Supporting Information

Structural Conformers of (1,3-Dithiol-2-ylidene)ethanethioamides: The Balance Between Thioamide Rotation and Preservation of Classical Sulfur-Sulfur Hypervalent Bonds.

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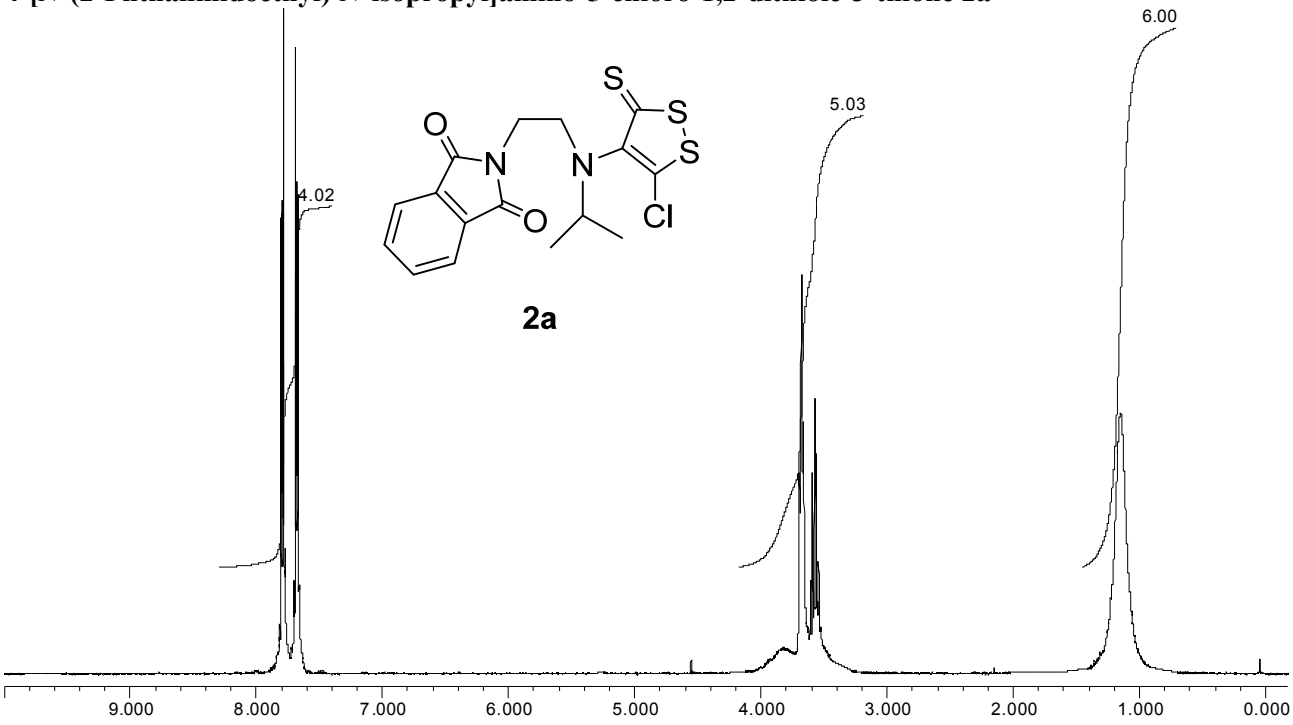
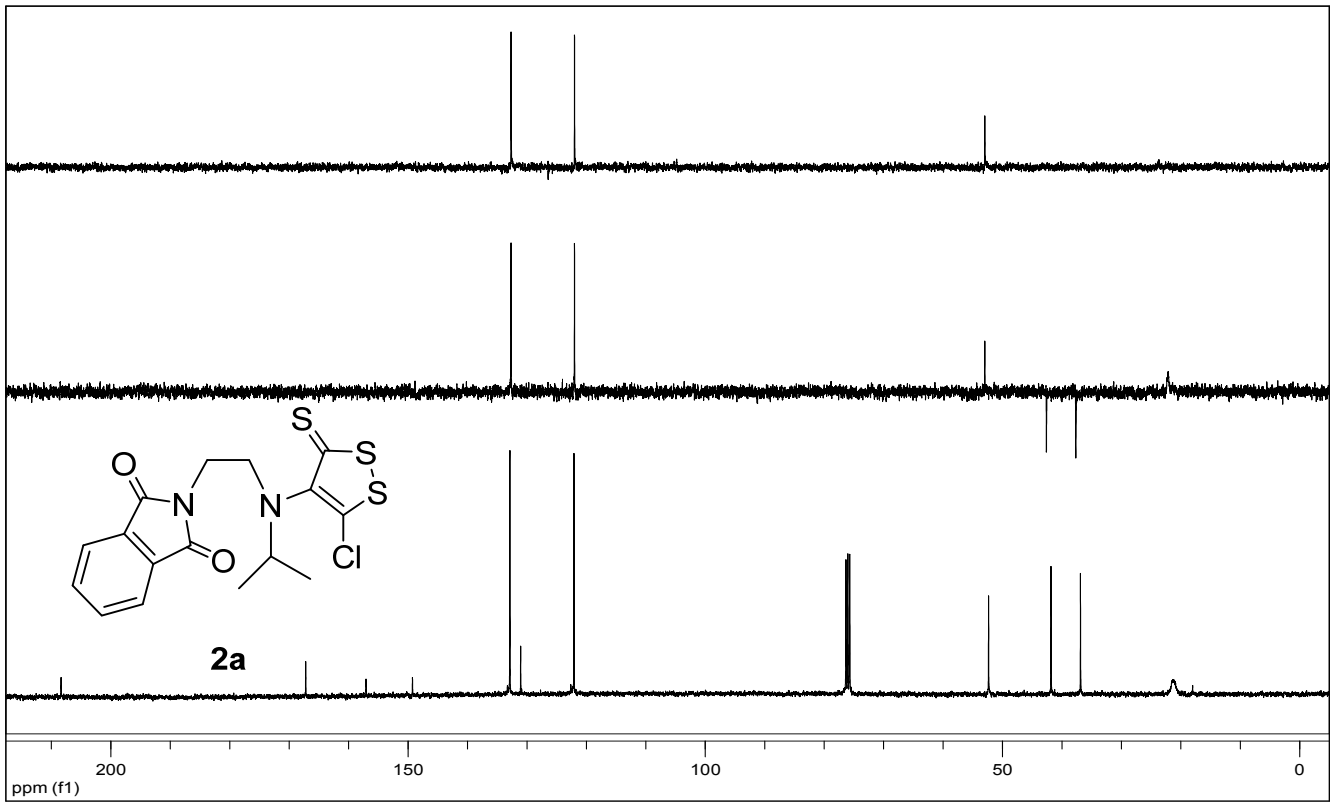
1.- Spectral description of all compounds

4-[*N*-(2-Phthalimidoethyl)-*N*-isopropyl]amino-5-chloro-1,2-dithiole-3-thione 2a

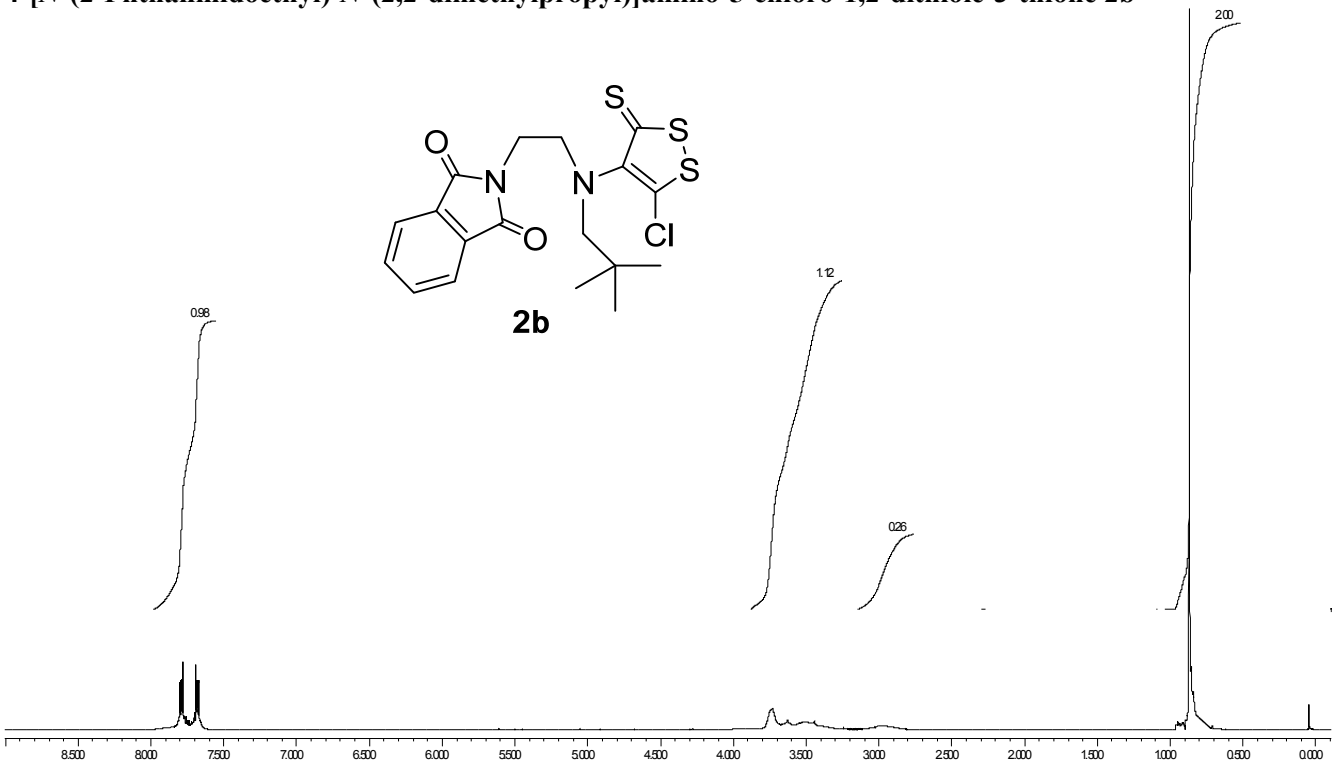


^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of 4-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-5-chloro-1,2-dithiole-3-thione 2a

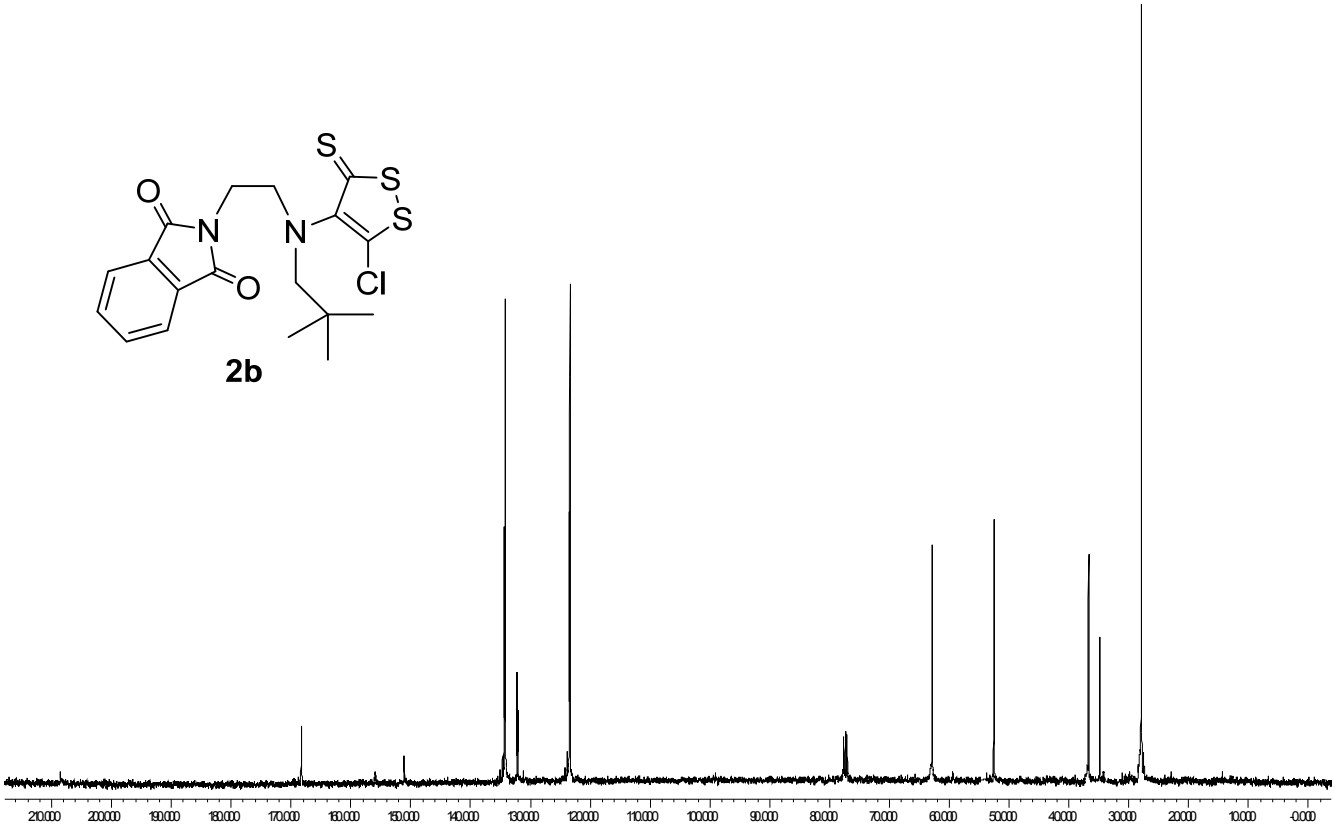


^{13}C NMR and DEPT spectra ($CDCl_3$, 100 MHz) of 4-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-5-chloro-1,2-dithiole-3-thione 2a

4-[*N*-(2-Phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-5-chloro-1,2-dithiole-3-thione 2b

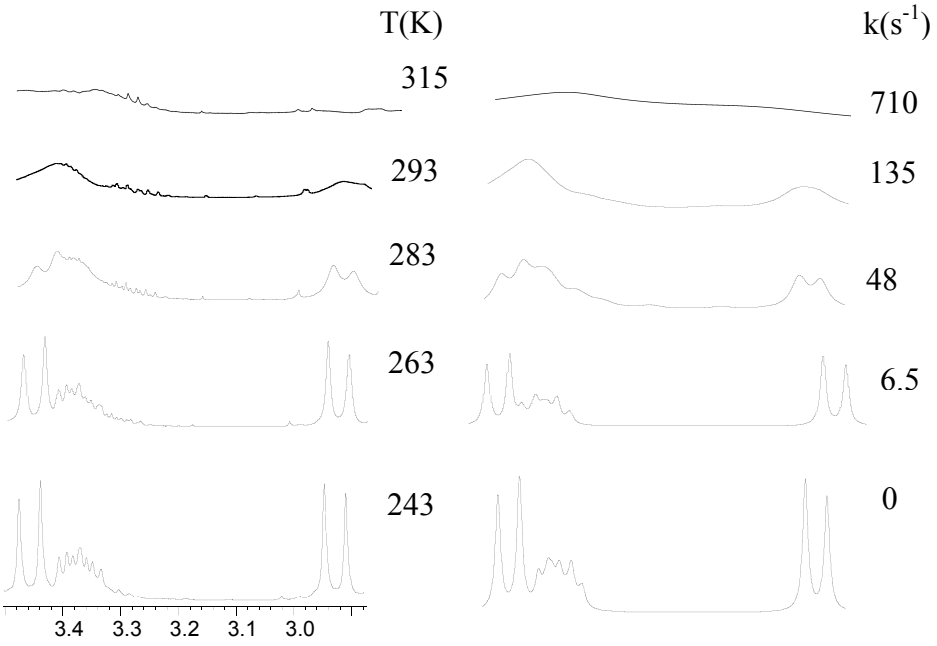


^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of 4-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-5-chloro-1,2-dithiole-3-thione 2b



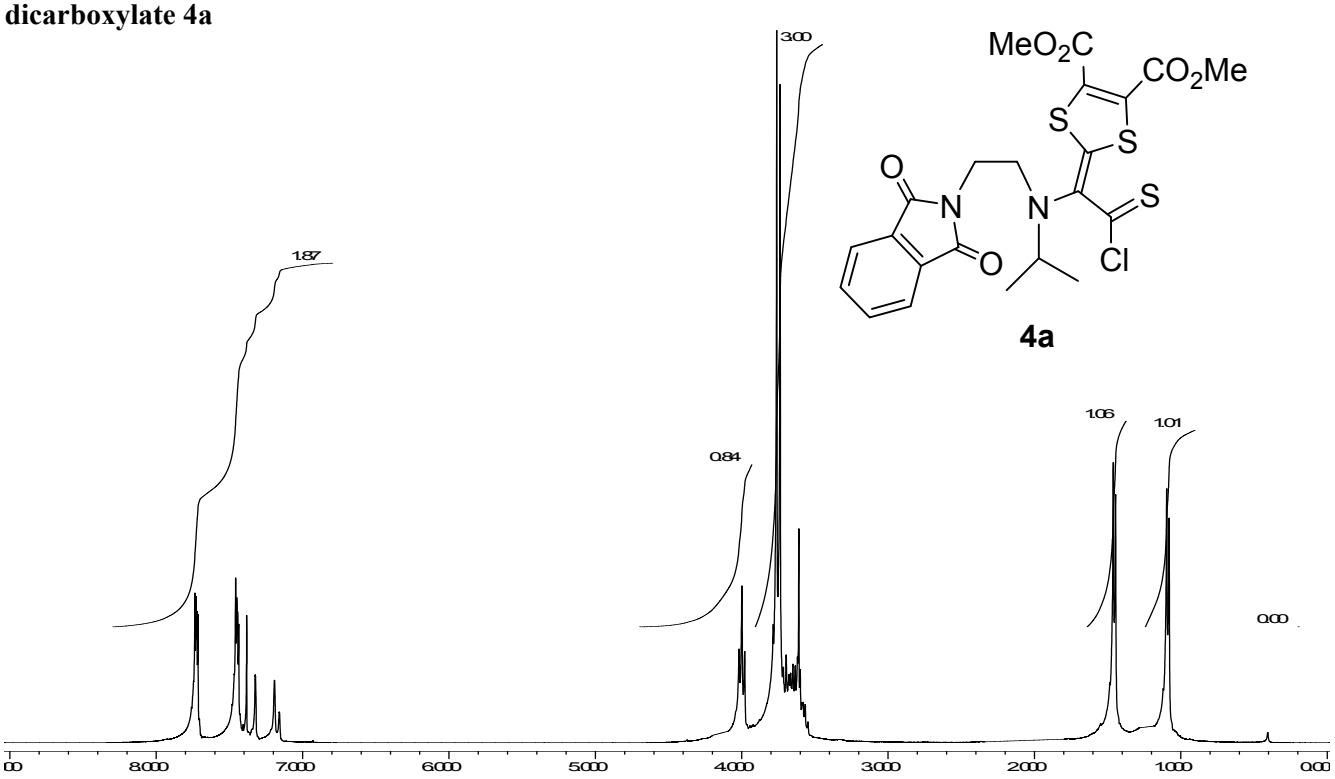
^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of 4-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-5-chloro-1,2-dithiole-3-thione 2b

Compound **2b** showed diastereomeric preferred conformations studied, in this case, by dynamic NMR of the neopentyl signals. The ^{1}H NMR spectrum of **2b** showed two broad signals at δ 2.9 and 3.4 in deuterated chloroform at room temperature, corresponding to slowly interchanging protons from the methylene group of the neopentyl group, and two protons from a methylene group of the phthalimidoethyl group. The signals were resolved in two doublets and one multiplet at –30ºC but the methylene protons from the neopentyl group only interchange at temperatures higher than 60ºC. Simulation of the signals with gNMR5.0.4.0 gave interchange constants k(s^{-1}) that were plotted as log k/T versus 1/T, giving a first order kinetics from which the free energy of transition was calculated to be $\Delta G^{\ddagger}$ = 14.54 ± 0.05 Kcal mol^{-1}. A similar value, 14.52 Kcal mol^{-1}, was obtained from the Eyring equation at the coalescence temperature T_c = 313 K (See next Figure). This energy was ascribed to a slow inversion-rotation process that places the phtalimidoethyl group in a diastereotopic environment.

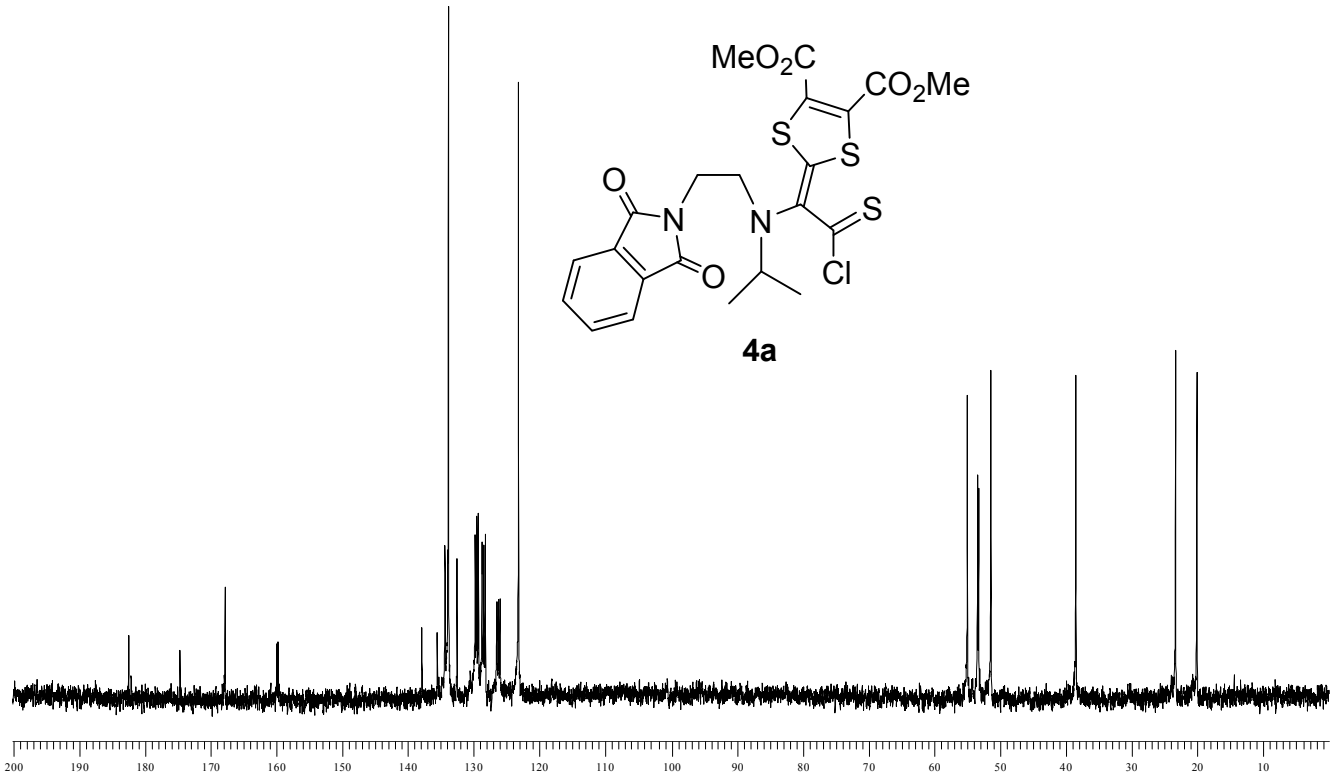


Dynamic NMR signals, simulation of the signals and interchange constants k(s^{-1}) of **2b**

Dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4a

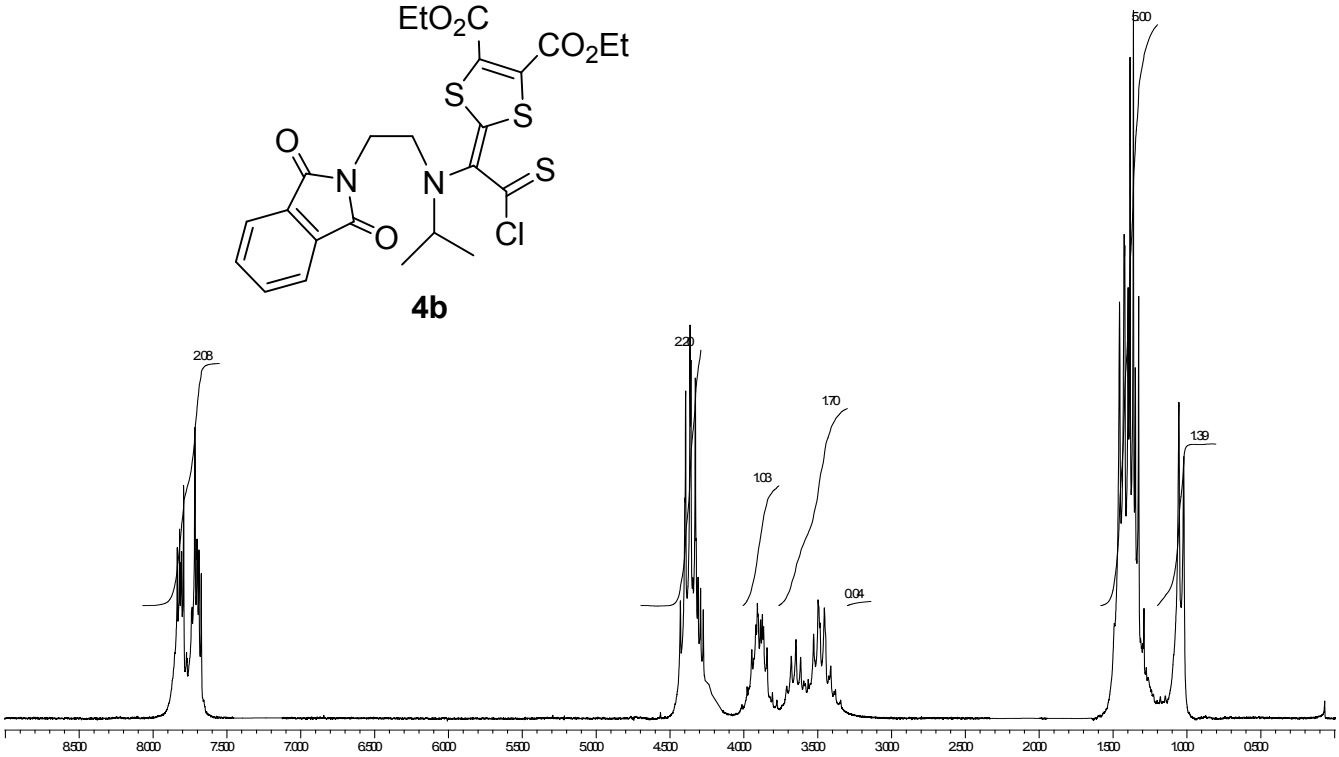


^{1}H NMR spectrum (C_6D_5Cl, 400 MHz) of dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4a

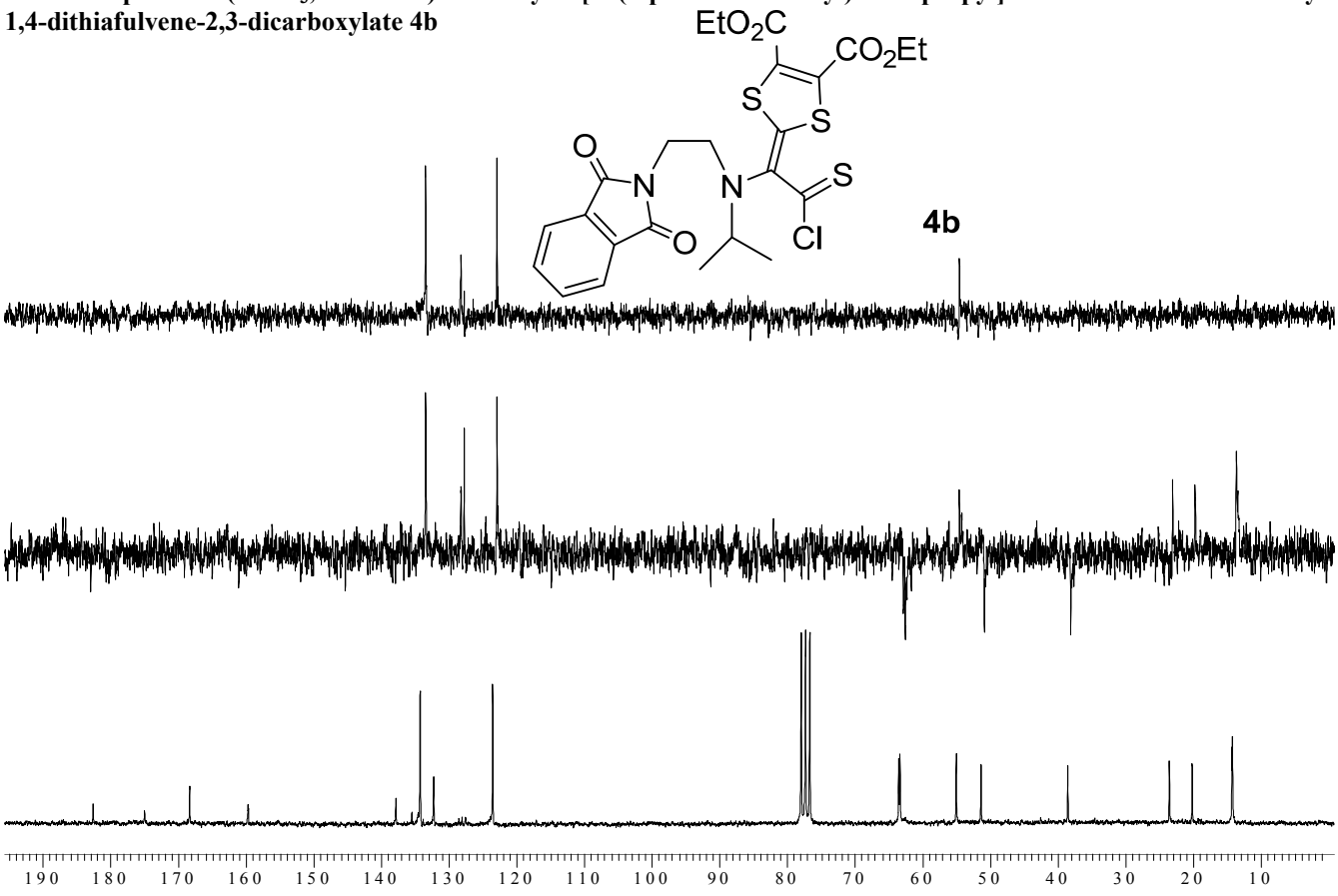


^{13}C NMR spectrum (C_6D_5Cl, 100 MHz) of dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4a

Diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4b

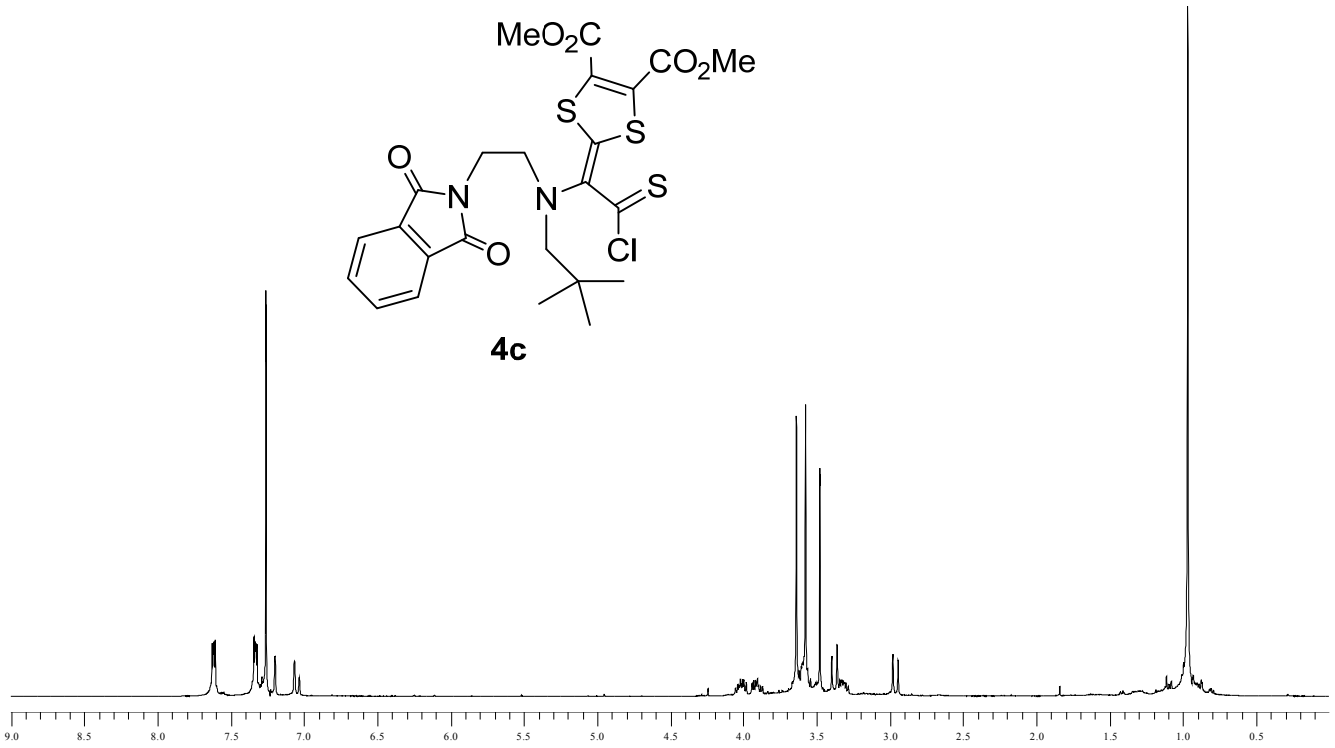


^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4b

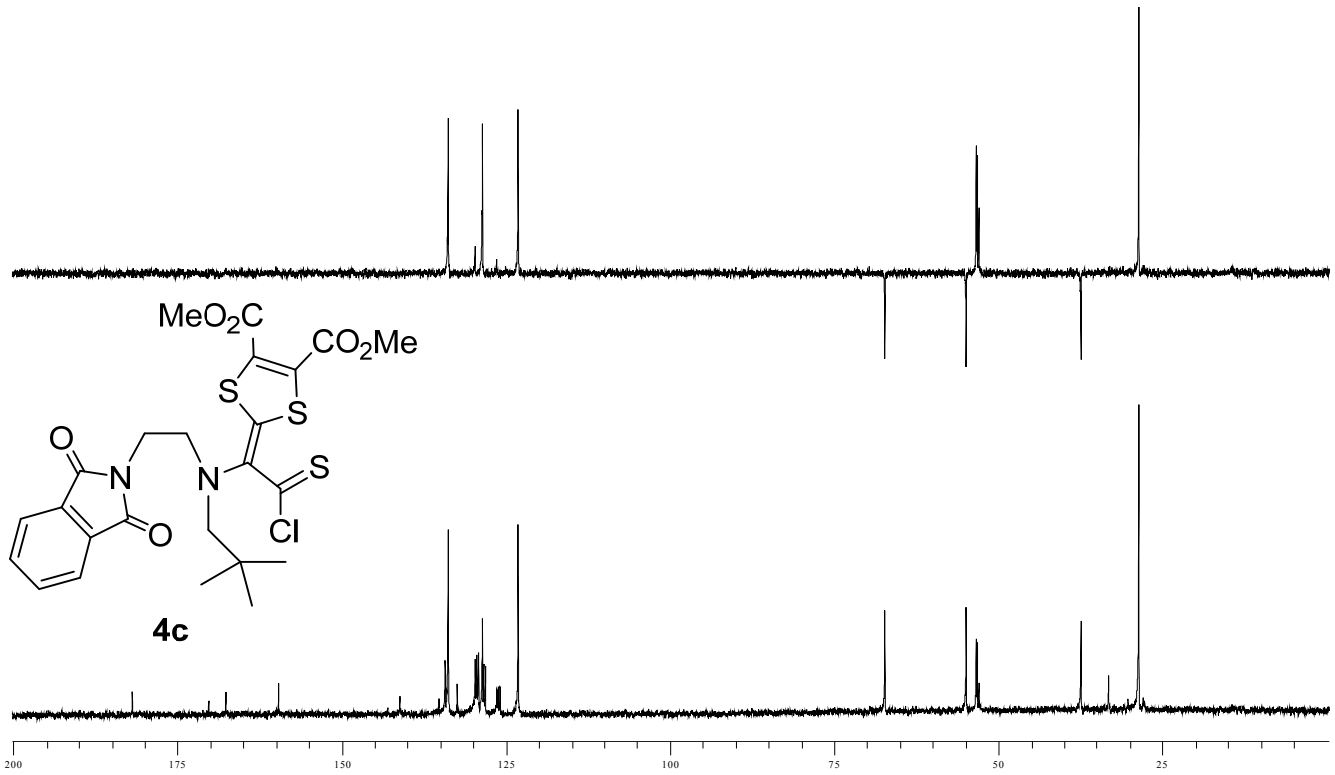


^{13}C NMR and DEPT spectra ($CDCl_3$, 100 MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4b

Dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4c

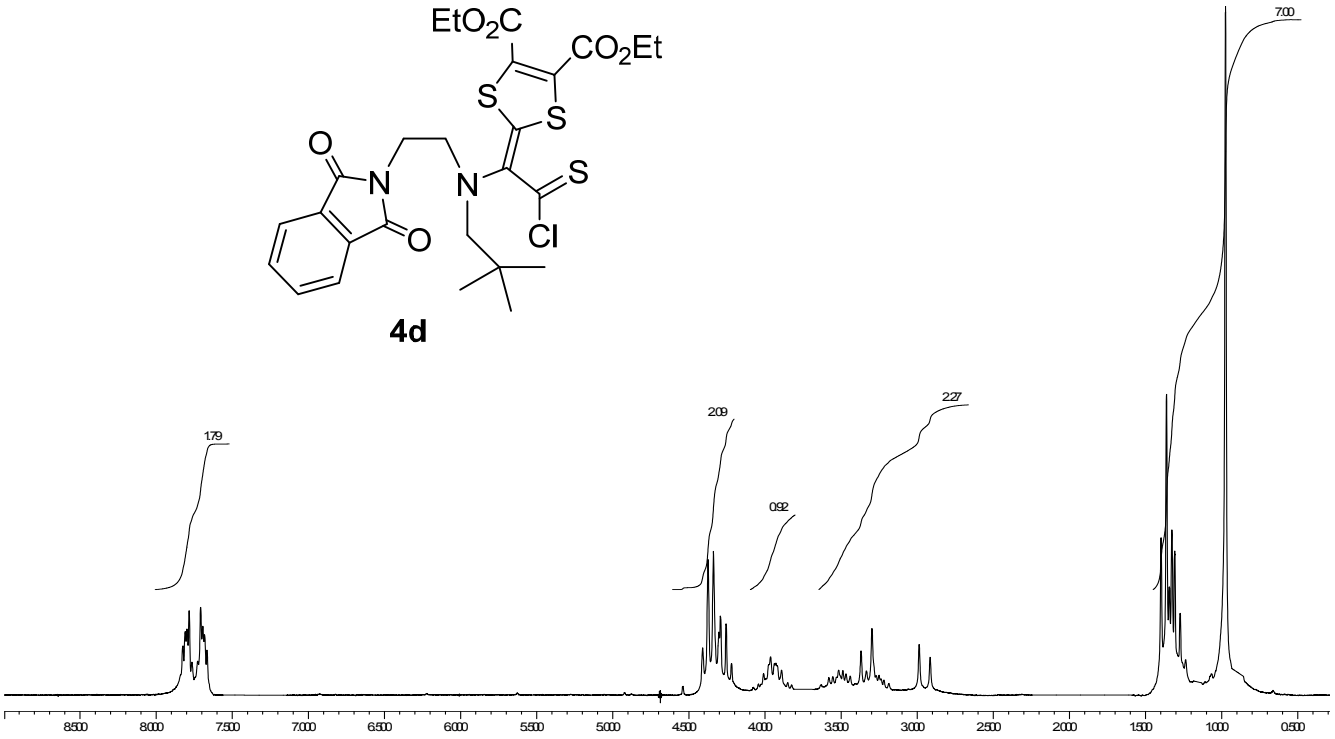


^{1}H NMR spectrum (C_6D_5Cl, 400 MHz) of dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4c

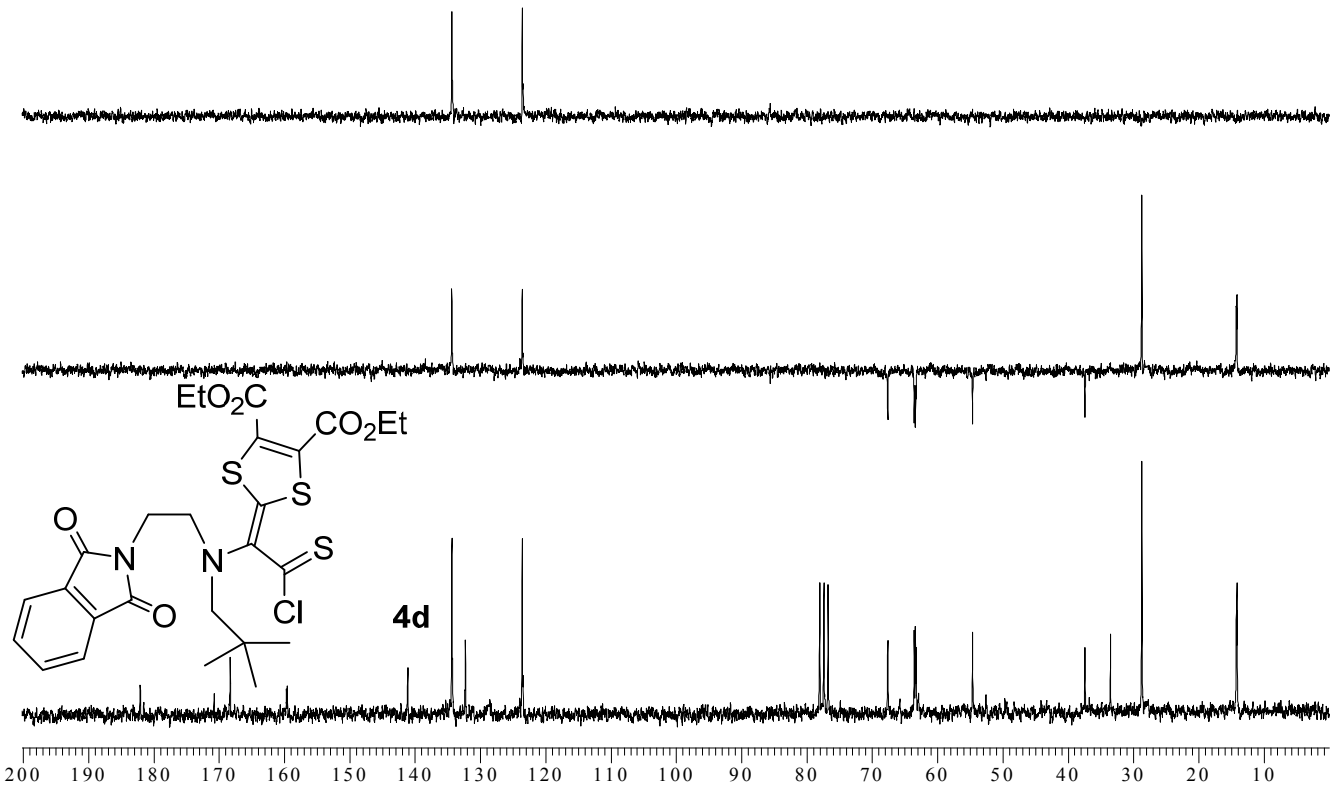


^{13}C NMR and DEPT spectra (C_6D_5Cl, 100 MHz) of dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4c

Diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4d

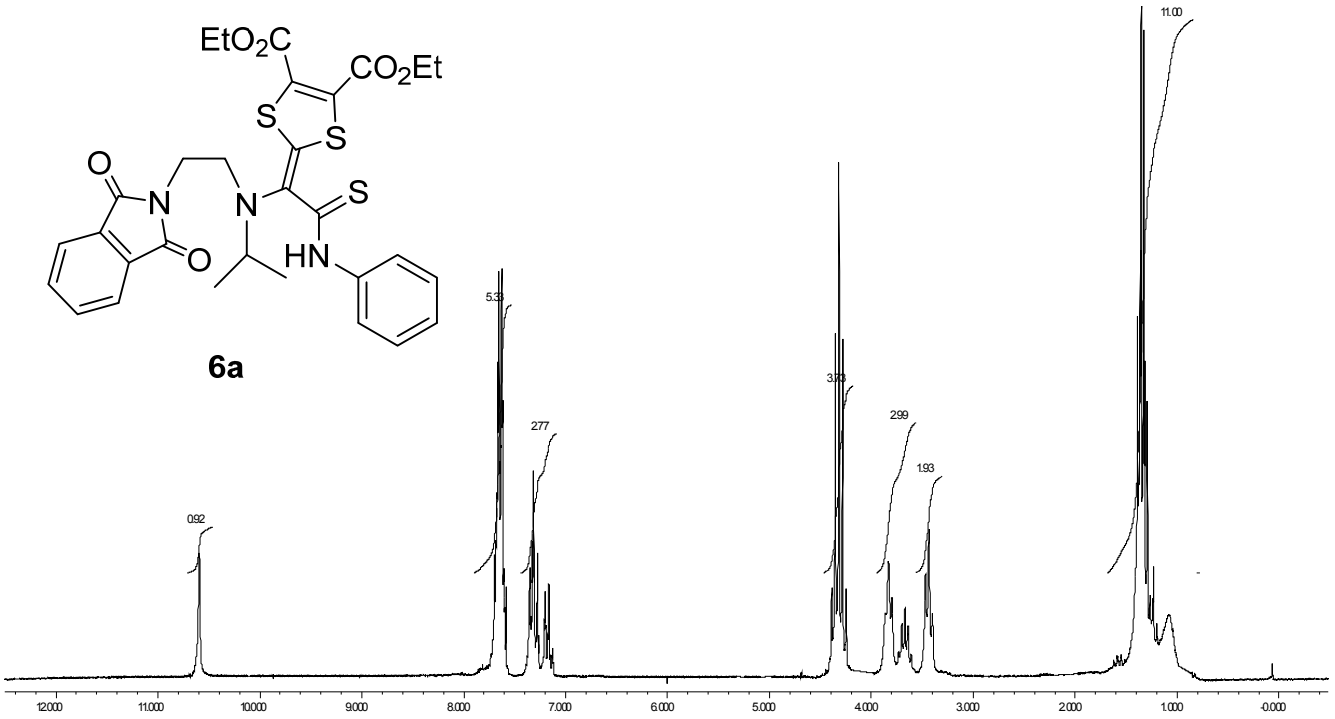


^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4d

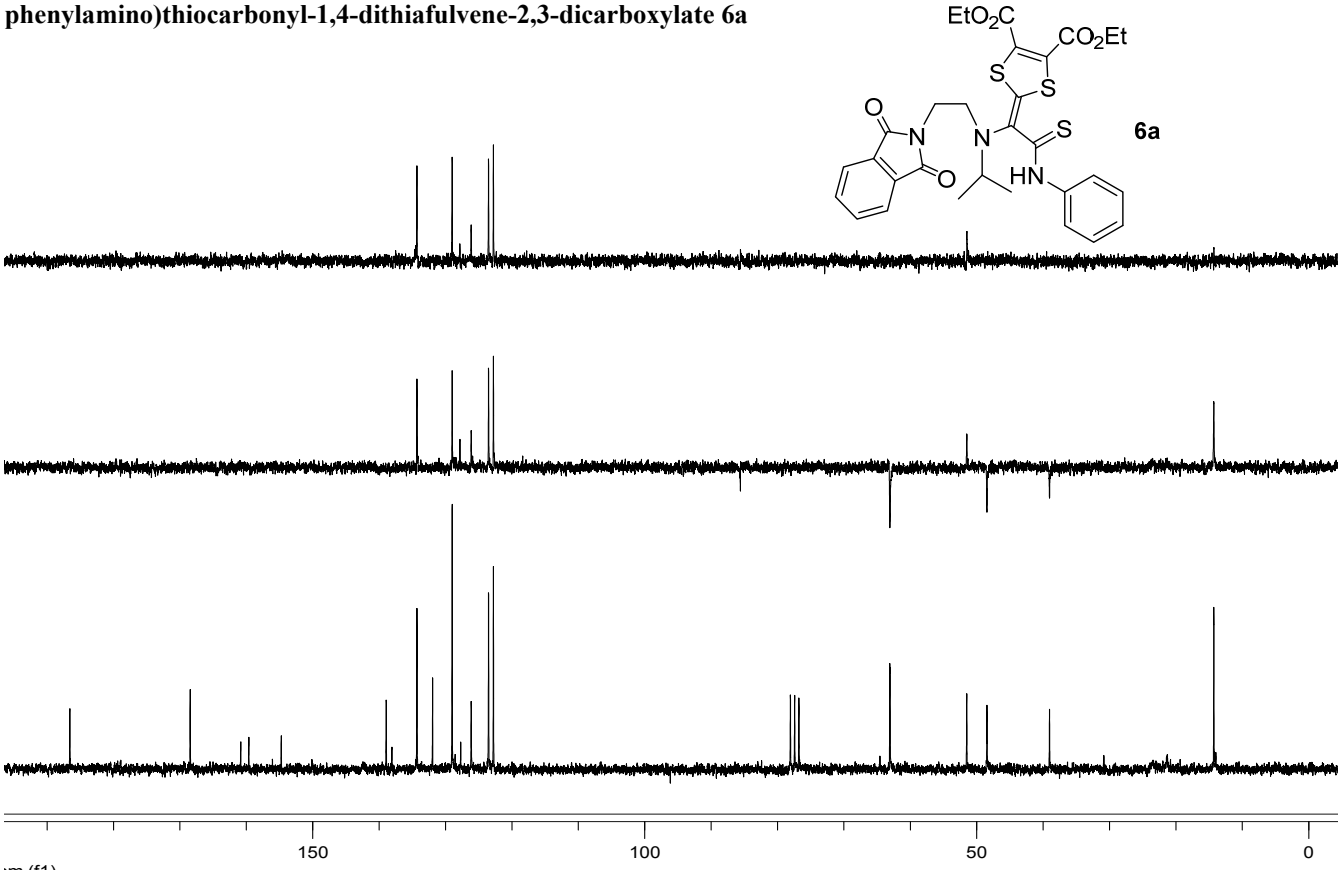


^{13}C NMR and DEPT spectra ($CDCl_3$, 100 MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-6-chlorothiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 4d

Diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-(*N*-phenylamino)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6a

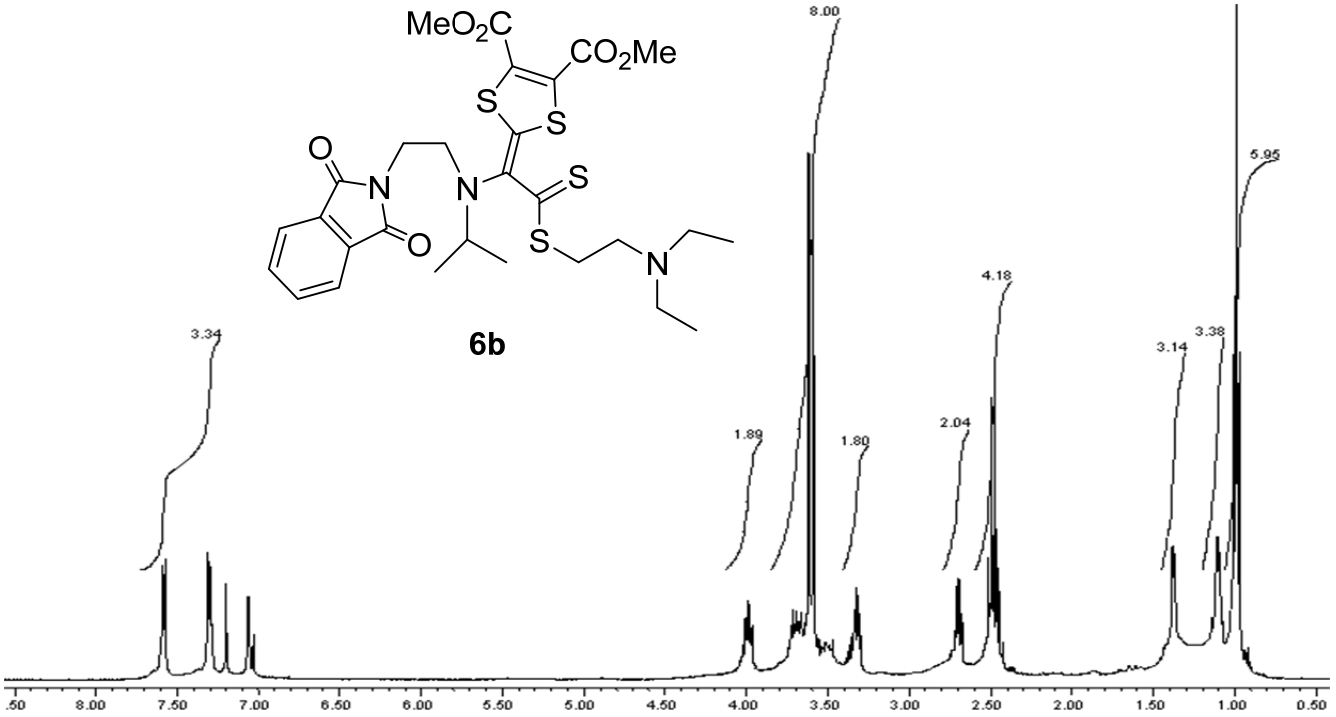


^{1}H NMR spectrum ($CDCl_3$, 400MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-(*N*-phenylamino)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6a

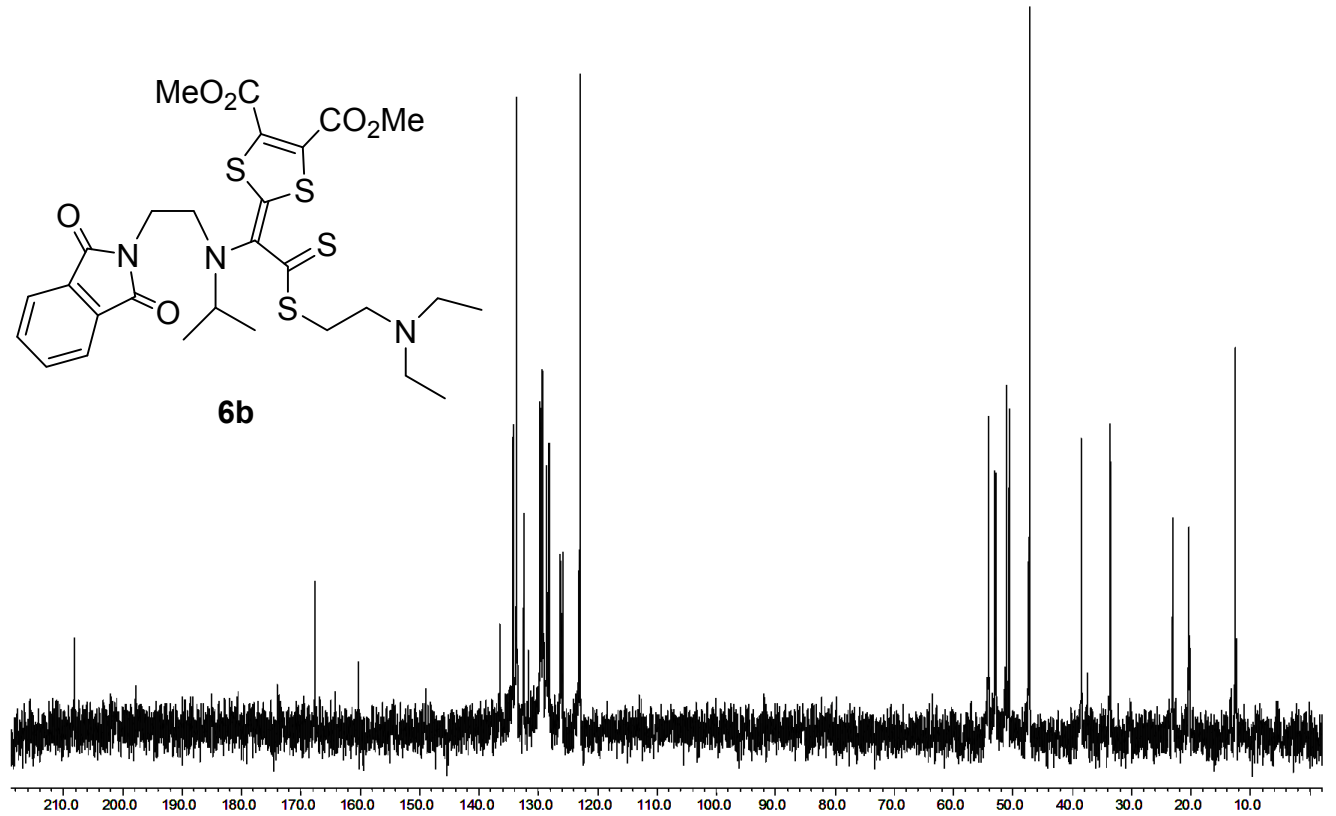


^{13}C NMR and DEPT spectra ($CDCl_3$, 100MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-(*N*-phenylamino)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6a

Dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-[2-(diethylamino)ethylmercapto]thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6b



^{1}H NMR spectrum (C_6D_5Cl, 400MHz) of dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-[2-(diethylamino)ethylmercapto]thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6b



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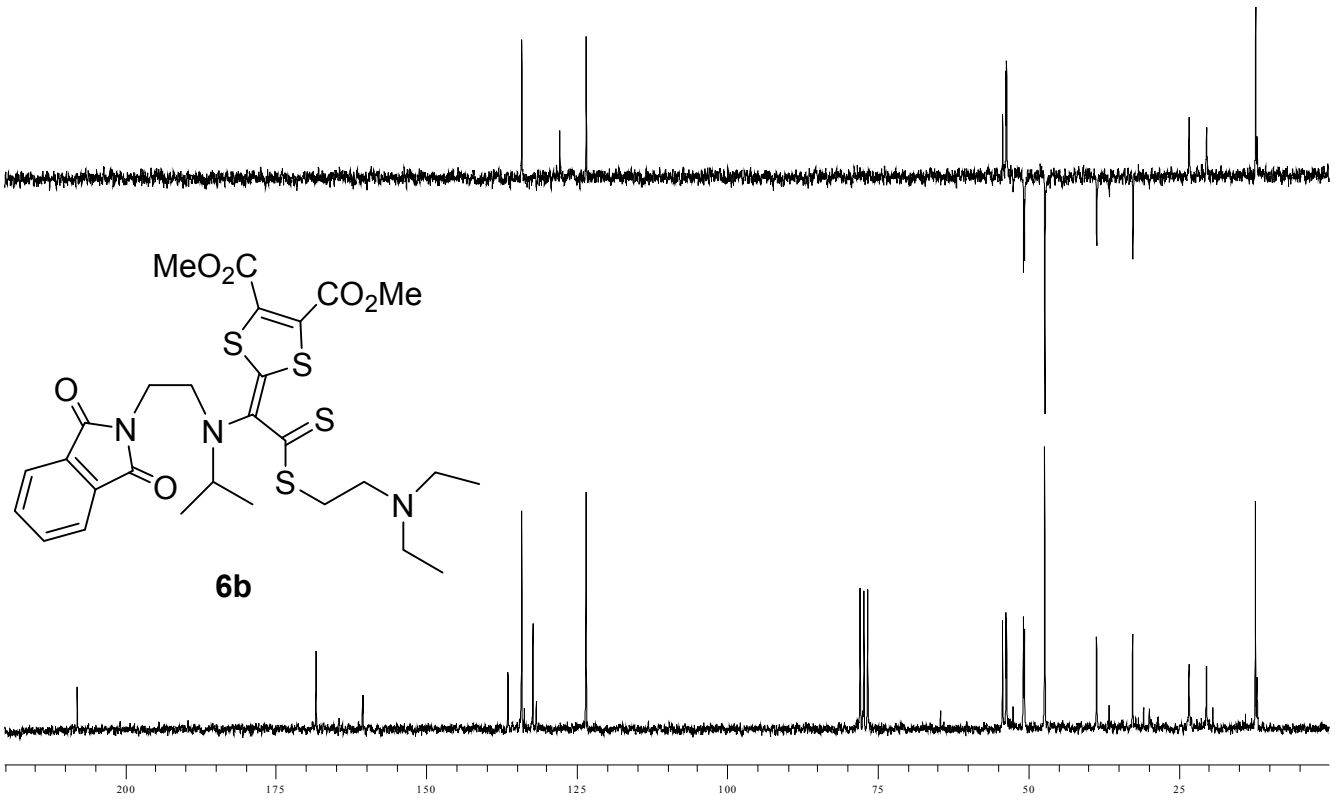
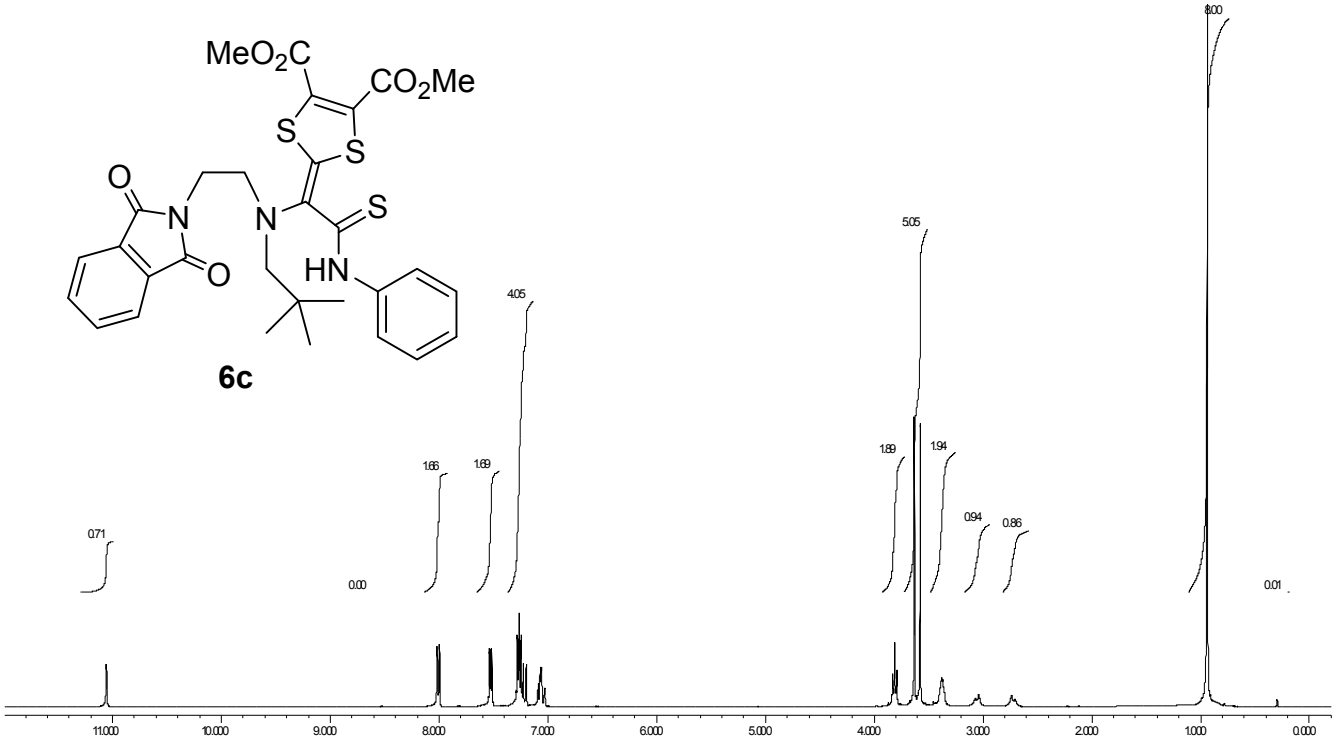
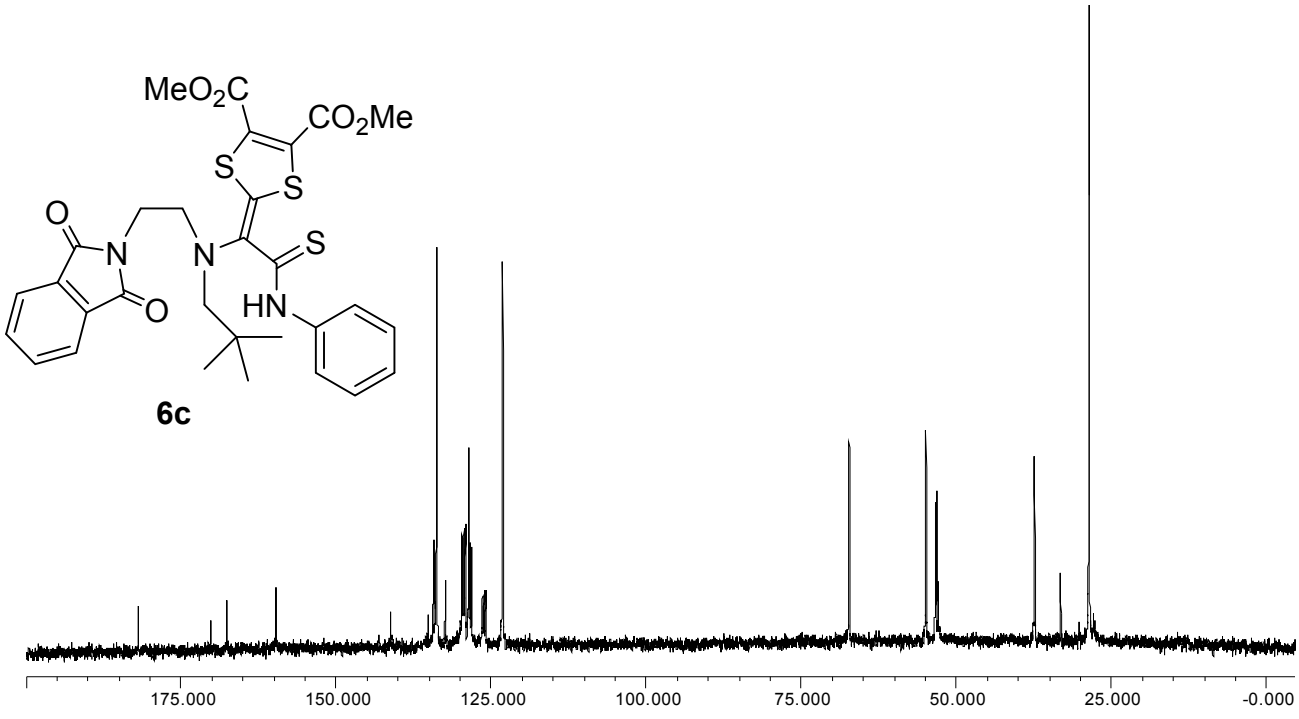


^{13}C NMR and DEPT spectra ($CDCl_3$, 100MHz) of dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-[2-(diethylamino)ethylmercapto]thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6b

Dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-2,2-dimethylpropyl)]amino-6-(*N*-phenylamino)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6c

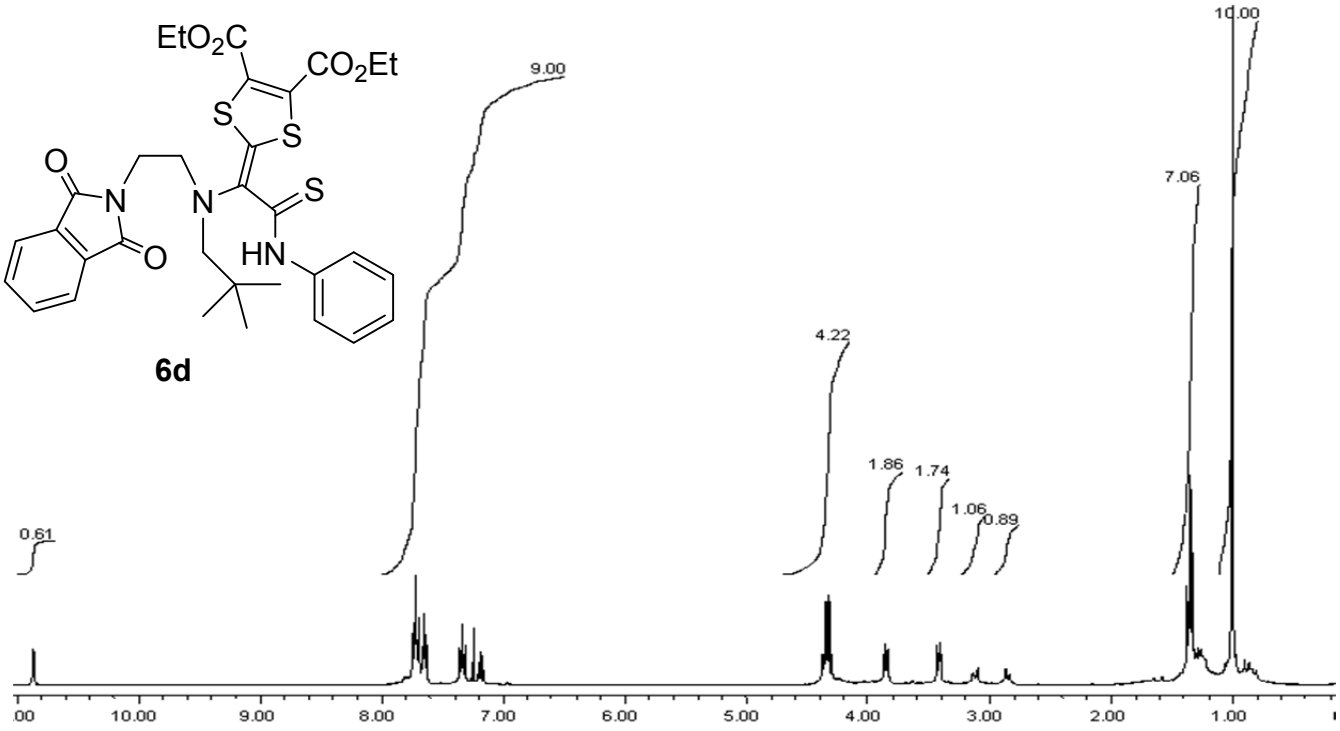


^{1}H NMR spectrum (C_6D_5Cl, 400MHz) of dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-2,2-dimethylpropyl)]amino-6-(*N*-phenylamino)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6c

