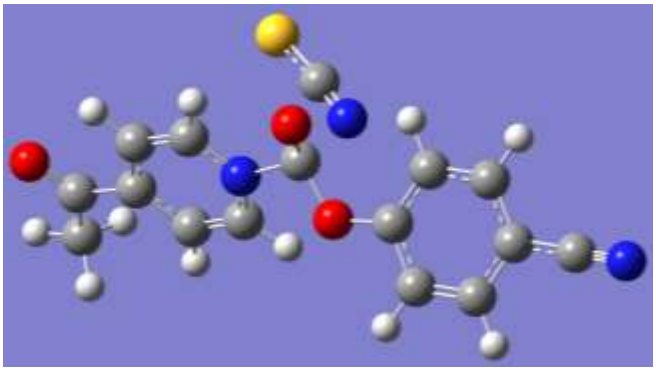
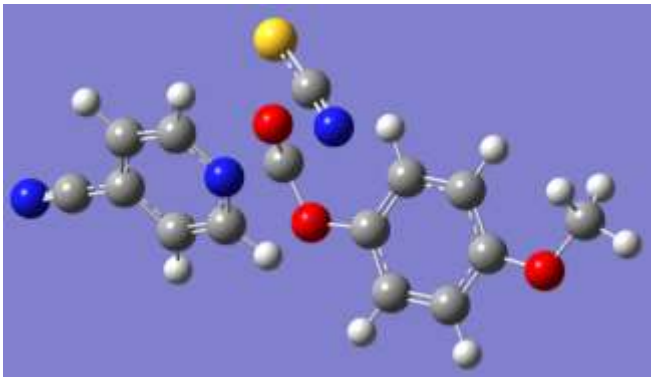
tsfD56.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.322447	0.246895	0.796146
2	8	0	0.544200	0.803114	1.839344
3	8	0	1.095775	-0.743374	0.229726
4	6	0	2.463858	-0.581295	0.134790
5	6	0	3.161462	-1.732969	-0.227344
6	6	0	3.124433	0.626988	0.346941
7	6	0	4.536872	-1.683279	-0.382398
8	1	0	2.615867	-2.655198	-0.380917
9	6	0	4.503338	0.669894	0.189931
10	1	0	2.576503	1.513266	0.623532
11	6	0	5.220429	-0.476957	-0.173951
12	1	0	5.087256	-2.572223	-0.662036
13	1	0	5.031026	1.601490	0.348782
14	7	0	0.275890	1.475742	-0.623213
15	6	0	-0.703961	2.133188	-0.791070
16	16	0	-2.079919	2.940192	-0.976376
17	6	0	-2.061627	0.229349	1.403107
18	6	0	-1.466984	-0.991769	-0.514889
19	6	0	-3.397886	-0.064967	1.208475
20	1	0	-1.672884	0.839796	2.206357
21	6	0	-2.788890	-1.299509	-0.758296
22	1	0	-0.649757	-1.294336	-1.150206
23	6	0	-3.780320	-0.842761	0.118119
24	1	0	-4.147656	0.316119	1.887674
25	1	0	-3.029547	-1.890195	-1.630603
26	7	0	-1.132344	-0.255089	0.562127
27	6	0	6.638682	-0.420992	-0.331635
28	7	0	7.786446	-0.379297	-0.460472
29	6	0	-5.252317	-1.133541	-0.079400
30	6	0	-5.682555	-1.827150	-1.347198
31	1	0	-5.363641	-1.257901	-2.225276
32	1	0	-5.230264	-2.821305	-1.415608
33	1	0	-6.766120	-1.924267	-1.348014
34	8	0	-6.039134	-0.797652	0.777556

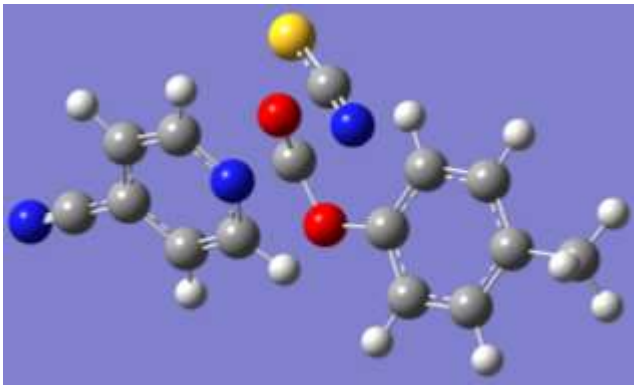
tsfD61.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.170436	0.107206	0.748875
2	8	0	-0.011936	0.649938	1.813051
3	8	0	0.607014	-0.873498	0.205486
4	6	0	1.987661	-0.694348	0.107172
5	6	0	2.686601	-1.797941	-0.378465
6	6	0	2.651453	0.477590	0.433053
7	6	0	4.059960	-1.728309	-0.539958
8	1	0	2.145638	-2.703316	-0.624755
9	6	0	4.036876	0.546288	0.266580
10	1	0	2.111495	1.331002	0.812016
11	6	0	4.746353	-0.551691	-0.218946
12	1	0	4.621348	-2.574567	-0.915042
13	1	0	4.540645	1.467547	0.522821
14	7	0	-0.223169	1.328954	-0.617060
15	6	0	-1.184109	2.017204	-0.769132
16	16	0	-2.537028	2.865771	-0.932412
17	6	0	-2.598086	0.073527	1.263872
18	6	0	-1.934102	-1.202815	-0.591651
19	6	0	-3.930084	-0.226411	1.037192
20	1	0	-2.237490	0.706805	2.063491
21	6	0	-3.240937	-1.535703	-0.872614
22	1	0	-1.091074	-1.521063	-1.185094
23	6	0	-4.260875	-1.049274	-0.039919
24	1	0	-4.692986	0.184856	1.682430
25	1	0	-3.469094	-2.160889	-1.724163
26	7	0	-1.642938	-0.431042	0.472267
27	8	0	6.097463	-0.578307	-0.413163
28	6	0	6.838701	0.595445	-0.114572
29	1	0	6.752529	0.862680	0.944249
30	1	0	7.876148	0.359736	-0.344440
31	1	0	6.512057	1.440014	-0.730870
32	6	0	-5.624836	-1.382414	-0.303945
33	7	0	-6.725274	-1.658260	-0.515569

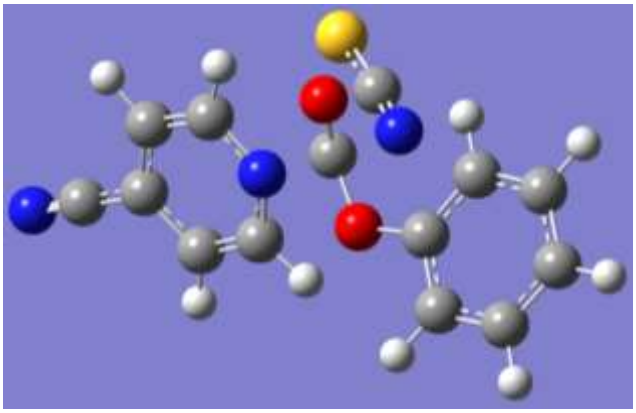
tsfD62.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.161694	0.222828	0.693073
2	8	0	0.302409	0.866174	1.701339
3	8	0	0.976187	-0.774113	0.236894
4	6	0	2.351652	-0.565369	0.146201
5	6	0	3.093467	-1.698172	-0.171922
6	6	0	2.968600	0.666530	0.321700
7	6	0	4.471799	-1.595647	-0.313841
8	1	0	2.585349	-2.645271	-0.306504
9	6	0	4.352332	0.744664	0.172907
10	1	0	2.391217	1.544665	0.564669
11	6	0	5.127988	-0.372254	-0.142059
12	1	0	5.044867	-2.482147	-0.563706
13	1	0	4.833833	1.707432	0.305345
14	7	0	0.059634	1.312753	-0.783574
15	6	0	-0.925846	1.952175	-0.984056
16	16	0	-2.310115	2.735147	-1.202699
17	6	0	-2.261298	0.148967	1.216395
18	6	0	-1.550341	-1.267684	-0.516310
19	6	0	-3.581086	-0.220598	1.023444
20	1	0	-1.924902	0.865884	1.953435
21	6	0	-2.843769	-1.673064	-0.760591
22	1	0	-0.696312	-1.607942	-1.081078
23	6	0	-3.881134	-1.150913	0.028010
24	1	0	-4.358504	0.219381	1.631321
25	1	0	-3.048503	-2.382112	-1.550134
26	7	0	-1.287882	-0.390626	0.471157
27	6	0	6.627350	-0.272849	-0.267689
28	1	0	7.003031	-0.917281	-1.066200
29	1	0	6.939875	0.750808	-0.483558
30	1	0	7.121235	-0.579646	0.660476
31	6	0	-5.231486	-1.558535	-0.198547
32	7	0	-6.320619	-1.894613	-0.379364

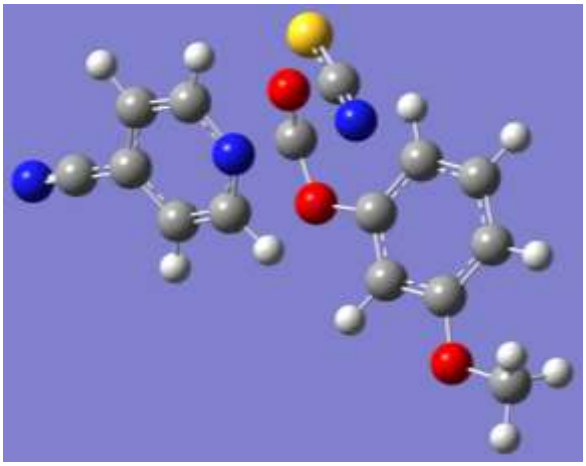
tsfD63.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.556607	0.125302	0.713249
2	8	0	0.744961	0.635537	1.787317
3	8	0	1.347117	-0.807055	0.100480
4	6	0	2.720550	-0.599671	-0.002359
5	6	0	3.441617	-1.705719	-0.442470
6	6	0	3.346729	0.610196	0.276527
7	6	0	4.818466	-1.600843	-0.607186
8	1	0	2.918557	-2.631670	-0.647329
9	6	0	4.727529	0.696621	0.105328
10	1	0	2.777402	1.460721	0.616762
11	6	0	5.467669	-0.397927	-0.333597
12	1	0	5.382145	-2.461051	-0.948446
13	1	0	5.223395	1.636007	0.319455
14	1	0	6.540227	-0.315687	-0.460719
15	7	0	0.403105	1.395990	-0.611682
16	6	0	-0.584493	2.059564	-0.681158
17	16	0	-1.970475	2.867713	-0.729649
18	6	0	-1.841309	-0.007497	1.320395
19	6	0	-1.209434	-1.194773	-0.605334
20	6	0	-3.170038	-0.348094	1.135806
21	1	0	-1.471404	0.609524	2.128285
22	6	0	-2.514079	-1.564207	-0.845879
23	1	0	-0.381221	-1.461824	-1.243098
24	6	0	-3.515692	-1.144704	0.043944
25	1	0	-3.919546	0.012405	1.825545
26	1	0	-2.754882	-2.167384	-1.709724
27	7	0	-0.901822	-0.449996	0.473969
28	6	0	-4.876565	-1.518708	-0.177295
29	7	0	-5.974199	-1.827779	-0.354844

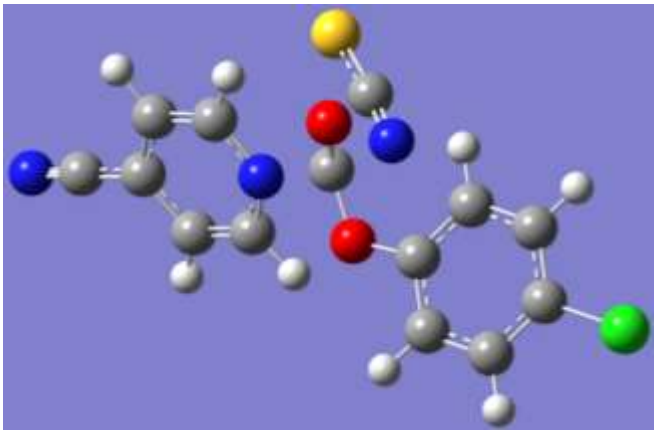
tsfD64.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.179679	0.477768	0.784099
2	8	0	-0.172501	1.142722	1.787489
3	8	0	0.790789	-0.389136	0.366798
4	6	0	2.118975	0.021236	0.295684
5	6	0	3.007844	-0.992789	-0.024899
6	6	0	2.541384	1.333074	0.500879
7	6	0	4.367366	-0.701209	-0.148602
8	1	0	2.659130	-2.005362	-0.178145
9	6	0	3.899257	1.599614	0.370897
10	1	0	1.840421	2.112816	0.750262
11	6	0	4.822432	0.604740	0.049903
12	1	0	4.250408	2.613298	0.523347
13	1	0	5.869728	0.854287	-0.040429
14	7	0	-0.391244	1.531563	-0.714473
15	6	0	-1.450593	2.028109	-0.940271
16	16	0	-2.925731	2.610517	-1.190967
17	6	0	-2.584576	0.059637	1.209810
18	6	0	-1.598279	-1.270459	-0.456281
19	6	0	-3.825389	-0.506830	0.975209
20	1	0	-2.390248	0.832486	1.941202
21	6	0	-2.805291	-1.870619	-0.738272
22	1	0	-0.680243	-1.490813	-0.978260
23	6	0	-3.941379	-1.492767	-0.004967
24	1	0	-4.684691	-0.174507	1.539673
25	1	0	-2.868503	-2.619113	-1.515319
26	7	0	-1.510703	-0.344147	0.517713
27	8	0	5.166656	-1.759683	-0.466071
28	6	0	6.561095	-1.527295	-0.609803
29	1	0	7.002001	-1.162133	0.323689
30	1	0	6.998326	-2.491146	-0.863653
31	1	0	6.764501	-0.812148	-1.413754
32	6	0	-5.205310	-2.102592	-0.272242
33	7	0	-6.223924	-2.601164	-0.486090

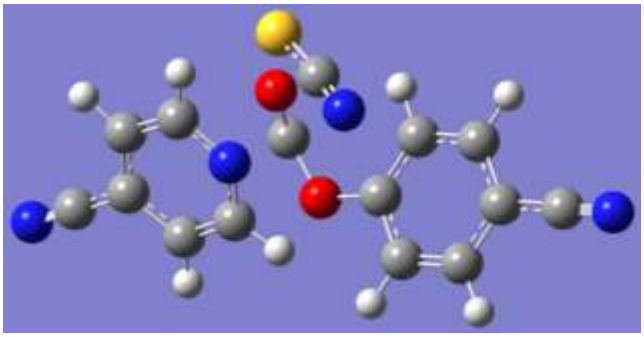
tsfD65.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.182822	0.167562	0.715349
2	8	0	-0.021924	0.702958	1.781530
3	8	0	0.639354	-0.765857	0.140960
4	6	0	2.009078	-0.537742	0.082679
5	6	0	2.769555	-1.643813	-0.283546
6	6	0	2.605334	0.693343	0.333999
7	6	0	4.149023	-1.525679	-0.403461
8	1	0	2.277229	-2.589924	-0.470074
9	6	0	3.988076	0.808064	0.213525
10	1	0	2.011985	1.548453	0.616515
11	6	0	4.748188	-0.295772	-0.152550
12	1	0	4.751297	-2.378701	-0.686203
13	1	0	4.468938	1.758191	0.404491
14	7	0	-0.308454	1.413555	-0.645842
15	6	0	-1.301640	2.065229	-0.746357
16	16	0	-2.695533	2.855379	-0.833507
17	6	0	-2.587466	0.025693	1.263261
18	6	0	-1.893588	-1.190268	-0.624081
19	6	0	-3.907179	-0.332293	1.050130
20	1	0	-2.245629	0.661102	2.069067
21	6	0	-3.187630	-1.576825	-0.891252
22	1	0	-1.047228	-1.459915	-1.236186
23	6	0	-4.216461	-1.152039	-0.035346
24	1	0	-4.677787	0.033240	1.713462
25	1	0	-3.399709	-2.197504	-1.750206
26	7	0	-1.621039	-0.423193	0.449991
27	17	0	6.492187	-0.138014	-0.300011
28	6	0	-5.567194	-1.543963	-0.284975
29	7	0	-6.656674	-1.867499	-0.485382

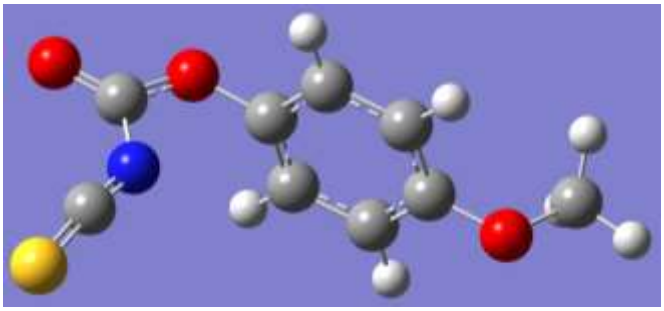
tsfD66.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.048603	0.145697	0.747945
2	8	0	0.119053	0.691449	1.806659
3	8	0	0.777162	-0.796623	0.181984
4	6	0	2.139195	-0.569105	0.109346
5	6	0	2.892106	-1.676239	-0.278319
6	6	0	2.740065	0.660367	0.368706
7	6	0	4.265851	-1.559496	-0.411129
8	1	0	2.391426	-2.616848	-0.468859
9	6	0	4.117666	0.770659	0.233096
10	1	0	2.149266	1.511616	0.666489
11	6	0	4.890678	-0.330693	-0.155255
12	1	0	4.859863	-2.413231	-0.710355
13	1	0	4.600155	1.719609	0.428489
14	7	0	-0.142133	1.391933	-0.645513
15	6	0	-1.126038	2.059943	-0.729390
16	16	0	-2.511508	2.867550	-0.785674
17	6	0	-2.450732	0.055723	1.268830
18	6	0	-1.752452	-1.195508	-0.596203
19	6	0	-3.772413	-0.287525	1.044530
20	1	0	-2.110999	0.695724	2.071439
21	6	0	-3.048220	-1.566544	-0.872371
22	1	0	-0.904503	-1.484631	-1.196609
23	6	0	-4.081064	-1.117197	-0.033114
24	1	0	-4.544928	0.098144	1.694072
25	1	0	-3.259216	-2.194764	-1.726078
26	7	0	-1.479900	-0.419327	0.473348
27	6	0	6.306960	-0.205429	-0.290341
28	7	0	7.453084	-0.107151	-0.400748
29	6	0	-5.433845	-1.494280	-0.292770
30	7	0	-6.525244	-1.805928	-0.501391

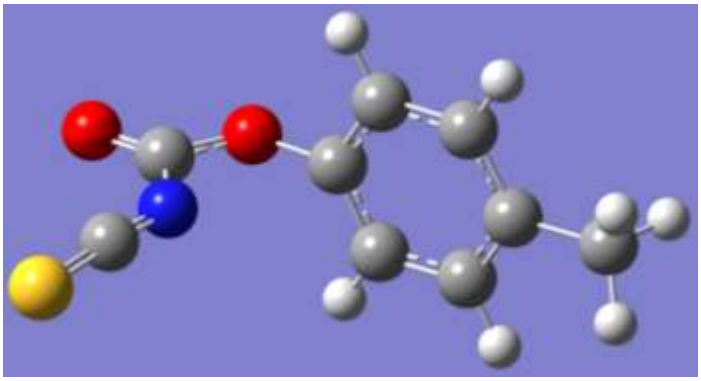
Carbncss1.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.036076	1.381087	0.000033
2	8	0	-3.005418	2.092170	0.000065
3	8	0	-0.794422	1.895031	0.000090
4	6	0	0.342073	1.060478	0.000061
5	6	0	0.911559	0.700375	-1.214115
6	6	0	0.911479	0.700179	1.214217
7	6	0	2.078399	-0.060381	-1.211055
8	1	0	0.448643	1.006777	-2.144091
9	6	0	2.078321	-0.060575	1.211109
10	1	0	0.448505	1.006433	2.144212
11	6	0	2.658058	-0.441802	0.000016
12	1	0	2.538566	-0.364891	-2.143371
13	1	0	2.538431	-0.365235	2.143405
14	7	0	-2.065832	-0.014029	-0.000064
15	6	0	-2.923039	-0.869375	-0.000103
16	16	0	-3.935719	-2.057604	-0.000161
17	8	0	3.780836	-1.243047	-0.000007
18	6	0	5.030418	-0.532145	-0.000016
19	1	0	5.121817	0.092104	0.894031
20	1	0	5.814386	-1.287820	-0.000034
21	1	0	5.121796	0.092123	-0.894053

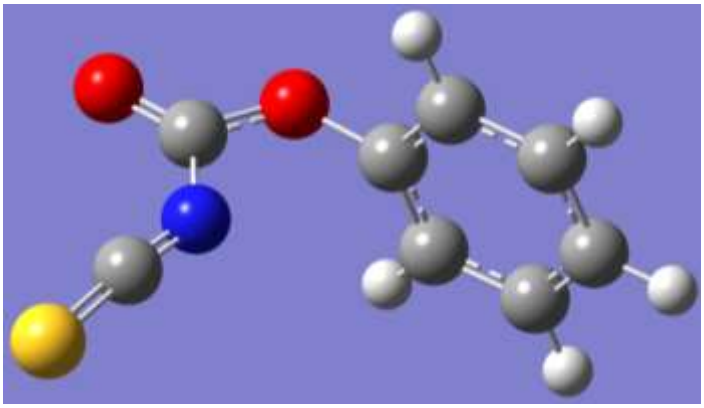
Carbncss2.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.579346	1.419590	-0.000783
2	8	0	2.521477	2.166944	-0.001494
3	8	0	0.319872	1.883860	-0.002692
4	6	0	-0.784836	1.005009	-0.001850
5	6	0	-1.342758	0.624321	1.210193
6	6	0	-1.340833	0.619576	-1.213270
7	6	0	-2.480096	-0.180873	1.200866
8	1	0	-0.894825	0.949385	2.141464
9	6	0	-2.478193	-0.185584	-1.202593
10	1	0	-0.891424	0.940989	-2.145097
11	6	0	-3.066797	-0.597869	-0.000520
12	1	0	-2.916619	-0.487115	2.145314
13	1	0	-2.913216	-0.495523	-2.146526
14	7	0	1.664989	0.025931	0.002009
15	6	0	2.554754	-0.794987	0.004315
16	16	0	3.613393	-1.943122	0.007392
17	6	0	-4.317641	-1.442396	0.000167
18	1	0	-4.367332	-2.078007	0.886666
19	1	0	-5.212357	-0.810634	-0.000938
20	1	0	-4.366748	-2.080322	-0.884694

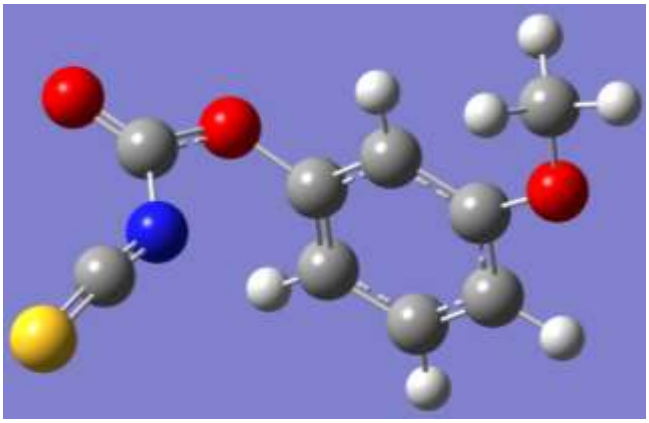
Carbncss3.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.955495	1.460184	0.000073
2	8	0	-1.756826	2.356216	0.000127
3	8	0	0.365323	1.706363	0.000122
4	6	0	1.306945	0.656203	0.000064
5	6	0	1.789777	0.190544	-1.215798
6	6	0	1.789700	0.190337	1.215878
7	6	0	2.779079	-0.792306	-1.208700
8	1	0	1.400119	0.590881	-2.143740
9	6	0	2.779002	-0.792511	1.208674
10	1	0	1.399985	0.590517	2.143863
11	6	0	3.272158	-1.284930	-0.000039
12	1	0	3.164821	-1.168383	-2.148848
13	1	0	3.164684	-1.168749	2.148783
14	1	0	4.042419	-2.047059	-0.000080
15	7	0	-1.272800	0.101669	-0.000047
16	6	0	-2.288270	-0.558127	-0.000114
17	16	0	-3.523922	-1.512115	-0.000208

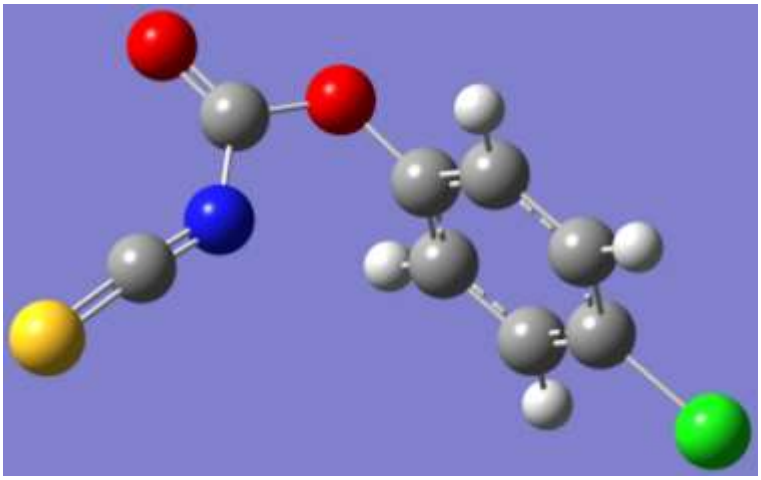
Carbncss4.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.625660	-1.111571	-0.937112
2	8	0	-2.475540	-1.576134	-1.649527
3	8	0	-0.387672	-1.631824	-0.899324
4	6	0	0.608077	-1.094694	-0.056550
5	6	0	0.741944	-1.592836	1.227759
6	6	0	1.471117	-0.148569	-0.599899
7	6	0	1.789040	-1.096868	2.010486
8	1	0	0.055741	-2.341046	1.602626
9	6	0	2.512648	0.332846	0.199305
10	1	0	1.318247	0.186548	-1.615822
11	6	0	2.666017	-0.145260	1.509390
12	1	0	1.919594	-1.463439	3.021680
13	1	0	3.479736	0.238020	2.112870
14	7	0	-1.801152	-0.016229	-0.090728
15	6	0	-2.708568	0.736444	0.185833
16	16	0	-3.798727	1.765482	0.621776
17	8	0	3.420053	1.258388	-0.210890
18	6	0	3.322402	1.775350	-1.542018
19	1	0	4.139169	2.486738	-1.642049
20	1	0	3.438647	0.978773	-2.282140
21	1	0	2.369447	2.289228	-1.695301

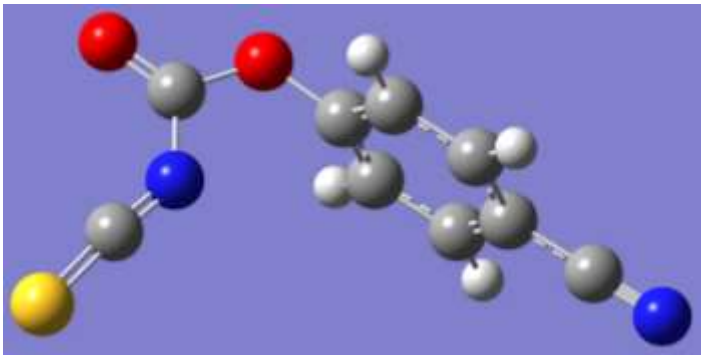
Carbncss5.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.036443	-1.360644	0.000008
2	8	0	3.036550	-2.026272	0.000013
3	8	0	0.819010	-1.935761	0.000017
4	6	0	-0.354152	-1.160378	0.000011
5	6	0	-0.942500	-0.831240	-1.213786
6	6	0	-0.942492	-0.831209	1.213803
7	6	0	-2.148145	-0.133524	-1.215116
8	1	0	-0.469057	-1.116257	-2.144917
9	6	0	-2.148137	-0.133493	1.215123
10	1	0	-0.469043	-1.116202	2.144938
11	6	0	-2.734386	0.208853	0.000001
12	1	0	-2.622677	0.135194	-2.149630
13	1	0	-2.622663	0.135249	2.149633
14	7	0	1.995784	0.032494	-0.000008
15	6	0	2.815264	0.925418	-0.000019
16	16	0	3.773592	2.156324	-0.000035
17	17	0	-4.258928	1.090801	-0.000005

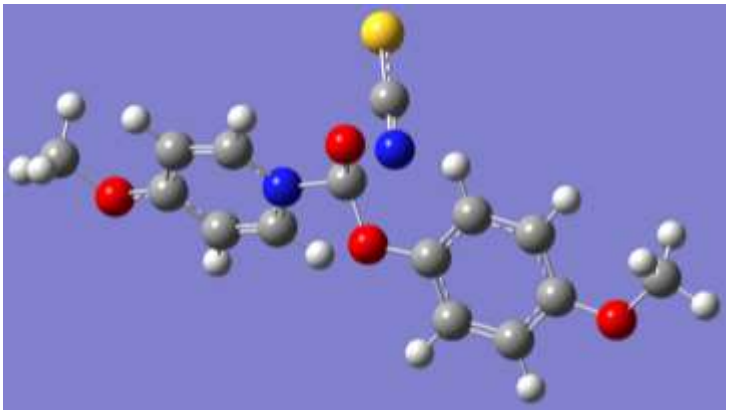
Carbncss6.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.892842	-1.347358	0.030640
2	8	0	-2.882994	-2.025894	0.052126
3	8	0	-0.666077	-1.909820	0.071290
4	6	0	0.496272	-1.127685	0.046714
5	6	0	1.066295	-0.737019	1.252701
6	6	0	1.093334	-0.853570	-1.178164
7	6	0	2.263383	-0.032866	1.232936
8	1	0	0.581261	-0.982834	2.188640
9	6	0	2.290441	-0.149487	-1.199284
10	1	0	0.628922	-1.188298	-2.096827
11	6	0	2.876705	0.264179	0.006460
12	1	0	2.722696	0.282958	2.160559
13	1	0	2.770563	0.076650	-2.142440
14	7	0	-1.862431	0.042903	-0.035663
15	6	0	-2.696083	0.922999	-0.087175
16	16	0	-3.671081	2.136733	-0.156262
17	6	0	4.110319	0.987764	-0.014512
18	7	0	5.107059	1.573124	-0.031492