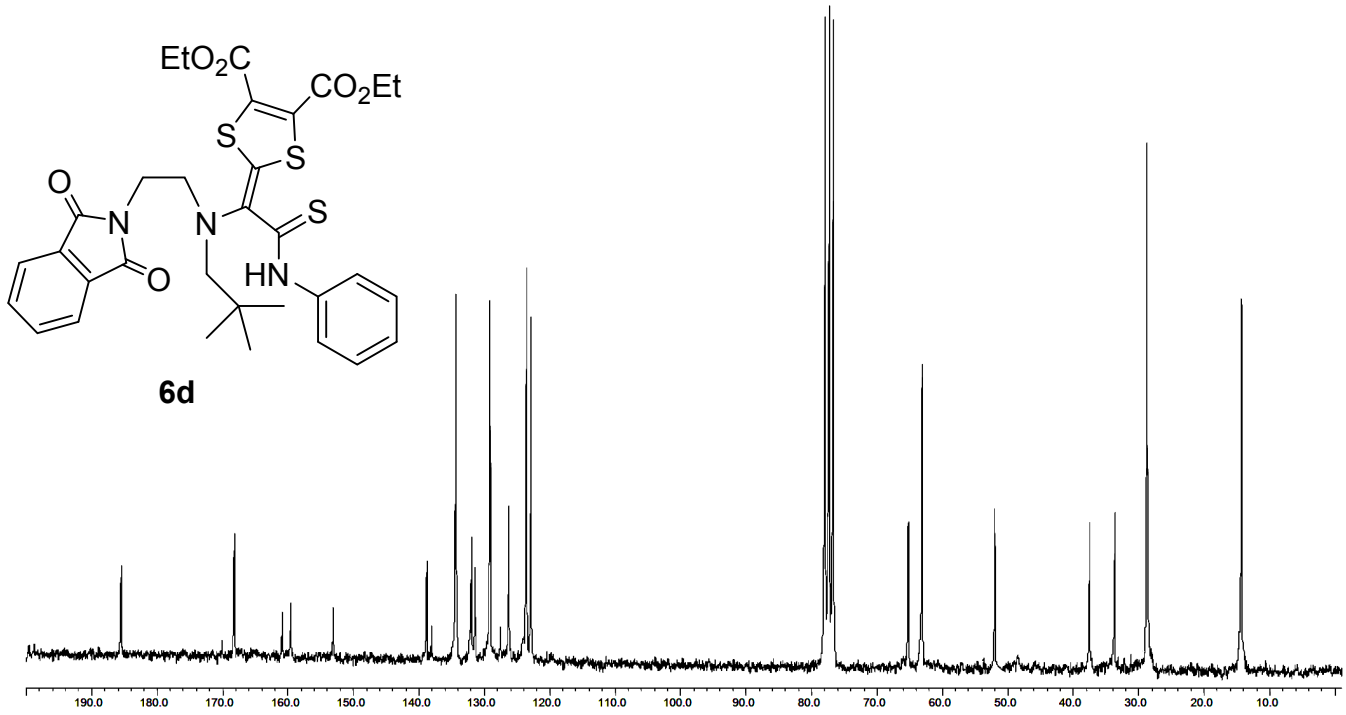


^{13}C NMR spectrum (C_6D_5Cl, 100MHz) of dimethyl 6-[*N*-(2-phthalimidoethyl)-*N*-2,2-dimethylpropyl)]amino-6-(*N*-phenylamino)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6c

Diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-6-(*N*-phenylamino)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6d

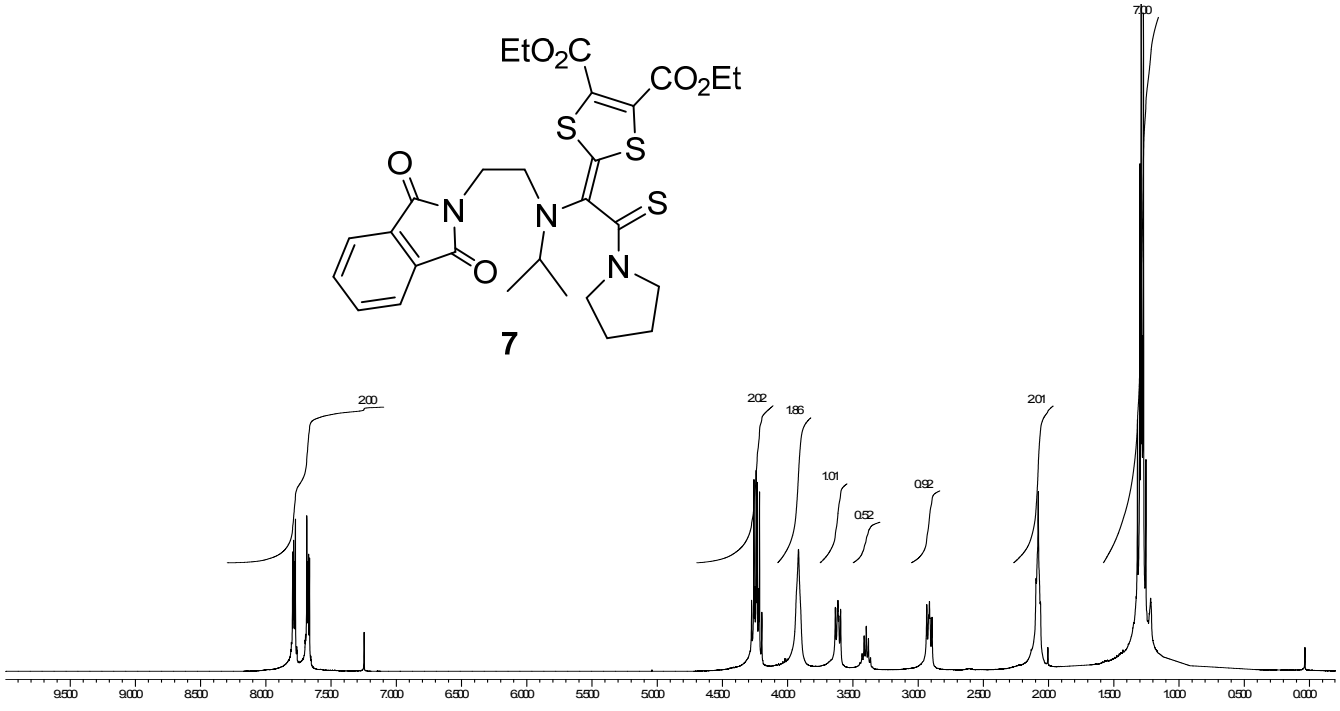


^{1}H NMR spectrum of ($CDCl_3$, 400MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-6-(*N*-phenylamino)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6d

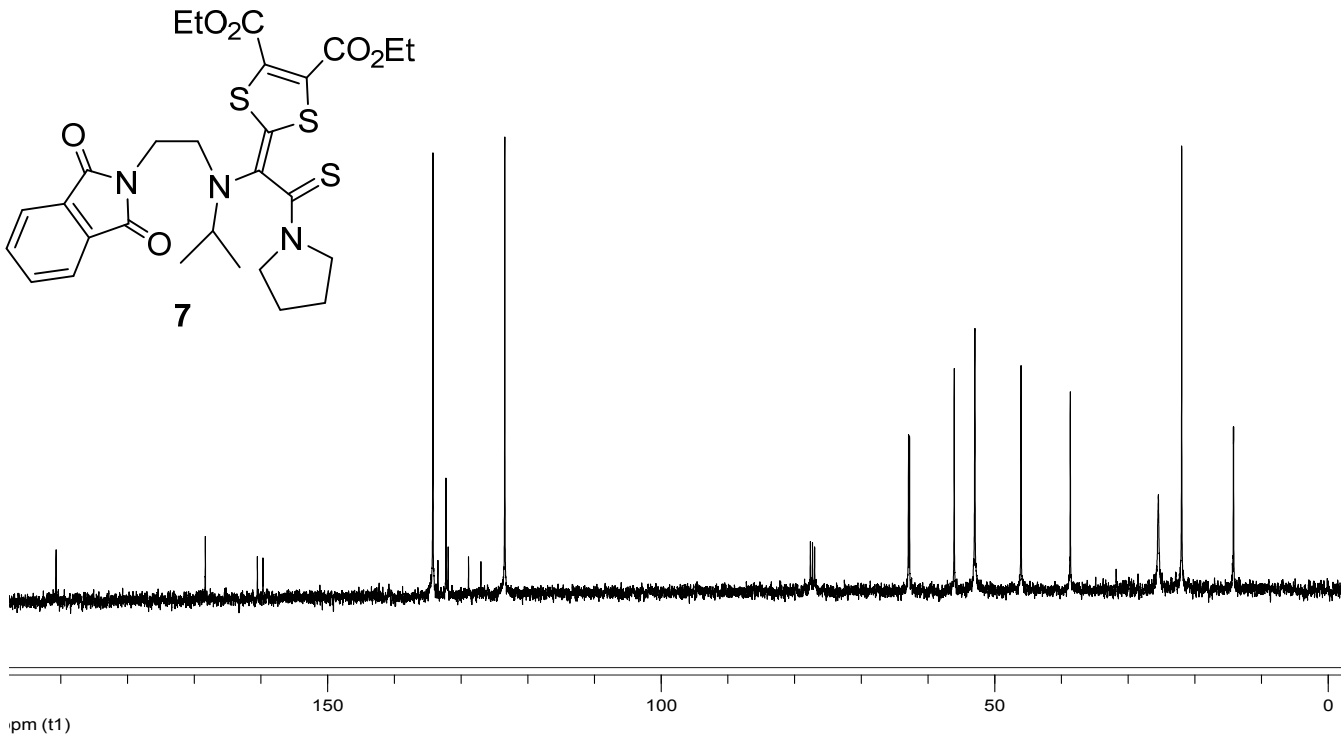


^{13}C NMR spectrum ($CDCl_3$, 100MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-(2,2-dimethylpropyl)]amino-6-(*N*-phenylamino)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 6d

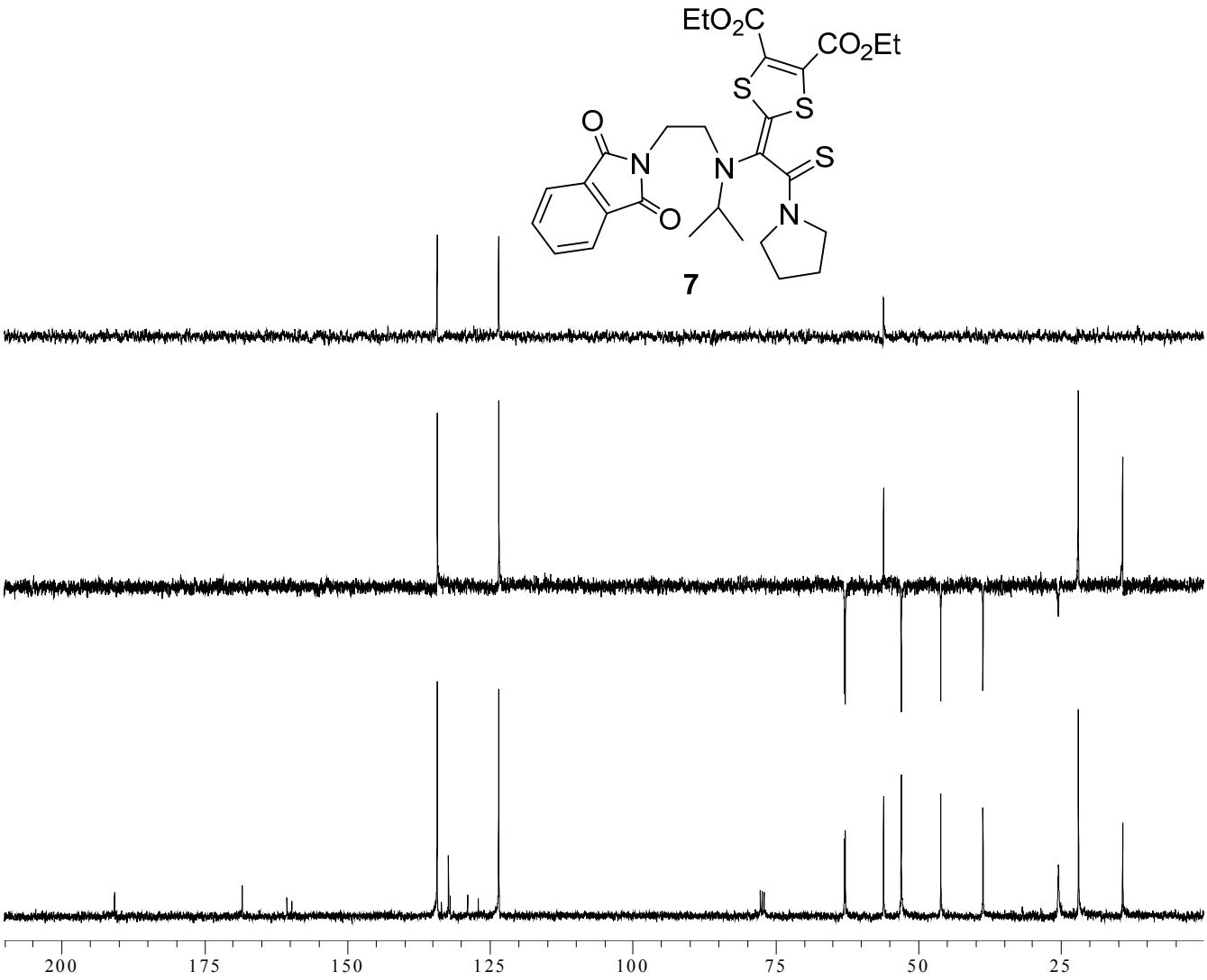
Diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-(pyrrolidin-1-yl)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 7



^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-(pyrrolidin-1-yl)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 7

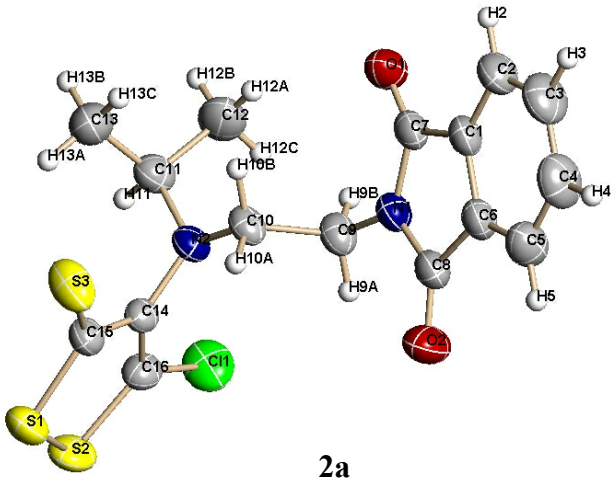


^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-(pyrrolidin-1-yl)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 7



^{13}C NMR and DEPT spectra ($CDCl_3$, 100 MHz) of diethyl 6-[*N*-(2-phthalimidoethyl)-*N*-isopropyl]amino-6-(pyrrolidin-1-yl)thiocarbonyl-1,4-dithiafulvene-2,3-dicarboxylate 7

2.- X-Ray Diffraction Structures



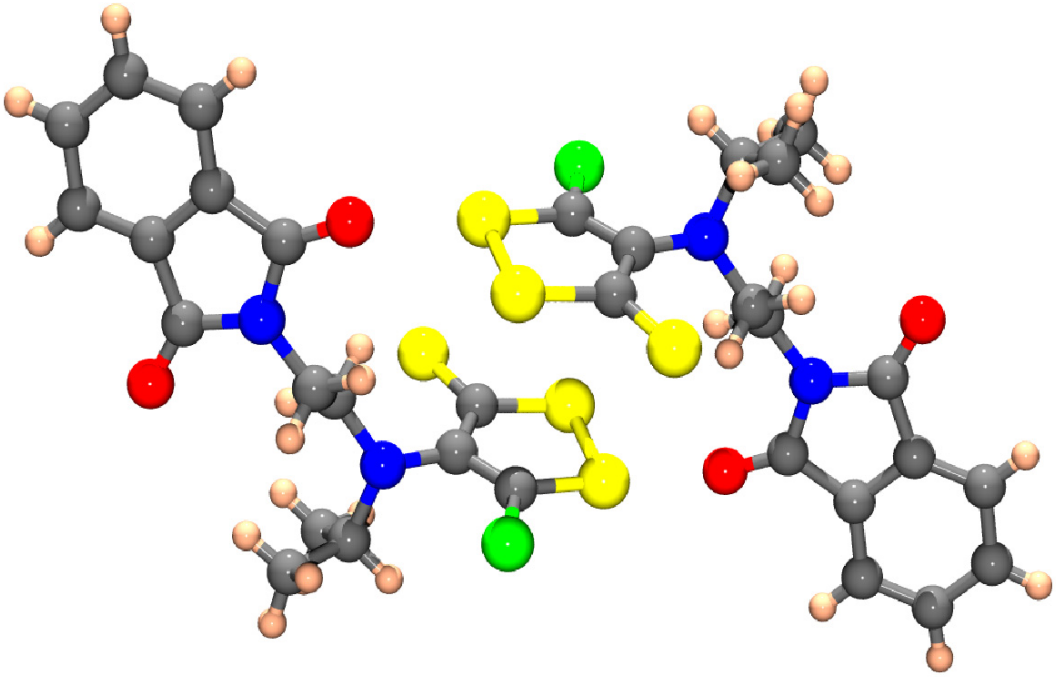
2a

Table 1A. Crystal data and structure refinement for **2a**.

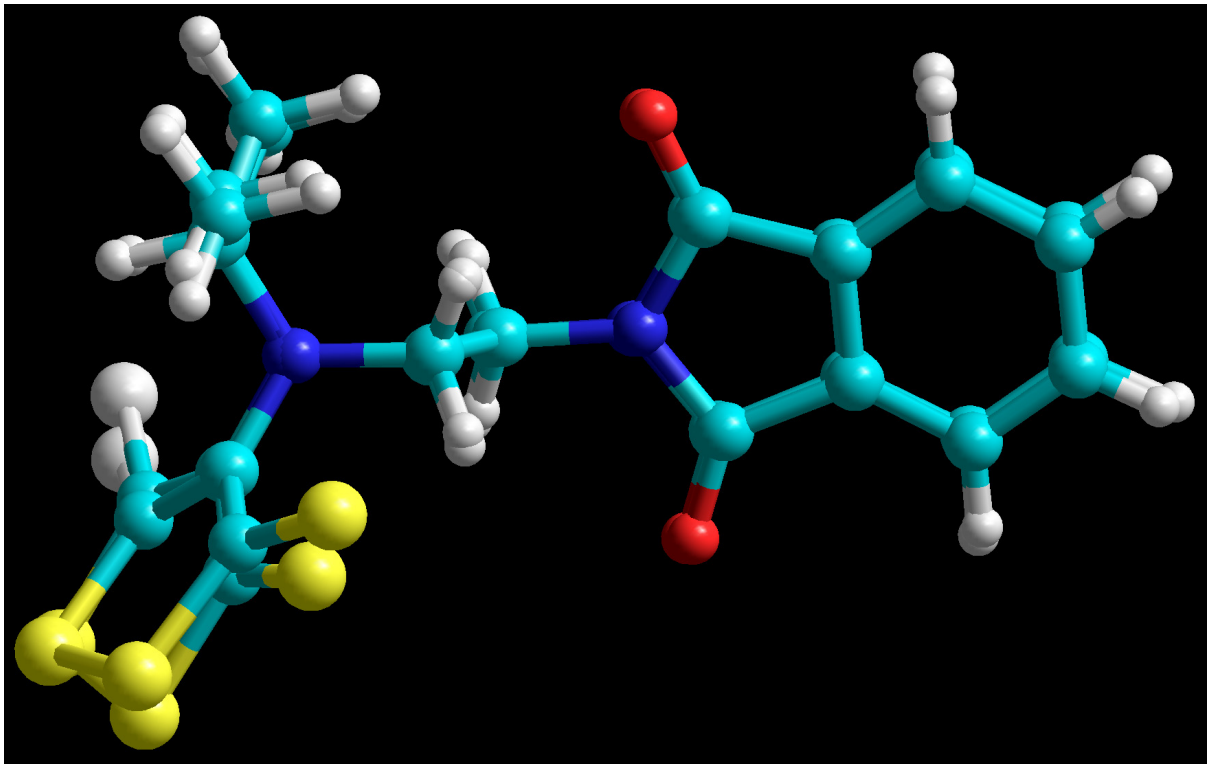
Identification code	CCDC 1010581	
Empirical formula	C16 H15 Cl N2 O2 S3	
Formula weight	398.93	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.900(3) Å	α = 63.212(5)°
	b = 11.409(4) Å	β = 86.744(6)°
	c = 11.512(4) Å	γ = 79.229(6)°
Volume	909.4(6) $Å^3$	
Z	2	
Density (calculated)	1.457 Mg/m^3	
Absorption coefficient	0.566 mm^{-1}	
F(000)	412	
Crystal size	0.40 x 0.30 x 0.10 mm	
θ range for data collection	2.03 to 25.00°	
Index ranges	-9<=h<=9, -13<=k<=13, -13<=l<=13	
Reflections collected	7535	
Independent reflections	3098 [R_{int} = 0.0154]	
Completeness to θ = 25.00°	96.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.945 and 0.855	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3098 / 0 / 219	
Goodness-of-fit on F^2	S = 1.082	
R indices [for 2721 reflections with I>2σ(I)]	R_1 = 0.0372, wR_2 = 0.1082	
R indices (for all 3098 data)	R_1 = 0.0424, wR_2 = 0.1108	
Weighting scheme	$w^{-1} = \sigma^2(F_o^2) + (aP)^2 + (bP)$, where $P = [\max(F_o^2, 0) + 2F_c^2]/3$ a = 0.0623, b = 0.2746	
Largest diff. peak and hole	0.254 and -0.252 $eÅ^{-3}$	

Table 1B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2a**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

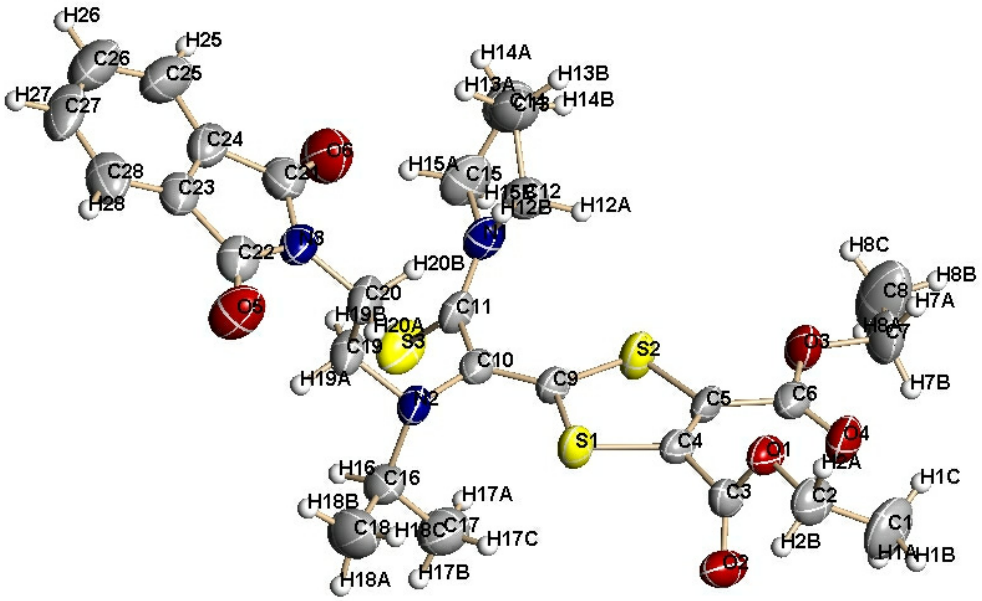
	x	y	z	U(eq)
Cl(1)	6643(1)	6105(1)	6763(1)	66(1)
S(1)	5357(1)	2807(1)	10409(1)	53(1)
S(2)	7262(1)	3699(1)	9216(1)	56(1)
S(3)	1686(1)	3496(1)	9857(1)	62(1)
O(1)	-1820(2)	8847(2)	5409(2)	54(1)
O(2)	984(2)	9043(2)	8655(2)	63(1)
N(1)	-51(2)	8770(2)	6976(2)	41(1)
N(2)	2903(2)	5728(2)	7134(2)	38(1)
C(1)	-2866(3)	9816(2)	6880(2)	41(1)
C(2)	-4603(3)	10315(2)	6607(2)	53(1)
C(3)	-5457(3)	10911(3)	7346(3)	64(1)
C(4)	-4605(4)	11008(3)	8294(3)	66(1)
C(5)	-2847(4)	10504(3)	8572(2)	58(1)
C(6)	-2004(3)	9902(2)	7844(2)	44(1)
C(7)	-1612(3)	9101(2)	6295(2)	41(1)
C(8)	-184(3)	9214(2)	7927(2)	44(1)
C(9)	1500(3)	7989(2)	6753(2)	44(1)
C(10)	1391(3)	6511(2)	7400(2)	39(1)
C(11)	2788(3)	5320(2)	6092(2)	47(1)
C(12)	2277(4)	6527(3)	4790(2)	65(1)
C(13)	1646(4)	4292(3)	6424(3)	63(1)
C(14)	4068(2)	4850(2)	8158(2)	34(1)
C(15)	3635(3)	3831(2)	9355(2)	41(1)
C(16)	5814(3)	4906(2)	8029(2)	43(1)



Crystal packing of 2a in the solid state, from single crystal X-ray diffraction analysis.



Superposition of structures 2a, from single crystal X-ray diffraction analysis and from DFT calculations.



7

Table 2A. Crystal data and structure refinement for **7**.

Identification code	CCDC 1010580	
Empirical formula	C28 H33 N3 O6 S3	
Formula weight	603.75	
Temperature	566(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 16.942(2) Å	α = 90°
	b = 14.3803(18) Å	β = 101.603(3)°
	c = 37.907(5) Å	γ = 90°
Volume	9046.8(19) $Å^3$	
Z	12	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	0.291 mm^{-1}	
F(000)	3816	
Crystal size	0.30 x 0.20 x 0.20 mm	
θ range for data collection	1.10 to 25.00°	
Index ranges	-20<=h<=20, -17<=k<=15, -42<=l<=45	
Reflections collected	66244	
Independent reflections	15913 [R_{int} = 0.0916]	
Completeness to θ = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.943 and 0.857	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15913 / 778 / 1093	
Goodness-of-fit on F^2	S = 0.922	
R indices [for 7448 reflections with I>2σ(I)]	R_1 = 0.0708, wR_2 = 0.1894	
R indices (for all 15913 data)	R_1 = 0.1545, wR_2 = 0.2262	

Weighting scheme	$w^{-1} = \sigma^2(F_o^2) + (aP)^2 + (bP)$, where $P = [\max(F_o^2, 0) + 2F_c^2]/3$ a = 0.1241, b = 0.0000
Largest diff. peak and hole	0.776 and -0.403 eÅ^{-3}

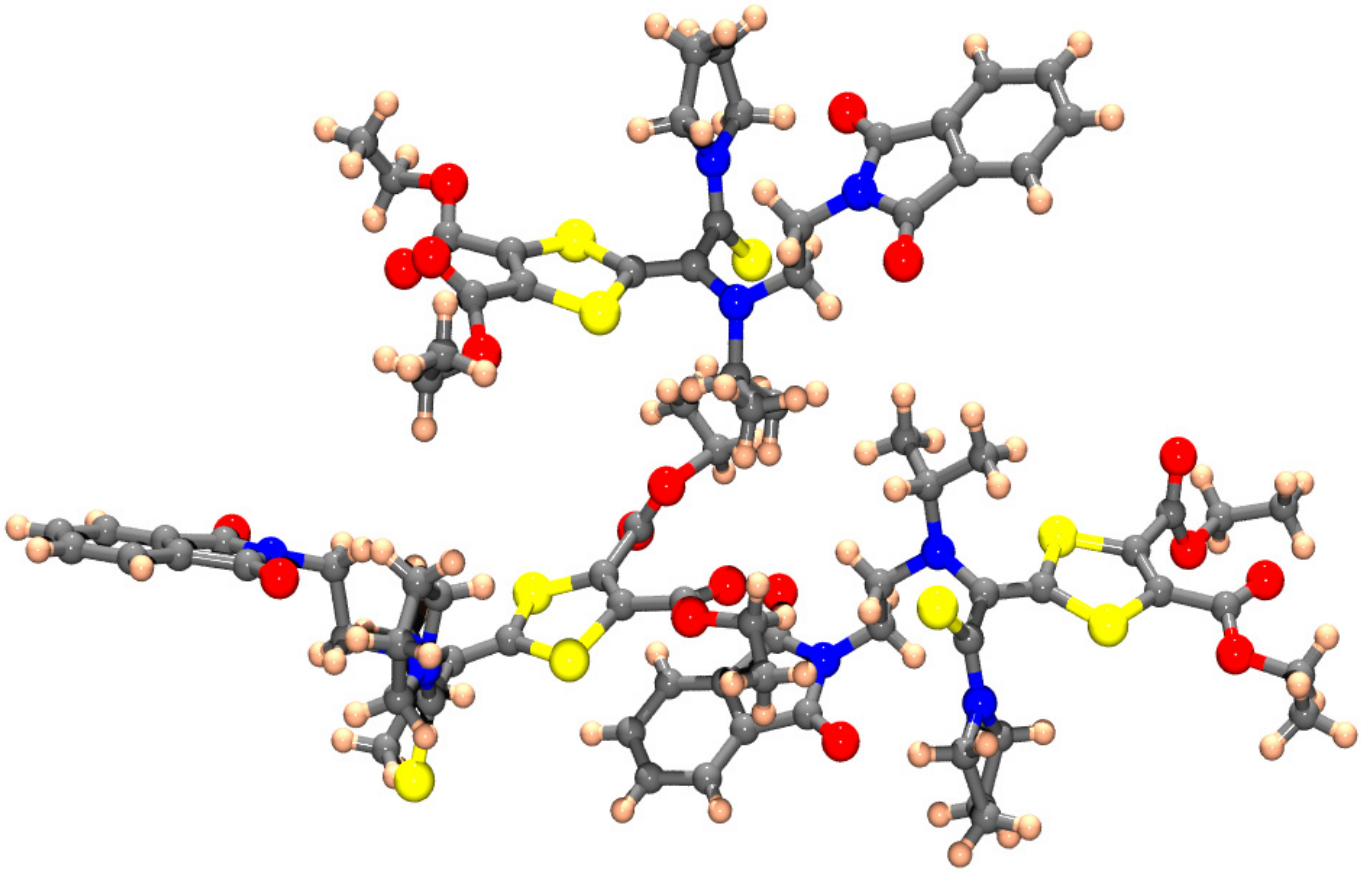
Table 2B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
S(1)	586(1)	2585(1)	2844(1)	51(1)
S(2)	668(1)	2562(1)	2074(1)	57(1)
S(3)	3013(1)	3883(1)	2308(1)	75(1)
N(1)	2593(2)	2141(3)	2157(1)	51(1)
N(2)	2311(2)	3060(3)	2990(1)	45(1)
N(3)	3842(2)	1226(3)	3332(1)	55(1)
O(2)	-1328(2)	2994(2)	2813(1)	63(1)
O(4)	-1667(2)	2259(2)	1925(1)	62(1)
O(5)	3924(2)	1286(3)	3944(1)	85(1)
O(6)	4151(2)	1061(3)	2774(1)	93(1)
C(3)	-1057(3)	2331(4)	2690(1)	46(1)
O(1)	-1328(2)	1471(2)	2685(1)	51(1)
C(2)	-2047(3)	1339(4)	2843(2)	63(2)
C(1)	-2784(3)	1610(5)	2586(2)	94(2)
C(4)	-303(2)	2398(3)	2536(1)	42(1)
C(5)	-276(2)	2373(3)	2187(1)	44(1)
C(6)	-983(3)	2262(3)	1885(1)	49(1)
O(3)	-755(2)	2176(3)	1573(1)	66(1)
C(7)	-1393(3)	2055(5)	1252(1)	79(2)
C(8)	-1069(4)	2227(6)	936(2)	134(3)
C(9)	1194(2)	2668(3)	2521(1)	42(1)
C(10)	1992(2)	2847(3)	2619(1)	43(1)
C(11)	2526(2)	2894(4)	2352(1)	47(1)
C(12)	2274(3)	1203(4)	2199(1)	61(1)
C(13)	2776(3)	561(4)	2019(2)	79(2)
C(14)	2992(4)	1163(5)	1729(2)	92(2)
C(15)	3115(3)	2115(5)	1891(2)	75(2)
C(16)	2299(3)	4064(4)	3106(1)	59(1)
C(17)	1651(3)	4642(4)	2890(2)	82(2)