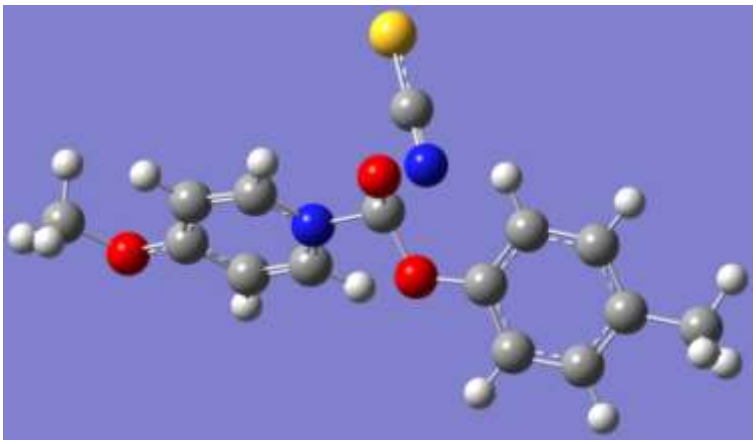
tssfD11.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.254014	0.046365	0.776795
2	8	0	-0.111294	0.499266	1.902531
3	8	0	0.492642	-1.016063	0.277871
4	6	0	1.869767	-0.905724	0.159072
5	6	0	2.469064	-1.865516	-0.659212
6	6	0	2.647451	0.055077	0.793418
7	6	0	3.842730	-1.864015	-0.840756
8	1	0	1.847959	-2.605568	-1.148618
9	6	0	4.032474	0.063283	0.600423
10	1	0	2.190356	0.792356	1.435249
11	6	0	4.636222	-0.895422	-0.213304
12	1	0	4.317008	-2.604775	-1.472752
13	1	0	4.619080	0.821979	1.098783
14	7	0	0.013303	1.266228	-0.443406
15	6	0	-0.562751	2.293243	-0.608574
16	16	0	-1.324752	3.686799	-0.862003
17	6	0	-2.675684	-0.082040	1.266680
18	6	0	-1.978708	-0.896958	-0.822690
19	6	0	-3.993404	-0.358701	0.980920
20	1	0	-2.347703	0.360153	2.196174
21	6	0	-3.266823	-1.197319	-1.170351
22	1	0	-1.136167	-1.070578	-1.472969
23	6	0	-4.310389	-0.929019	-0.262223
24	1	0	-4.745393	-0.128513	1.719227
25	1	0	-3.486756	-1.633514	-2.134325
26	7	0	-1.698284	-0.351947	0.385805
27	8	0	-5.537615	-1.239178	-0.662939
28	6	0	-6.653770	-0.980853	0.213816
29	1	0	-6.723992	0.085383	0.433984
30	1	0	-7.530863	-1.306267	-0.337553
31	1	0	-6.554481	-1.558504	1.134024
32	8	0	5.979155	-0.971655	-0.455496
33	6	0	6.828398	-0.006518	0.164743
34	1	0	7.839477	-0.251177	-0.153646
35	1	0	6.577734	1.007282	-0.161265
36	1	0	6.763640	-0.067282	1.255070

tssfD12.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.077607	0.056831	0.731522
2	8	0	0.231642	0.452316	1.876759
3	8	0	0.836374	-0.965542	0.168187
4	6	0	2.217030	-0.874939	0.129756
5	6	0	2.854439	-1.938329	-0.509616
6	6	0	2.963075	0.175259	0.658186
7	6	0	4.239717	-1.949884	-0.617396
8	1	0	2.255429	-2.741980	-0.920503
9	6	0	4.353257	0.145769	0.532754
10	1	0	2.478493	0.999000	1.158348
11	6	0	5.017956	-0.907743	-0.097447
12	1	0	4.722974	-2.781507	-1.118981
13	1	0	4.928239	0.969809	0.941510
14	7	0	0.295599	1.340918	-0.430085
15	6	0	-0.283268	2.376899	-0.508183
16	16	0	-1.048925	3.784090	-0.643354
17	6	0	-2.331015	-0.146852	1.248822
18	6	0	-1.651763	-0.834069	-0.891903
19	6	0	-3.647489	-0.434177	0.968033
20	1	0	-1.996892	0.251596	2.195715
21	6	0	-2.939225	-1.140904	-1.236076
22	1	0	-0.816597	-0.954926	-1.563349
23	6	0	-3.973273	-0.942667	-0.299461
24	1	0	-4.391833	-0.259003	1.728809
25	1	0	-3.166029	-1.528484	-2.219038
26	7	0	-1.362897	-0.349370	0.340109
27	8	0	-5.200533	-1.254876	-0.698255
28	6	0	-6.306640	-1.068215	0.208888
29	1	0	-6.394650	-0.017128	0.487733
30	1	0	-7.186222	-1.381912	-0.345288
31	1	0	-6.179429	-1.692651	1.094424
32	6	0	6.522634	-0.939781	-0.195325
33	1	0	6.949087	0.055488	-0.056248
34	1	0	6.952494	-1.593914	0.570581
35	1	0	6.849027	-1.319623	-1.166502

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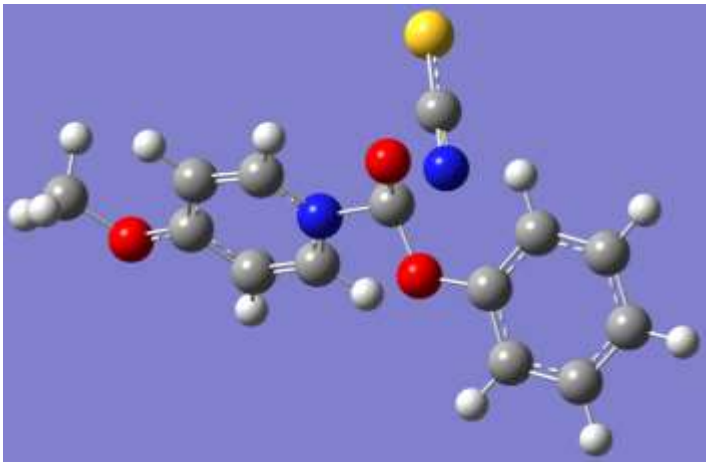
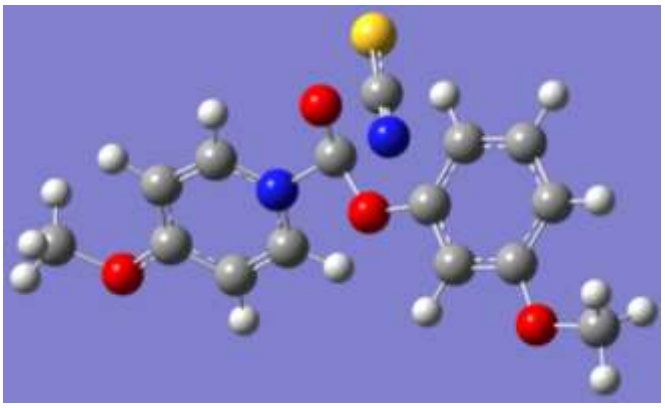
tssfD13.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.447412	-0.010897	0.702165
2	8	0	0.637373	0.370735	1.845555
3	8	0	1.154753	-1.059591	0.118822
4	6	0	2.535928	-1.038654	0.073796
5	6	0	3.111603	-2.147402	-0.548354
6	6	0	3.332108	-0.013713	0.583572
7	6	0	4.494994	-2.232506	-0.662588
8	1	0	2.466811	-2.926368	-0.936336
9	6	0	4.718547	-0.112778	0.455782
10	1	0	2.886600	0.838078	1.072472
11	6	0	5.307150	-1.213765	-0.161630
12	1	0	4.937197	-3.095688	-1.145969
13	1	0	5.338700	0.684094	0.849610
14	1	0	6.384649	-1.279341	-0.251144
15	7	0	0.707616	1.276599	-0.462050
16	6	0	0.179123	2.340816	-0.512355
17	16	0	-0.520145	3.785618	-0.608505
18	6	0	-1.958709	-0.103366	1.248151
19	6	0	-1.337176	-0.811985	-0.903846
20	6	0	-3.290082	-0.328116	0.981895
21	1	0	-1.595652	0.275028	2.192556
22	6	0	-2.641291	-1.057865	-1.233125
23	1	0	-0.516792	-0.967810	-1.586101
24	6	0	-3.653937	-0.816411	-0.283282
25	1	0	-4.016510	-0.121649	1.752128
26	1	0	-2.897370	-1.430451	-2.214688
27	7	0	-1.011512	-0.346734	0.326848
28	8	0	-4.898503	-1.070921	-0.668062
29	6	0	-5.984253	-0.837677	0.252982
30	1	0	-6.020016	0.214945	0.537308
31	1	0	-6.883753	-1.107613	-0.292162
32	1	0	-5.875686	-1.471765	1.134134

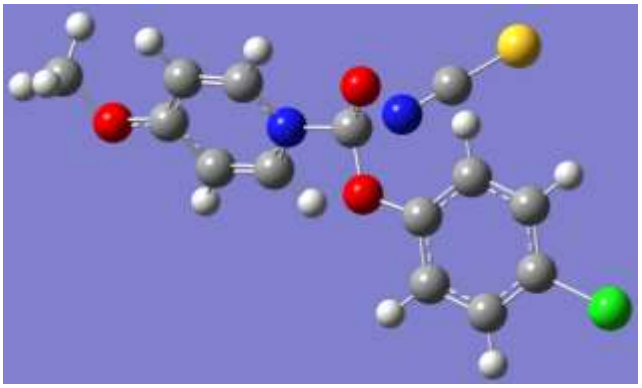
tssfD14.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.246217	0.389011	0.733380
2	8	0	-0.192957	0.903333	1.837929
3	8	0	0.684936	-0.541150	0.276839
4	6	0	2.037311	-0.260011	0.312027
5	6	0	2.846641	-1.310463	-0.103718
6	6	0	2.585409	0.962894	0.707289
7	6	0	4.233858	-1.151323	-0.129478
8	1	0	2.403729	-2.249910	-0.408361
9	6	0	3.969783	1.100552	0.668825
10	1	0	1.958078	1.774328	1.037912
11	6	0	4.807498	0.063976	0.258132
12	1	0	4.411192	2.043153	0.970836
13	7	0	-0.198164	1.592076	-0.550281
14	6	0	-0.843798	2.584039	-0.662195
15	16	0	-1.697970	3.935095	-0.843391
16	6	0	-2.597708	-0.178432	1.225229
17	6	0	-1.753459	-0.876736	-0.853492
18	6	0	-3.837185	-0.706859	0.945190
19	1	0	-2.362535	0.332284	2.147594
20	6	0	-2.959199	-1.424048	-1.194115
21	1	0	-0.892497	-0.894782	-1.502528
22	6	0	-4.036010	-1.348243	-0.288169
23	1	0	-4.620782	-0.613077	1.680764
24	1	0	-3.090215	-1.909084	-2.150887
25	7	0	-1.585273	-0.269833	0.346713
26	8	0	-5.178451	-1.897878	-0.681226
27	6	0	-6.323040	-1.852963	0.195816
28	1	0	-6.608512	-0.818613	0.393087
29	1	0	-7.116014	-2.362198	-0.343657
30	1	0	-6.107015	-2.377748	1.127589
31	1	0	5.877664	0.210764	0.246255
32	8	0	4.942859	-2.238349	-0.547986
33	6	0	6.367738	-2.140402	-0.587576
34	1	0	6.776135	-1.941976	0.407242
35	1	0	6.721052	-3.106855	-0.940262
36	1	0	6.689631	-1.357896	-1.280268

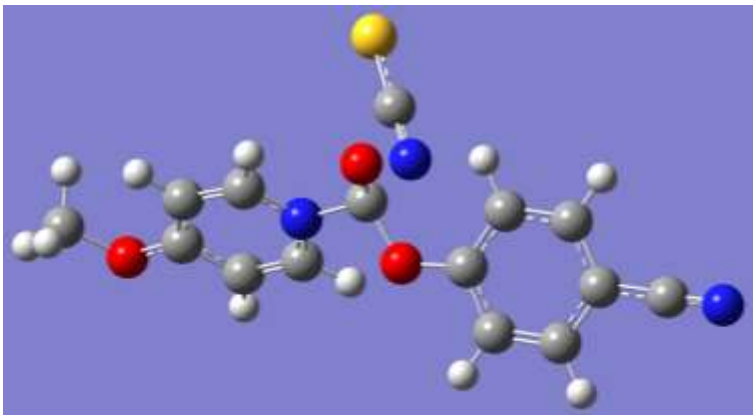
tssfD15.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.404799	0.197213	0.670287
2	8	0	-0.269635	0.706904	1.768160
3	8	0	0.418652	-0.822829	0.186412
4	6	0	1.789070	-0.664666	0.136324
5	6	0	2.461922	-1.660142	-0.572315
6	6	0	2.492832	0.383248	0.727446
7	6	0	3.844901	-1.613800	-0.697212
8	1	0	1.894467	-2.462976	-1.025563
9	6	0	3.879444	0.435030	0.592315
10	1	0	1.979774	1.147303	1.289354
11	6	0	4.541511	-0.559891	-0.114092
12	1	0	4.433072	1.248248	1.042694
13	7	0	-0.253288	1.390917	-0.647512
14	6	0	0.304029	2.439718	-0.658820
15	16	0	1.044343	3.869197	-0.704675
16	6	0	-2.769208	-0.179855	1.240284
17	6	0	-2.072567	-0.832296	-0.907415
18	6	0	-4.058001	-0.591270	0.991567
19	1	0	-2.455827	0.261721	2.174870
20	6	0	-3.332391	-1.262246	-1.218954
21	1	0	-1.244335	-0.882996	-1.595712
22	6	0	-4.360632	-1.148061	-0.261965
23	1	0	-4.799841	-0.474618	1.765926
24	1	0	-3.542686	-1.682861	-2.191911
25	7	0	-1.805217	-0.305025	0.312002
26	8	0	-5.559867	-1.581139	-0.628502
27	6	0	-6.660874	-1.487989	0.299761
28	1	0	-6.843230	-0.446399	0.567843
29	1	0	-7.517009	-1.891623	-0.232412
30	1	0	-6.457150	-2.085337	1.189588
31	1	0	4.369972	-2.383946	-1.246335
32	17	0	6.296665	-0.488936	-0.274916

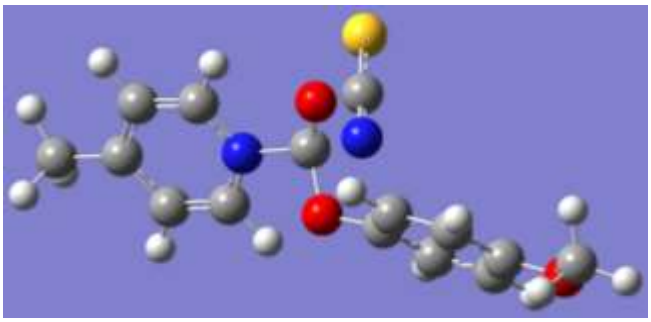
tssfD16.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.117731	0.066089	0.714840
2	8	0	0.057418	0.467101	1.848878
3	8	0	0.678748	-0.915505	0.117862
4	6	0	2.042987	-0.794436	0.098906
5	6	0	2.712276	-1.877938	-0.477883
6	6	0	2.750534	0.306294	0.588013
7	6	0	4.092557	-1.867587	-0.570672
8	1	0	2.136196	-2.715502	-0.849093
9	6	0	4.135346	0.314847	0.489779
10	1	0	2.234374	1.137480	1.039924
11	6	0	4.816190	-0.765986	-0.086339
12	1	0	4.691978	1.164232	0.864107
13	7	0	0.062333	1.397613	-0.484339
14	6	0	-0.549871	2.416798	-0.509303
15	16	0	-1.367372	3.802084	-0.566540
16	6	0	-2.501000	-0.182535	1.249563
17	6	0	-1.819354	-0.839070	-0.904265
18	6	0	-3.811656	-0.492478	0.972305
19	1	0	-2.171739	0.214246	2.198487
20	6	0	-3.101967	-1.167078	-1.242411
21	1	0	-0.987206	-0.936034	-1.582865
22	6	0	-4.134877	-0.996855	-0.298224
23	1	0	-4.554947	-0.337745	1.738461
24	1	0	-3.326894	-1.549959	-2.227565
25	7	0	-1.532366	-0.359902	0.332541
26	8	0	-5.356312	-1.329100	-0.692450
27	6	0	-6.462757	-1.173086	0.221355
28	1	0	-6.571296	-0.126246	0.508316
29	1	0	-7.337423	-1.501158	-0.332089
30	1	0	-6.317776	-1.801958	1.100826
31	1	0	4.612977	-2.705017	-1.016545
32	6	0	6.238792	-0.748036	-0.178989
33	7	0	7.393123	-0.733641	-0.254568

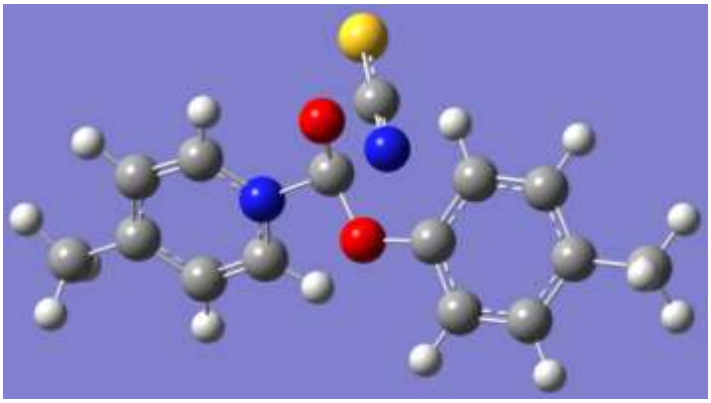
tssfD21.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.549794	0.223216	0.275660
2	8	0	-0.318277	1.047057	1.143822
3	8	0	0.219289	-0.925648	0.079583
4	6	0	1.596992	-0.732483	-0.015730
5	6	0	2.193773	-0.790904	-1.273038
6	6	0	2.365397	-0.548129	1.123807
7	6	0	3.570609	-0.660580	-1.385965
8	1	0	1.575932	-0.935809	-2.149429
9	6	0	3.750778	-0.413158	1.015882
10	1	0	1.887317	-0.510522	2.093477
11	6	0	4.356474	-0.467506	-0.242687
12	1	0	4.054615	-0.705819	-2.353809
13	1	0	4.336446	-0.271415	1.912973
14	7	0	-0.515261	0.955083	-1.309890
15	6	0	-1.185168	1.833422	-1.749498
16	16	0	-2.077499	3.015864	-2.377486
17	6	0	-2.896303	0.208604	1.062126
18	6	0	-2.351304	-1.291847	-0.658728
19	6	0	-4.210752	-0.212015	1.045979
20	1	0	-2.509665	0.972530	1.720767
21	6	0	-3.649792	-1.743327	-0.708404
22	1	0	-1.566443	-1.658719	-1.300983
23	6	0	-4.618937	-1.208086	0.153859
24	1	0	-4.913327	0.242627	1.731101
25	1	0	-3.909345	-2.511573	-1.424480
26	7	0	-1.998559	-0.334015	0.224184
27	8	0	5.698925	-0.348534	-0.455251
28	6	0	6.546299	-0.148620	0.676916
29	1	0	6.481064	-0.991183	1.371250
30	1	0	7.557621	-0.079729	0.282282
31	1	0	6.293329	0.778520	1.199152
32	6	0	-6.031968	-1.702247	0.123102
33	1	0	-6.378676	-1.824671	-0.904743
34	1	0	-6.087818	-2.683939	0.604335
35	1	0	-6.703738	-1.025816	0.650598

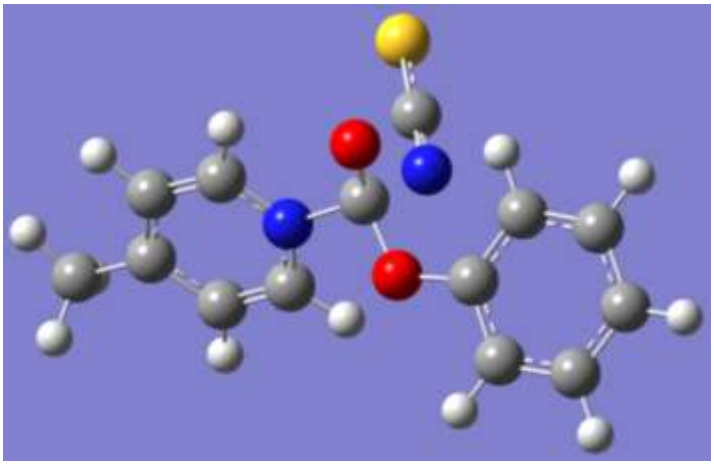
tssfD22.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.231998	-0.048357	0.801752
2	8	0	-0.079477	0.321220	1.953208
3	8	0	0.561969	-1.005036	0.187836
4	6	0	1.936647	-0.844020	0.125306
5	6	0	2.610110	-1.846978	-0.571060
6	6	0	2.640254	0.220504	0.681881
7	6	0	3.991600	-1.783773	-0.707631
8	1	0	2.042441	-2.662113	-1.003144
9	6	0	4.026774	0.266773	0.526557
10	1	0	2.126229	0.997666	1.225385
11	6	0	4.728382	-0.725690	-0.160614
12	1	0	4.504234	-2.568451	-1.253594
13	1	0	4.569188	1.101789	0.956956
14	7	0	-0.104882	1.297278	-0.331050
15	6	0	-0.752628	2.294138	-0.360432
16	16	0	-1.614747	3.650460	-0.428030
17	6	0	-2.627935	-0.355778	1.336669
18	6	0	-1.941625	-0.978714	-0.820260
19	6	0	-3.933690	-0.696401	1.045658
20	1	0	-2.299428	0.039480	2.286755
21	6	0	-3.228155	-1.331505	-1.153699
22	1	0	-1.107514	-1.052626	-1.499861
23	6	0	-4.264758	-1.197116	-0.216637
24	1	0	-4.689881	-0.567368	1.807924
25	1	0	-3.425481	-1.709338	-2.148003
26	7	0	-1.664984	-0.505325	0.413450
27	6	0	6.230270	-0.678291	-0.288937
28	1	0	6.607310	0.337141	-0.152632
29	1	0	6.708617	-1.312313	0.465091
30	1	0	6.556057	-1.036537	-1.268331
31	6	0	-5.668465	-1.582690	-0.566817
32	1	0	-5.982467	-1.085169	-1.487652
33	1	0	-5.725120	-2.660207	-0.746819
34	1	0	-6.365198	-1.326405	0.230201

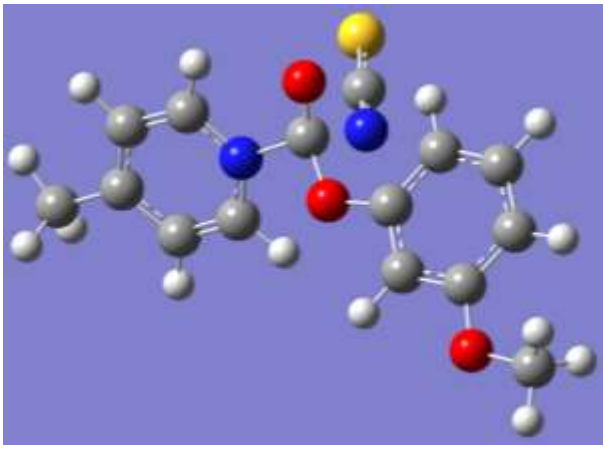
tssfD23.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.143761	-0.038845	0.732166
2	8	0	0.337353	0.384714	1.857554
3	8	0	0.887322	-1.056755	0.152527
4	6	0	2.265429	-0.966239	0.071104
5	6	0	2.880771	-2.055862	-0.545932
6	6	0	3.018689	0.108463	0.541007
7	6	0	4.263390	-2.071163	-0.695604
8	1	0	2.267639	-2.874399	-0.902366
9	6	0	4.404605	0.079066	0.377713
10	1	0	2.541424	0.945240	1.025864
11	6	0	5.033525	-1.001882	-0.235342
12	1	0	4.737631	-2.919408	-1.174952
13	1	0	4.992224	0.914556	0.739988
14	1	0	6.110250	-1.013131	-0.352911
15	7	0	0.303650	1.244521	-0.479249
16	6	0	-0.308360	2.261906	-0.546819
17	16	0	-1.123764	3.643567	-0.665956
18	6	0	-2.249266	-0.209864	1.323884
19	6	0	-1.632361	-0.978421	-0.807474
20	6	0	-3.573724	-0.507867	1.074139
21	1	0	-1.885958	0.221551	2.245067
22	6	0	-2.939064	-1.291505	-1.098749
23	1	0	-0.815741	-1.125681	-1.496233
24	6	0	-3.950598	-1.060885	-0.152952
25	1	0	-4.308596	-0.304897	1.841132
26	1	0	-3.171642	-1.713635	-2.067296
27	7	0	-1.311544	-0.451696	0.393841
28	6	0	-5.376414	-1.399597	-0.458845
29	1	0	-5.696272	-0.902043	-1.377925
30	1	0	-5.478421	-2.476098	-0.622755
31	1	0	-6.041245	-1.105294	0.352113

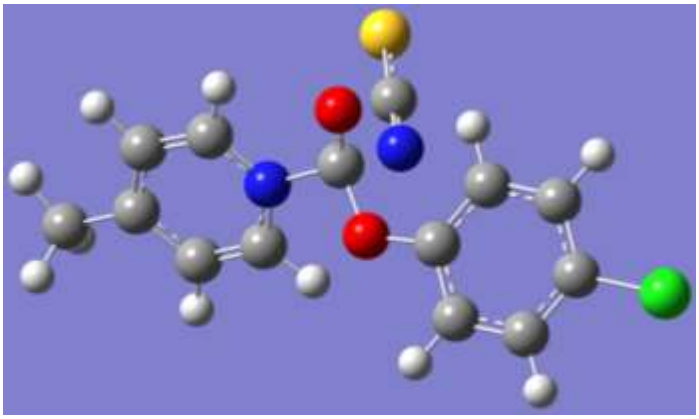
tssfD24.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.536431	0.267188	0.776720
2	8	0	-0.519138	0.808744	1.866992
3	8	0	0.468225	-0.571733	0.315456
4	6	0	1.788572	-0.159733	0.319212
5	6	0	2.687407	-1.131966	-0.101687
6	6	0	2.220650	1.116270	0.687989
7	6	0	4.051482	-0.837501	-0.160056
8	1	0	2.332666	-2.114217	-0.385901
9	6	0	3.583611	1.388668	0.617581
10	1	0	1.522978	1.866981	1.021115
11	6	0	4.510321	0.433498	0.200865
12	1	0	3.936128	2.374219	0.898466
13	1	0	5.560381	0.684524	0.164147
14	7	0	-0.633151	1.455956	-0.535325
15	6	0	-1.474396	2.276437	-0.717324
16	16	0	-2.600767	3.392092	-0.991902
17	6	0	-2.835851	-0.471140	1.299409
18	6	0	-1.934332	-1.195981	-0.744190
19	6	0	-4.026111	-1.115423	1.030287
20	1	0	-2.642468	0.100729	2.195071
21	6	0	-3.101803	-1.854428	-1.052483
22	1	0	-1.073271	-1.172948	-1.393136
23	6	0	-4.185599	-1.829271	-0.161219
24	1	0	-4.828082	-1.054747	1.753321
25	1	0	-3.169853	-2.385531	-1.992484
26	7	0	-1.820534	-0.525304	0.421952
27	8	0	4.854996	-1.854978	-0.581822
28	6	0	6.261448	-1.615668	-0.662063
29	1	0	6.674264	-1.362989	0.318486
30	1	0	6.700345	-2.547084	-1.012839
31	1	0	6.484503	-0.815295	-1.372953
32	6	0	-5.456826	-2.554300	-0.476488
33	1	0	-5.748026	-2.392854	-1.516181
34	1	0	-5.307893	-3.630674	-0.343888
35	1	0	-6.269424	-2.239456	0.177347

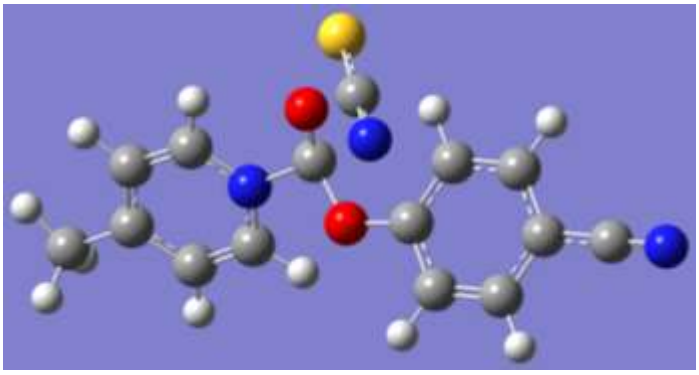
tssfD25.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.554263	-0.032567	0.788447
2	8	0	-0.392766	0.335423	1.936860
3	8	0	0.273537	-0.945635	0.147898
4	6	0	1.635465	-0.733886	0.086463
5	6	0	2.346747	-1.721515	-0.594887
6	6	0	2.293909	0.366373	0.632984
7	6	0	3.724877	-1.615331	-0.736494
8	1	0	1.813383	-2.565871	-1.012669
9	6	0	3.676093	0.474310	0.485832
10	1	0	1.749503	1.127405	1.168694
11	6	0	4.377269	-0.512816	-0.193654
12	1	0	4.280207	-2.379243	-1.264170
13	1	0	4.196506	1.325585	0.904364
14	7	0	-0.486129	1.343070	-0.348402
15	6	0	-1.180542	2.308520	-0.350529
16	16	0	-2.109521	3.622020	-0.378700
17	6	0	-2.925488	-0.418186	1.345496
18	6	0	-2.239255	-1.002624	-0.823983
19	6	0	-4.221787	-0.797664	1.063019
20	1	0	-2.601876	-0.019811	2.295789
21	6	0	-3.516821	-1.393548	-1.147733
22	1	0	-1.410467	-1.043363	-1.512638
23	6	0	-4.548357	-1.299601	-0.200200
24	1	0	-4.974746	-0.697620	1.832740
25	1	0	-3.711377	-1.769274	-2.143293
26	7	0	-1.966084	-0.530421	0.411768
27	17	0	6.126415	-0.368551	-0.370645
28	6	0	-5.941309	-1.730553	-0.538902
29	1	0	-6.264027	-1.279925	-1.480280
30	1	0	-5.970618	-2.816047	-0.673645
31	1	0	-6.646355	-1.460503	0.246185