C(18)	2232(4)	4085(5)	3504(2)	93(2)
C(19)	3101(3)	2646(3)	3128(1)	53(1)
C(20)	3035(3)	1629(3)	3217(2)	60(1)
C(21)	4340(3)	1004(4)	3099(2)	62(2)
C(22)	4225(3)	1136(4)	3690(2)	57(1)
C(23)	5055(3)	802(3)	3686(2)	56(1)
C(24)	5113(3)	714(4)	3327(2)	63(2)
C(25)	5813(4)	426(4)	3228(2)	87(2)
C(26)	6455(4)	245(5)	3503(2)	104(2)
C(27)	6410(4)	334(4)	3855(2)	94(2)
C(28)	5695(4)	603(4)	3958(2)	75(2)
S(5)	6183(1)	7781(1)	3976(1)	57(1)
S(4)	5899(1)	7525(1)	4712(1)	69(1)
S(6)	3593(1)	6463(1)	4393(1)	94(1)
N(4)	3945(2)	8218(4)	4522(1)	62(1)
N(5)	4408(2)	7382(3)	3742(1)	48(1)
N(6)	2854(2)	9151(3)	3356(1)	54(1)
O(7)	8159(2)	7741(4)	5011(1)	129(2)
O(9)	8120(3)	9004(4)	4429(2)	148(3)
O(11)	2467(2)	9331(3)	3899(1)	86(1)
O(12)	2843(2)	9084(3)	2748(1)	78(1)
C(31)	7502(4)	7962(5)	5000(2)	80(2)
O(8)	7225(3)	8245(5)	5273(1)	161(3)
C(30)	7747(6)	7921(10)	5666(3)	253(8)
C(29)	8093(7)	8669(9)	5709(4)	311(12)
C(32)	6857(3)	7918(4)	4668(2)	56(1)
C(33)	6973(3)	8048(3)	4332(1)	52(1)
C(34)	7734(3)	8435(5)	4253(2)	78(2)
O(10)	7887(2)	8069(3)	3960(1)	93(1)
C(35)	8714(5)	8304(6)	3875(2)	128(3)
C(36)	8600(5)	9060(6)	3663(2)	128(3)
C(37)	5477(3)	7600(3)	4247(1)	49(1)
C(38)	4679(3)	7500(3)	4113(1)	45(1)
C(39)	4084(3)	7444(4)	4356(1)	56(1)
C(40)	3326(4)	8286(5)	4747(2)	90(2)
C(41)	3418(6)	9235(6)	4894(2)	140(3)
C(42)	3930(4)	9768(6)	4706(3)	142(4)
C(43)	4340(4)	9128(4)	4508(2)	74(2)
C(44)	4652(3)	6548(4)	3563(2)	71(2)

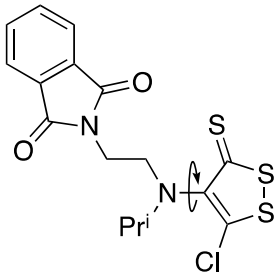
C(45)	4132(4)	5727(5)	3561(2)	114(3)
C(46)	4764(4)	6798(5)	3188(2)	99(2)
C(47)	3609(3)	7754(3)	3589(1)	51(1)
C(48)	3651(3)	8768(3)	3488(2)	61(2)
C(49)	2504(3)	9233(3)	2992(2)	53(1)
C(50)	2315(3)	9369(4)	3576(2)	61(1)
C(51)	1558(3)	9647(3)	3328(1)	53(1)
C(52)	832(3)	9935(4)	3406(2)	68(2)
C(53)	208(3)	10128(4)	3113(2)	74(2)
C(54)	318(3)	10045(4)	2765(2)	67(2)
C(55)	1051(3)	9745(3)	2689(2)	61(1)
C(56)	1665(3)	9557(3)	2976(2)	52(1)
S(7)	7371(1)	2899(1)	3609(1)	69(1)
S(8)	7284(1)	2516(1)	4363(1)	67(1)
S(9)	9688(1)	1901(1)	3706(1)	77(1)
N(7)	9309(2)	3655(3)	3777(1)	50(1)
N(8)	9074(2)	2268(3)	4486(1)	47(1)
N(9)	10545(2)	3947(3)	5000(1)	52(1)
O(13)	5592(3)	2410(4)	4482(1)	111(2)
O(15)	5041(3)	3037(4)	3512(2)	156(3)
O(17)	10765(2)	3314(3)	5567(1)	74(1)
O(18)	10725(2)	4698(3)	4485(1)	95(1)
C(59)	5696(3)	2962(4)	4281(2)	81(2)
O(14)	5295(3)	3678(4)	4190(2)	156(3)
C(58)	4397(7)	3585(9)	4309(3)	226(6)
C(57)	4630(5)	4095(6)	4571(3)	142(3)
C(60)	6419(3)	2901(4)	4081(2)	65(2)
C(61)	6442(3)	3072(4)	3744(2)	60(2)
C(62)	5748(4)	3286(5)	3454(2)	100(2)
O(16)	5879(3)	3654(5)	3190(1)	171(3)
C(63)	5241(5)	3833(8)	2868(2)	175(5)
C(64)	5384(5)	3551(8)	2570(2)	185(5)
C(65)	7899(3)	2679(3)	4046(1)	50(1)
C(66)	8711(3)	2588(3)	4142(1)	47(1)
C(67)	9229(3)	2776(4)	3868(1)	47(1)
C(68)	8919(3)	4482(4)	3898(1)	62(2)
C(69)	9270(4)	5274(4)	3736(2)	90(2)
C(70)	9755(5)	4947(5)	3505(2)	130(3)
C(71)	9847(3)	3938(4)	3536(2)	67(2)

C(72)	8928(3)	1288(4)	4590(2)	66(2)
C(73)	8818(4)	1271(5)	4976(2)	103(2)
C(74)	9571(3)	603(4)	4527(2)	88(2)
C(75)	9853(3)	2660(3)	4651(1)	49(1)
C(76)	9760(3)	3530(3)	4859(1)	57(1)
C(77)	10982(3)	4462(4)	4796(2)	62(2)
C(78)	10997(3)	3775(4)	5339(2)	54(1)
C(79)	11786(3)	4243(3)	5359(1)	49(1)
C(80)	12459(3)	4289(4)	5628(2)	65(2)
C(81)	13115(3)	4768(4)	5561(2)	80(2)
C(82)	13103(4)	5189(5)	5233(2)	88(2)
C(83)	12433(4)	5140(4)	4962(2)	84(2)
C(84)	11774(3)	4662(4)	5029(1)	56(1)

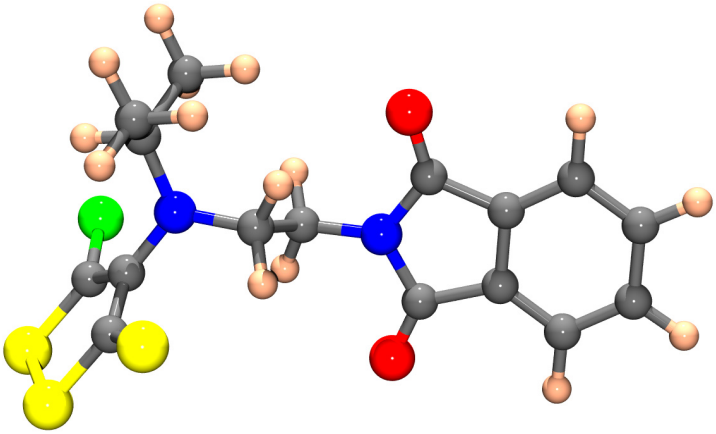


The three independent conformations found in the X-ray diffraction structure of 7

3.- Coordinates of all stationary points



2a, rotation of the 1,2-dithiole-3-thione ring



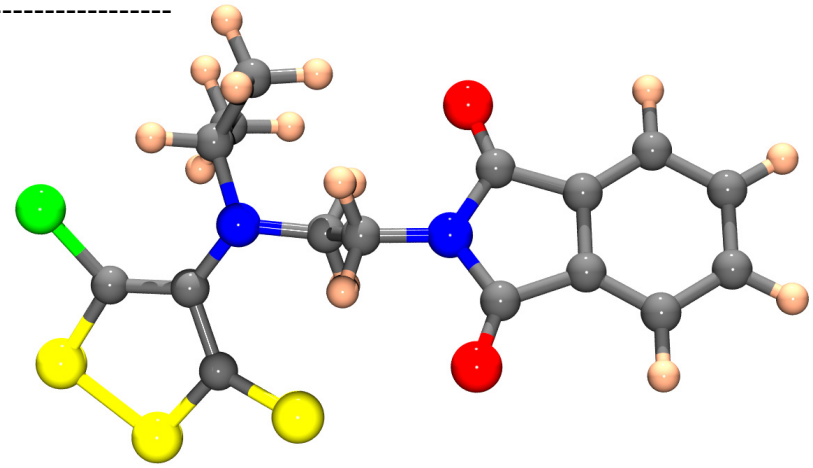
2a_rot1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.156096	-1.010161	-0.385851
2	6	0	-4.395220	0.312888	-0.007213
3	6	0	-5.654779	0.737835	0.388385
4	6	0	-6.683855	-0.213438	0.394154
5	6	0	-6.444013	-1.540178	0.014610
6	6	0	-5.167417	-1.959136	-0.383859
7	6	0	-2.714130	-1.139576	-0.753577
8	6	0	-3.111999	1.068400	-0.116633
9	1	0	-5.829466	1.768632	0.680869
10	1	0	-7.684342	0.080985	0.698205
11	1	0	-7.262121	-2.254706	0.030178
12	1	0	-4.970268	-2.984806	-0.680007
13	8	0	-2.106143	-2.117258	-1.139450
14	8	0	-2.888220	2.240052	0.124657
15	7	0	-2.162341	0.141590	-0.570680
16	6	0	-0.764616	0.476384	-0.805259
17	1	0	-0.357957	-0.289268	-1.470396
18	1	0	-0.727943	1.442827	-1.312519
19	6	0	0.036054	0.530645	0.512882
20	1	0	-0.457205	1.221806	1.202000
21	1	0	0.014229	-0.453674	0.988079
22	7	0	1.414623	0.963157	0.299072
23	6	0	2.406945	-0.003131	0.115416
24	6	0	2.738862	-1.006757	1.126011
25	6	0	3.165292	-0.058477	-1.033359
26	16	0	2.096651	-1.218298	2.639863
27	16	0	4.002164	-2.130964	0.635451
28	16	0	4.449060	-1.219168	-1.229823
29	17	0	2.942465	1.007235	-2.377869
30	6	0	1.814639	2.351622	0.639595
31	6	0	1.824687	2.609725	2.155746
32	6	0	0.958153	3.386473	-0.102657
33	1	0	2.843642	2.450275	0.276204

2a_rot1

34	1	0	2.458453	1.884863	2.673713
35	1	0	2.202504	3.618147	2.362895
36	1	0	0.816909	2.540386	2.580500
37	1	0	1.028494	3.246927	-1.185993
38	1	0	-0.097705	3.328465	0.185088
39	1	0	1.308769	4.396715	0.136337



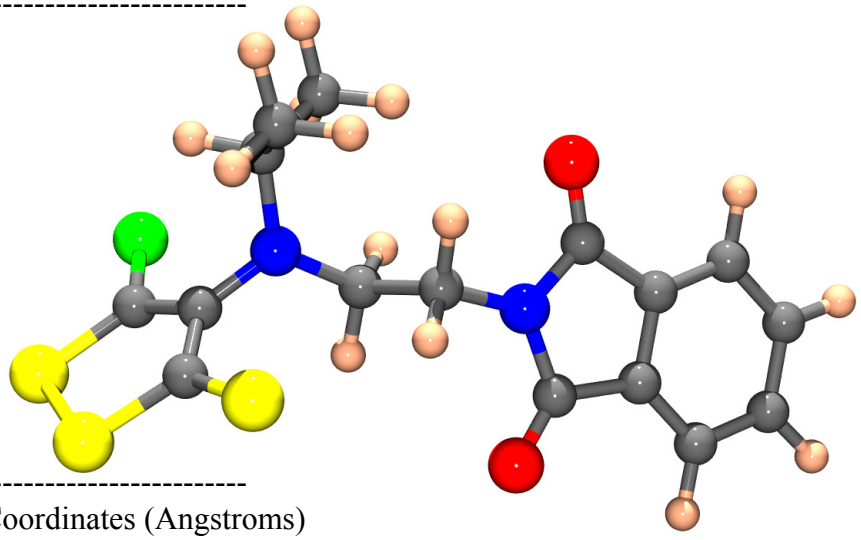
2a_TS1

Standard orientation:

2a_TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.380747	-0.767448	-0.233853
2	6	0	-4.417477	0.560490	0.193898
3	6	0	-5.572811	1.123586	0.715721
4	6	0	-6.707154	0.305227	0.798749
5	6	0	-6.670334	-1.027663	0.369089
6	6	0	-5.498007	-1.585702	-0.158045
7	6	0	-3.008347	-1.058125	-0.745720
8	6	0	-3.067882	1.157769	-0.026024
9	1	0	-5.590629	2.158255	1.043985
10	1	0	-7.631405	0.709317	1.202017
11	1	0	-7.566604	-1.636699	0.445797
12	1	0	-5.457705	-2.616652	-0.495743
13	8	0	-2.581380	-2.082564	-1.233738
14	8	0	-2.695513	2.295658	0.201727
15	7	0	-2.276237	0.136119	-0.566038
16	6	0	-0.884523	0.311845	-0.971308
17	1	0	-0.598743	-0.591542	-1.510964
18	1	0	-0.825509	1.166714	-1.649288
19	6	0	0.033254	0.528897	0.246953
20	1	0	-0.358278	1.362264	0.831146
21	1	0	-0.001685	-0.347755	0.887083
22	7	0	1.422398	0.861912	-0.131662
23	6	0	2.457340	-0.069182	0.012566
24	6	0	2.199334	-1.516905	0.202111
25	6	0	3.829265	0.177276	-0.093336
26	16	0	0.848824	-2.473601	-0.019874
27	16	0	3.583379	-2.482276	0.662565
28	16	0	5.040145	-1.008143	0.356454
29	17	0	4.674114	1.576373	-0.730177

30	6	0	1.708377	2.323369	0.011761
31	6	0	1.865380	2.727209	1.487313
32	6	0	0.691687	3.202953	-0.729378
33	1	0	2.650152	2.513078	-0.483854
34	1	0	2.629040	2.118152	1.982915
35	1	0	2.174012	3.776366	1.556386
36	1	0	0.927594	2.621420	2.044170
37	1	0	0.661837	2.947600	-1.793988
38	1	0	-0.323558	3.148217	-0.326977
39	1	0	1.021861	4.244702	-0.648976

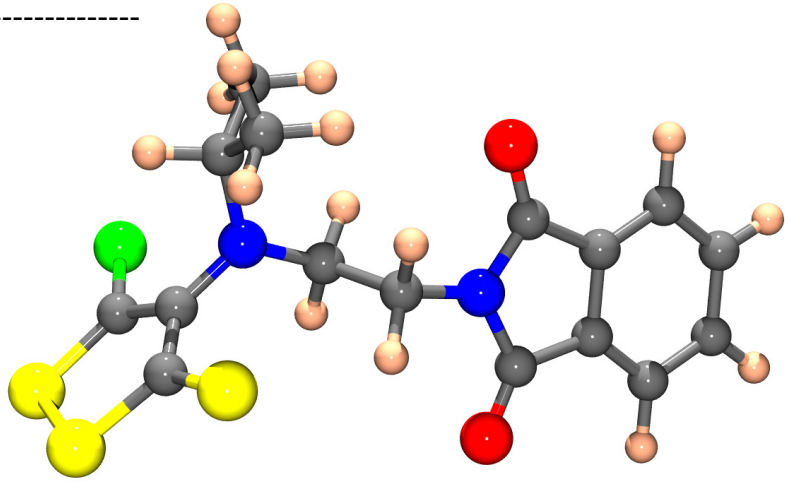


2a_rot2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.219067	-0.994893	-0.351272
2	6	0	4.474527	0.348914	-0.069284
3	6	0	5.716236	0.917793	-0.310744
4	6	0	6.710357	0.090430	-0.850346
5	6	0	6.454023	-1.257207	-1.133494
6	6	0	5.195446	-1.821859	-0.886160
7	6	0	2.801861	-1.290152	0.018711
8	6	0	3.228322	0.953224	0.488398
9	1	0	5.903851	1.963478	-0.087165
10	1	0	7.696381	0.498976	-1.052764
11	1	0	7.245162	-1.873286	-1.551467
12	1	0	4.985895	-2.865116	-1.101402
13	8	0	2.185046	-2.331349	-0.081000
14	8	0	3.028325	2.098038	0.849264
15	7	0	2.284477	-0.084494	0.524125
16	6	0	0.924635	0.082229	1.019725
17	1	0	0.624063	-0.830502	1.536245
18	1	0	0.952579	0.903423	1.737259
19	6	0	-0.056229	0.393389	-0.131671
20	1	0	0.396708	1.161689	-0.772424
21	1	0	-0.164596	-0.505979	-0.744329
22	7	0	-1.389404	0.813321	0.291406
23	6	0	-2.485923	0.015965	-0.047908
24	6	0	-2.823560	-1.190618	0.704022
25	6	0	-3.323363	0.303983	-1.101129

26	16	0	-2.053882	-1.844108	2.015739
27	16	0	-4.242308	-2.040704	0.105913
28	16	0	-4.726897	-0.668319	-1.450366
29	17	0	-3.082739	1.643444	-2.171042
30	6	0	-1.645189	2.143687	0.900596
31	6	0	-0.677376	3.220442	0.393005
32	6	0	-1.678775	2.088871	2.438330
33	1	0	-2.649309	2.433688	0.568196
34	1	0	-0.707774	3.300884	-0.698699
35	1	0	-0.973382	4.188935	0.810047
36	1	0	0.358275	3.035916	0.698353
37	1	0	-2.376301	1.321640	2.786704
38	1	0	-0.693431	1.859845	2.857115
39	1	0	-1.998994	3.057462	2.841977



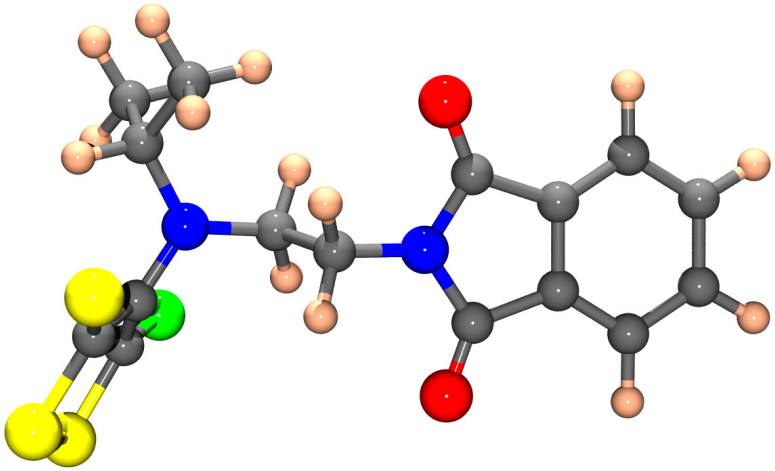
2a_TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.209192	-1.065877	-0.236134
2	6	0	4.405497	0.299832	-0.019347
3	6	0	5.633247	0.902168	-0.250662
4	6	0	6.675382	0.085860	-0.710628
5	6	0	6.478788	-1.283940	-0.927243
6	6	0	5.233632	-1.882355	-0.691304
7	6	0	2.791121	-1.395558	0.100894
8	6	0	3.118093	0.884558	0.460622
9	1	0	5.774583	1.964860	-0.079217
10	1	0	7.652220	0.520632	-0.902773
11	1	0	7.306222	-1.890748	-1.284033
12	1	0	5.069937	-2.942882	-0.855925
13	8	0	2.219684	-2.465226	0.040271
14	8	0	2.860220	2.038346	0.749836
15	7	0	2.211749	-0.184316	0.518904
16	6	0	0.827076	-0.034396	0.948505
17	1	0	0.474637	-1.009669	1.287120
18	1	0	0.811911	0.654292	1.794509
19	6	0	-0.052949	0.509476	-0.200144
20	1	0	0.467105	1.357463	-0.656561
21	1	0	-0.136270	-0.262194	-0.973596

2a_TS2

22	7	0	-1.393484	0.924047	0.196135
23	6	0	-2.465035	0.056476	-0.048306
24	6	0	-2.930233	-0.909568	0.944312
25	6	0	-3.150835	0.045863	-1.240875
26	16	0	-2.352143	-1.201443	2.468913
27	16	0	-4.291962	-1.889107	0.417755
28	16	0	-4.489322	-1.032128	-1.524735
29	17	0	-2.762877	1.081964	-2.571135
30	6	0	-1.680302	2.299127	0.680737
31	6	0	-0.963693	3.381015	-0.142933
32	6	0	-1.394958	2.494486	2.180473
33	1	0	-2.758778	2.427071	0.528393
34	1	0	-1.140504	3.256449	-1.215647
35	1	0	-1.340434	4.366004	0.153765
36	1	0	0.116757	3.380340	0.039565
37	1	0	-1.873165	1.714367	2.777379
38	1	0	-0.318236	2.476439	2.384077
39	1	0	-1.773454	3.470951	2.507354

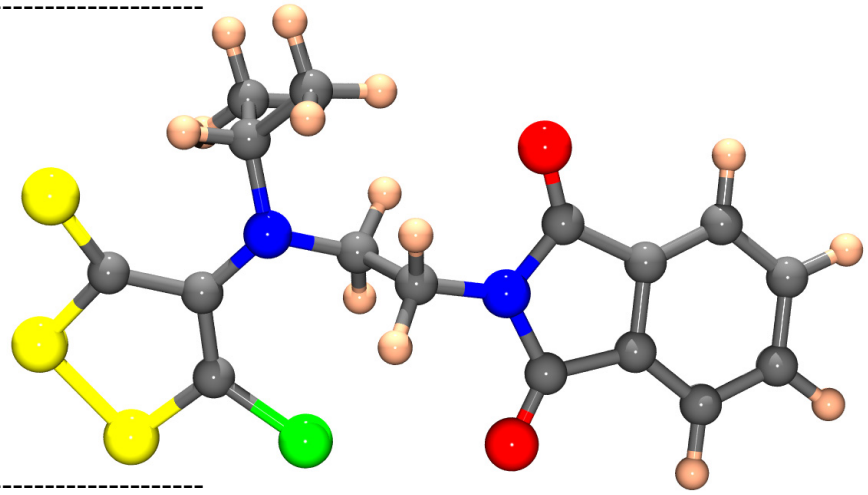


2a_rot3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.122797	-1.015193	-0.356572
2	6	0	-4.379539	0.321554	-0.043470
3	6	0	-5.650673	0.753855	0.304349
4	6	0	-6.673236	-0.204124	0.329056
5	6	0	-6.415861	-1.544560	0.014571
6	6	0	-5.127475	-1.971033	-0.334979
7	6	0	-2.671152	-1.150046	-0.681984
8	6	0	-3.099045	1.081373	-0.156884
9	1	0	-5.839092	1.795359	0.545992
10	1	0	-7.682547	0.095917	0.596223
11	1	0	-7.229499	-2.263806	0.042484
12	1	0	-4.916763	-3.007273	-0.580806
13	8	0	-2.045659	-2.142194	-0.997102
14	8	0	-2.887921	2.262605	0.044251
15	7	0	-2.133424	0.143132	-0.551502
16	6	0	-0.733643	0.477539	-0.777290
17	1	0	-0.310493	-0.304793	-1.411290

18	1	0	-0.690187	1.426931	-1.313651
19	6	0	0.044284	0.575853	0.552318
20	1	0	-0.452739	1.301284	1.203184
21	1	0	-0.011844	-0.392308	1.060150
22	7	0	1.431372	0.981721	0.363409
23	6	0	2.409626	0.019592	0.117011
24	6	0	3.140722	0.007506	-1.150188
25	6	0	2.758335	-0.977350	1.001348
26	16	0	2.984506	1.037458	-2.438323
27	16	0	4.332326	-1.277013	-1.286765
28	16	0	3.913215	-2.212670	0.575677
29	17	0	2.104213	-1.127718	2.598297
30	6	0	1.842807	2.385136	0.609286
31	6	0	1.903581	2.701899	2.113727
32	6	0	0.969784	3.392066	-0.149477
33	1	0	2.856915	2.462162	0.204314
34	1	0	2.571735	2.009486	2.635812
35	1	0	2.273946	3.721445	2.272924
36	1	0	0.912522	2.634678	2.578304
37	1	0	1.020574	3.203332	-1.225308
38	1	0	-0.079254	3.354275	0.166013
39	1	0	1.333076	4.408460	0.039723



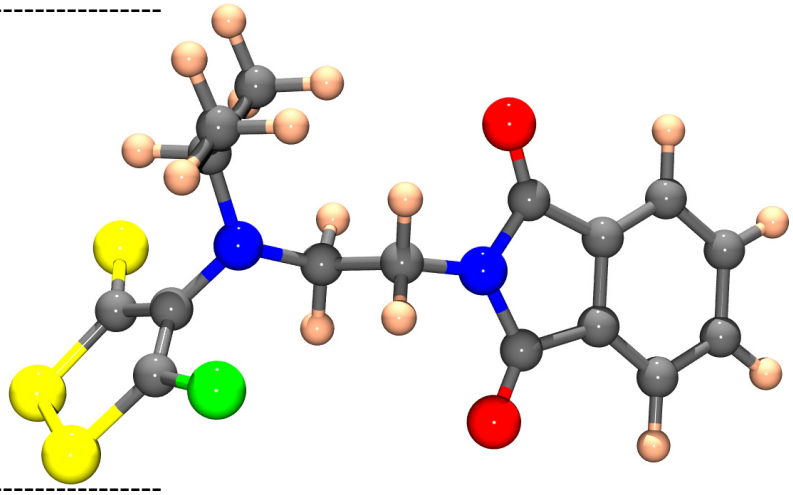
2a_TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.298786	-0.797146	-0.155984
2	6	0	-4.423117	0.571312	0.092434
3	6	0	-5.623778	1.127544	0.508221
4	6	0	-6.713159	0.260951	0.669793
5	6	0	-6.588517	-1.111789	0.420204
6	6	0	-5.370513	-1.663408	0.000585
7	6	0	-2.895532	-1.071058	-0.585371
8	6	0	-3.101908	1.213419	-0.168415
9	1	0	-5.709385	2.192953	0.698202
10	1	0	-7.670842	0.658489	0.993491
11	1	0	-7.451532	-1.757757	0.554039
12	1	0	-5.262895	-2.725460	-0.196772
13	8	0	-2.388246	-2.129718	-0.897704

2a_TS3

14	8	0	-2.787509	2.384728	-0.069466
15	7	0	-2.243181	0.176460	-0.567297
16	6	0	-0.852507	0.388077	-0.952615
17	1	0	-0.544924	-0.479291	-1.536639
18	1	0	-0.809158	1.273819	-1.589782
19	6	0	0.051067	0.591084	0.281037
20	1	0	-0.355649	1.426747	0.852531
21	1	0	-0.001537	-0.276721	0.937535
22	7	0	1.442850	0.918318	-0.063811
23	6	0	2.445268	-0.051461	0.029420
24	6	0	3.884439	0.262402	-0.112116
25	6	0	2.248643	-1.430755	0.152182
26	16	0	4.731147	1.570713	-0.724545
27	16	0	4.984796	-1.014693	0.358462
28	16	0	3.551108	-2.533042	0.536411
29	17	0	0.793606	-2.354101	-0.135529
30	6	0	1.758451	2.366836	0.141169
31	6	0	1.828676	2.732064	1.632003
32	6	0	0.812118	3.279520	-0.648136
33	1	0	2.745457	2.527294	-0.278079
34	1	0	2.554219	2.099517	2.154899
35	1	0	2.154290	3.772760	1.740617
36	1	0	0.861097	2.637000	2.139064
37	1	0	0.843548	3.037264	-1.715937
38	1	0	-0.229178	3.242727	-0.311952
39	1	0	1.155672	4.313634	-0.533811



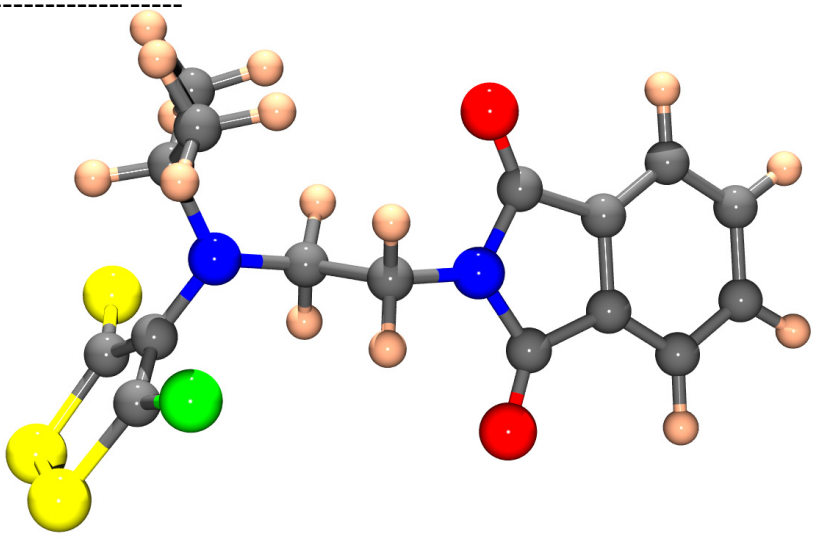
2a_rot4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.190847	-1.048288	0.221781
2	6	0	-4.450936	0.317817	0.089625
3	6	0	-5.687640	0.855468	0.413756
4	6	0	-6.671686	-0.026407	0.880631
5	6	0	-6.411021	-1.396192	1.013005
6	6	0	-5.157661	-1.929267	0.682764
7	6	0	-2.781754	-1.300273	-0.204910
8	6	0	-3.216107	0.980747	-0.425104
9	1	0	-5.878822	1.918855	0.307761

2a_rot4

10	1	0	-7.653127	0.356967	1.144972
11	1	0	-7.194263	-2.054524	1.377982
12	1	0	-4.944764	-2.989241	0.781411
13	8	0	-2.164272	-2.346040	-0.238111
14	8	0	-3.022607	2.155387	-0.673687
15	7	0	-2.272269	-0.046575	-0.583619
16	6	0	-0.916627	0.172978	-1.066042
17	1	0	-0.610171	-0.711876	-1.627912
18	1	0	-0.952494	1.028243	-1.743971
19	6	0	0.065613	0.441828	0.092601
20	1	0	-0.359088	1.208898	0.749794
21	1	0	0.158744	-0.470069	0.689428
22	7	0	1.397581	0.821615	-0.377652
23	6	0	2.478685	0.039984	0.053441
24	6	0	3.130919	0.269894	1.339349
25	6	0	2.981911	-1.002622	-0.686925
26	16	0	2.750469	1.399519	2.489672
27	16	0	4.476325	-0.816371	1.672033
28	16	0	4.314812	-1.966358	-0.109185
29	17	0	2.365751	-1.483349	-2.228361
30	6	0	1.705264	2.217501	-0.803459
31	6	0	0.738340	3.259544	-0.228873
32	6	0	1.798042	2.321324	-2.335159
33	1	0	2.696864	2.444348	-0.394270
34	1	0	0.737712	3.234168	0.864454
35	1	0	1.068302	4.255484	-0.543700
36	1	0	-0.289058	3.126932	-0.586224
37	1	0	2.508757	1.592470	-2.737051
38	1	0	0.825664	2.139976	-2.807024
39	1	0	2.133173	3.323386	-2.629432



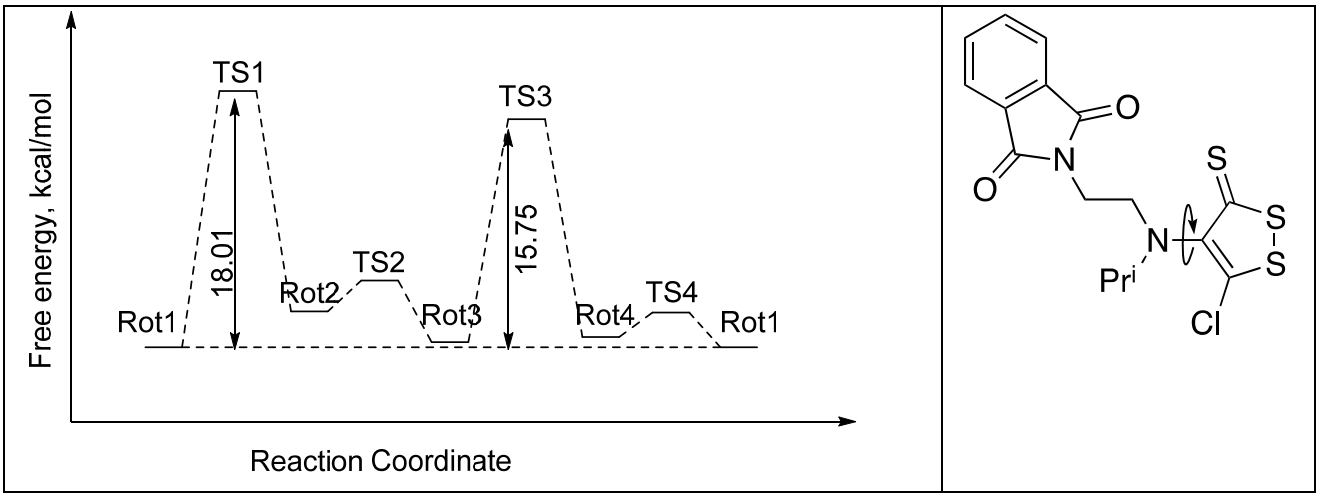
2a_TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.174657	-1.091889	-0.007441
2	6	0	-4.399013	0.285494	0.052211
3	6	0	-5.633850	0.804543	0.411788

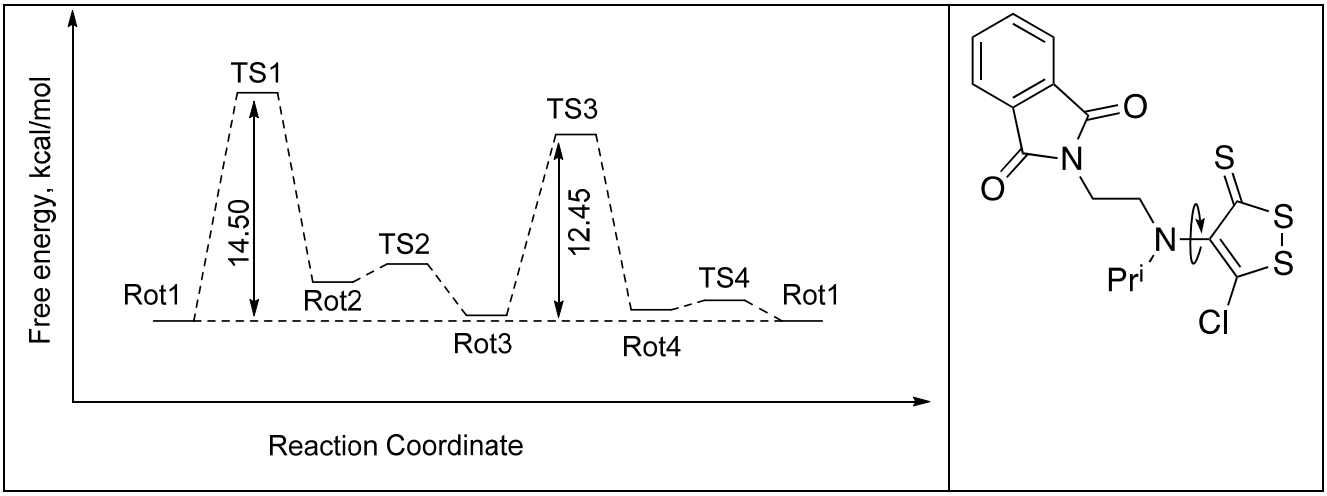
2a_TS4

4	6	0	-6.653515	-0.107962	0.714299
5	6	0	-6.428715	-1.489142	0.654354
6	6	0	-5.176901	-2.003219	0.289814
7	6	0	-2.757645	-1.318846	-0.422721
8	6	0	-3.131497	0.981136	-0.320516
9	1	0	-5.797012	1.876985	0.454993
10	1	0	-7.634718	0.260040	1.000527
11	1	0	-7.238971	-2.171506	0.895122
12	1	0	-4.991529	-3.071778	0.240556
13	8	0	-2.166971	-2.366592	-0.591886
14	8	0	-2.900148	2.173471	-0.387968
15	7	0	-2.206025	-0.037259	-0.596073
16	6	0	-0.828447	0.219665	-0.992247
17	1	0	-0.465112	-0.673178	-1.505550
18	1	0	-0.832651	1.055115	-1.695943
19	6	0	0.057843	0.553594	0.226709
20	1	0	-0.427311	1.341999	0.807402
21	1	0	0.114218	-0.325168	0.877115
22	7	0	1.409248	0.962404	-0.151522
23	6	0	2.445301	0.047379	0.082769
24	6	0	2.964546	-0.200709	1.425467
25	6	0	3.037911	-0.680715	-0.921317
26	16	0	2.480564	0.483185	2.854406
27	16	0	4.260404	-1.389871	1.493414
28	16	0	4.336079	-1.796320	-0.592807
29	17	0	2.578361	-0.593648	-2.585807
30	6	0	1.772239	2.401857	-0.293425
31	6	0	1.065672	3.319365	0.715933
32	6	0	1.555716	2.915204	-1.727350
33	1	0	2.846496	2.445073	-0.078919
34	1	0	1.184688	2.949932	1.738014
35	1	0	1.507328	4.320335	0.655808
36	1	0	-0.002728	3.423658	0.494443
37	1	0	2.088416	2.300186	-2.457594
38	1	0	0.491043	2.916100	-1.987982
39	1	0	1.917412	3.946710	-1.817440



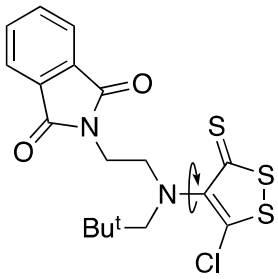
Calculated free energy values for the rotation of the 1,2-dithiole-3-thione ring in compound **2a**, level of theory: B3LYP/6-31G(d) (kcal/mol):

	Rot1	TS1	Rot2	TS2	Rot3	TS3	Rot4	TS4	Rot1
G	0	18.01	2.34	3.17	0.04	15.75	1.24	2.27	0

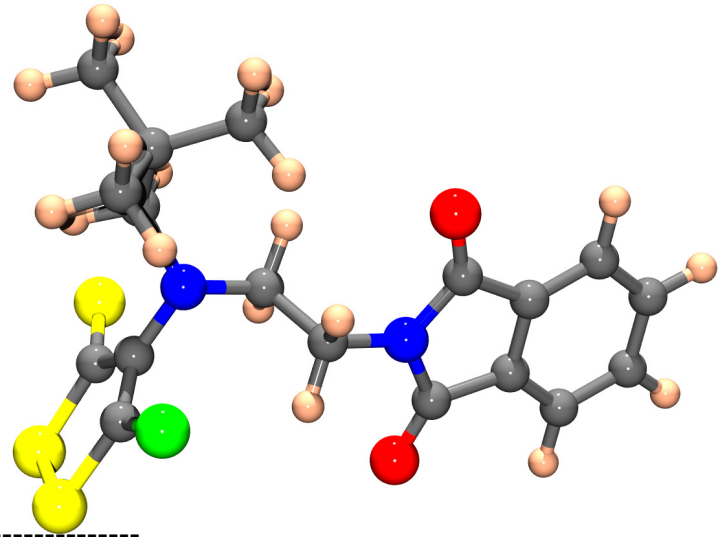


Calculated free energy values for the rotation of the 1,2-dithiole-3-thione ring in compound **2a** with solvation, level of theory: PCM/B3LYP/6-311++G(2d,p) (kcal/mol):

	Rot1	TS1	Rot2	TS2	Rot3	TS3	Rot4	TS4	Rot1
G	0	14.50	2.19	2.54	0.18	12.45	1.30	1.71	0



2b, rotation of the 1,2-dithiole-3-thione ring



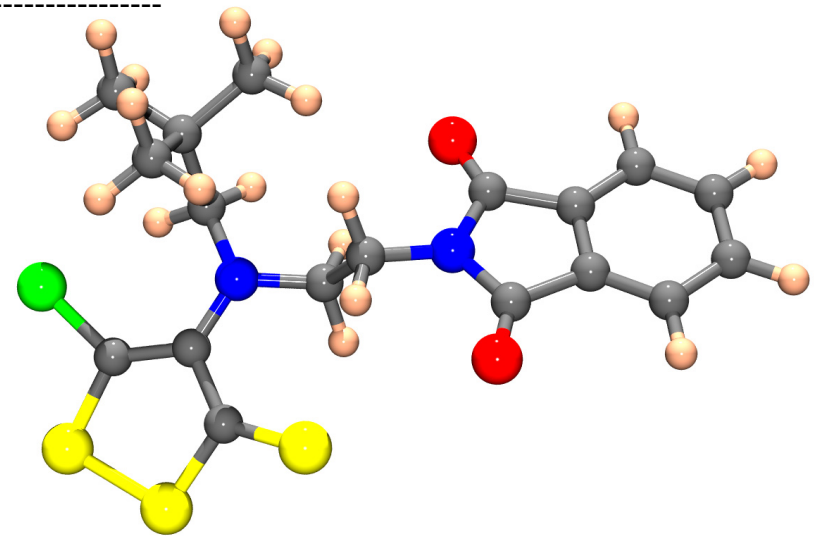
2b_rot1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.300950	-0.978452	-0.064883
2	6	0	-4.457823	0.409311	-0.054519
3	6	0	-5.690570	0.997979	0.185258
4	6	0	-6.777910	0.145236	0.418447
5	6	0	-6.620489	-1.246561	0.407861
6	6	0	-5.370569	-1.831220	0.163656
7	6	0	-2.867911	-1.286259	-0.350897
8	6	0	-3.128940	1.031941	-0.330961
9	1	0	-5.801511	2.077927	0.190763
10	1	0	-7.759601	0.568707	0.610956
11	1	0	-7.482432	-1.881468	0.592358
12	1	0	-5.236921	-2.908535	0.153057
13	8	0	-2.321564	-2.365907	-0.454199
14	8	0	-2.834491	2.209061	-0.410667
15	7	0	-2.235235	-0.037972	-0.494434
16	6	0	-0.818509	0.129870	-0.784789
17	1	0	-0.474277	-0.813414	-1.215022
18	1	0	-0.708958	0.919859	-1.532027
19	6	0	-0.020377	0.484378	0.480072
20	1	0	-0.413083	1.416714	0.889069
21	1	0	-0.172563	-0.295666	1.238015
22	7	0	1.410264	0.689575	0.189044
23	6	0	2.156544	-0.511318	0.105734
24	6	0	2.521533	-1.289819	1.285572
25	6	0	2.569575	-1.033073	-1.095846
26	16	0	2.184129	-0.981914	2.878994
27	16	0	3.449994	-2.746849	0.930609
28	16	0	3.478989	-2.518778	-1.176010
29	17	0	2.253607	-0.321405	-2.638318
30	6	0	2.071860	1.801293	0.917806
31	1	0	1.600346	1.929504	1.900926
32	1	0	3.105145	1.495986	1.113164
33	6	0	2.110865	3.174017	0.194149
34	6	0	2.862158	3.070723	-1.143003
35	6	0	0.698484	3.737315	-0.048006
36	6	0	2.873649	4.133141	1.132148

2b_rot1

37	1	0	2.947283	4.057516	-1.613962
38	1	0	3.878828	2.682045	-1.000659
39	1	0	2.341641	2.407594	-1.838617
40	1	0	0.140010	3.842643	0.890632
41	1	0	0.760307	4.732670	-0.504727
42	1	0	0.107265	3.107372	-0.719939
43	1	0	2.940413	5.133443	0.688671
44	1	0	2.370116	4.231644	2.101834
45	1	0	3.896376	3.782524	1.319276



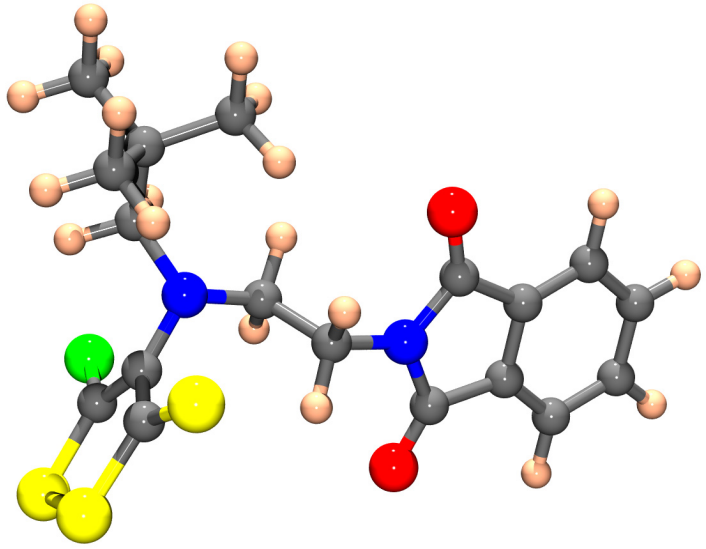
2b_TS1

Standard orientation:

2b_TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.580507	-0.770122	0.204024
2	6	0	4.548929	0.471935	-0.431818
3	6	0	5.679740	1.012531	-1.026301
4	6	0	6.860992	0.261436	-0.964898
5	6	0	6.892868	-0.984961	-0.326036
6	6	0	5.744752	-1.520899	0.272407
7	6	0	3.218020	-1.057285	0.744183
8	6	0	3.163768	1.015526	-0.322015
9	1	0	5.643891	1.980376	-1.516839
10	1	0	7.768042	0.650529	-1.418777
11	1	0	7.824259	-1.543198	-0.294343
12	1	0	5.758055	-2.484737	0.771785
13	8	0	2.843636	-2.014817	1.387145
14	8	0	2.727440	2.077578	-0.727664
15	7	0	2.421740	0.045949	0.367845
16	6	0	1.016243	0.204731	0.727666
17	1	0	0.779822	-0.587049	1.437408
18	1	0	0.892959	1.170388	1.219957
19	6	0	0.109746	0.109833	-0.516993
20	1	0	0.486938	0.814361	-1.262512
21	1	0	0.193746	-0.888109	-0.941461
22	7	0	-1.309441	0.455730	-0.276257
23	6	0	-2.296101	-0.539642	-0.263283
24	6	0	-1.959946	-1.957081	0.020881

25	6	0	-3.675491	-0.382310	-0.416839
26	16	0	-0.603576	-2.700520	0.645715
27	16	0	-3.230149	-3.121048	-0.275562
28	16	0	-4.770991	-1.739863	-0.588364
29	17	0	-4.665518	1.065670	-0.404819
30	6	0	-1.637339	1.859154	-0.633259
31	1	0	-0.908331	2.170141	-1.388739
32	1	0	-2.593817	1.867886	-1.143960
33	6	0	-1.645308	2.955760	0.495752
34	6	0	-2.012673	2.370868	1.869809
35	6	0	-0.279395	3.672585	0.569485
36	6	0	-2.685760	4.025187	0.094334
37	1	0	-2.041783	3.169357	2.620850
38	1	0	-2.997269	1.891270	1.857738
39	1	0	-1.283618	1.624847	2.201676
40	1	0	-0.062224	4.191103	-0.372541
41	1	0	-0.287776	4.424830	1.367349
42	1	0	0.559285	2.998839	0.755004
43	1	0	-2.637130	4.880876	0.777842
44	1	0	-2.494451	4.403319	-0.918260
45	1	0	-3.707359	3.634172	0.121574



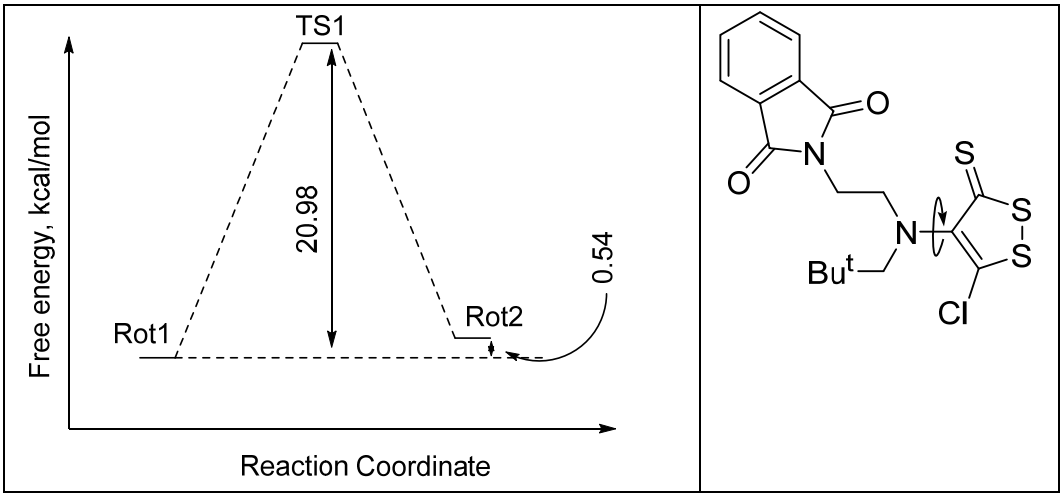
2b_rot2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.315760	-0.961927	0.055301
2	6	0	-4.471798	0.411361	-0.145473
3	6	0	-5.711157	1.024363	-0.036224
4	6	0	-6.806715	0.211271	0.283755
5	6	0	-6.650288	-1.166078	0.485070
6	6	0	-5.393313	-1.775402	0.372788
7	6	0	-2.874258	-1.302820	-0.136815
8	6	0	-3.134070	0.991328	-0.469429
9	1	0	-5.821012	2.092677	-0.195284
10	1	0	-7.794175	0.654350	0.377179

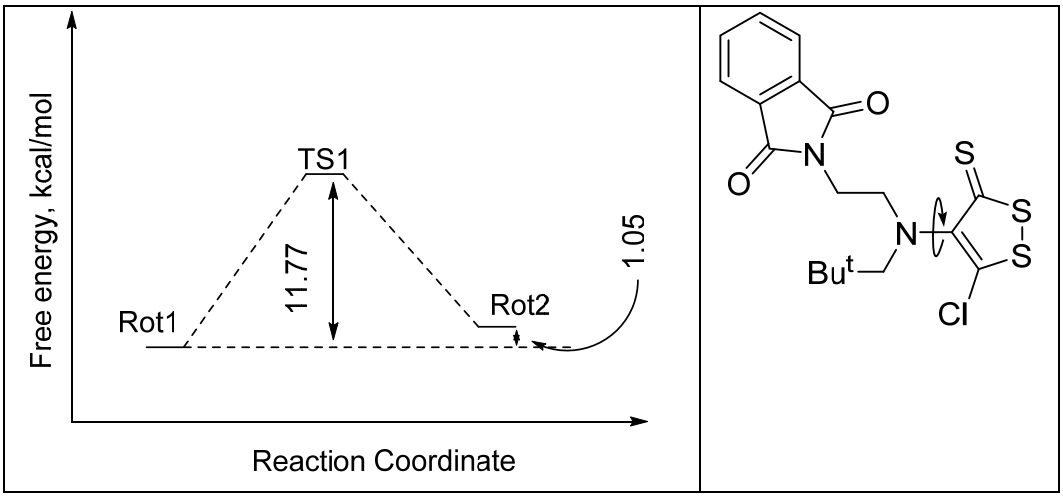
2b_rot2

11	1	0	-7.518815	-1.770292	0.731530
12	1	0	-5.260758	-2.842027	0.525687
13	8	0	-2.324622	-2.382703	-0.051402
14	8	0	-2.835082	2.146012	-0.704077
15	7	0	-2.237908	-0.089483	-0.451839
16	6	0	-0.816673	0.034989	-0.746706
17	1	0	-0.476209	-0.943777	-1.089945
18	1	0	-0.691942	0.752526	-1.559789
19	6	0	-0.035118	0.497292	0.492910
20	1	0	-0.439393	1.460406	0.808966
21	1	0	-0.210423	-0.219029	1.311226
22	7	0	1.400341	0.688540	0.232729
23	6	0	2.142133	-0.501886	0.053822
24	6	0	2.499084	-0.955421	-1.286875
25	6	0	2.568866	-1.310682	1.080015
26	16	0	2.142057	-0.281802	-2.755845
27	16	0	3.443503	-2.439429	-1.317492
28	16	0	3.523826	-2.740022	0.787054
29	17	0	2.232605	-1.008047	2.753701
30	6	0	2.055183	1.776062	0.996011
31	1	0	1.537734	1.911520	1.957298
32	1	0	3.073209	1.450898	1.236026
33	6	0	2.156516	3.152762	0.285368
34	6	0	3.030128	3.044219	-0.975191
35	6	0	0.770443	3.706608	-0.089911
36	6	0	2.825149	4.112916	1.290979
37	1	0	3.127175	4.022725	-1.461172
38	1	0	4.041526	2.695495	-0.728391
39	1	0	2.597946	2.345039	-1.696317
40	1	0	0.123327	3.809461	0.790803
41	1	0	0.869895	4.701981	-0.539222
42	1	0	0.256401	3.070136	-0.816688
43	1	0	2.941864	5.109816	0.850527
44	1	0	2.226955	4.221517	2.204714
45	1	0	3.822730	3.759799	1.581692



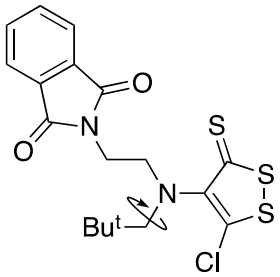
Calculated free energy values for the rotation of the 1,2-dithiole-3-thione ring in compound **2b**, level of theory: B3LYP/6-31G(d) (kcal/mol):

	Rot1	TS1	Rot2
G	0	20,98	0,54



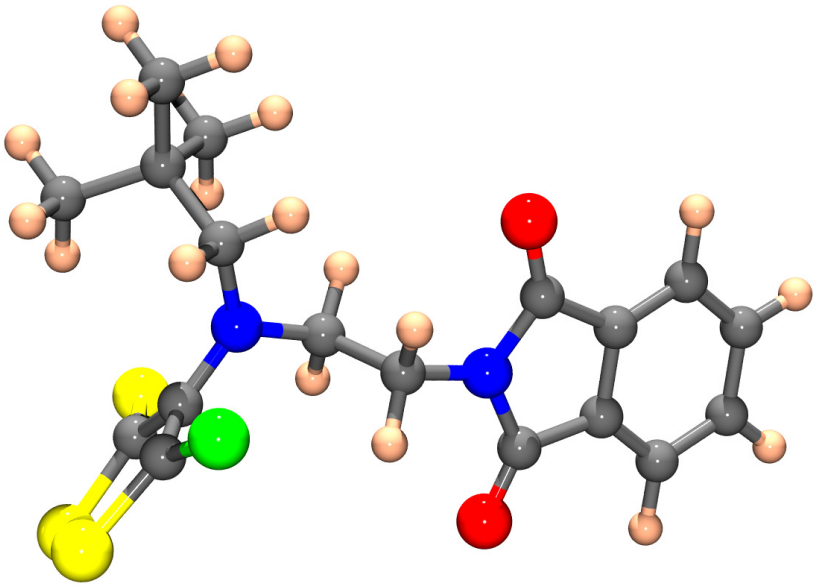
Calculated free energy values for the rotation of the 1,2-dithiole-3-thione ring in compound **2b** with solvation, level of theory: PCM/B3LYP/6-311++G(2d,p) (kcal/mol):

	Rot1	TS1	Rot2
G	0	11,77	1,05



2b, rotation of the neopentyl group

2b_rot3

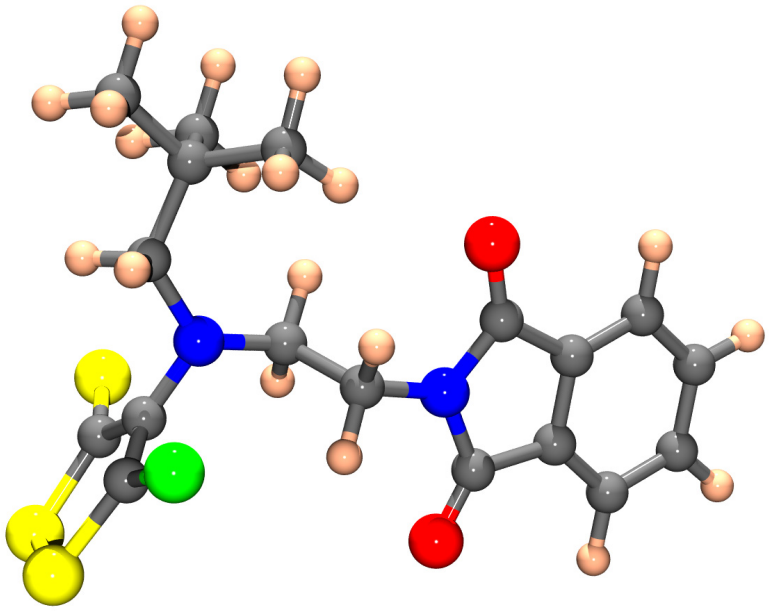


2b_rot3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.446099	-0.943510	0.049390
2	6	0	-4.583717	0.429521	-0.167793
3	6	0	-5.801465	1.071923	-0.000562
4	6	0	-6.894212	0.289375	0.396199
5	6	0	-6.756266	-1.087371	0.613922
6	6	0	-5.521167	-1.726887	0.441753
7	6	0	-3.025228	-1.320442	-0.214976
8	6	0	-3.254154	0.973759	-0.574852
9	1	0	-5.897110	2.139690	-0.171883
10	1	0	-7.864675	0.756422	0.538192
11	1	0	-7.621780	-1.667246	0.921702
12	1	0	-5.402790	-2.793128	0.608113
13	8	0	-2.494516	-2.410473	-0.144820
14	8	0	-2.941716	2.116048	-0.850800
15	7	0	-2.381797	-0.126117	-0.586124
16	6	0	-0.968341	-0.027751	-0.917675
17	1	0	-0.645561	-1.015354	-1.255769
18	1	0	-0.868202	0.681174	-1.744120
19	6	0	-0.131168	0.433562	0.295289
20	1	0	-0.541432	1.371804	0.677286
21	1	0	-0.213385	-0.304511	1.097200
22	7	0	1.279174	0.638161	-0.030467
23	6	0	2.132572	-0.466264	-0.005423
24	6	0	2.492732	-1.091942	1.268779
25	6	0	2.686023	-1.059011	-1.119335
26	16	0	2.009027	-0.677625	2.798339
27	16	0	3.578723	-2.465158	1.120411
28	16	0	3.840011	-2.359867	-0.983686
29	17	0	2.313463	-0.608088	-2.751274
30	6	0	1.672129	1.908231	-0.658692
31	1	0	2.391580	1.714854	-1.460601
32	1	0	0.779739	2.325728	-1.142019
33	6	0	2.279912	2.989297	0.278505

34	6	0	1.322411	3.329585	1.433803
35	6	0	3.628984	2.514693	0.847693
36	6	0	2.506678	4.243932	-0.588590
37	1	0	1.748333	4.120707	2.062769
38	1	0	0.355517	3.690301	1.059905
39	1	0	1.147164	2.456292	2.070330
40	1	0	4.333837	2.258759	0.045831
41	1	0	4.089187	3.305729	1.452030
42	1	0	3.505485	1.638773	1.491770
43	1	0	2.951695	5.048948	0.007685
44	1	0	3.185791	4.037489	-1.425882
45	1	0	1.564029	4.620338	-1.005411



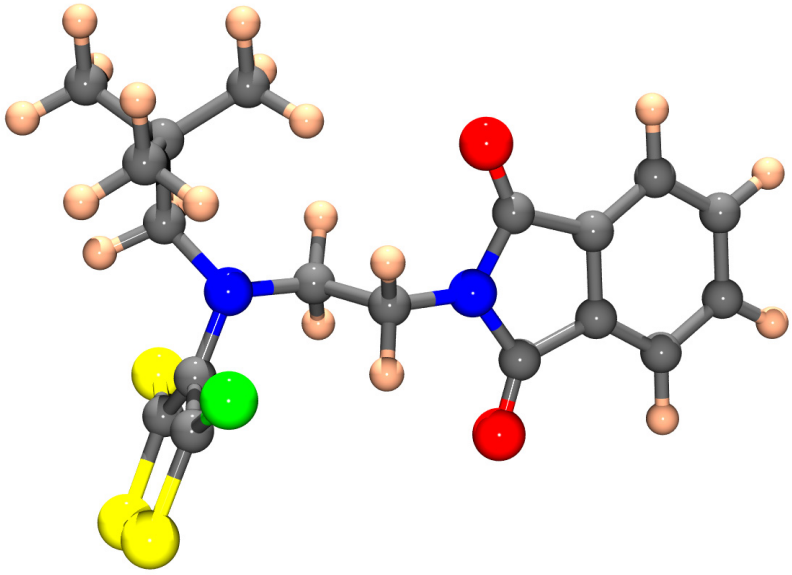
2b_TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.190142	-1.170096	-0.035612
2	6	0	-4.411644	0.208419	-0.062588
3	6	0	-5.658442	0.748726	0.214987
4	6	0	-6.693176	-0.144101	0.524916
5	6	0	-6.471140	-1.526805	0.551975
6	6	0	-5.207150	-2.062265	0.269634
7	6	0	-2.758248	-1.420479	-0.377896
8	6	0	-3.127112	0.880539	-0.419154
9	1	0	-5.819307	1.822112	0.191290
10	1	0	-7.684183	0.240641	0.748485
11	1	0	-7.293282	-2.193472	0.796368
12	1	0	-5.023726	-3.132116	0.288056
13	8	0	-2.165521	-2.476412	-0.468070
14	8	0	-2.895833	2.069016	-0.542938
15	7	0	-2.193168	-0.149627	-0.595892
16	6	0	-0.796125	0.069572	-0.948052
17	1	0	-0.421692	-0.875754	-1.347126
18	1	0	-0.751477	0.827692	-1.734236

2b_TS3

19	6	0	0.040064	0.512246	0.271485
20	1	0	-0.359483	1.448029	0.653943
21	1	0	-0.078688	-0.229296	1.070755
22	7	0	1.452500	0.667706	-0.056060
23	6	0	2.244752	-0.483962	0.045724
24	6	0	2.626400	-1.032257	1.343061
25	6	0	2.758198	-1.134792	-1.049030
26	16	0	2.238681	-0.455225	2.846040
27	16	0	3.627578	-2.478366	1.245278
28	16	0	3.786646	-2.531438	-0.874942
29	17	0	2.460200	-0.643977	-2.680138
30	6	0	2.239549	1.923868	-0.126412
31	1	0	3.054145	1.841531	0.606978
32	1	0	2.710982	1.960787	-1.119459
33	6	0	1.577136	3.307928	0.105036
34	6	0	0.447340	3.612845	-0.900606
35	6	0	1.103277	3.500878	1.560599
36	6	0	2.714299	4.328112	-0.148991
37	1	0	0.169637	4.671952	-0.835691
38	1	0	0.782198	3.424809	-1.928725
39	1	0	-0.466169	3.037679	-0.730460
40	1	0	1.926252	3.323962	2.262752
41	1	0	0.750711	4.529145	1.705914
42	1	0	0.286170	2.833033	1.844748
43	1	0	2.353078	5.347336	0.028306
44	1	0	3.567044	4.155280	0.518550
45	1	0	3.076406	4.277083	-1.182845



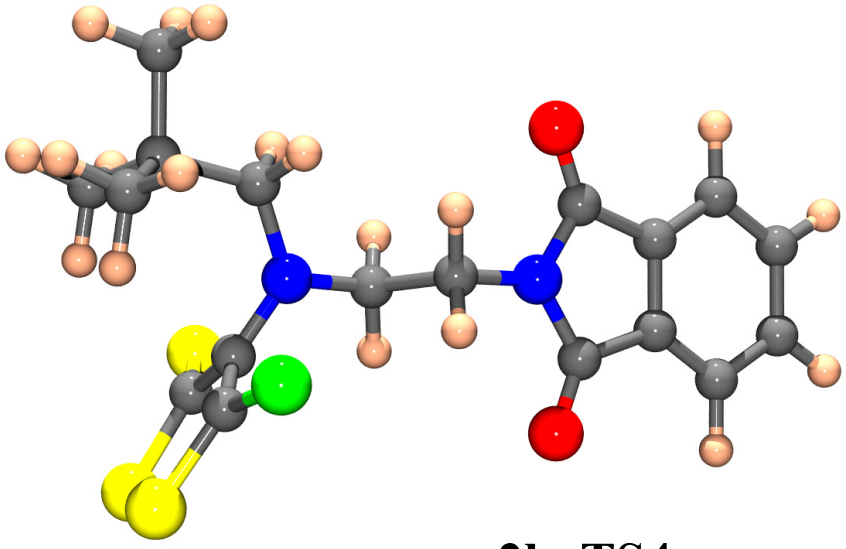
2b_rot4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.286238	-1.028324	-0.057063
2	6	0	-4.461416	0.357261	-0.068363

2b_rot4

3	6	0	-5.702857	0.933382	0.156477
4	6	0	-6.780158	0.070089	0.397239
5	6	0	-6.604487	-1.319506	0.408496
6	6	0	-5.345838	-1.891430	0.179204
7	6	0	-2.847820	-1.321154	-0.332272
8	6	0	-3.139761	0.993141	-0.348510
9	1	0	-5.827828	2.011750	0.144979
10	1	0	-7.768276	0.483496	0.578399
11	1	0	-7.459018	-1.962795	0.598354
12	1	0	-5.198275	-2.966959	0.185467
13	8	0	-2.286196	-2.394561	-0.416923
14	8	0	-2.861575	2.173050	-0.445383
15	7	0	-2.231275	-0.066901	-0.492277
16	6	0	-0.816003	0.116361	-0.780153
17	1	0	-0.464893	-0.811105	-1.238547
18	1	0	-0.714529	0.928706	-1.503970
19	6	0	-0.013163	0.438489	0.490890
20	1	0	-0.419833	1.344442	0.943294
21	1	0	-0.139682	-0.374057	1.218280
22	7	0	1.408659	0.682518	0.188593
23	6	0	2.187270	-0.497208	0.100158
24	6	0	2.572432	-1.271215	1.276276
25	6	0	2.620104	-0.997628	-1.103334
26	16	0	2.227397	-0.979340	2.871059
27	16	0	3.539231	-2.701524	0.914463
28	16	0	3.571959	-2.456148	-1.190467
29	17	0	2.293130	-0.279925	-2.640314
30	6	0	2.052775	1.813773	0.901583
31	1	0	1.645305	1.894986	1.917988
32	1	0	3.111447	1.557642	1.015346
33	6	0	1.976034	3.204724	0.215362
34	6	0	2.579920	3.158780	-1.197321
35	6	0	0.533100	3.740130	0.144155
36	6	0	2.810963	4.159481	1.095303
37	1	0	2.591364	4.160665	-1.643425
38	1	0	3.613814	2.790681	-1.178476
39	1	0	2.001313	2.502159	-1.852162
40	1	0	0.074553	3.788708	1.140030
41	1	0	0.528363	4.756720	-0.267667
42	1	0	-0.115274	3.130879	-0.493161
43	1	0	2.789896	5.176642	0.687223
44	1	0	2.422224	4.203779	2.120281
45	1	0	3.860056	3.842468	1.147689

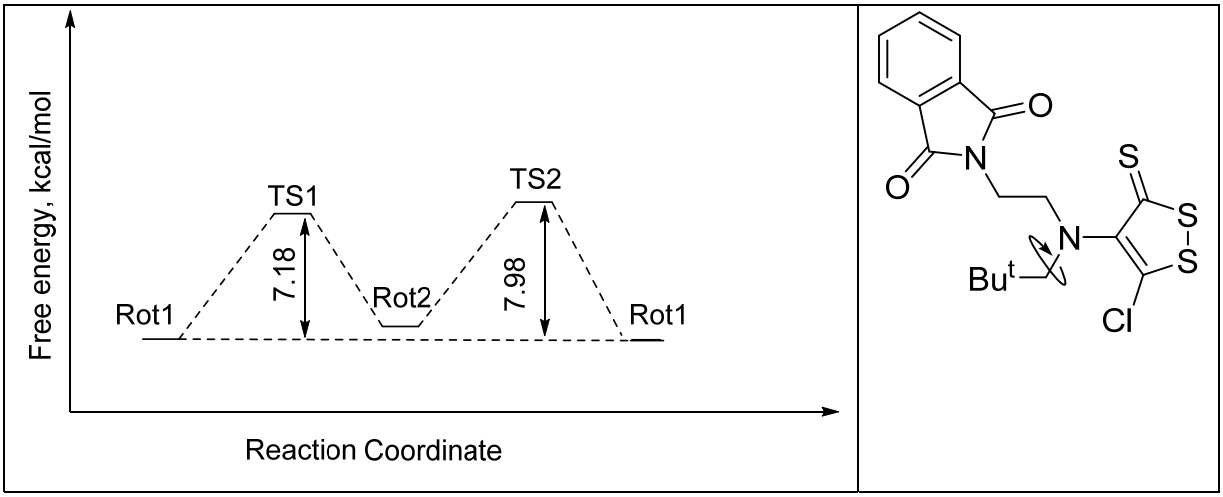


2b_TS4

Standard orientation:

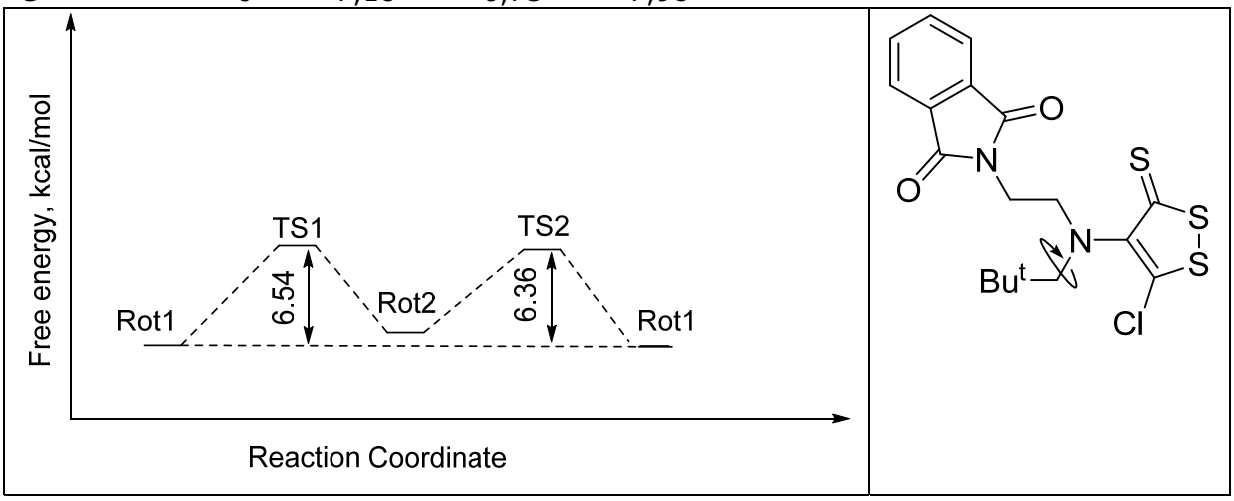
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.588410	-0.775025	-0.155811
2	6	0	-4.765642	0.595479	0.047124
3	6	0	-5.992443	1.119884	0.425980
4	6	0	-7.052650	0.219977	0.599284
5	6	0	-6.874886	-1.154416	0.395729
6	6	0	-5.631088	-1.673939	0.012361
7	6	0	-3.167514	-1.009432	-0.551656
8	6	0	-3.464268	1.279980	-0.214642
9	1	0	-6.118926	2.186955	0.580868
10	1	0	-8.028878	0.592474	0.896519
11	1	0	-7.715939	-1.827052	0.538216
12	1	0	-5.482050	-2.737242	-0.148202
13	8	0	-2.605938	-2.054296	-0.815336
14	8	0	-3.193490	2.462883	-0.152317
15	7	0	-2.565622	0.259897	-0.570736
16	6	0	-1.165782	0.486726	-0.898931
17	1	0	-0.882498	-0.226914	-1.676199
18	1	0	-1.091340	1.500435	-1.299461
19	6	0	-0.255804	0.315967	0.336173
20	1	0	-0.615259	0.972964	1.140015
21	1	0	-0.341973	-0.712303	0.696336
22	7	0	1.145629	0.607876	0.037718
23	6	0	2.040306	-0.462547	0.085873
24	6	0	2.386257	-1.115208	1.347816
25	6	0	2.552261	-1.057339	-1.044166
26	16	0	1.861354	-0.731713	2.869868
27	16	0	3.482364	-2.482135	1.176617
28	16	0	3.660713	-2.397542	-0.943237
29	17	0	2.152329	-0.567147	-2.652317
30	6	0	1.478277	2.050906	0.037629
31	1	0	1.016624	2.502065	-0.853242
32	1	0	0.956882	2.484015	0.904222
33	6	0	2.937959	2.579772	0.091413
34	6	0	3.695347	2.133481	1.355482

35	6	0	3.759194	2.227270	-1.163443
36	6	0	2.788274	4.119755	0.140747
37	1	0	4.638415	2.687394	1.438001
38	1	0	3.110603	2.322885	2.262215
39	1	0	3.943405	1.069475	1.338692
40	1	0	3.222242	2.491570	-2.082000
41	1	0	4.704639	2.782921	-1.157855
42	1	0	4.010905	1.165025	-1.211082
43	1	0	3.775461	4.594494	0.166892
44	1	0	2.257211	4.502215	-0.739316
45	1	0	2.239053	4.441499	1.033379



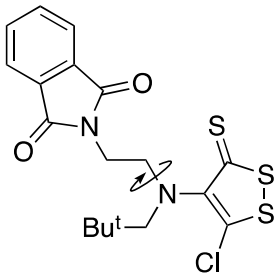
Calculated free energy values for the rotation of the neopentil group in compound **2b**, level of theory: B3LYP/6-31G(d) (kcal/mol):

	2b_rot3	2b_TS3	2b_rot4	2b_TS4
G	0	7,18	0,73	7,98

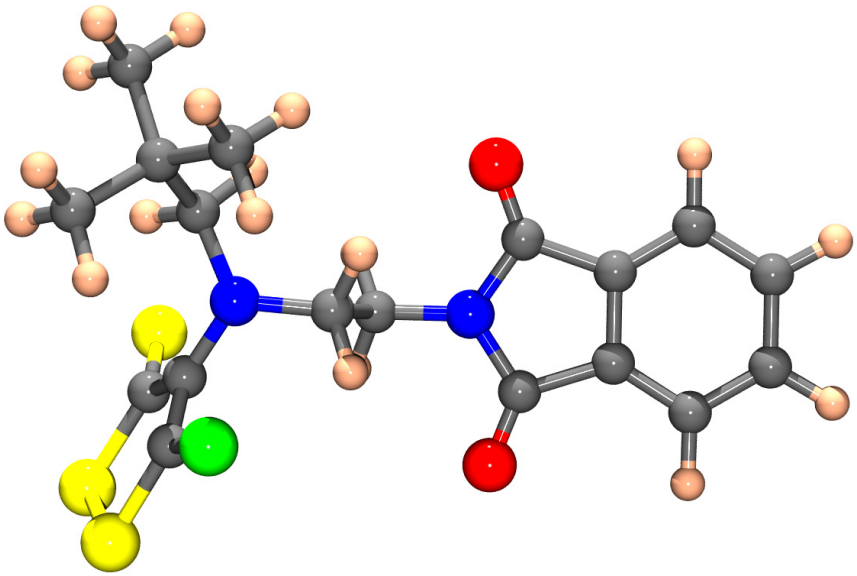


Calculated free energy values for the rotation of the neopentil group in compound **2b** with solvatation, level of theory: PCM/B3LYP/6-311++G(2d,p) (kcal/mol):

	2b_rot3	2b_TS3	2b_rot4	2b_TS4
G	0	6,54	0,56	6,36



2b, rotation of the phthalimidoethyl group



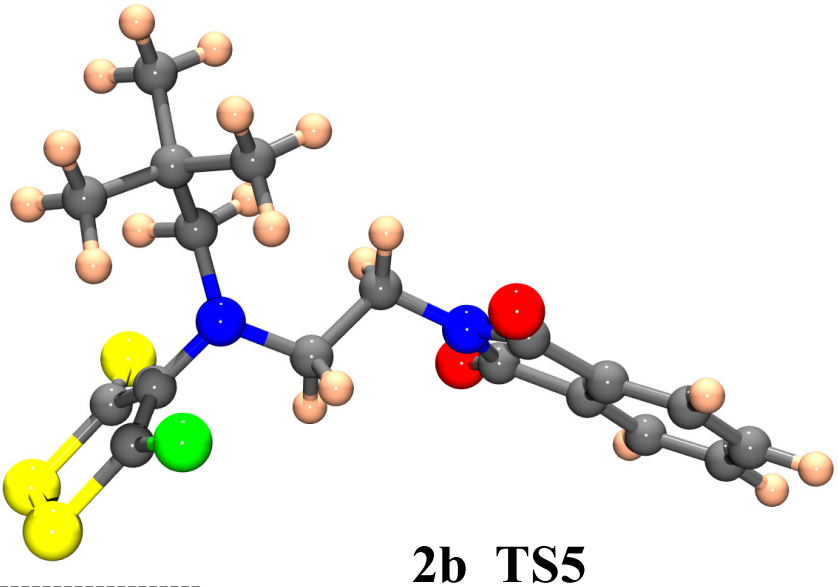
2b_rot5

2b_rot5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.579398	0.415430	0.235355
2	6	0	-4.401232	-0.918507	-0.138630
3	6	0	-5.456923	-1.688588	-0.603384
4	6	0	-6.715292	-1.076858	-0.683504
5	6	0	-6.893997	0.260638	-0.307987
6	6	0	-5.820232	1.030355	0.159530
7	6	0	-3.260827	0.955832	0.682444
8	6	0	-2.963406	-1.272290	0.059167
9	1	0	-5.306835	-2.724478	-0.891513
10	1	0	-7.567086	-1.647668	-1.042309
11	1	0	-7.881728	0.706936	-0.381071
12	1	0	-5.947566	2.067748	0.453214
13	8	0	-2.980697	2.072468	1.072259
14	8	0	-2.395335	-2.324474	-0.156690
15	7	0	-2.354541	-0.110813	0.563546
16	6	0	-0.939668	-0.009290	0.893184
17	1	0	-0.840896	0.706065	1.712413
18	1	0	-0.607054	-0.989008	1.242660
19	6	0	-0.113846	0.443408	-0.330490
20	1	0	-0.215558	-0.306205	-1.121477
21	1	0	-0.533121	1.377264	-0.715939
22	7	0	1.304078	0.663483	-0.046253
23	6	0	2.138648	-0.457854	0.036904
24	6	0	2.598667	-1.022578	1.304151
25	6	0	2.544190	-1.145019	-1.086839
26	16	0	2.235892	-0.555880	2.854525
27	16	0	3.680556	-2.400700	1.127750
28	16	0	3.529207	-2.577159	-0.979865
29	17	0	2.117425	-0.686515	-2.699122

30	6	0	1.688761	1.932922	0.593900
31	1	0	0.796228	2.349356	1.077020
32	1	0	2.399367	1.729102	1.399314
33	6	0	2.298927	3.011740	-0.342599
34	6	0	3.645030	2.532525	-0.915430
35	6	0	1.340429	3.360964	-1.494551
36	6	0	2.535479	4.265262	0.523359
37	1	0	4.348763	2.271573	-0.114873
38	1	0	3.518986	1.654951	-1.557180
39	1	0	4.108700	3.320540	-1.521229
40	1	0	0.378561	3.730539	-1.116818
41	1	0	1.769391	4.146320	-2.128761
42	1	0	1.149157	2.489195	-2.129381
43	1	0	2.981271	5.069743	-0.073468
44	1	0	1.596292	4.644060	0.945327
45	1	0	3.216030	4.053344	1.357505



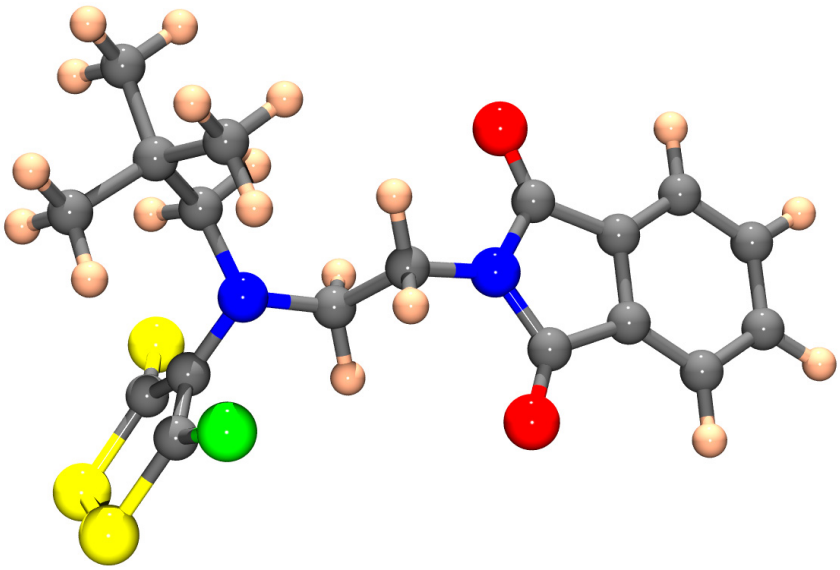
2b_TS5

Standard orientation:

2b_TS5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.533340	0.198183	0.560225
2	6	0	4.529116	-0.685496	-0.521316
3	6	0	5.622128	-1.491301	-0.803829
4	6	0	6.735587	-1.386475	0.040479
5	6	0	6.739867	-0.500077	1.125171
6	6	0	5.630528	0.310261	1.401352
7	6	0	3.222348	0.912013	0.587342
8	6	0	3.216016	-0.564185	-1.222310
9	1	0	5.608227	-2.174078	-1.647728
10	1	0	7.610838	-2.001747	-0.147792
11	1	0	7.618345	-0.441326	1.761506
12	1	0	5.622995	1.001266	2.238632
13	8	0	2.825221	1.760909	1.360715
14	8	0	2.815438	-1.148119	-2.208193
15	7	0	2.492834	0.404137	-0.501338

16	6	0	1.150958	0.847090	-0.851211
17	1	0	1.089932	1.912442	-0.620253
18	1	0	1.035077	0.695783	-1.926639
19	6	0	0.108655	0.043792	-0.058705
20	1	0	0.216718	-1.008020	-0.355785
21	1	0	0.374527	0.119326	1.003620
22	7	0	-1.295795	0.464033	-0.247372
23	6	0	-2.222413	-0.532612	0.092144
24	6	0	-2.777982	-1.450144	-0.899792
25	6	0	-2.581864	-0.788932	1.394237
26	16	0	-2.447170	-1.545040	-2.520128
27	16	0	-3.929933	-2.610263	-0.239840
28	16	0	-3.675955	-2.083954	1.801214
29	17	0	-1.987452	0.106770	2.748400
30	6	0	-1.711577	1.513123	-1.193487
31	1	0	-0.880631	1.727053	-1.870811
32	1	0	-2.508310	1.115507	-1.831026
33	6	0	-2.204002	2.853458	-0.576099
34	6	0	-3.508307	2.643077	0.214779
35	6	0	-1.137307	3.475961	0.339788
36	6	0	-2.486035	3.804427	-1.756914
37	1	0	-4.281902	2.177841	-0.409289
38	1	0	-3.351719	2.009647	1.092580
39	1	0	-3.901700	3.603553	0.569465
40	1	0	-0.227616	3.731774	-0.217992
41	1	0	-1.509762	4.402361	0.793562
42	1	0	-0.859488	2.793961	1.150083
43	1	0	-2.852933	4.772282	-1.395659
44	1	0	-1.580039	3.991344	-2.347153
45	1	0	-3.245809	3.391578	-2.432412



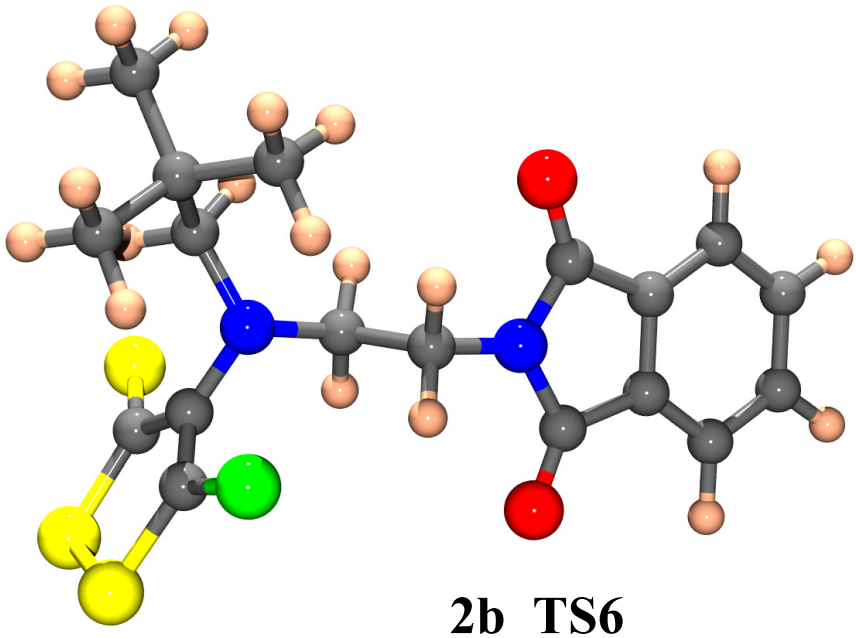
2b_rot6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.485412	-0.871039	-0.344170
2	6	0	-4.684852	0.349680	0.304686

2b_rot6

3	6	0	-5.906816	0.678131	0.872573
4	6	0	-6.938809	-0.264517	0.771649
5	6	0	-6.738869	-1.488729	0.120978
6	6	0	-5.500181	-1.810542	-0.449906
7	6	0	-3.075913	-0.914870	-0.835934
8	6	0	-3.410186	1.125374	0.245462
9	1	0	-6.050670	1.629769	1.374820
10	1	0	-7.910365	-0.044158	1.204802
11	1	0	-7.558384	-2.199146	0.059341
12	1	0	-5.333879	-2.756312	-0.956329
13	8	0	-2.500585	-1.797618	-1.441704
14	8	0	-3.162419	2.229705	0.687252
15	7	0	-2.503748	0.309649	-0.454204
16	6	0	-1.124472	0.683656	-0.730171
17	1	0	-0.868889	0.342850	-1.736278
18	1	0	-1.080783	1.774157	-0.702913
19	6	0	-0.157539	0.070547	0.296354
20	1	0	-0.501154	0.310358	1.312048
21	1	0	-0.186962	-1.017258	0.189954
22	7	0	1.228008	0.526367	0.081867
23	6	0	2.197157	-0.496191	0.187289
24	6	0	2.674241	-1.015997	1.463152
25	6	0	2.687091	-1.130940	-0.928383
26	16	0	2.195745	-0.612072	2.998475
27	16	0	3.909482	-2.267334	1.310902
28	16	0	3.865305	-2.408701	-0.804128
29	17	0	2.195001	-0.765391	-2.542823
30	6	0	1.562209	1.849596	0.659972
31	1	0	0.614998	2.286137	0.996470
32	1	0	2.175041	1.724220	1.560470
33	6	0	2.260055	2.875069	-0.273182
34	6	0	3.664606	2.394644	-0.684944
35	6	0	1.418202	3.156176	-1.528680
36	6	0	2.403541	4.174899	0.545878
37	1	0	4.276267	2.151118	0.192749
38	1	0	3.621109	1.510341	-1.327292
39	1	0	4.186848	3.179561	-1.245494
40	1	0	0.437219	3.571745	-1.264973
41	1	0	1.920543	3.886031	-2.175165
42	1	0	1.258871	2.243255	-2.110671
43	1	0	2.896218	4.953435	-0.048272
44	1	0	1.425459	4.561979	0.857628
45	1	0	3.004867	4.014782	1.449340

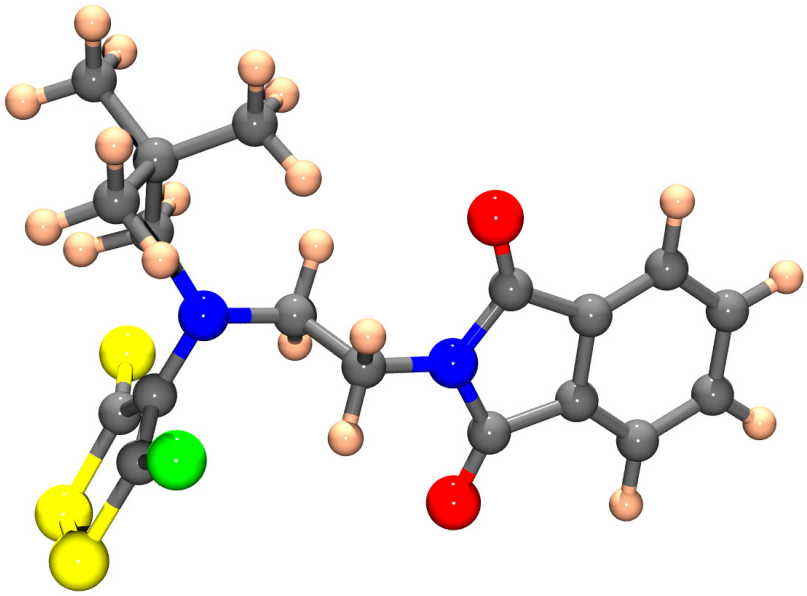


2b_TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.418277	-0.903600	-0.230287
2	6	0	-4.593116	0.431198	0.142450
3	6	0	-5.819315	0.906474	0.583098
4	6	0	-6.881523	-0.005824	0.641042
5	6	0	-6.706142	-1.344261	0.267276
6	6	0	-5.462929	-1.814271	-0.177050
7	6	0	-2.997052	-1.090562	-0.650203
8	6	0	-3.288373	1.138230	-0.026041
9	1	0	-5.943875	1.945846	0.870844
10	1	0	-7.857359	0.328464	0.981791
11	1	0	-7.548627	-2.027735	0.323849
12	1	0	-5.315732	-2.849487	-0.469044
13	8	0	-2.438309	-2.095925	-1.041624
14	8	0	-3.010882	2.301518	0.192133
15	7	0	-2.392541	0.169985	-0.507982
16	6	0	-0.990676	0.440026	-0.795861
17	1	0	-0.675520	-0.259648	-1.572319
18	1	0	-0.920127	1.458597	-1.181504
19	6	0	-0.122699	0.283486	0.466655
20	1	0	-0.520755	0.939968	1.247020
21	1	0	-0.218248	-0.744203	0.834861
22	7	0	1.296693	0.610423	0.237944
23	6	0	2.152577	-0.509230	0.173591
24	6	0	2.591190	-1.213982	1.374964
25	6	0	2.574521	-1.052128	-1.015079
26	16	0	2.188232	-0.906049	2.952415
27	16	0	3.670030	-2.571871	1.061897
28	16	0	3.617222	-2.448551	-1.055083
29	17	0	2.134491	-0.454644	-2.576303
30	6	0	1.834691	1.826479	0.892243
31	1	0	1.046880	2.215881	1.546729
32	1	0	2.663719	1.544993	1.551686

33	6	0	2.316138	2.982560	-0.024955
34	6	0	3.600617	2.594022	-0.779406
35	6	0	1.226330	3.398672	-1.026652
36	6	0	2.629886	4.170394	0.908626
37	1	0	4.397864	2.305475	-0.082691
38	1	0	3.430361	1.760750	-1.467016
39	1	0	3.969438	3.439486	-1.373002
40	1	0	0.287829	3.653553	-0.517774
41	1	0	1.543773	4.279487	-1.597970
42	1	0	1.019683	2.595620	-1.740985
43	1	0	3.020415	5.019318	0.335362
44	1	0	1.732353	4.510748	1.439661
45	1	0	3.383241	3.901664	1.659733



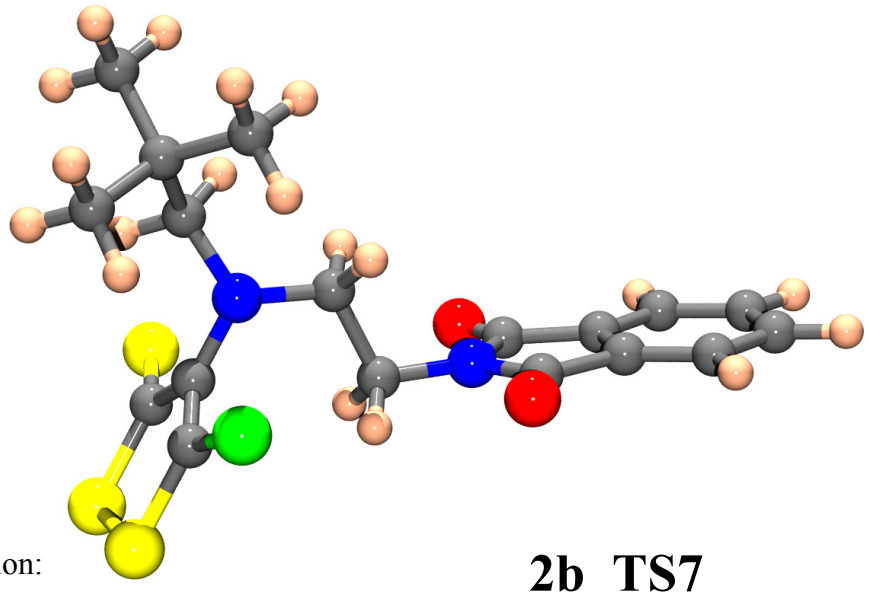
2b_rot7

Standard orientation:

2b_rot7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.301188	-0.978042	-0.064245
2	6	0	-4.457862	0.409753	-0.055022
3	6	0	-5.690581	0.998792	0.183981
4	6	0	-6.778103	0.146396	0.417584
5	6	0	-6.620883	-1.245431	0.408146
6	6	0	-5.370989	-1.830469	0.164713
7	6	0	-2.868140	-1.286289	-0.349754
8	6	0	-3.128838	1.031973	-0.331708
9	1	0	-5.801371	2.078761	0.188580
10	1	0	-7.759781	0.570164	0.609506
11	1	0	-7.482966	-1.880064	0.592932
12	1	0	-5.237502	-2.907812	0.154997
13	8	0	-2.321927	-2.366093	-0.452089
14	8	0	-2.834185	2.208981	-0.412244
15	7	0	-2.235272	-0.038207	-0.494232
16	6	0	-0.818483	0.129205	-0.784499

17	1	0	-0.474343	-0.814459	-1.213958
18	1	0	-0.708729	0.918627	-1.532305
19	6	0	-0.020517	0.484604	0.480207
20	1	0	-0.413254	1.417304	0.888359
21	1	0	-0.172884	-0.294839	1.238746
22	7	0	1.410188	0.689627	0.189331
23	6	0	2.156284	-0.511342	0.105578
24	6	0	2.521258	-1.290259	1.285151
25	6	0	2.569105	-1.032823	-1.096193
26	16	0	2.183903	-0.982850	2.878672
27	16	0	3.449577	-2.747263	0.929686
28	16	0	3.478305	-2.518630	-1.176873
29	17	0	2.253028	-0.320719	-2.638447
30	6	0	2.071826	1.800965	0.918622
31	1	0	1.599507	1.929446	1.901318
32	1	0	3.104778	1.495146	1.114914
33	6	0	2.112079	3.173641	0.194954
34	6	0	2.865870	3.070222	-1.140792
35	6	0	0.700100	3.736731	-0.049940
36	6	0	2.873030	4.132940	1.134250
37	1	0	3.882397	2.681897	-0.996469
38	1	0	2.346812	2.406749	-1.837173
39	1	0	2.951553	4.056900	-1.611892
40	1	0	0.139865	3.842243	0.887625
41	1	0	0.762651	4.731960	-0.506833
42	1	0	0.110269	3.106480	-0.722809
43	1	0	2.941340	5.132954	0.690355
44	1	0	2.367182	4.232238	2.102648
45	1	0	3.895141	3.781973	1.324079



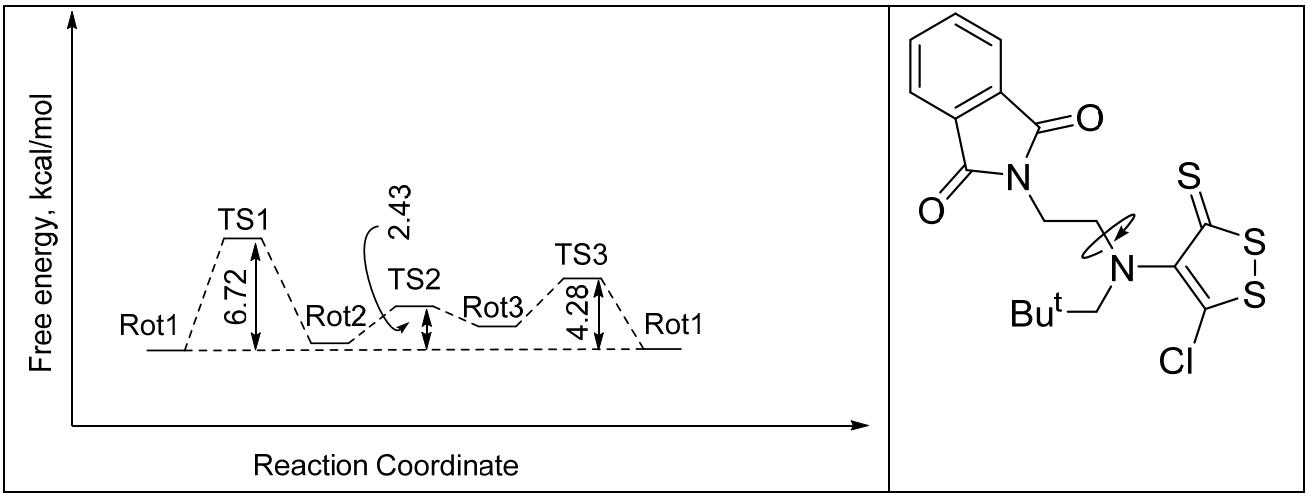
2b_TS7

Standard orientation:

2b_TS7

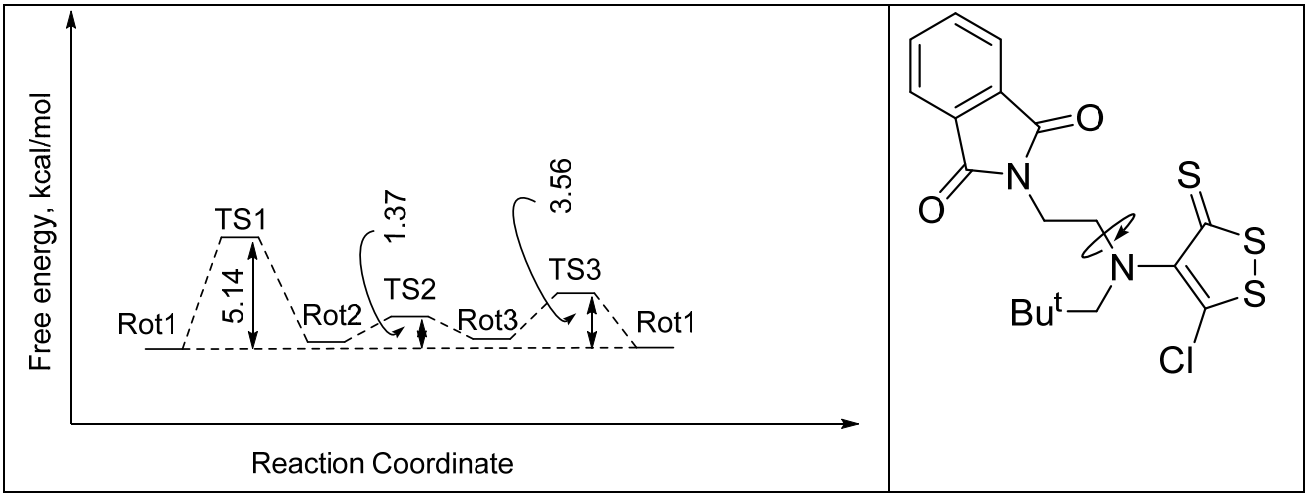
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.431763	-0.255647	-0.688474
2	6	0	4.407920	0.010620	0.682249

3	6	0	5.570393	0.280508	1.389202
4	6	0	6.775366	0.276724	0.673973
5	6	0	6.799238	0.009559	-0.700942
6	6	0	5.618970	-0.262510	-1.405604
7	6	0	3.030951	-0.502725	-1.143454
8	6	0	2.991313	-0.058982	1.148863
9	1	0	5.540213	0.485715	2.454830
10	1	0	7.707231	0.484018	1.192377
11	1	0	7.749237	0.013630	-1.227803
12	1	0	5.625459	-0.471630	-2.470871
13	8	0	2.620568	-0.767166	-2.254904
14	8	0	2.542061	0.105144	2.265648
15	7	0	2.232191	-0.369641	0.006995
16	6	0	0.787152	-0.542968	0.021755
17	1	0	0.538516	-1.322232	-0.703026
18	1	0	0.522118	-0.878488	1.026382
19	6	0	0.085724	0.776740	-0.332886
20	1	0	0.457509	1.551885	0.348317
21	1	0	0.395248	1.053450	-1.350249
22	7	0	-1.386717	0.728464	-0.279431
23	6	0	-2.042815	-0.485796	-0.030239
24	6	0	-2.471728	-1.381980	-1.102184
25	6	0	-2.298330	-0.931598	1.246177
26	16	0	-2.215201	-1.231618	-2.731007
27	16	0	-3.349381	-2.805132	-0.543320
28	16	0	-3.110067	-2.446563	1.536951
29	17	0	-1.826523	-0.081437	2.674136
30	6	0	-2.091610	1.746559	-1.077980
31	1	0	-1.417581	2.071396	-1.882183
32	1	0	-2.947742	1.276467	-1.572521
33	6	0	-2.599139	3.001361	-0.315381
34	6	0	-3.752484	2.628657	0.633287
35	6	0	-1.466287	3.668492	0.483647
36	6	0	-3.122758	3.984753	-1.381518
37	1	0	-4.584498	2.169961	0.083922
38	1	0	-3.425149	1.926281	1.405584
39	1	0	-4.141036	3.520637	1.139764
40	1	0	-0.623370	3.939711	-0.164746
41	1	0	-1.822756	4.587902	0.963990
42	1	0	-1.093509	3.004957	1.270906
43	1	0	-3.534917	4.884501	-0.909696
44	1	0	-2.322715	4.300987	-2.062403
45	1	0	-3.918174	3.532108	-1.986710



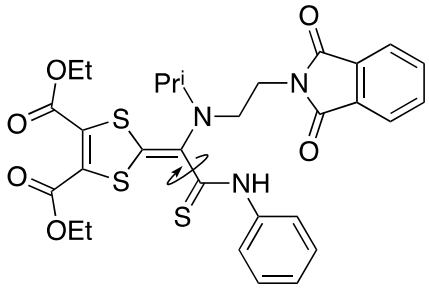
Calculated free energy values for the rotation of the phthalimidoethyl group in compound **2b**, level of theory: B3LYP/6-31G(d) (kcal/mol):

	2b_rot5	2b_TS5	2b_rot6	2b_TS6	2b_rot7	2b_TS7
G	0	6,72	0,84	2,43	1,34	4,28

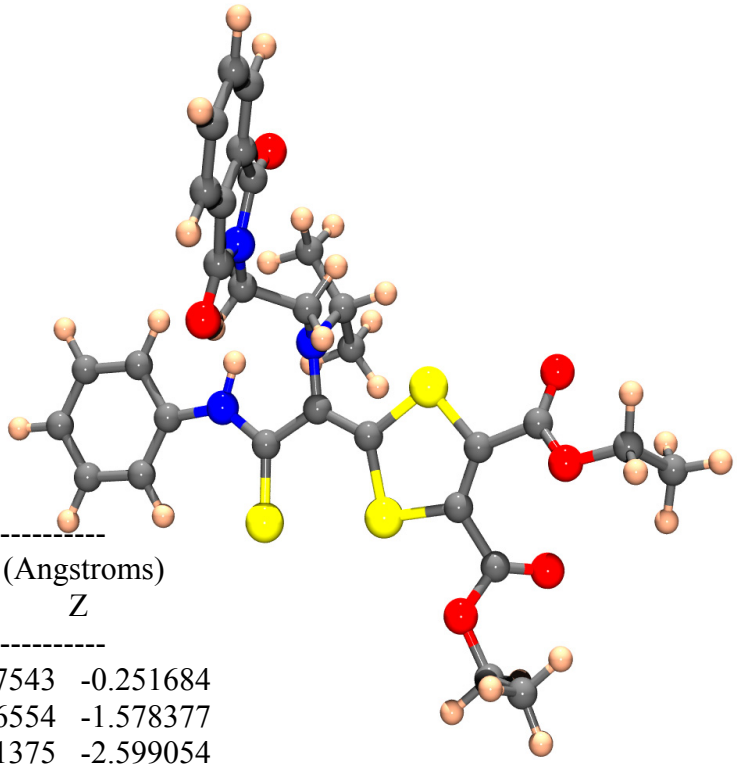


Calculated free energy values for the rotation of the phthalimidoethyl group in compound **2b** with solvation, level of theory: PCM/B3LYP/6-311++G(2d,p) (kcal/mol):

	2b_rot5	2b_TS5	2b_rot6	2b_TS6	2b_rot7	2b_TS7
G	0	5,14	0,86	1,37	0,84	3,56



6a, rotation of the thiocarboxamide group.