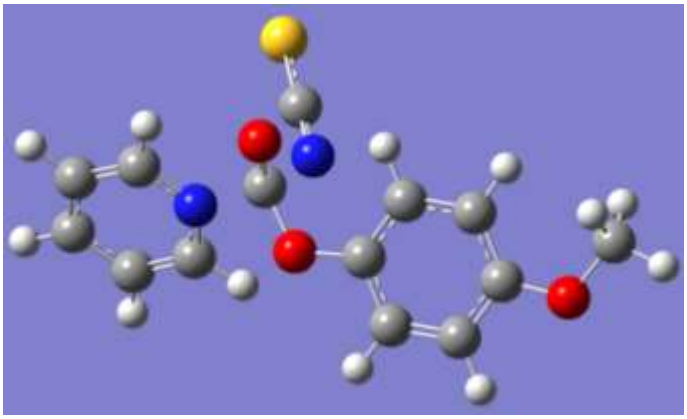
tssfD26.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.420544	-0.008455	0.761522
2	8	0	-0.250655	0.419102	1.884414
3	8	0	0.408525	-0.952315	0.160690
4	6	0	1.766035	-0.765251	0.112199
5	6	0	2.474439	-1.820074	-0.469939
6	6	0	2.427349	0.373455	0.576975
7	6	0	3.850356	-1.742417	-0.592941
8	1	0	1.932523	-2.688213	-0.821766
9	6	0	3.807646	0.449451	0.448264
10	1	0	1.880088	1.182717	1.032140
11	6	0	4.528397	-0.601770	-0.133937
12	1	0	4.401913	-2.557209	-1.043222
13	1	0	4.329392	1.328801	0.802989
14	7	0	-0.330731	1.326825	-0.465838
15	6	0	-1.030948	2.287197	-0.505921
16	16	0	-1.972510	3.590931	-0.581675
17	6	0	-2.792580	-0.326302	1.320199
18	6	0	-2.098565	-1.031828	-0.812460
19	6	0	-4.091696	-0.700471	1.046228
20	1	0	-2.471314	0.115460	2.251741
21	6	0	-3.379261	-1.419490	-1.125418
22	1	0	-1.266309	-1.119197	-1.492315
23	6	0	-4.416395	-1.261867	-0.192338
24	1	0	-4.848703	-0.549649	1.803530
25	1	0	-3.572016	-1.842551	-2.102108
26	7	0	-1.827101	-0.501234	0.400827
27	6	0	5.946071	-0.513719	-0.258795
28	7	0	7.096183	-0.442239	-0.360696
29	6	0	-5.812771	-1.689019	-0.520015
30	1	0	-6.122309	-1.280139	-1.484617
31	1	0	-5.856259	-2.779263	-0.602605
32	1	0	-6.519204	-1.371539	0.245762

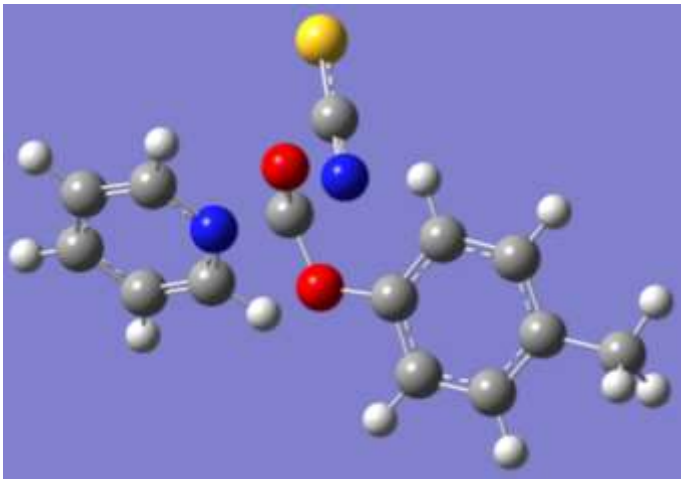
tssfD31.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.904422	-0.171682	0.722843
2	8	0	-0.804411	0.259742	1.856914
3	8	0	-0.059332	-1.114624	0.172965
4	6	0	1.307815	-0.879925	0.108717
5	6	0	2.031207	-1.834783	-0.608293
6	6	0	1.957986	0.201146	0.689268
7	6	0	3.404098	-1.707256	-0.743068
8	1	0	1.507027	-2.669704	-1.056607
9	6	0	3.342796	0.333091	0.545382
10	1	0	1.406996	0.938107	1.252300
11	6	0	4.071624	-0.618415	-0.167827
12	1	0	3.974843	-2.442713	-1.296523
13	1	0	3.829960	1.182875	1.001915
14	7	0	-0.803428	1.135725	-0.475505
15	6	0	-1.494901	2.099703	-0.557058
16	16	0	-2.418423	3.410449	-0.692700
17	6	0	-3.307939	-0.526906	1.200215
18	6	0	-2.526330	-1.254221	-0.897263
19	6	0	-4.594618	-0.927258	0.890162
20	1	0	-3.017950	-0.066597	2.133332
21	6	0	-3.792514	-1.671630	-1.253227
22	1	0	-1.664477	-1.338352	-1.539933
23	6	0	-4.842436	-1.507863	-0.350014
24	1	0	-5.382970	-0.782325	1.615101
25	1	0	-3.948700	-2.115624	-2.226169
26	1	0	-5.842531	-1.827271	-0.613369
27	7	0	-2.314379	-0.701078	0.313602
28	8	0	5.424214	-0.576391	-0.356307
29	6	0	6.146636	0.516968	0.209899
30	1	0	6.047329	0.533059	1.299221
31	1	0	7.188622	0.355868	-0.057905
32	1	0	5.805693	1.470661	-0.203561

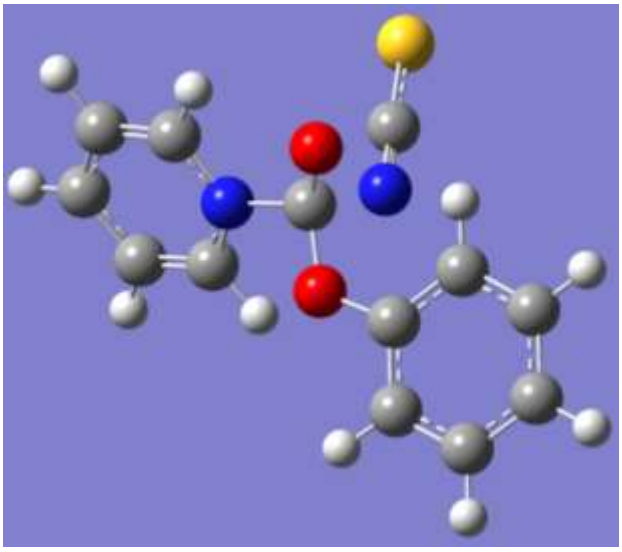
tssfD32.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.564381	-0.155049	0.708081
2	8	0	-0.488955	0.270745	1.845290
3	8	0	0.337451	-1.037684	0.146500
4	6	0	1.692295	-0.742527	0.120558
5	6	0	2.481299	-1.692028	-0.528501
6	6	0	2.269640	0.397064	0.670741
7	6	0	3.853293	-1.498499	-0.623605
8	1	0	2.009074	-2.568950	-0.954371
9	6	0	3.650586	0.573605	0.557721
10	1	0	1.665934	1.132384	1.179177
11	6	0	4.466280	-0.360623	-0.081980
12	1	0	4.457028	-2.243360	-1.130987
13	1	0	4.095629	1.465673	0.984961
14	7	0	-0.549051	1.170483	-0.482745
15	6	0	-1.278836	2.107990	-0.531580
16	16	0	-2.255075	3.384150	-0.621991
17	6	0	-2.936496	-0.674104	1.184865
18	6	0	-2.115983	-1.311412	-0.927299
19	6	0	-4.194103	-1.156102	0.871894
20	1	0	-2.674904	-0.210935	2.124918
21	6	0	-3.352228	-1.808315	-1.286127
22	1	0	-1.253293	-1.326147	-1.574124
23	6	0	-4.407054	-1.731789	-0.377024
24	1	0	-4.987366	-1.077325	1.601682
25	1	0	-3.481873	-2.245393	-2.266053
26	1	0	-5.383986	-2.114568	-0.642694
27	7	0	-1.937083	-0.765309	0.292228
28	6	0	5.958516	-0.166283	-0.180897
29	1	0	6.492985	-0.910188	0.418163
30	1	0	6.304010	-0.273646	-1.212763
31	1	0	6.252111	0.822864	0.174645

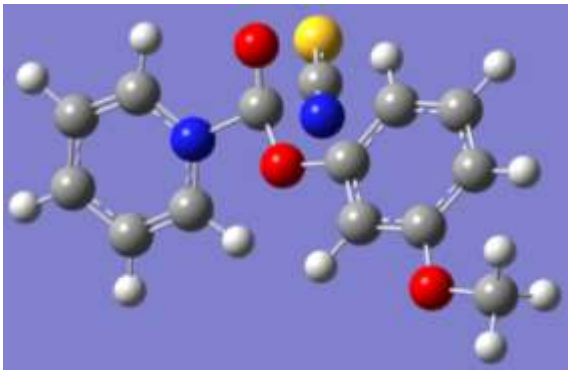
tssfD33.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.184096	-0.156918	0.689387
2	8	0	-0.087655	0.280086	1.819790
3	8	0	0.706088	-1.048289	0.120856
4	6	0	2.061544	-0.767305	0.078780
5	6	0	2.833393	-1.745057	-0.548731
6	6	0	2.647892	0.386076	0.596332
7	6	0	4.208319	-1.567915	-0.659960
8	1	0	2.346146	-2.628245	-0.943049
9	6	0	4.028468	0.549752	0.471455
10	1	0	2.048922	1.136289	1.087948
11	6	0	4.813538	-0.417864	-0.150827
12	1	0	4.805541	-2.329255	-1.147579
13	1	0	4.487654	1.446411	0.871065
14	1	0	5.884280	-0.279517	-0.238138
15	7	0	-0.176689	1.162715	-0.520232
16	6	0	-0.905124	2.101729	-0.560629
17	16	0	-1.881836	3.378548	-0.637736
18	6	0	-2.552911	-0.644580	1.199492
19	6	0	-1.761990	-1.319002	-0.913024
20	6	0	-3.818471	-1.117961	0.906751
21	1	0	-2.276608	-0.171208	2.130140
22	6	0	-3.006924	-1.808504	-1.250965
23	1	0	-0.907070	-1.350924	-1.569388
24	6	0	-4.050864	-1.708744	-0.331607
25	1	0	-4.602777	-1.020977	1.643965
26	1	0	-3.151707	-2.257724	-2.223240
27	1	0	-5.034401	-2.085308	-0.581290
28	7	0	-1.564078	-0.758247	0.297185

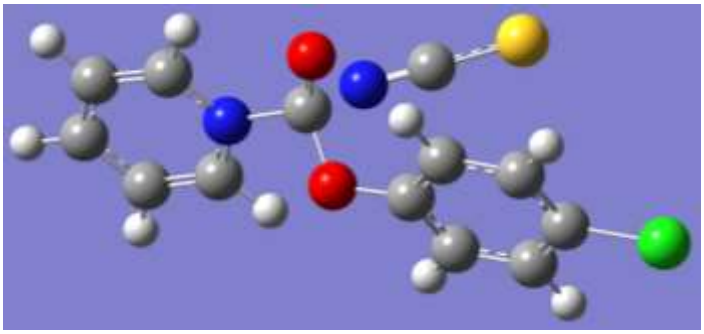
tssfD34.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.870239	-0.006311	0.735307
2	8	0	-0.948519	0.489769	1.842141
3	8	0	0.231701	-0.697932	0.267973
4	6	0	1.496207	-0.136701	0.325827
5	6	0	2.509066	-0.976243	-0.119550
6	6	0	1.767751	1.159487	0.767985
7	6	0	3.830422	-0.523437	-0.128449
8	1	0	2.276722	-1.976581	-0.461123
9	6	0	3.091023	1.590458	0.746720
10	1	0	0.980130	1.805976	1.118647
11	6	0	4.130467	0.771365	0.307032
12	1	0	3.320716	2.594135	1.084664
13	1	0	5.144564	1.143315	0.308669
14	7	0	-1.080507	1.226681	-0.546474
15	6	0	-1.992463	1.978779	-0.675215
16	16	0	-3.217097	3.004588	-0.872108
17	6	0	-3.095782	-0.997914	1.144898
18	6	0	-2.041036	-1.561302	-0.883288
19	6	0	-4.200778	-1.759635	0.813009
20	1	0	-2.992926	-0.435469	2.061148
21	6	0	-3.119369	-2.336144	-1.258292
22	1	0	-1.161107	-1.423902	-1.491203
23	6	0	-4.214836	-2.439159	-0.401188
24	1	0	-5.031927	-1.813649	1.501635
25	1	0	-3.097433	-2.847094	-2.210397
26	1	0	-5.070330	-3.040520	-0.680307
27	7	0	-2.051652	-0.920609	0.303134
28	8	0	4.755041	-1.416872	-0.581055
29	6	0	6.124513	-1.010441	-0.619198
30	1	0	6.490480	-0.765804	0.381782
31	1	0	6.675202	-1.863233	-1.009896
32	1	0	6.261343	-0.151299	-1.281646

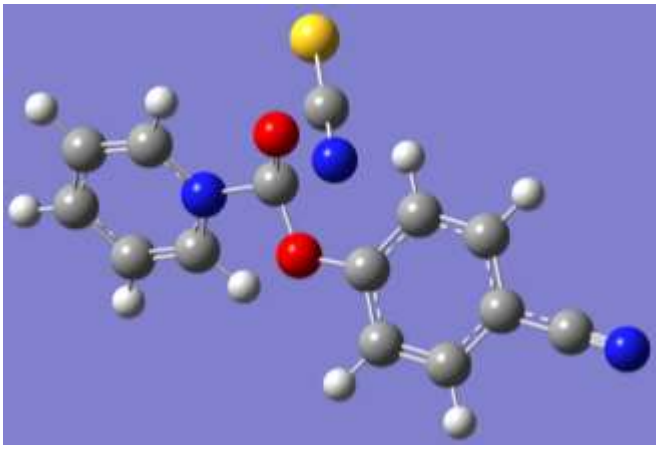
tssfD35.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.103745	-0.092312	0.601117
2	8	0	-1.100807	0.643490	1.565186
3	8	0	-0.125326	-1.048509	0.334082
4	6	0	1.194642	-0.621782	0.252580
5	6	0	1.881829	-0.946661	-0.911776
6	6	0	1.817694	0.065887	1.289687
7	6	0	3.212316	-0.568331	-1.055804
8	1	0	1.369996	-1.479638	-1.702400
9	6	0	3.146746	0.455079	1.144279
10	1	0	1.270840	0.304357	2.189529
11	6	0	3.826240	0.137182	-0.026396
12	1	0	3.756648	-0.808580	-1.959186
13	1	0	3.645663	0.996464	1.936991
14	7	0	-1.058821	0.871454	-0.942951
15	6	0	-0.253850	1.694447	-1.240048
16	16	0	0.803372	2.830210	-1.681754
17	6	0	-3.436321	-0.658222	1.153691
18	6	0	-2.522980	-1.635721	-0.784082
19	6	0	-4.645432	-1.291348	0.936005
20	1	0	-3.233460	0.003570	1.982614
21	6	0	-3.709211	-2.290959	-1.043553
22	1	0	-1.648639	-1.707589	-1.410480
23	6	0	-4.785920	-2.118986	-0.174300
24	1	0	-5.458075	-1.132473	1.630495
25	1	0	-3.784458	-2.921941	-1.917704
26	1	0	-5.724757	-2.623260	-0.363577
27	7	0	-2.413629	-0.845923	0.302436
28	17	0	5.506899	0.635122	-0.208059

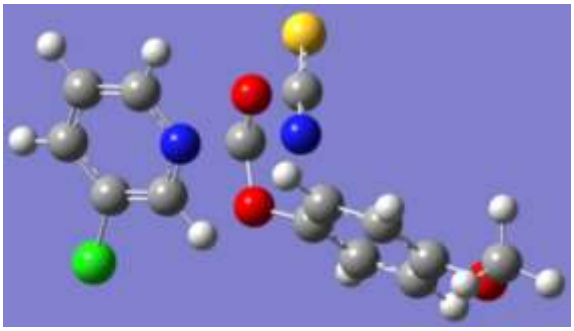
tssfD36.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.737066	-0.150059	0.687332
2	8	0	-0.633174	0.303484	1.806252
3	8	0	0.179862	-1.017579	0.110811
4	6	0	1.519759	-0.719660	0.098758
5	6	0	2.327749	-1.719543	-0.448572
6	6	0	2.070297	0.475174	0.565665
7	6	0	3.695819	-1.530603	-0.532925
8	1	0	1.868866	-2.633020	-0.803667
9	6	0	3.443199	0.662193	0.476544
10	1	0	1.445206	1.242971	0.991635
11	6	0	4.264154	-0.333406	-0.069447
12	1	0	4.325496	-2.302228	-0.955836
13	1	0	3.880693	1.585382	0.833712
14	7	0	-0.745670	1.187061	-0.560004
15	6	0	-1.556344	2.054705	-0.628896
16	16	0	-2.653368	3.228062	-0.737697
17	6	0	-3.091678	-0.644144	1.193046
18	6	0	-2.280615	-1.345188	-0.906057
19	6	0	-4.351076	-1.130300	0.897632
20	1	0	-2.826964	-0.155198	2.118709
21	6	0	-3.519827	-1.846972	-1.244154
22	1	0	-1.422521	-1.379831	-1.557791
23	6	0	-4.570746	-1.740800	-0.333422
24	1	0	-5.141188	-1.027036	1.627667
25	1	0	-3.654866	-2.310778	-2.210886
26	1	0	-5.550104	-2.127099	-0.584437
27	7	0	-2.094294	-0.765398	0.298637
28	6	0	5.673334	-0.131768	-0.152935
29	7	0	6.816506	0.031417	-0.220966

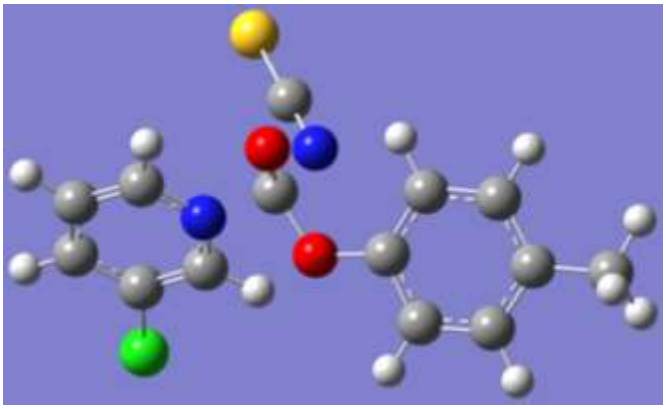
tssfD41.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.350293	0.480254	0.597530
2	8	0	-0.023020	1.481281	1.199874
3	8	0	0.351559	-0.710701	0.603380
4	6	0	1.711880	-0.636392	0.292153
5	6	0	2.132511	-1.147873	-0.932388
6	6	0	2.625157	-0.126159	1.201772
7	6	0	3.483509	-1.145211	-1.247359
8	1	0	1.400810	-1.540722	-1.626045
9	6	0	3.985163	-0.116285	0.886658
10	1	0	2.282072	0.262003	2.151110
11	6	0	4.417128	-0.625630	-0.341304
12	1	0	3.833329	-1.539796	-2.193279
13	1	0	4.687117	0.284303	1.603867
14	7	0	-0.475890	0.812679	-1.157066
15	6	0	-1.206630	1.584244	-1.690837
16	16	0	-2.194211	2.618180	-2.430838
17	6	0	-2.636203	0.814880	1.500815
18	6	0	-2.265323	-1.136542	0.236012
19	6	0	-3.968043	0.481516	1.675377
20	1	0	-2.169790	1.705153	1.895749
21	6	0	-3.588864	-1.502508	0.389669
22	1	0	-1.543304	-1.713191	-0.319391
23	6	0	-4.459339	-0.691359	1.117051
24	1	0	-4.610664	1.137995	2.244337
25	1	0	-5.496463	-0.973992	1.237523
26	7	0	-1.829884	0.005296	0.798614
27	8	0	5.720143	-0.662454	-0.741558
28	6	0	6.713076	-0.137020	0.140941
29	1	0	6.736350	-0.692310	1.082909
30	1	0	7.662639	-0.257075	-0.375820
31	1	0	6.537497	0.923353	0.343020
32	17	0	-4.147359	-2.978785	-0.337475

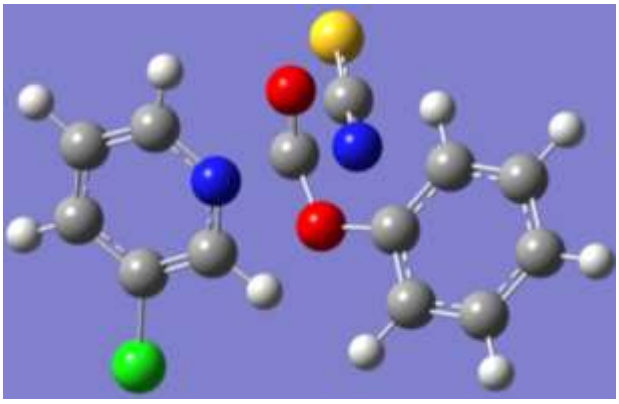
tssfD42.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.015297	0.355502	0.937800
2	8	0	0.274185	0.985085	1.934073
3	8	0	0.660571	-0.749812	0.478890
4	6	0	2.036728	-0.710770	0.292184
5	6	0	2.602696	-1.919267	-0.109368
6	6	0	2.827263	0.421689	0.456647
7	6	0	3.970271	-1.992848	-0.343792
8	1	0	1.965344	-2.785535	-0.237946
9	6	0	4.198274	0.324912	0.211757
10	1	0	2.394202	1.359458	0.767440
11	6	0	4.795981	-0.872372	-0.186184
12	1	0	4.401465	-2.937311	-0.657573
13	1	0	4.811042	1.211082	0.336797
14	7	0	-0.002462	1.410922	-0.519556
15	6	0	-0.704181	2.351033	-0.716763
16	16	0	-1.653771	3.618065	-1.003465
17	6	0	-2.357224	0.374123	1.751867
18	6	0	-1.925800	-0.850309	-0.212937
19	6	0	-3.704377	0.065356	1.681013
20	1	0	-1.906620	0.979768	2.523966
21	6	0	-3.263953	-1.178556	-0.316906
22	1	0	-1.174866	-1.165736	-0.919361
23	6	0	-4.172833	-0.721295	0.637032
24	1	0	-4.376728	0.441164	2.438866
25	1	0	-5.221407	-0.974623	0.557738
26	7	0	-1.513967	-0.090433	0.818162
27	6	0	6.283081	-0.967976	-0.417158
28	1	0	6.784194	-1.428650	0.440594
29	1	0	6.509361	-1.581255	-1.292724
30	1	0	6.724500	0.019038	-0.566902
31	17	0	-3.792231	-2.160069	-1.650006

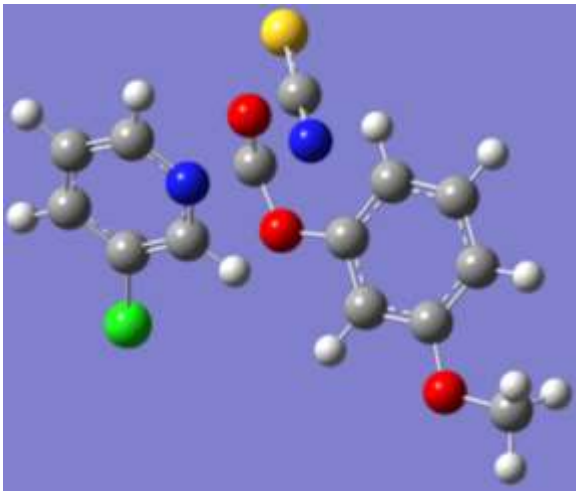
tssfD43.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.376135	0.258264	0.884251
2	8	0	0.750978	0.869422	1.862514
3	8	0	0.958252	-0.891264	0.402247
4	6	0	2.325796	-0.951908	0.176331
5	6	0	2.794032	-2.212849	-0.190047
6	6	0	3.189919	0.135992	0.274841
7	6	0	4.146888	-2.388840	-0.461024
8	1	0	2.094190	-3.036359	-0.259392
9	6	0	4.543843	-0.058235	-0.003126
10	1	0	2.823595	1.108661	0.562613
11	6	0	5.029285	-1.311425	-0.368793
12	1	0	4.509780	-3.369513	-0.744854
13	1	0	5.219934	0.785393	0.071290
14	1	0	6.082794	-1.448739	-0.579631
15	7	0	0.397822	1.307990	-0.587497
16	6	0	-0.175458	2.342065	-0.718068
17	16	0	-0.949487	3.739508	-0.912450
18	6	0	-1.921210	0.438527	1.790498
19	6	0	-1.652136	-0.809261	-0.189255
20	6	0	-3.287970	0.222810	1.772624
21	1	0	-1.400489	1.010766	2.543670
22	6	0	-3.012413	-1.045944	-0.239403
23	1	0	-0.953055	-1.173309	-0.924845
24	6	0	-3.849686	-0.528539	0.748693
25	1	0	-3.902698	0.642156	2.556121
26	1	0	-4.915361	-0.709938	0.710975
27	7	0	-1.149137	-0.080587	0.824036
28	17	0	-3.658246	-1.988820	-1.548023

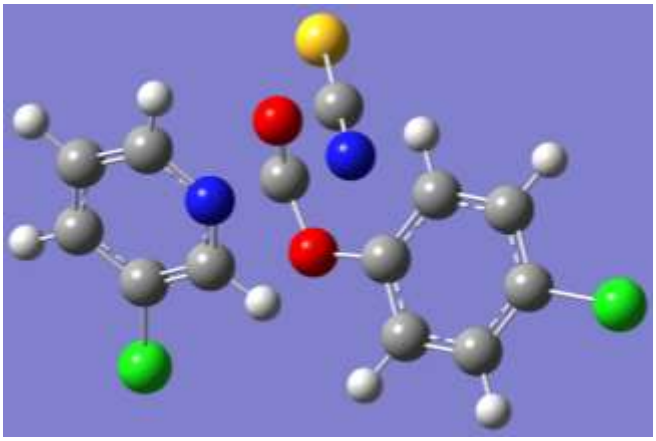
tssfD44.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.389095	0.626963	0.965373
2	8	0	-0.296860	1.395225	1.898510
3	8	0	0.539204	-0.332118	0.634994
4	6	0	1.874041	0.000467	0.457461
5	6	0	2.688054	-1.080938	0.149207
6	6	0	2.385435	1.295132	0.556513
7	6	0	4.053173	-0.878437	-0.067188
8	1	0	2.268179	-2.075516	0.073383
9	6	0	3.747513	1.473479	0.332301
10	1	0	1.749080	2.129848	0.801084
11	6	0	4.593165	0.408751	0.023223
12	1	0	4.164073	2.471318	0.402925
13	1	0	5.645471	0.589562	-0.140664
14	7	0	-0.536763	1.524561	-0.602192
15	6	0	-1.406390	2.279152	-0.900005
16	16	0	-2.581538	3.295829	-1.321345
17	6	0	-2.717800	0.197922	1.691992
18	6	0	-1.917203	-1.072135	-0.123299
19	6	0	-3.958994	-0.407824	1.603306
20	1	0	-2.455796	0.955924	2.414953
21	6	0	-3.142961	-1.698342	-0.241419
22	1	0	-1.076801	-1.274814	-0.767492
23	6	0	-4.183255	-1.369906	0.627395
24	1	0	-4.740004	-0.124073	2.294007
25	1	0	-5.144784	-1.856627	0.535070
26	7	0	-1.741019	-0.149760	0.840653
27	8	0	4.773812	-1.996624	-0.361814
28	6	0	6.177293	-1.854559	-0.591614
29	1	0	6.682353	-1.458851	0.293825
30	1	0	6.544836	-2.856019	-0.803893
31	1	0	6.371591	-1.203680	-1.448466
32	17	0	-3.366181	-2.890445	-1.485336

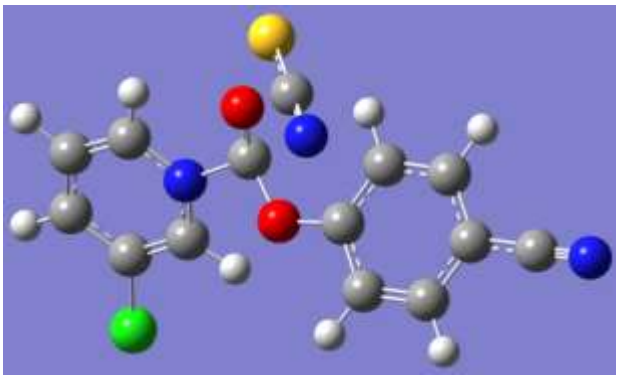
tssfD45.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.347589	0.391628	0.947422
2	8	0	-0.081226	1.062459	1.920827
3	8	0	0.380642	-0.694207	0.514775
4	6	0	1.747339	-0.596009	0.324401
5	6	0	2.366699	-1.787631	-0.048464
6	6	0	2.482658	0.578472	0.464456
7	6	0	3.735669	-1.813555	-0.284988
8	1	0	1.771628	-2.685826	-0.152984
9	6	0	3.855593	0.551424	0.223778
10	1	0	2.006750	1.500492	0.757669
11	6	0	4.468008	-0.638655	-0.146083
12	1	0	4.222555	-2.735405	-0.573862
13	1	0	4.437678	1.457458	0.328168
14	7	0	-0.363246	1.413581	-0.558682
15	6	0	-1.108520	2.316288	-0.770793
16	16	0	-2.120513	3.530835	-1.072523
17	6	0	-2.689512	0.360967	1.736139
18	6	0	-2.191391	-0.921503	-0.176927
19	6	0	-4.023832	0.002968	1.661237
20	1	0	-2.270520	1.010157	2.490244
21	6	0	-3.515660	-1.300556	-0.282057
22	1	0	-1.422321	-1.235875	-0.863766
23	6	0	-4.451643	-0.838950	0.643284
24	1	0	-4.718030	0.383916	2.396424
25	1	0	-5.489746	-1.131613	0.561875
26	7	0	-1.818428	-0.109228	0.829784
27	17	0	6.205704	-0.662903	-0.443950
28	17	0	-3.992692	-2.350671	-1.581089

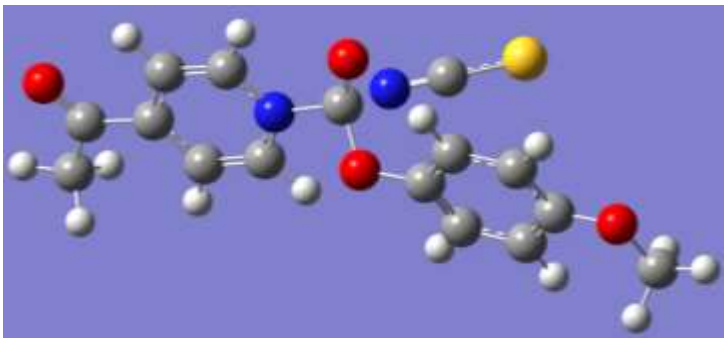
tssfD46.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.219353	0.365749	0.965194
2	8	0	0.057375	1.030113	1.936895
3	8	0	0.506067	-0.721815	0.519942
4	6	0	1.866124	-0.635541	0.335401
5	6	0	2.474605	-1.836863	-0.034122
6	6	0	2.609157	0.536838	0.476680
7	6	0	3.838529	-1.873643	-0.265537
8	1	0	1.868024	-2.727050	-0.137067
9	6	0	3.976884	0.496374	0.240690
10	1	0	2.136184	1.461177	0.765808
11	6	0	4.600460	-0.702419	-0.129392
12	1	0	4.315736	-2.801708	-0.551420
13	1	0	4.563690	1.399605	0.345250
14	7	0	-0.210224	1.406624	-0.560759
15	6	0	-0.960471	2.307942	-0.760742
16	16	0	-1.983833	3.518886	-1.041352
17	6	0	-2.561229	0.377905	1.726901
18	6	0	-2.062394	-0.913410	-0.182020
19	6	0	-3.900391	0.044440	1.634170
20	1	0	-2.141186	1.019026	2.487062
21	6	0	-3.391827	-1.267532	-0.303629
22	1	0	-1.291643	-1.241068	-0.860497
23	6	0	-4.330678	-0.788807	0.610250
24	1	0	-4.596602	0.438077	2.360659
25	1	0	-5.372959	-1.061866	0.515368
26	7	0	-1.686723	-0.108385	0.830777
27	6	0	6.006495	-0.732780	-0.366598
28	7	0	7.146733	-0.757795	-0.559186
29	17	0	-3.871937	-2.307770	-1.608725