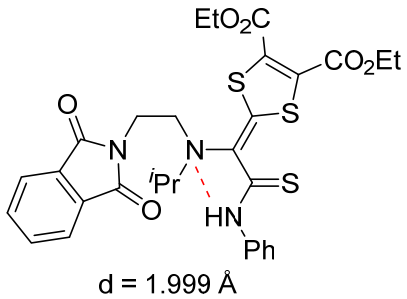
6a_rot1 (0 Kcal/mol)

6a_rot1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.636555	-3.647543	-0.251684
2	6	0	-4.285772	-3.386554	-1.578377
3	6	0	-4.600001	-4.271375	-2.599054
4	6	0	-5.284895	-5.442713	-2.248560
5	6	0	-5.635964	-5.704750	-0.918119
6	6	0	-5.314105	-4.803812	0.105823
7	6	0	-4.160230	-2.510173	0.589091
8	6	0	-3.576093	-2.073267	-1.627086
9	1	0	-4.323379	-4.058012	-3.626911
10	1	0	-5.548810	-6.160501	-3.020036
11	1	0	-6.166494	-6.621778	-0.678030
12	1	0	-5.581968	-4.996612	1.140060
13	8	0	-4.262530	-2.348569	1.791154
14	8	0	-3.111982	-1.486672	-2.582630
15	7	0	-3.545144	-1.613225	-0.296465
16	6	0	-2.945520	-0.356404	0.126986
17	1	0	-3.607403	0.095595	0.870643
18	6	0	-1.539737	-0.566781	0.724009
19	1	0	-1.592774	-1.354510	1.483447
20	1	0	-0.878523	-0.931453	-0.068827
21	7	0	-0.988525	0.660507	1.326679
22	6	0	-0.905060	0.662007	2.821000
23	6	0	-2.309055	0.560769	3.435904
24	6	0	-0.183605	1.905163	3.346992
25	1	0	-0.338301	-0.223652	3.151765
26	1	0	-2.860075	-0.320858	3.094768
27	1	0	-2.226406	0.492694	4.526555
28	1	0	-2.903733	1.453255	3.201302
29	1	0	0.851529	1.963359	3.001484
30	1	0	-0.698774	2.823833	3.044589
31	1	0	-0.169695	1.871924	4.441344
32	6	0	0.003484	1.359598	0.544802
33	6	0	1.265735	0.824353	0.400757
34	16	0	2.621218	1.476252	-0.541163
35	16	0	1.641092	-0.691670	1.232113
36	6	0	3.284175	-0.859103	0.632552

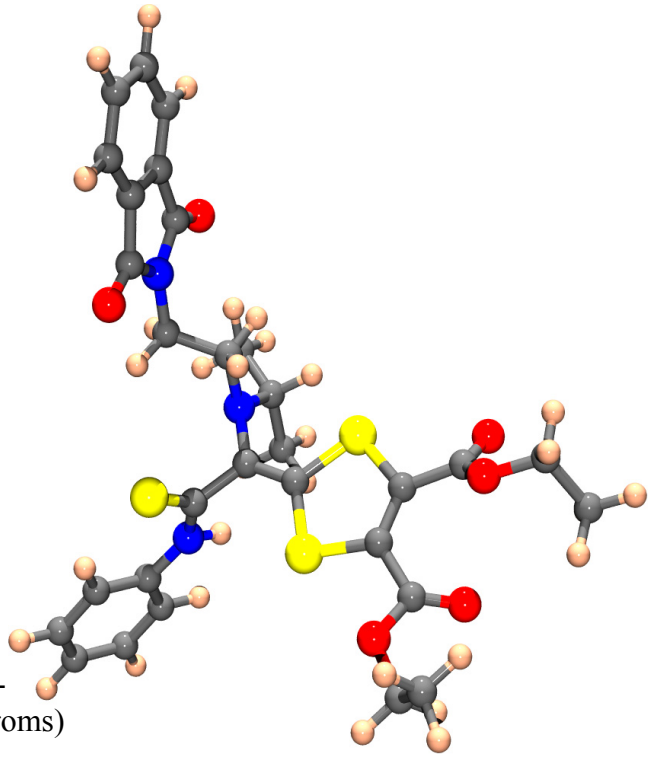
37	6	0	3.744077	0.145934	-0.144341
38	6	0	-0.420288	2.623056	-0.083400
39	16	0	0.613623	3.524415	-1.060832
40	7	0	-1.703964	2.950012	0.224220
41	1	0	-2.108363	2.243560	0.840529
42	6	0	-2.562765	4.017058	-0.096742
43	6	0	-3.830775	3.980333	0.516756
44	6	0	-2.257141	5.078885	-0.962741
45	6	0	-4.768188	4.977014	0.274803
46	1	0	-4.076294	3.160731	1.189365
47	6	0	-3.209697	6.072331	-1.194734
48	1	0	-1.290958	5.121690	-1.443320
49	6	0	-4.463164	6.034801	-0.585618
50	1	0	-5.738829	4.926304	0.760715
51	1	0	-2.958018	6.887682	-1.867810
52	1	0	-5.193259	6.815909	-0.777139
53	6	0	5.152997	0.311879	-0.618551
54	8	0	6.139266	-0.023192	0.000417
55	8	0	5.167289	0.954121	-1.803072
56	6	0	3.958258	-2.110516	1.085338
57	8	0	3.645510	-2.672764	2.117597
58	8	0	4.864010	-2.550543	0.205577
59	6	0	6.469150	1.279748	-2.355674
60	6	0	7.032446	0.116758	-3.157073
61	1	0	7.134580	1.561657	-1.536177
62	1	0	6.277568	2.150059	-2.986911
63	1	0	7.979149	0.414281	-3.622320
64	1	0	7.223000	-0.742876	-2.508586
65	1	0	6.338474	-0.182461	-3.948962
66	6	0	5.658463	-3.698726	0.605274
67	6	0	6.834513	-3.272957	1.470303
68	1	0	5.988050	-4.129392	-0.342764
69	1	0	5.009648	-4.409571	1.122510
70	1	0	7.478720	-4.137646	1.667227
71	1	0	7.422007	-2.500122	0.966915
72	1	0	6.486474	-2.878659	2.429218
73	1	0	-2.899286	0.291434	-0.751750



d = 1.999 Å

6a

The optimized structure of compound **6a** displays a distance of 1.999 Å between the hydrogen atom of the thioamide and the amine nitrogen atom, which is in the range of the hydrogen bond interactions and it can be classified as a moderate-weak hydrogen bond.



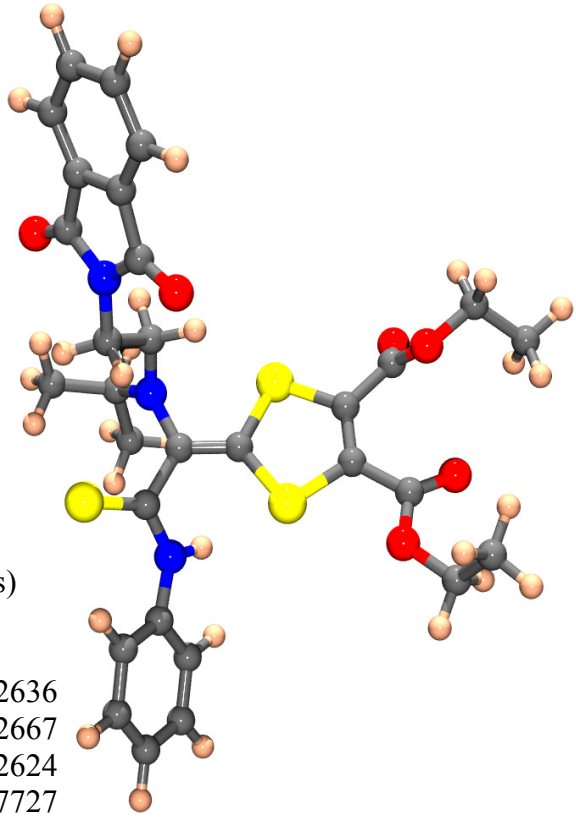
6a_TS1 (13 Kcal/mol)

6a_TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.103756	-1.929478	-0.108909
2	6	0	-5.833545	-1.675001	-1.454522
3	6	0	-6.547122	-2.297466	-2.467844
4	6	0	-7.552993	-3.196808	-2.089380
5	6	0	-7.823825	-3.452406	-0.738940
6	6	0	-7.097305	-2.817061	0.276986
7	6	0	-5.168515	-1.108833	0.716251
8	6	0	-4.720958	-0.680025	-1.529877
9	1	0	-6.328708	-2.090884	-3.511041
10	1	0	-8.133612	-3.704797	-2.854291
11	1	0	-8.610204	-4.154754	-0.477113
12	1	0	-7.298789	-3.006854	1.326778
13	8	0	-5.082099	-1.043727	1.929562
14	8	0	-4.202246	-0.191987	-2.511589
15	7	0	-4.377266	-0.395605	-0.193044
16	6	0	-3.331855	0.539509	0.210875
17	1	0	-3.724139	1.161174	1.018725
18	6	0	-2.057918	-0.195352	0.674488
19	1	0	-2.338458	-0.984614	1.382600
20	1	0	-1.600945	-0.682852	-0.192730
21	7	0	-1.078216	0.707106	1.307157
22	6	0	-0.978931	0.599914	2.787967
23	6	0	-2.330529	0.919336	3.444558
24	6	0	0.094307	1.525614	3.367617
25	1	0	-0.710868	-0.434466	3.068707
26	1	0	-3.133151	0.255619	3.112389
27	1	0	-2.243097	0.809138	4.531729
28	1	0	-2.623494	1.953399	3.226376
29	1	0	1.090891	1.319213	2.966115
30	1	0	-0.162647	2.577242	3.186431
31	1	0	0.143089	1.384835	4.452143
32	6	0	0.082947	0.988925	0.523949

33	6	0	1.136598	0.150196	0.403905
34	16	0	2.569107	0.491533	-0.607929
35	16	0	1.217465	-1.418808	1.244761
36	6	0	2.795444	-1.880340	0.615201
37	6	0	3.428963	-0.999509	-0.193007
38	6	0	0.034013	2.263259	-0.293520
39	16	0	-0.551425	2.219621	-1.852678
40	7	0	0.485061	3.338580	0.401083
41	1	0	0.816556	3.103156	1.330104
42	6	0	0.588853	4.721483	0.120297
43	6	0	1.199264	5.501953	1.118803
44	6	0	0.126715	5.339346	-1.050700
45	6	0	1.347637	6.873879	0.952386
46	1	0	1.561029	5.025660	2.028256
47	6	0	0.283398	6.718208	-1.201894
48	1	0	-0.342547	4.747360	-1.823122
49	6	0	0.889463	7.492574	-0.213506
50	1	0	1.822580	7.458816	1.735113
51	1	0	-0.078444	7.187138	-2.112909
52	1	0	1.004607	8.564319	-0.347199
53	6	0	4.826393	-1.142173	-0.690409
54	8	0	5.676741	-1.846031	-0.188270
55	8	0	5.025584	-0.332661	-1.750554
56	6	0	3.262622	-3.226452	1.080645
57	8	0	3.087771	-3.612391	2.218515
58	8	0	3.789335	-3.946618	0.085271
59	6	0	6.360815	-0.309275	-2.317528
60	6	0	6.541373	-1.420418	-3.339701
61	1	0	7.085506	-0.390633	-1.503942
62	1	0	6.435841	0.678564	-2.777192
63	1	0	7.528266	-1.333134	-3.808335
64	1	0	6.473714	-2.401090	-2.860461
65	1	0	5.780237	-1.354802	-4.123482
66	6	0	4.328806	-5.248474	0.439869
67	6	0	5.740935	-5.130700	0.991391
68	1	0	4.306675	-5.802067	-0.501402
69	1	0	3.652765	-5.721493	1.156304
70	1	0	6.155926	-6.132951	1.149369
71	1	0	6.384124	-4.586331	0.294815
72	1	0	5.740274	-4.603154	1.949055
73	1	0	-3.110831	1.171898	-0.650792



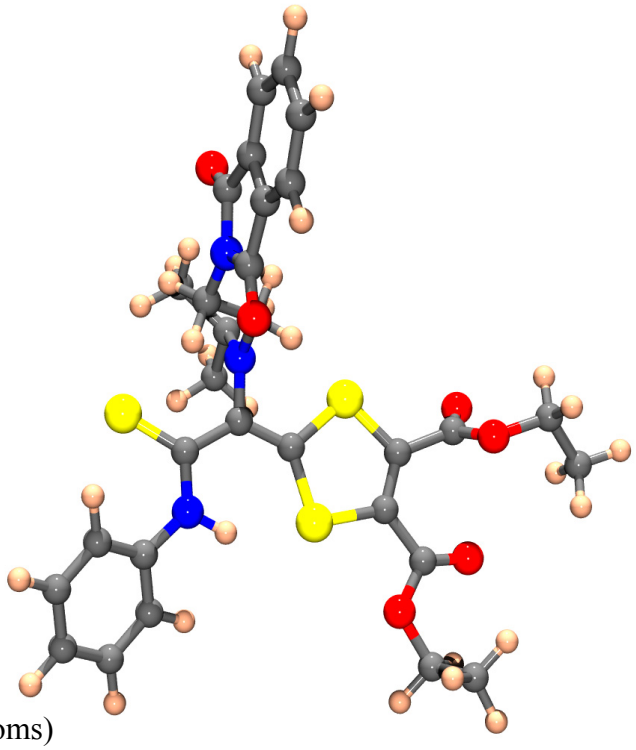
6a_rot2 (8 Kcal/mol)

6a_rot2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.285209	0.213424	-0.452636
2	6	0	5.639800	0.885314	-1.492667
3	6	0	6.302692	1.820973	-2.272624
4	6	0	7.650258	2.068570	-1.977727
5	6	0	8.297585	1.394483	-0.934437
6	6	0	7.618092	0.451083	-0.151920
7	6	0	5.300966	-0.712189	0.184577
8	6	0	4.225212	0.405919	-1.553239
9	1	0	5.791024	2.337150	-3.079155
10	1	0	8.203542	2.794420	-2.567063
11	1	0	9.343040	1.607776	-0.730032
12	1	0	8.109470	-0.077495	0.659172
13	8	0	5.459656	-1.463198	1.128976
14	8	0	3.336469	0.745758	-2.308341
15	7	0	4.106149	-0.550975	-0.531091
16	6	0	2.882602	-1.286834	-0.226193
17	1	0	3.160031	-2.301206	0.058838
18	6	0	2.098544	-0.581836	0.902332
19	1	0	2.786783	-0.385913	1.732511
20	1	0	1.778963	0.396499	0.522929
21	7	0	0.958415	-1.312615	1.449418
22	6	0	1.185355	-2.069030	2.707882
23	6	0	2.184381	-3.231072	2.576346
24	6	0	-0.130556	-2.537805	3.335468
25	1	0	1.628942	-1.340583	3.404829
26	1	0	3.163186	-2.883115	2.231548
27	1	0	2.332335	-3.700488	3.556864
28	1	0	1.818030	-3.989215	1.878014
29	1	0	-0.841462	-1.711767	3.445873
30	1	0	-0.601797	-3.335666	2.751957
31	1	0	0.074249	-2.940021	4.333032
32	6	0	-0.256514	-1.372501	0.734385
33	6	0	-0.995727	-0.220152	0.647229
34	16	0	-2.382682	0.102674	-0.433119
35	16	0	-0.514631	1.194588	1.614491

36	6	0	-1.718252	2.290197	0.956791
37	6	0	-2.586278	1.797577	0.045619
38	6	0	-0.705499	-2.638671	0.070224
39	16	0	0.358066	-3.644878	-0.729634
40	7	0	-2.047636	-2.851309	0.216256
41	1	0	-2.485463	-2.229457	0.887159
42	6	0	-2.957116	-3.798260	-0.307073
43	6	0	-4.228322	-3.819426	0.295110
44	6	0	-2.691332	-4.662076	-1.379877
45	6	0	-5.212866	-4.690176	-0.158199
46	1	0	-4.440651	-3.148542	1.125347
47	6	0	-3.690405	-5.528935	-1.823882
48	1	0	-1.718951	-4.656326	-1.849615
49	6	0	-4.948664	-5.554844	-1.222706
50	1	0	-6.186880	-4.692137	0.323185
51	1	0	-3.472430	-6.193578	-2.655445
52	1	0	-5.714279	-6.238845	-1.577335
53	6	0	-3.739165	2.549535	-0.513062
54	8	0	-4.159519	3.600051	-0.073220
55	8	0	-4.276061	1.880887	-1.553776
56	6	0	-1.666442	3.686677	1.513314
57	8	0	-1.668931	3.907937	2.705280
58	8	0	-1.523868	4.595380	0.544543
59	6	0	-5.443672	2.470885	-2.181886
60	6	0	-5.043266	3.478531	-3.247648
61	1	0	-6.059451	2.930816	-1.405380
62	1	0	-5.973058	1.617381	-2.610912
63	1	0	-5.939576	3.853720	-3.754635
64	1	0	-4.520911	4.328453	-2.799613
65	1	0	-4.392137	3.015982	-3.996061
66	6	0	-1.491152	5.988799	0.959772
67	6	0	-2.894393	6.548629	1.129633
68	1	0	-0.950957	6.486511	0.151453
69	1	0	-0.912467	6.062208	1.883701
70	1	0	-2.833738	7.620348	1.352075
71	1	0	-3.481194	6.409639	0.217707
72	1	0	-3.413068	6.052388	1.953988
73	1	0	2.289931	-1.338039	-1.139957



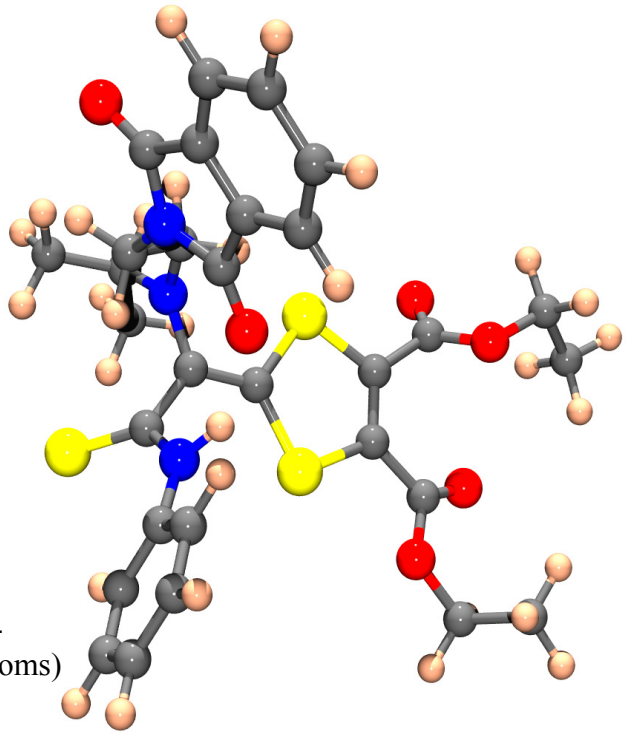
6a_TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.972551	-1.609303	-0.611272
2	6	0	-5.388109	-1.367723	-1.856132
3	6	0	-5.908056	-1.914946	-3.019574
4	6	0	-7.046980	-2.722833	-2.899697
5	6	0	-7.633209	-2.964891	-1.650872
6	6	0	-7.099227	-2.407435	-0.481174
7	6	0	-5.176591	-0.885431	0.425207
8	6	0	-4.203747	-0.479064	-1.652123
9	1	0	-5.445531	-1.720201	-3.982319
10	1	0	-7.483927	-3.169112	-3.788628
11	1	0	-8.515934	-3.595252	-1.589984
12	1	0	-7.545099	-2.588221	0.492079
13	8	0	-5.345196	-0.849449	1.629613
14	8	0	-3.425370	-0.043879	-2.477455
15	7	0	-4.152028	-0.227891	-0.270851
16	6	0	-3.141613	0.603470	0.377301
17	1	0	-3.624380	1.166725	1.175595
18	6	0	-1.994424	-0.273693	0.927830
19	1	0	-2.432145	-1.060861	1.553160
20	1	0	-1.521347	-0.776426	0.073299
21	7	0	-0.977445	0.407956	1.719289
22	6	0	-1.098378	0.355120	3.203201
23	6	0	-2.445079	0.881312	3.725569
24	6	0	0.064572	1.068818	3.896368
25	1	0	-1.042708	-0.711405	3.480452
26	1	0	-3.293492	0.337416	3.298106
27	1	0	-2.487043	0.743052	4.813005
28	1	0	-2.558511	1.944588	3.499902
29	1	0	1.036711	0.663723	3.598976
30	1	0	0.048700	2.142861	3.688226
31	1	0	-0.032999	0.931654	4.978353

6a_TS2 (14 Kcal/mol)

32	6	0	0.068977	1.083620	1.028789
33	6	0	1.122418	0.253172	0.717518
34	16	0	2.631537	0.547340	-0.177020
35	16	0	0.995787	-1.419479	1.307043
36	6	0	2.517385	-1.981737	0.643752
37	6	0	3.287877	-1.092288	-0.019364
38	6	0	-0.065865	2.533394	0.706234
39	16	0	-1.345115	3.433915	1.311007
40	7	0	0.908065	3.089058	-0.074825
41	1	0	1.700442	2.513006	-0.317674
42	6	0	1.088310	4.426690	-0.526575
43	6	0	2.403943	4.910480	-0.556955
44	6	0	0.045331	5.224019	-1.014159
45	6	0	2.675638	6.182094	-1.057422
46	1	0	3.211456	4.290603	-0.174004
47	6	0	0.328107	6.497563	-1.506084
48	1	0	-0.968797	4.849824	-1.006795
49	6	0	1.636361	6.984730	-1.529497
50	1	0	3.699578	6.545366	-1.069839
51	1	0	-0.486896	7.110623	-1.880941
52	1	0	1.843786	7.979400	-1.913928
53	6	0	4.642790	-1.370851	-0.551745
54	8	0	5.265168	-2.392143	-0.342877
55	8	0	5.093662	-0.323865	-1.271622
56	6	0	2.848673	-3.426576	0.920133
57	8	0	2.951720	-3.862018	2.045113
58	8	0	2.910244	-4.132397	-0.211753
59	6	0	6.429287	-0.437630	-1.830813
60	6	0	6.402522	-1.139305	-3.179094
61	1	0	7.059768	-0.968128	-1.113614
62	1	0	6.767558	0.596989	-1.919390
63	1	0	7.410013	-1.144543	-3.610322
64	1	0	6.070854	-2.175664	-3.069980
65	1	0	5.733138	-0.623146	-3.874508
66	6	0	3.237381	-5.544811	-0.078650
67	6	0	4.738754	-5.759404	0.021971
68	1	0	2.822737	-5.991536	-0.984871
69	1	0	2.713378	-5.940524	0.794776
70	1	0	4.951229	-6.834769	0.032839
71	1	0	5.254870	-5.307072	-0.829262
72	1	0	5.133374	-5.318234	0.940642
73	1	0	-2.773057	1.307629	-0.369286



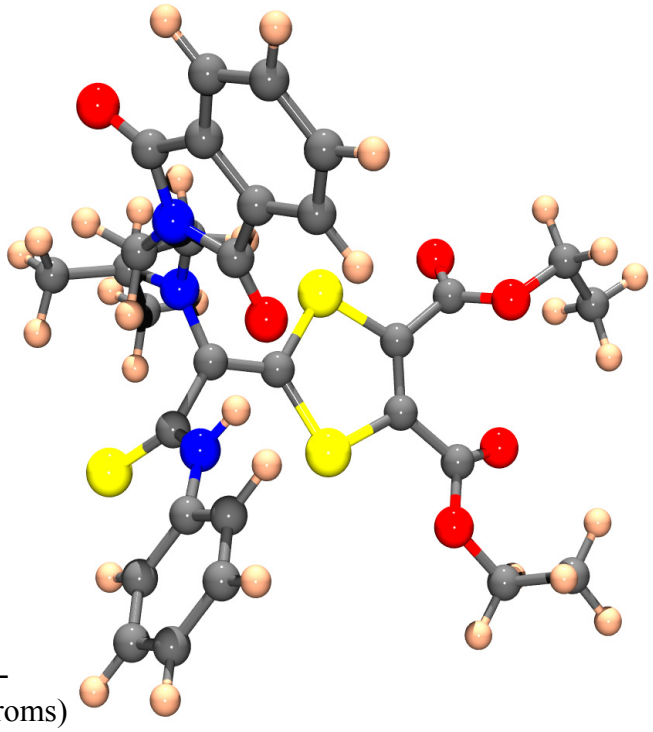
6a_rot3 (7 Kcal/mol)

6a_rot3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.120977	-2.362543	-1.196175
2	6	0	-4.194947	-1.680905	-1.989330
3	6	0	-4.207288	-1.785461	-3.372113
4	6	0	-5.190204	-2.602447	-3.947520
5	6	0	-6.119678	-3.284406	-3.152459
6	6	0	-6.097251	-3.172788	-1.755243
7	6	0	-4.836102	-2.041282	0.234070
8	6	0	-3.292512	-0.908975	-1.087133
9	1	0	-3.481625	-1.253646	-3.979658
10	1	0	-5.232807	-2.709752	-5.027606
11	1	0	-6.869493	-3.910164	-3.627978
12	1	0	-6.812715	-3.697303	-1.129585
13	8	0	-5.402731	-2.426489	1.234775
14	8	0	-2.348088	-0.192876	-1.388279
15	7	0	-3.733464	-1.161218	0.211637
16	6	0	-3.104084	-0.596175	1.400868
17	1	0	-3.825859	-0.688138	2.214068
18	6	0	-1.764667	-1.312043	1.727461
19	1	0	-1.971701	-2.226760	2.295535
20	1	0	-1.316197	-1.623876	0.775667
21	7	0	-0.785221	-0.523647	2.460939
22	6	0	-0.717602	-0.674041	3.936494
23	6	0	-1.989341	-0.211587	4.667776
24	6	0	0.528199	-0.003694	4.519977
25	1	0	-0.619442	-1.757807	4.106115
26	1	0	-2.877763	-0.741118	4.305433
27	1	0	-1.900242	-0.425415	5.740019
28	1	0	-2.143933	0.862905	4.537860
29	1	0	1.445414	-0.388515	4.064393
30	1	0	0.490677	1.081121	4.385366
31	1	0	0.574211	-0.212566	5.594254
32	6	0	-0.137036	0.493400	1.705343
33	6	0	1.032055	0.151585	1.097479
34	16	0	2.041994	1.187647	0.057731

35	16	0	1.703941	-1.474452	1.364306
36	6	0	3.164865	-1.216880	0.418668
37	6	0	3.342998	-0.001751	-0.147143
38	6	0	-0.726595	1.863067	1.496937
39	16	0	-1.069980	2.877876	2.775569
40	7	0	-0.916535	2.144365	0.175238
41	1	0	-0.941752	1.322558	-0.424930
42	6	0	-1.312513	3.332512	-0.490276
43	6	0	-1.948733	3.175195	-1.732566
44	6	0	-1.040817	4.620275	-0.007725
45	6	0	-2.319393	4.292767	-2.475424
46	1	0	-2.153863	2.174982	-2.104100
47	6	0	-1.418597	5.729304	-0.763903
48	1	0	-0.543997	4.749580	0.943249
49	6	0	-2.060121	5.577436	-1.993958
50	1	0	-2.814380	4.156243	-3.433217
51	1	0	-1.203845	6.723624	-0.381733
52	1	0	-2.352664	6.449721	-2.571715
53	6	0	4.573688	0.430205	-0.858624
54	8	0	5.642063	-0.143966	-0.811600
55	8	0	4.346934	1.576134	-1.534414
56	6	0	4.092603	-2.397651	0.367761
57	8	0	4.429842	-3.002079	1.363372
58	8	0	4.398761	-2.731190	-0.891201
59	6	0	5.474904	2.157273	-2.236951
60	6	0	5.622711	1.559780	-3.627432
61	1	0	6.374731	2.003033	-1.636857
62	1	0	5.241213	3.223353	-2.277900
63	1	0	6.433491	2.067212	-4.162581
64	1	0	5.864722	0.495079	-3.566200
65	1	0	4.700025	1.681979	-4.203580
66	6	0	5.326600	-3.837186	-1.060135
67	6	0	6.769494	-3.377741	-0.922715
68	1	0	5.112292	-4.202979	-2.066888
69	1	0	5.079128	-4.612833	-0.331185
70	1	0	7.441001	-4.213921	-1.150151
71	1	0	6.982271	-2.555279	-1.610814
72	1	0	6.972649	-3.037917	0.096146
73	1	0	-2.930492	0.465247	1.214906



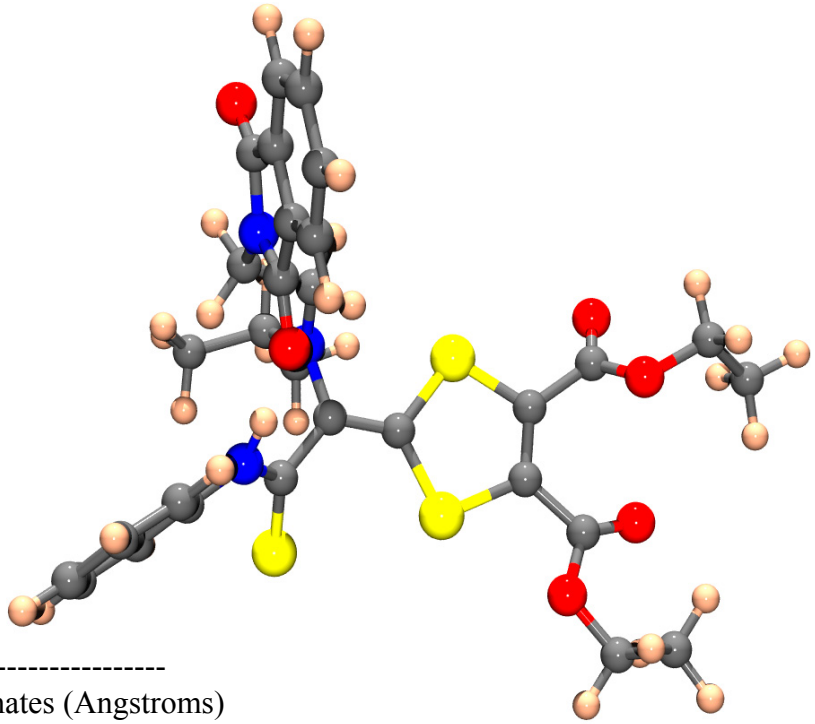
6a_TS3 (9 Kcal/mol)

6a_TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.972784	-2.623623	-0.900612
2	6	0	-4.027541	-2.045318	-1.751322
3	6	0	-3.983160	-2.351866	-3.103039
4	6	0	-4.928464	-3.266528	-3.587247
5	6	0	-5.877029	-3.845117	-2.734897
6	6	0	-5.912063	-3.529134	-1.369537
7	6	0	-4.751423	-2.088248	0.475536
8	6	0	-3.177058	-1.127804	-0.940768
9	1	0	-3.243319	-1.898512	-3.755391
10	1	0	-4.926339	-3.532224	-4.640458
11	1	0	-6.596753	-4.550626	-3.140040
12	1	0	-6.642831	-3.972377	-0.700252
13	8	0	-5.349370	-2.334877	1.501181
14	8	0	-2.233301	-0.441852	-1.309061
15	7	0	-3.664639	-1.194184	0.362899
16	6	0	-3.086321	-0.452207	1.478736
17	1	0	-3.820968	-0.481630	2.285070
18	6	0	-1.720615	-1.056797	1.911047
19	1	0	-1.901588	-1.898390	2.590461
20	1	0	-1.242342	-1.469433	1.014898
21	7	0	-0.781538	-0.145244	2.547717
22	6	0	-0.807422	-0.030894	4.027389
23	6	0	-2.038948	0.700683	4.591072
24	6	0	0.491154	0.570658	4.571140
25	1	0	-0.859775	-1.072814	4.377789
26	1	0	-2.973198	0.235808	4.257297
27	1	0	-2.027419	0.656107	5.687105
28	1	0	-2.044349	1.751479	4.289635
29	1	0	1.363924	-0.004359	4.247330
30	1	0	0.610984	1.609300	4.249862
31	1	0	0.462831	0.555293	5.666140

32	6	0	-0.106103	0.760068	1.677851
33	6	0	1.068045	0.346204	1.140807
34	16	0	2.071282	1.268274	-0.007173
35	16	0	1.747225	-1.238091	1.588181
36	6	0	3.175150	-1.103322	0.567720
37	6	0	3.345544	0.041006	-0.133371
38	6	0	-0.663399	2.114322	1.286242
39	16	0	-0.665842	3.380187	2.374081
40	7	0	-1.088492	2.138665	-0.005930
41	1	0	-1.116745	1.221572	-0.450899
42	6	0	-1.567638	3.164817	-0.859555
43	6	0	-1.944031	2.752051	-2.152145
44	6	0	-1.668047	4.521003	-0.513888
45	6	0	-2.411186	3.677687	-3.078135
46	1	0	-1.874109	1.701806	-2.419809
47	6	0	-2.137149	5.435928	-1.458134
48	1	0	-1.386930	4.848556	0.475840
49	6	0	-2.511065	5.029040	-2.737777
50	1	0	-2.697524	3.339851	-4.070575
51	1	0	-2.209229	6.483518	-1.178108
52	1	0	-2.876324	5.752665	-3.461117
53	6	0	4.557764	0.384687	-0.921801
54	8	0	5.626650	-0.184575	-0.842325
55	8	0	4.314173	1.452789	-1.710451
56	6	0	4.082847	-2.298612	0.611075
57	8	0	4.419412	-2.821424	1.652503
58	8	0	4.372815	-2.745146	-0.616525
59	6	0	5.424387	1.955588	-2.496132
60	6	0	5.530738	1.225195	-3.825675
61	1	0	6.340000	1.854003	-1.908877
62	1	0	5.194237	3.014305	-2.634224
63	1	0	6.326477	1.674510	-4.430803
64	1	0	5.772313	0.170175	-3.668702
65	1	0	4.591843	1.295316	-4.384077
66	6	0	5.286754	-3.871875	-0.696943
67	6	0	6.735610	-3.419747	-0.604810
68	1	0	5.062981	-4.317166	-1.669049
69	1	0	5.034395	-4.581736	0.094712
70	1	0	7.396535	-4.278890	-0.768881
71	1	0	6.952220	-2.656741	-1.357163
72	1	0	6.949158	-3.002683	0.382793
73	1	0	-2.960422	0.586364	1.165741