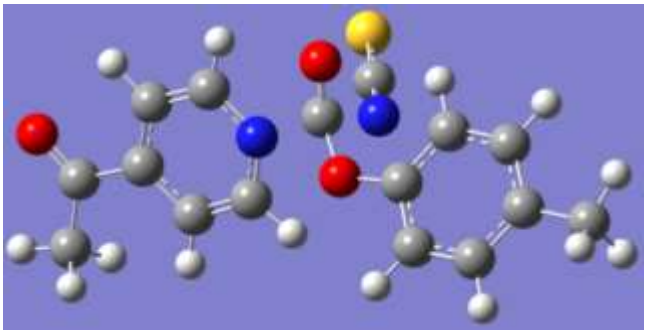
tssfD51.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.246142	0.025769	0.943093
2	8	0	-0.055028	0.406161	2.078774
3	8	0	0.405180	-1.039211	0.340323
4	6	0	1.800812	-1.010456	0.303918
5	6	0	2.571707	-0.934966	1.462969
6	6	0	2.399936	-1.099480	-0.942629
7	6	0	3.954825	-0.926380	1.356031
8	1	0	2.093464	-0.872748	2.429546
9	6	0	3.789829	-1.103691	-1.052408
10	1	0	1.780211	-1.153885	-1.828578
11	6	0	4.572380	-1.005841	0.101367
12	1	0	4.575310	-0.862058	2.241354
13	1	0	4.240642	-1.170249	-2.032078
14	7	0	0.089494	1.359672	-0.245709
15	6	0	1.104559	1.970733	-0.346285
16	16	0	2.450035	2.845557	-0.512204
17	6	0	-2.662118	0.000930	1.471043
18	6	0	-2.043101	-0.543895	-0.730234
19	6	0	-3.998050	-0.156685	1.163026
20	1	0	-2.288943	0.286551	2.443502
21	6	0	-3.366162	-0.711978	-1.089169
22	1	0	-1.219409	-0.668871	-1.414467
23	6	0	-4.366878	-0.516509	-0.133902
24	1	0	-4.751221	0.001223	1.921372
25	1	0	-3.591518	-0.987804	-2.108616
26	7	0	-1.725400	-0.197916	0.529160
27	8	0	5.935527	-0.986596	0.105580
28	6	0	6.614858	-1.048125	-1.149628
29	1	0	6.347439	-0.197414	-1.782728
30	1	0	7.676172	-1.008494	-0.914810
31	1	0	6.390429	-1.981831	-1.672975
32	6	0	-5.841245	-0.674509	-0.452266
33	8	0	-6.652154	-0.520236	0.439020
34	6	0	-6.237864	-1.013925	-1.860306
35	1	0	-5.863176	-0.258406	-2.556401
36	1	0	-5.805927	-1.974072	-2.156901
37	1	0	-7.322318	-1.067679	-1.926806

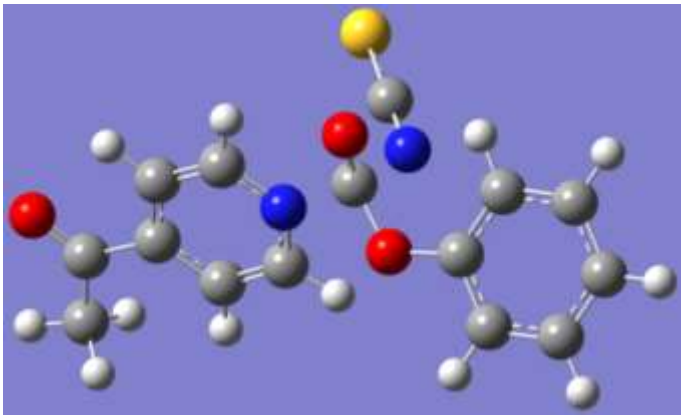
tssfD52.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.377332	0.300380	0.698325
2	8	0	0.612600	0.937248	1.706077
3	8	0	1.037472	-0.848447	0.324183
4	6	0	2.420766	-0.864563	0.207961
5	6	0	2.953805	-2.083370	-0.209244
6	6	0	3.252513	0.219671	0.466573
7	6	0	4.327561	-2.214708	-0.367483
8	1	0	2.285988	-2.913491	-0.404642
9	6	0	4.629901	0.065962	0.295166
10	1	0	2.846268	1.161939	0.799261
11	6	0	5.193563	-1.141054	-0.121309
12	1	0	4.732570	-3.168133	-0.689252
13	1	0	5.275154	0.913787	0.498142
14	7	0	0.566458	1.313306	-0.765278
15	6	0	-0.043800	2.300619	-1.026452
16	16	0	-0.865763	3.632459	-1.398159
17	6	0	-2.021576	0.473356	1.292746
18	6	0	-1.491605	-0.861462	-0.568965
19	6	0	-3.368844	0.231876	1.115730
20	1	0	-1.608806	1.091242	2.076576
21	6	0	-2.827565	-1.135698	-0.785413
22	1	0	-0.697079	-1.244263	-1.189382
23	6	0	-3.789460	-0.585281	0.065983
24	1	0	-4.090996	0.672861	1.787559
25	1	0	-3.094294	-1.772054	-1.616179
26	7	0	-1.122310	-0.076596	0.459612
27	6	0	6.681566	-1.287967	-0.316715
28	1	0	7.053011	-2.206934	0.144103
29	1	0	6.935368	-1.333607	-1.380695
30	1	0	7.222168	-0.445584	0.118359
31	6	0	-5.273869	-0.837773	-0.108567
32	8	0	-6.051977	-0.316216	0.665188
33	6	0	-5.721190	-1.724932	-1.234812
34	1	0	-5.403933	-1.309878	-2.195724
35	1	0	-5.269729	-2.716686	-1.142697
36	1	0	-6.805254	-1.813299	-1.216499

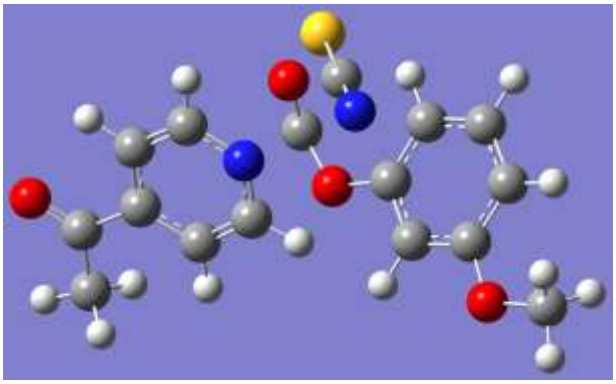
tssfD53.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.742675	0.056918	0.784778
2	8	0	1.012364	0.507077	1.879805
3	8	0	1.346888	-1.044030	0.217909
4	6	0	2.725526	-1.109336	0.087528
5	6	0	3.191441	-2.272359	-0.524595
6	6	0	3.606885	-0.115586	0.507590
7	6	0	4.557831	-2.444597	-0.718829
8	1	0	2.478613	-3.023207	-0.842300
9	6	0	4.974394	-0.303043	0.300293
10	1	0	3.242239	0.779180	0.986809
11	6	0	5.456981	-1.459349	-0.307840
12	1	0	4.918177	-3.348972	-1.194508
13	1	0	5.663549	0.468240	0.623727
14	1	0	6.521011	-1.592999	-0.460155
15	7	0	0.983557	1.291242	-0.499751
16	6	0	0.407457	2.328010	-0.593006
17	16	0	-0.371076	3.728447	-0.736437
18	6	0	-1.642432	0.265820	1.410789
19	6	0	-1.178958	-0.793283	-0.637191
20	6	0	-3.000046	0.129207	1.204311
21	1	0	-1.199968	0.731844	2.278830
22	6	0	-2.526995	-0.958052	-0.886522
23	1	0	-0.404363	-1.118085	-1.313238
24	6	0	-3.460668	-0.493190	0.043635
25	1	0	-3.699600	0.500710	1.939104
26	1	0	-2.824529	-1.444197	-1.803687
27	7	0	-0.771084	-0.197878	0.498651
28	6	0	-4.956128	-0.634942	-0.160036
29	6	0	-5.447694	-1.336869	-1.393452
30	1	0	-6.535088	-1.365914	-1.382997
31	1	0	-5.104598	-0.815589	-2.291663
32	1	0	-5.053070	-2.355904	-1.436432
33	8	0	-5.707219	-0.178589	0.678853

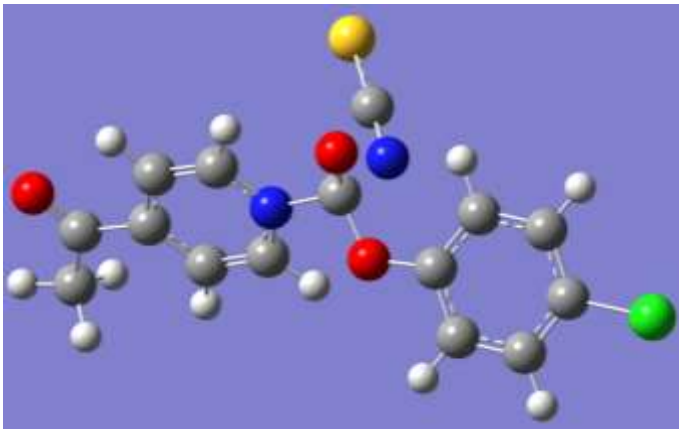
tssfD54.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.071042	0.537898	0.806628
2	8	0	0.203188	1.118394	1.864588
3	8	0	0.915403	-0.447104	0.340377
4	6	0	2.287079	-0.248350	0.312656
5	6	0	3.014858	-1.374770	-0.046969
6	6	0	2.914583	0.966370	0.593704
7	6	0	4.407342	-1.300696	-0.130410
8	1	0	2.507231	-2.306002	-0.262334
9	6	0	4.302326	1.017370	0.501274
10	1	0	2.345585	1.836859	0.876126
11	6	0	5.062470	-0.096037	0.145029
12	1	0	4.807965	1.951774	0.714516
13	1	0	6.138096	-0.015045	0.087667
14	7	0	0.077069	1.691809	-0.568167
15	6	0	-0.739166	2.526982	-0.795825
16	16	0	-1.842396	3.650632	-1.124541
17	6	0	-2.311704	0.234042	1.403298
18	6	0	-1.583626	-0.795502	-0.581560
19	6	0	-3.600033	-0.214504	1.194159
20	1	0	-2.002014	0.831327	2.248179
21	6	0	-2.856987	-1.264697	-0.836027
22	1	0	-0.742423	-0.974312	-1.232110
23	6	0	-3.888903	-0.975240	0.061101
24	1	0	-4.378489	0.025095	1.904036
25	1	0	-3.020527	-1.846291	-1.731340
26	7	0	-1.341536	-0.066680	0.523617
27	8	0	5.037405	-2.455095	-0.487495
28	6	0	6.463282	-2.443979	-0.583358
29	1	0	6.919796	-2.197877	0.379295
30	1	0	6.747869	-3.452632	-0.874445
31	1	0	6.800855	-1.734260	-1.343623
32	6	0	-5.312046	-1.451546	-0.150490
33	6	0	-5.639358	-2.185441	-1.418951
34	1	0	-6.701338	-2.420397	-1.437139
35	1	0	-5.379770	-1.578237	-2.290442
36	1	0	-5.060413	-3.111360	-1.481827
37	8	0	-6.140146	-1.222932	0.708665

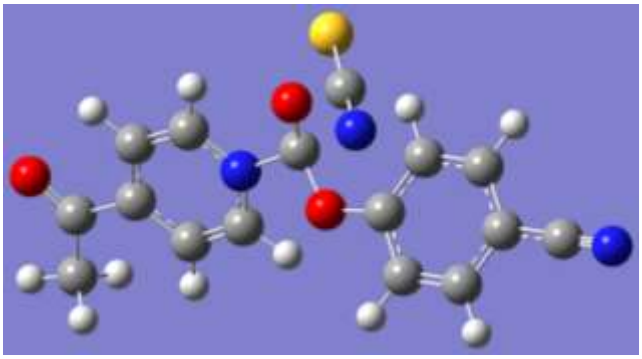
tssfD55.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.035985	0.232225	0.793945
2	8	0	0.259369	0.719645	1.882273
3	8	0	0.753340	-0.806766	0.238069
4	6	0	2.130342	-0.738056	0.137050
5	6	0	2.725956	-1.865823	-0.425798
6	6	0	2.900543	0.351757	0.536504
7	6	0	4.104338	-1.912226	-0.593954
8	1	0	2.104729	-2.698182	-0.730926
9	6	0	4.283203	0.305082	0.363673
10	1	0	2.443029	1.222722	0.977718
11	6	0	4.871107	-0.821339	-0.196341
12	1	0	4.572189	-2.784602	-1.030230
13	1	0	4.891787	1.146048	0.668734
14	7	0	0.168261	1.477426	-0.513945
15	6	0	-0.493730	2.461757	-0.605528
16	16	0	-1.387823	3.792037	-0.746220
17	6	0	-2.354158	0.198609	1.413303
18	6	0	-1.778310	-0.798024	-0.638795
19	6	0	-3.689467	-0.077364	1.201963
20	1	0	-1.964972	0.703978	2.284733
21	6	0	-3.101474	-1.098540	-0.893060
22	1	0	-0.973026	-1.038131	-1.314330
23	6	0	-4.080340	-0.737704	0.036801
24	1	0	-4.425414	0.216189	1.936467
25	1	0	-3.345538	-1.606908	-1.814085
26	7	0	-1.436942	-0.169020	0.501557
27	17	0	6.621060	-0.872124	-0.407285
28	6	0	-5.552746	-1.031758	-0.173182
29	6	0	-5.967380	-1.744126	-1.428429
30	1	0	-5.680557	-1.161725	-2.308703
31	1	0	-5.466437	-2.713507	-1.501124
32	1	0	-7.045502	-1.888751	-1.422795
33	8	0	-6.346648	-0.682398	0.677402

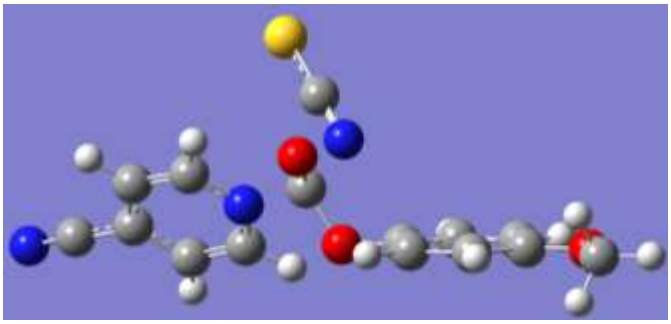
tssfD56.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.169439	0.196708	0.803736
2	8	0	0.405376	0.697332	1.880296
3	8	0	0.885903	-0.849677	0.251044
4	6	0	2.256163	-0.796718	0.161712
5	6	0	2.845087	-1.954165	-0.352453
6	6	0	3.030252	0.306068	0.525133
7	6	0	4.218802	-2.016509	-0.506869
8	1	0	2.215370	-2.790312	-0.626967
9	6	0	4.408064	0.240595	0.365970
10	1	0	2.572460	1.195935	0.925443
11	6	0	5.011518	-0.914958	-0.147536
12	1	0	4.680411	-2.910644	-0.904561
13	1	0	5.018467	1.090300	0.642715
14	7	0	0.319786	1.439723	-0.541765
15	6	0	-0.349415	2.419060	-0.634302
16	16	0	-1.257848	3.740695	-0.772175
17	6	0	-2.215002	0.214359	1.410462
18	6	0	-1.642971	-0.827807	-0.621920
19	6	0	-3.552950	-0.042483	1.194398
20	1	0	-1.823939	0.728101	2.275929
21	6	0	-2.969271	-1.109937	-0.878701
22	1	0	-0.838627	-1.092330	-1.289183
23	6	0	-3.947655	-0.716284	0.038319
24	1	0	-4.288363	0.276491	1.918747
25	1	0	-3.216136	-1.629932	-1.792419
26	7	0	-1.297656	-0.185068	0.510674
27	6	0	6.427853	-0.972800	-0.304120
28	7	0	7.576530	-1.020233	-0.431535
29	6	0	-5.424033	-0.988668	-0.175697
30	6	0	-5.843358	-1.718610	-1.419023
31	1	0	-5.541539	-1.158833	-2.308914
32	1	0	-5.358792	-2.697677	-1.469375
33	1	0	-6.923817	-1.844618	-1.417155
34	8	0	-6.216177	-0.608190	0.662895

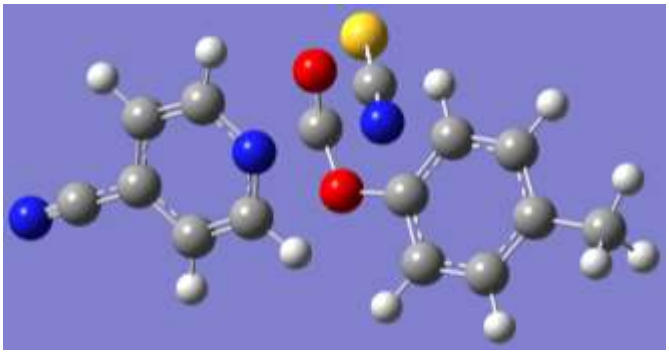
tssfD61.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.297932	0.318062	0.298341
2	8	0	-0.020073	1.217518	1.063847
3	8	0	0.411344	-0.860034	0.170356
4	6	0	1.797227	-0.737715	0.027190
5	6	0	2.351983	-0.909018	-1.237962
6	6	0	2.600883	-0.515069	1.133818
7	6	0	3.729622	-0.853522	-1.392161
8	1	0	1.703458	-1.081388	-2.086593
9	6	0	3.987419	-0.456497	0.983238
10	1	0	2.151555	-0.389865	2.109947
11	6	0	4.554763	-0.624750	-0.283397
12	1	0	4.184309	-0.986348	-2.366042
13	1	0	4.603608	-0.284753	1.854196
14	7	0	-0.332766	0.911539	-1.381450
15	6	0	-1.147370	1.640665	-1.852382
16	16	0	-2.258278	2.609485	-2.494131
17	6	0	-2.654419	0.575710	1.024740
18	6	0	-2.177160	-1.279789	-0.340174
19	6	0	-3.996063	0.247041	1.063498
20	1	0	-2.226510	1.432618	1.524534
21	6	0	-3.501435	-1.664299	-0.336949
22	1	0	-1.405716	-1.815008	-0.870281
23	6	0	-4.425622	-0.890118	0.374996
24	1	0	-4.685346	0.865949	1.618728
25	1	0	-3.805119	-2.546674	-0.880686
26	7	0	-1.787981	-0.184745	0.339383
27	8	0	5.894014	-0.587419	-0.535697
28	6	0	6.782009	-0.364609	0.560934
29	1	0	6.692709	-1.159600	1.306666
30	1	0	7.783939	-0.373016	0.137648
31	1	0	6.591165	0.604249	1.030969
32	6	0	-5.807187	-1.261331	0.391550
33	7	0	-6.920970	-1.560780	0.404363

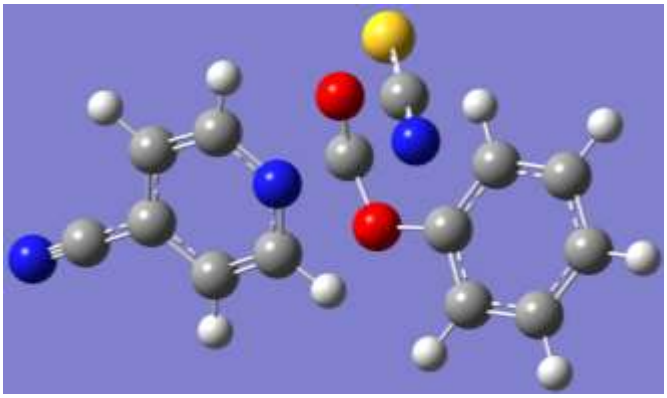
tssfD62.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000470	0.038031	0.815171
2	8	0	0.154536	0.480103	1.934087
3	8	0	0.748533	-0.958283	0.244173
4	6	0	2.132071	-0.850360	0.162909
5	6	0	2.755968	-1.896138	-0.514451
6	6	0	2.877495	0.196162	0.694403
7	6	0	4.137705	-1.892099	-0.658877
8	1	0	2.152830	-2.699571	-0.919223
9	6	0	4.264149	0.181807	0.531730
10	1	0	2.398295	1.002450	1.227388
11	6	0	4.919252	-0.850978	-0.141223
12	1	0	4.615664	-2.711538	-1.184681
13	1	0	4.843405	0.998889	0.947714
14	7	0	0.143890	1.345822	-0.422358
15	6	0	-0.572530	2.291768	-0.511926
16	16	0	-1.544851	3.566210	-0.645835
17	6	0	-2.427816	-0.023181	1.307239
18	6	0	-1.745432	-0.995622	-0.723669
19	6	0	-3.754274	-0.295039	1.032214
20	1	0	-2.085567	0.472023	2.204232
21	6	0	-3.049195	-1.298303	-1.054810
22	1	0	-0.904631	-1.226996	-1.357824
23	6	0	-4.069964	-0.944044	-0.163948
24	1	0	-4.519127	-0.006222	1.737955
25	1	0	-3.263613	-1.797105	-1.988529
26	7	0	-1.467801	-0.378620	0.440556
27	6	0	6.415928	-0.842737	-0.325139
28	1	0	6.843622	-1.830871	-0.138196
29	1	0	6.683401	-0.561514	-1.348940
30	1	0	6.893330	-0.130212	0.349846
31	6	0	-5.432813	-1.242413	-0.481186
32	7	0	-6.531342	-1.483066	-0.737344

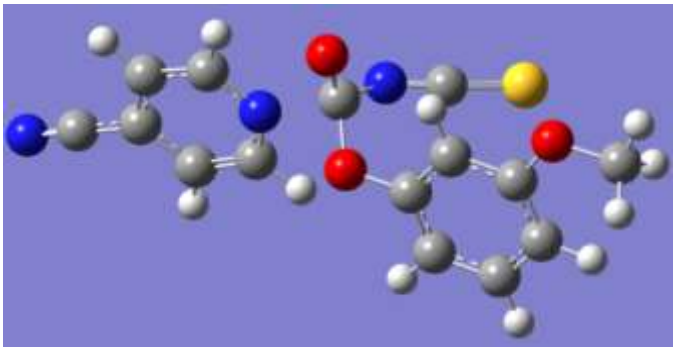
tssfD63.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.374784	-0.003982	0.747596
2	8	0	0.594349	0.439432	1.854370
3	8	0	1.049271	-1.045534	0.161722
4	6	0	2.433923	-1.033328	0.064093
5	6	0	2.975921	-2.158129	-0.555564
6	6	0	3.247383	0.000313	0.521543
7	6	0	4.353966	-2.251693	-0.718810
8	1	0	2.313194	-2.941169	-0.902484
9	6	0	4.627735	-0.108551	0.345237
10	1	0	2.822237	0.865684	1.004914
11	6	0	5.187169	-1.226105	-0.269434
12	1	0	4.774892	-3.126428	-1.200034
13	1	0	5.265474	0.693478	0.697815
14	1	0	6.260247	-1.298911	-0.397378
15	7	0	0.550266	1.285236	-0.514134
16	6	0	-0.108293	2.274515	-0.576791
17	16	0	-1.003833	3.607203	-0.673148
18	6	0	-2.031360	0.080883	1.317800
19	6	0	-1.472375	-0.952517	-0.721244
20	6	0	-3.379195	-0.119541	1.090012
21	1	0	-1.632460	0.566520	2.196363
22	6	0	-2.801261	-1.185580	-1.005023
23	1	0	-0.667702	-1.237894	-1.379744
24	6	0	-3.770281	-0.765010	-0.085600
25	1	0	-4.102622	0.219905	1.816519
26	1	0	-3.074282	-1.682741	-1.924188
27	7	0	-1.121978	-0.338497	0.425071
28	6	0	-5.157486	-0.991745	-0.352678
29	7	0	-6.275661	-1.174727	-0.568268

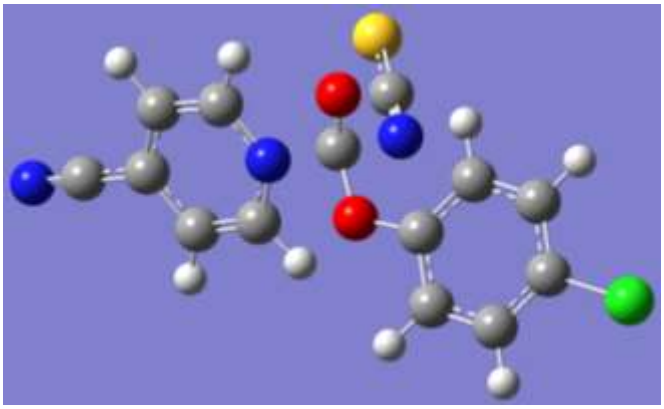
tssfD64.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.365140	0.202720	0.963750
2	8	0	-0.347428	0.193076	2.180905
3	8	0	0.323700	-0.771271	0.195525
4	6	0	1.644978	-0.482676	-0.121539
5	6	0	2.538406	-0.038825	0.842882
6	6	0	2.032616	-0.666492	-1.448401
7	6	0	3.852801	0.260836	0.467835
8	1	0	2.228472	0.098110	1.869697
9	6	0	3.346545	-0.383702	-1.798493
10	1	0	1.308693	-1.007718	-2.176501
11	6	0	4.263505	0.088435	-0.857057
12	1	0	3.666815	-0.515919	-2.825054
13	1	0	5.274958	0.312517	-1.163484
14	7	0	-0.346804	1.483465	0.256606
15	6	0	0.484478	2.245920	-0.150393
16	16	0	1.478040	3.341385	-0.713844
17	6	0	-2.929780	-0.589028	1.375983
18	6	0	-2.363797	-0.500364	-0.881008
19	6	0	-4.222138	-1.000537	1.084764
20	1	0	-2.566910	-0.438698	2.385912
21	6	0	-3.631067	-0.907234	-1.262668
22	1	0	-1.583049	-0.288857	-1.599133
23	6	0	-4.573720	-1.160763	-0.258665
24	1	0	-4.930280	-1.189673	1.878686
25	1	0	-3.877304	-1.024776	-2.308208
26	7	0	-2.048883	-0.352990	0.408070
27	8	0	4.657016	0.713694	1.468861
28	6	0	6.014046	1.034268	1.154270
29	1	0	6.066033	1.835757	0.412498
30	1	0	6.461950	1.370544	2.086601
31	1	0	6.549841	0.155022	0.786236
32	6	0	-5.895529	-1.584735	-0.608700
33	7	0	-6.960849	-1.926524	-0.890777

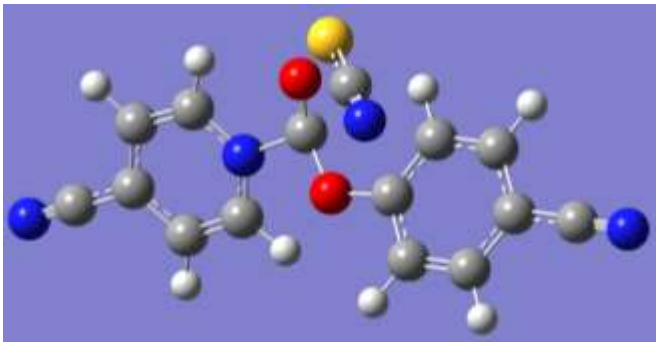
tssfD65.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.318291	0.095047	0.789685
2	8	0	-0.149775	0.545811	1.901859
3	8	0	0.460917	-0.872909	0.201360
4	6	0	1.834655	-0.724553	0.122946
5	6	0	2.494930	-1.781067	-0.501497
6	6	0	2.539089	0.376785	0.602435
7	6	0	3.875727	-1.743576	-0.651407
8	1	0	1.922509	-2.623577	-0.867917
9	6	0	3.924057	0.414660	0.447156
10	1	0	2.029669	1.191929	1.091074
11	6	0	4.577828	-0.641002	-0.174382
12	1	0	4.394965	-2.560230	-1.134814
13	1	0	4.483160	1.265257	0.813687
14	7	0	-0.238079	1.412122	-0.459419
15	6	0	-1.052649	2.272498	-0.576423
16	16	0	-2.167553	3.419151	-0.740985
17	6	0	-2.728893	-0.020712	1.315429
18	6	0	-2.046131	-1.016694	-0.705251
19	6	0	-4.051141	-0.329071	1.060577
20	1	0	-2.389620	0.500049	2.198816
21	6	0	-3.345862	-1.356064	-1.014482
22	1	0	-1.208227	-1.239710	-1.345985
23	6	0	-4.364830	-1.008536	-0.118879
24	1	0	-4.814613	-0.043741	1.769193
25	1	0	-3.558600	-1.877787	-1.935966
26	7	0	-1.769583	-0.370870	0.444497
27	17	0	6.329816	-0.584964	-0.362382
28	6	0	-5.723676	-1.343752	-0.415152
29	7	0	-6.819082	-1.613947	-0.654613

tssfD66.



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.184716	0.065500	0.790713
2	8	0	0.002158	0.497108	1.904916
3	8	0	0.590548	-0.893287	0.173009
4	6	0	1.959187	-0.767247	0.113741
5	6	0	2.611451	-1.852712	-0.474270
6	6	0	2.670131	0.341279	0.573711
7	6	0	3.988896	-1.836518	-0.606185
8	1	0	2.028131	-2.695014	-0.822423
9	6	0	4.051927	0.355011	0.436415
10	1	0	2.161636	1.174776	1.030384
11	6	0	4.719680	-0.727901	-0.150402
12	1	0	4.500622	-2.674534	-1.060619
13	1	0	4.615142	1.209820	0.787389
14	7	0	-0.094268	1.419259	-0.454429
15	6	0	-0.911325	2.281865	-0.531667
16	16	0	-2.034819	3.427648	-0.636514
17	6	0	-2.586780	-0.022708	1.319545
18	6	0	-1.919210	-0.996056	-0.719019
19	6	0	-3.912635	-0.311013	1.061627
20	1	0	-2.241020	0.479711	2.210794
21	6	0	-3.223350	-1.314025	-1.030354
22	1	0	-1.086183	-1.219058	-1.365853
23	6	0	-4.236589	-0.968600	-0.127315
24	1	0	-4.671139	-0.027119	1.776089
25	1	0	-3.443878	-1.818349	-1.959633
26	7	0	-1.632318	-0.372162	0.441406
27	6	0	6.139487	-0.704468	-0.284430
28	7	0	7.290785	-0.685789	-0.393709
29	6	0	-5.599716	-1.283510	-0.425751
30	7	0	-6.698591	-1.537552	-0.666883