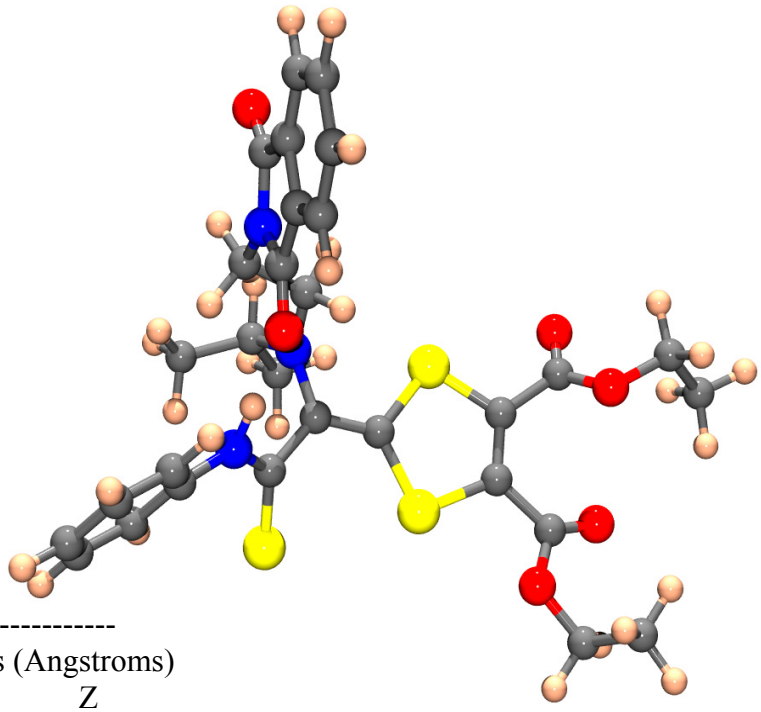
6a_rot4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.453094	3.541689	-0.302588
2	6	0	3.928794	2.773066	-1.345947
3	6	0	4.048023	3.167490	-2.670044
4	6	0	4.718923	4.371528	-2.925199
5	6	0	5.244924	5.141306	-1.880460
6	6	0	5.118227	4.733572	-0.545022
7	6	0	4.160467	2.845552	0.986576
8	6	0	3.283732	1.570013	-0.749917
9	1	0	3.635950	2.564109	-3.472876
10	1	0	4.832962	4.714433	-3.949484
11	1	0	5.759626	6.069812	-2.110220
12	1	0	5.522620	5.323227	0.271789
13	8	0	4.443804	3.170966	2.119537
14	8	0	2.703565	0.649390	-1.309350
15	7	0	3.460084	1.674514	0.627397
16	6	0	2.956350	0.671941	1.556274
17	1	0	3.472675	0.834169	2.504903
18	6	0	1.412174	0.770309	1.718805
19	1	0	1.197638	1.556458	2.457187
20	1	0	0.986952	1.103970	0.768641
21	7	0	0.732964	-0.459850	2.091085
22	6	0	0.990936	-1.029916	3.432797
23	6	0	2.144183	-2.051693	3.481916
24	6	0	-0.281630	-1.630175	4.044807
25	1	0	1.283029	-0.165092	4.046060
26	1	0	3.079048	-1.639005	3.090529
27	1	0	2.325226	-2.360137	4.518609
28	1	0	1.897809	-2.949431	2.905971
29	1	0	-1.084665	-0.888799	4.095120
30	1	0	-0.635100	-2.485354	3.459168
31	1	0	-0.073808	-1.981406	5.061597
32	6	0	-0.004089	-1.199471	1.118596

6a_rot4 (6 Kcal/mol)

33	6	0	-1.266972	-0.783559	0.828952
34	16	0	-2.384756	-1.529156	-0.334019
35	16	0	-1.915300	0.669992	1.618719
36	6	0	-3.381684	0.757659	0.646307
37	6	0	-3.606300	-0.247839	-0.231628
38	6	0	0.586739	-2.417481	0.469140
39	16	0	-0.171416	-3.906160	0.578377
40	7	0	1.755253	-2.165962	-0.181675
41	1	0	1.940520	-1.184709	-0.386998
42	6	0	2.667809	-3.050108	-0.816285
43	6	0	3.370812	-2.554811	-1.925869
44	6	0	2.937238	-4.343105	-0.346594
45	6	0	4.321165	-3.348815	-2.563711
46	1	0	3.167094	-1.549633	-2.282055
47	6	0	3.890085	-5.126436	-0.996297
48	1	0	2.404816	-4.731371	0.510308
49	6	0	4.583724	-4.641006	-2.106021
50	1	0	4.854412	-2.953861	-3.424384
51	1	0	4.089975	-6.128011	-0.625102
52	1	0	5.321022	-5.262078	-2.606988
53	6	0	-4.863983	-0.448910	-1.006493
54	8	0	-5.940691	0.037621	-0.732739
55	8	0	-4.645912	-1.298999	-2.031691
56	6	0	-4.228854	1.955573	0.939723
57	8	0	-4.374347	2.382868	2.067510
58	8	0	-4.707248	2.523756	-0.173453
59	6	0	-5.796311	-1.664572	-2.835129
60	6	0	-6.034723	-0.652235	-3.944636
61	1	0	-6.665775	-1.751932	-2.179303
62	1	0	-5.539182	-2.648130	-3.234249
63	1	0	-6.860749	-0.989673	-4.581166
64	1	0	-6.298849	0.323222	-3.526737
65	1	0	-5.142033	-0.541555	-4.568447
66	6	0	-5.611058	3.645834	0.008831
67	6	0	-7.027642	3.172853	0.295376
68	1	0	-5.548649	4.185194	-0.939059
69	1	0	-5.225259	4.277538	0.812838
70	1	0	-7.703241	4.035713	0.324001
71	1	0	-7.367473	2.480310	-0.479223
72	1	0	-7.076802	2.664011	1.261812
73	1	0	3.237382	-0.312046	1.174823



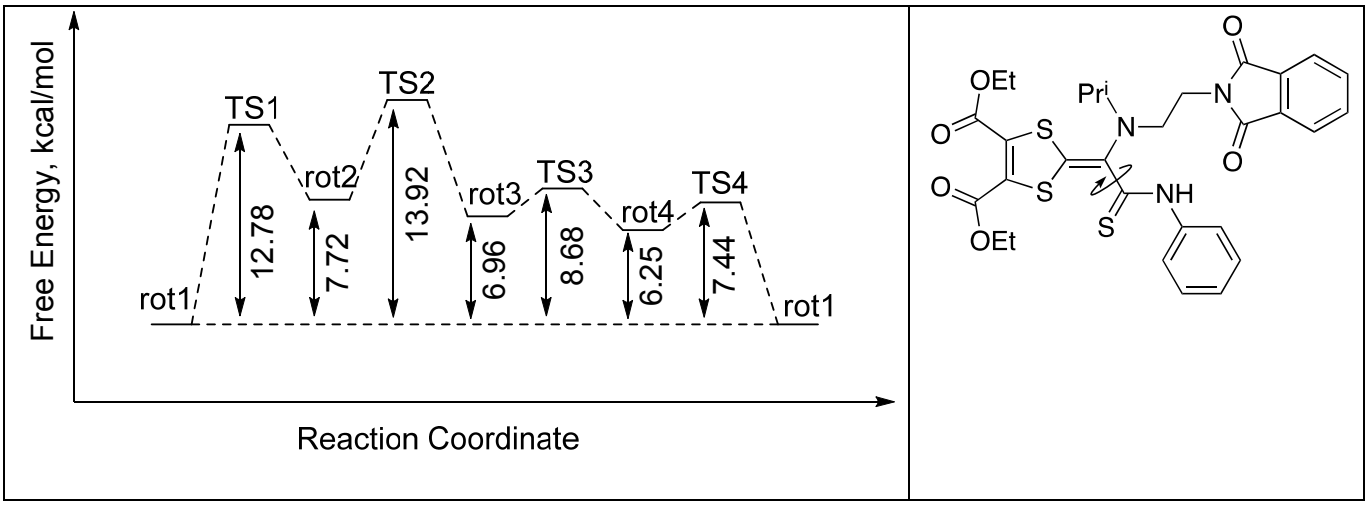
6a_TS4 (7 Kcal/mol)

6a_TS4

Standard orientation:

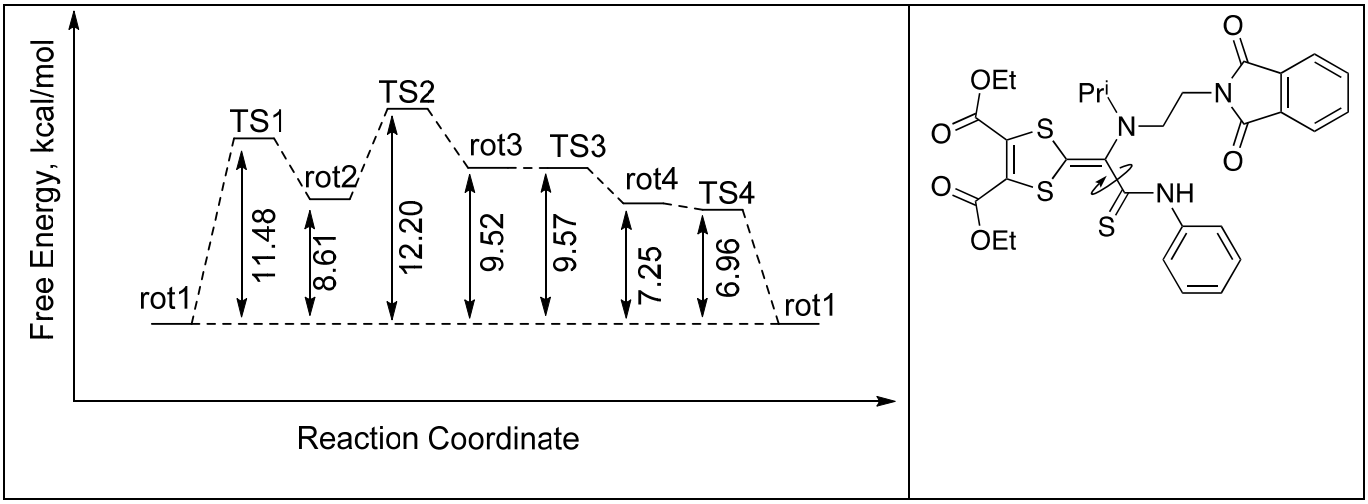
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.476544	3.582040	-0.316635
2	6	0	4.045571	2.764245	-1.365474
3	6	0	4.239982	3.120417	-2.691544
4	6	0	4.889836	4.336688	-2.942952
5	6	0	5.322499	5.155602	-1.892737
6	6	0	5.120113	4.786457	-0.555417
7	6	0	4.121203	2.918176	0.973968
8	6	0	3.399281	1.560144	-0.772508
9	1	0	3.899945	2.479098	-3.498709
10	1	0	5.060816	4.650583	-3.968619
11	1	0	5.823108	6.092481	-2.119656
12	1	0	5.451762	5.414309	0.265697
13	8	0	4.320154	3.288217	2.111316
14	8	0	2.885271	0.602865	-1.333652
15	7	0	3.481594	1.715070	0.609769
16	6	0	2.949708	0.724156	1.534074
17	1	0	3.406613	0.920702	2.506605
18	6	0	1.397728	0.787597	1.607004
19	1	0	1.125295	1.601607	2.295324
20	1	0	1.016560	1.065919	0.621053
21	7	0	0.739254	-0.449704	1.993335
22	6	0	0.987506	-0.989072	3.349831
23	6	0	2.109555	-2.043817	3.416117
24	6	0	-0.294557	-1.538811	3.990203
25	1	0	1.308761	-0.117810	3.938545
26	1	0	3.049827	-1.674172	2.996192
27	1	0	2.296684	-2.325350	4.459358
28	1	0	1.826675	-2.951081	2.872374
29	1	0	-1.076639	-0.775296	4.034671
30	1	0	-0.679261	-2.396033	3.427451
31	1	0	-0.084059	-1.874920	5.011523
32	6	0	-0.021164	-1.201929	1.049022

33	6	0	-1.293737	-0.785354	0.783329
34	16	0	-2.458500	-1.547630	-0.318647
35	16	0	-1.897980	0.696692	1.550120
36	6	0	-3.388155	0.787624	0.615378
37	6	0	-3.651719	-0.237481	-0.228366
38	6	0	0.556085	-2.422782	0.408135
39	16	0	-0.282669	-3.873192	0.382585
40	7	0	1.791175	-2.218823	-0.129978
41	1	0	2.036561	-1.245911	-0.302420
42	6	0	2.707205	-3.137384	-0.706155
43	6	0	3.517723	-2.666457	-1.750910
44	6	0	2.879177	-4.445138	-0.231704
45	6	0	4.478603	-3.499071	-2.320556
46	1	0	3.387840	-1.650614	-2.111695
47	6	0	3.842995	-5.267286	-0.813226
48	1	0	2.265129	-4.814055	0.578097
49	6	0	4.644380	-4.805727	-1.858942
50	1	0	5.096035	-3.122462	-3.131787
51	1	0	3.966840	-6.279920	-0.438857
52	1	0	5.390038	-5.456375	-2.307238
53	6	0	-4.932140	-0.442814	-0.966383
54	8	0	-6.001167	0.042962	-0.663879
55	8	0	-4.741969	-1.298452	-1.992242
56	6	0	-4.202158	2.008864	0.901190
57	8	0	-4.275227	2.488750	2.015198
58	8	0	-4.742576	2.531413	-0.205612
59	6	0	-5.914370	-1.671652	-2.759795
60	6	0	-6.185231	-0.668019	-3.869771
61	1	0	-6.764760	-1.754955	-2.078930
62	1	0	-5.667173	-2.657883	-3.158575
63	1	0	-7.028119	-1.011342	-4.480521
64	1	0	-6.439093	0.310274	-3.452089
65	1	0	-5.310407	-0.560916	-4.518978
66	6	0	-5.627765	3.667832	-0.020940
67	6	0	-7.026138	3.219100	0.373737
68	1	0	-5.621354	4.161764	-0.995212
69	1	0	-5.189944	4.333337	0.727225
70	1	0	-7.696265	4.086324	0.398239
71	1	0	-7.413559	2.489988	-0.342832
72	1	0	-7.019065	2.761112	1.366544
73	1	0	3.276164	-0.261033	1.193523



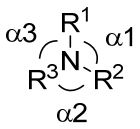
Calculated free energy values for the rotation of the thiocarboxamide group in compound **6a**, level of theory: B3LYP/6-31G(d) (kcal/mol):

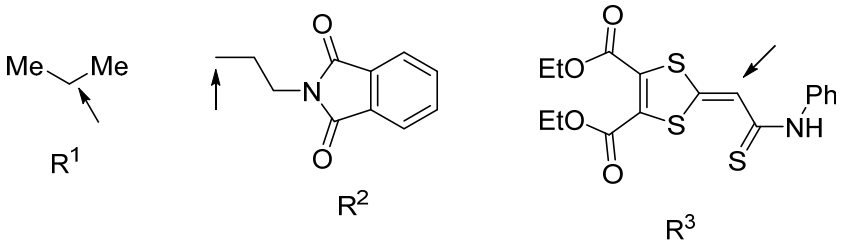
	6a_rot1	6a_TS1	6a_rot2	6a_TS2	6a_rot3	6a_TS3	6a_rot4	6a_TS4
ΔG	0	12,78	7,72	13,92	6,96	8,68	6,25	7,44



Calculated free energy values for the rotation of the thiocarboxamide group in compound **6a** with solvation, level of theory: PCM/B3LYP/6-311++G(2d,p) (kcal/mol):

	6a_rot1	6a_TS1	6a_rot2	6a_TS2	6a_rot3	6a_TS3	6a_rot4	6a_TS4
ΔG	0	11,48	8,61	12,20	9,52	9,57	7,25	6,96





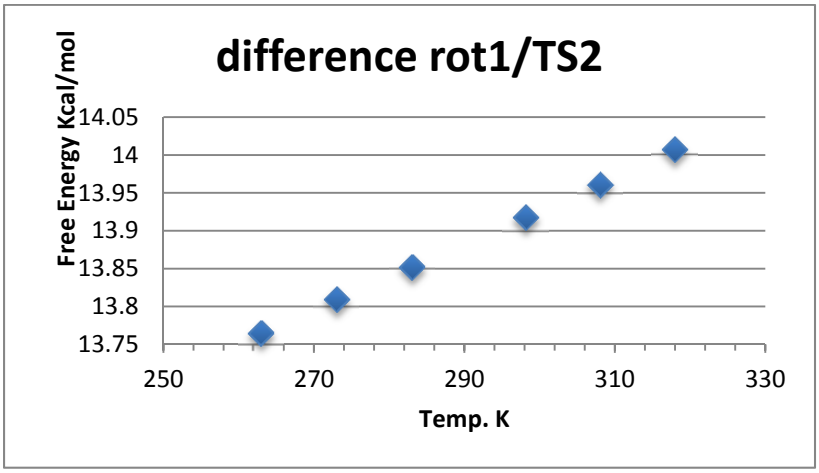
Angles around the amine nitrogen atom of the calculated structures for the rotation of the thiocarboxamide fragment in **6a**.

	Rot1	TS1	Rot2	TS2	Rot3	TS3	Rot4	TS4
α1	115.46	115.29	116.92	117.87	118.46	118.23	118.46	118.52
α2	116.02	115.18	120.24	118.11	115.22	115.88	120.36	120.94
α3	120.13	120.37	122.63	124.02	125.40	124.58	120.53	120.24
Sum	351.61	350.84	359.79	360	359.08	358.69	359.35	359.7

A study of the difference on energies between the rotamer 1 (ground state, rot1) and the highest transition state in **6a** when this difference has been calculated at different temperatures has been performed. The calculations show that there is not big change when the temperature rises from 263K to 318K.

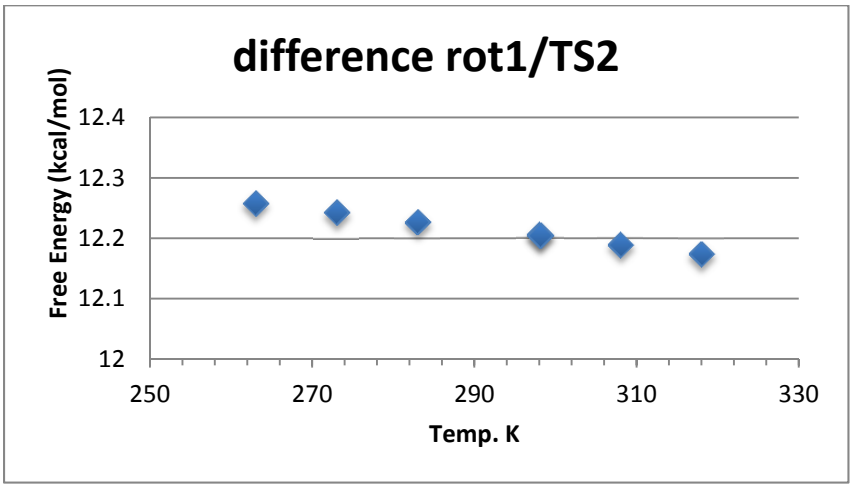
Difference of free energies between the rotamer 1 and the TS2 with the temperature. Calculations performed in gas phase at the B3LYP/6-31G(d) level of theory.

Temp (K)	rot1	TS	dif a.u.	dif kcal/mol
263	-2971,554754	-2971,532818	0,021936	13,765046
273	-2971,558695	-2971,536688	0,022007	13,80959917
283	-2971,562717	-2971,540642	0,022075	13,85226981
298.15	-2971,568971	-2971,546791	0,022180	13,91815829
308	-2971,573140	-2971,550891	0,022249	13,96145644
318	-2971,577455	-2971,555134	0,022321	14,00663712

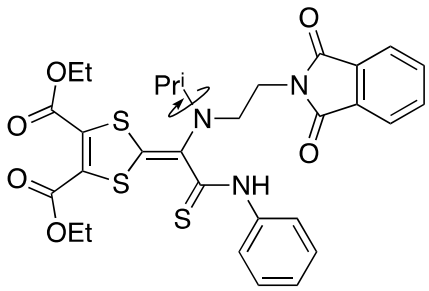


Difference of free energies between the rotamer 1 and the TS2 with the temperature. Calculations performed in solution (PCM, solvent=chloroform) at the B3LYP/6-311G(2d,p) level of theory.

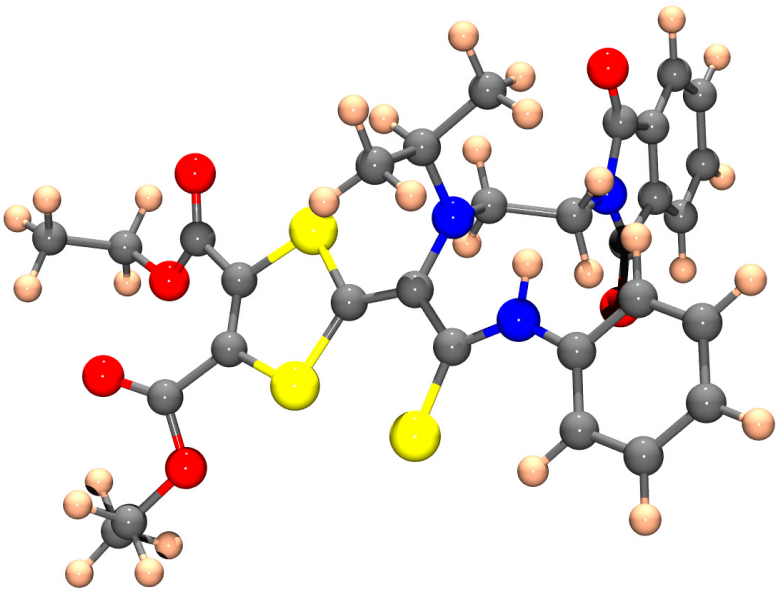
Temp (K)	rot1	TS	dif a.u.	dif kcal/mol
263	-2972,667829	-2972,648296	0,019533	12,25714093
273	-2972,664928	-2972,645418	0,019510	12,24270822
283	-2972,662026	-2972,642541	0,019485	12,22702048
298	-2972,657675	-2972,638225	0,019450	12,20505765
298.15	-2972,657631	-2972,638182	0,019449	12,20443015
308	-2972,654773	-2972,635348	0,019425	12,18936992
318	-2972,651872	-2972,632470	0,019402	12,1749372



Although there is no influence of the temperature in the difference of energies of the conformers, the temperature is very important to overcome the barriers of the dynamic process observed.



6a, rotation of the isopropyl group.



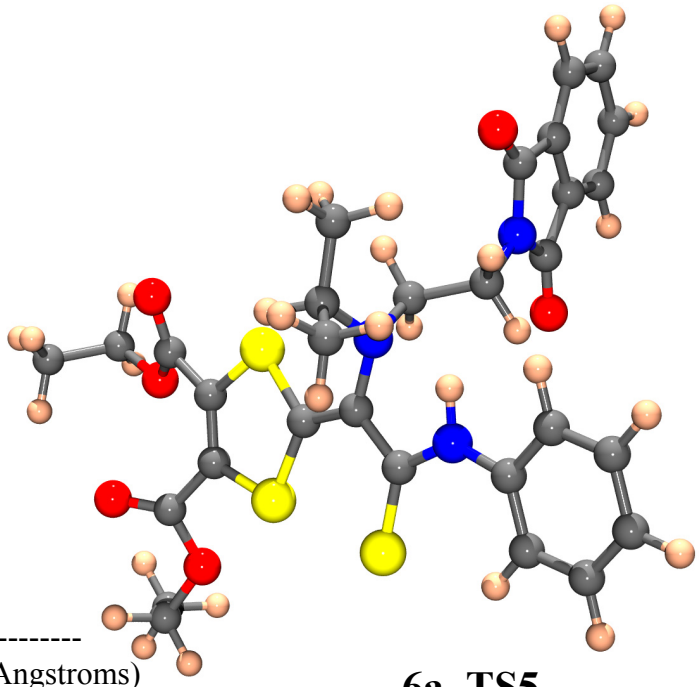
6a_rot1

6a_rot1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.636555	-3.647543	-0.251684
2	6	0	-4.285772	-3.386554	-1.578377
3	6	0	-4.600001	-4.271375	-2.599054
4	6	0	-5.284895	-5.442713	-2.248560
5	6	0	-5.635964	-5.704750	-0.918119
6	6	0	-5.314105	-4.803812	0.105823
7	6	0	-4.160230	-2.510173	0.589091
8	6	0	-3.576093	-2.073267	-1.627086
9	1	0	-4.323379	-4.058012	-3.626911
10	1	0	-5.548810	-6.160501	-3.020036
11	1	0	-6.166494	-6.621778	-0.678030
12	1	0	-5.581968	-4.996612	1.140060
13	8	0	-4.262530	-2.348569	1.791154
14	8	0	-3.111982	-1.486672	-2.582630
15	7	0	-3.545144	-1.613225	-0.296465
16	6	0	-2.945520	-0.356404	0.126986
17	1	0	-3.607403	0.095595	0.870643
18	6	0	-1.539737	-0.566781	0.724009
19	1	0	-1.592774	-1.354510	1.483447
20	1	0	-0.878523	-0.931453	-0.068827
21	7	0	-0.988525	0.660507	1.326679
22	6	0	-0.905060	0.662007	2.821000
23	6	0	-2.309055	0.560769	3.435904
24	6	0	-0.183605	1.905163	3.346992
25	1	0	-0.338301	-0.223652	3.151765
26	1	0	-2.860075	-0.320858	3.094768
27	1	0	-2.226406	0.492694	4.526555
28	1	0	-2.903733	1.453255	3.201302
29	1	0	0.851529	1.963359	3.001484
30	1	0	-0.698774	2.823833	3.044589
31	1	0	-0.169695	1.871924	4.441344

32	6	0	0.003484	1.359598	0.544802
33	6	0	1.265735	0.824353	0.400757
34	16	0	2.621218	1.476252	-0.541163
35	16	0	1.641092	-0.691670	1.232113
36	6	0	3.284175	-0.859103	0.632552
37	6	0	3.744077	0.145934	-0.144341
38	6	0	-0.420288	2.623056	-0.083400
39	16	0	0.613623	3.524415	-1.060832
40	7	0	-1.703964	2.950012	0.224220
41	1	0	-2.108363	2.243560	0.840529
42	6	0	-2.562765	4.017058	-0.096742
43	6	0	-3.830775	3.980333	0.516756
44	6	0	-2.257141	5.078885	-0.962741
45	6	0	-4.768188	4.977014	0.274803
46	1	0	-4.076294	3.160731	1.189365
47	6	0	-3.209697	6.072331	-1.194734
48	1	0	-1.290958	5.121690	-1.443320
49	6	0	-4.463164	6.034801	-0.585618
50	1	0	-5.738829	4.926304	0.760715
51	1	0	-2.958018	6.887682	-1.867810
52	1	0	-5.193259	6.815909	-0.777139
53	6	0	5.152997	0.311879	-0.618551
54	8	0	6.139266	-0.023192	0.000417
55	8	0	5.167289	0.954121	-1.803072
56	6	0	3.958258	-2.110516	1.085338
57	8	0	3.645510	-2.672764	2.117597
58	8	0	4.864010	-2.550543	0.205577
59	6	0	6.469150	1.279748	-2.355674
60	6	0	7.032446	0.116758	-3.157073
61	1	0	7.134580	1.561657	-1.536177
62	1	0	6.277568	2.150059	-2.986911
63	1	0	7.979149	0.414281	-3.622320
64	1	0	7.223000	-0.742876	-2.508586
65	1	0	6.338474	-0.182461	-3.948962
66	6	0	5.658463	-3.698726	0.605274
67	6	0	6.834513	-3.272957	1.470303
68	1	0	5.988050	-4.129392	-0.342764
69	1	0	5.009648	-4.409571	1.122510
70	1	0	7.478720	-4.137646	1.667227
71	1	0	7.422007	-2.500122	0.966915
72	1	0	6.486474	-2.878659	2.429218
73	1	0	-2.899286	0.291434	-0.751750



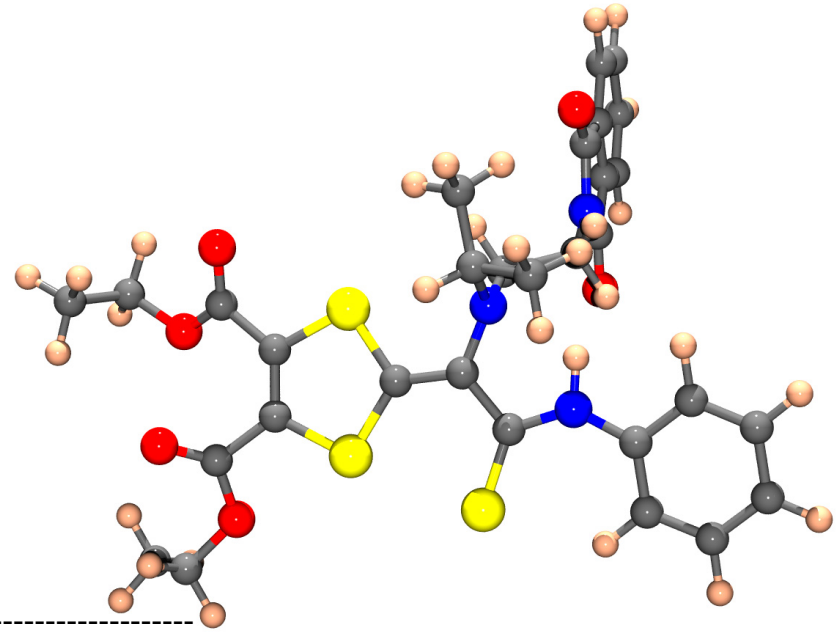
6a_TS5

6a_TS5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.838362	-3.482705	-0.300396
2	6	0	-4.352131	-3.247699	-1.588691
3	6	0	-4.619399	-4.118435	-2.634659
4	6	0	-5.398260	-5.248120	-2.350006
5	6	0	-5.885500	-5.483865	-1.058119
6	6	0	-5.610044	-4.597546	-0.008218
7	6	0	-4.380377	-2.370028	0.583078
8	6	0	-3.567406	-1.977038	-1.569389
9	1	0	-4.237159	-3.925656	-3.632296
10	1	0	-5.629034	-5.953727	-3.143058
11	1	0	-6.486494	-6.368782	-0.868934
12	1	0	-5.982920	-4.770238	0.996623
13	8	0	-4.585454	-2.196261	1.768830
14	8	0	-2.979062	-1.422561	-2.475295
15	7	0	-3.636550	-1.511802	-0.243857
16	6	0	-3.000119	-0.293098	0.230399
17	1	0	-3.582126	0.057886	1.086012
18	6	0	-1.531180	-0.526864	0.642122
19	1	0	-1.484016	-1.415146	1.276908
20	1	0	-0.954012	-0.750848	-0.259772
21	7	0	-0.945626	0.648202	1.315138
22	6	0	-0.792681	0.684508	2.808874
23	6	0	-1.694424	-0.320704	3.534823
24	6	0	-1.047782	2.102666	3.338980
25	1	0	0.245731	0.427102	3.064258
26	1	0	-1.406813	-1.359455	3.351189
27	1	0	-1.603849	-0.149808	4.612654
28	1	0	-2.750690	-0.207184	3.268114
29	1	0	-0.430706	2.847684	2.828476
30	1	0	-2.101087	2.387287	3.224083
31	1	0	-0.803365	2.146101	4.406295
32	6	0	0.066435	1.366161	0.574794

33	6	0	1.319843	0.807765	0.434701
34	16	0	2.726480	1.494960	-0.399599
35	16	0	1.616100	-0.795545	1.124106
36	6	0	3.276334	-0.957641	0.575505
37	6	0	3.795647	0.099978	-0.086103
38	6	0	-0.320726	2.655049	-0.023737
39	16	0	0.773130	3.609398	-0.877853
40	7	0	-1.627601	2.957553	0.198357
41	1	0	-2.062316	2.241448	0.780305
42	6	0	-2.467142	4.037756	-0.129129
43	6	0	-3.753325	4.002618	0.445251
44	6	0	-2.128917	5.106012	-0.974755
45	6	0	-4.675771	5.009468	0.187812
46	1	0	-4.025012	3.176809	1.099819
47	6	0	-3.066679	6.109588	-1.222585
48	1	0	-1.149200	5.145991	-1.427384
49	6	0	-4.337440	6.075128	-0.650024
50	1	0	-5.660764	4.960469	0.644110
51	1	0	-2.789768	6.930185	-1.879157
52	1	0	-5.055620	6.864315	-0.853101
53	6	0	5.225662	0.260873	-0.491317
54	8	0	6.174974	-0.193754	0.109305
55	8	0	5.309449	1.045981	-1.583630
56	6	0	3.895098	-2.269144	0.929020
57	8	0	3.543915	-2.905251	1.904332
58	8	0	4.795719	-2.667957	0.025035
59	6	0	6.642466	1.376743	-2.052120
60	6	0	7.176839	0.302725	-2.986541
61	1	0	7.292569	1.513314	-1.184709
62	1	0	6.512490	2.331482	-2.566134
63	1	0	8.148967	0.612558	-3.386780
64	1	0	7.309866	-0.642395	-2.452673
65	1	0	6.493189	0.143247	-3.826349
66	6	0	5.535109	-3.880054	0.330385
67	6	0	6.711032	-3.586123	1.248738
68	1	0	5.864787	-4.236058	-0.648120
69	1	0	4.847818	-4.606932	0.769921
70	1	0	7.317017	-4.491255	1.371270
71	1	0	7.337452	-2.793803	0.829675
72	1	0	6.361936	-3.270402	2.235896
73	1	0	-3.056930	0.447720	-0.571858



6a_rot6

6a_rot6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.900280	-3.428378	-0.313299
2	6	0	-4.690388	-2.960748	-1.612847
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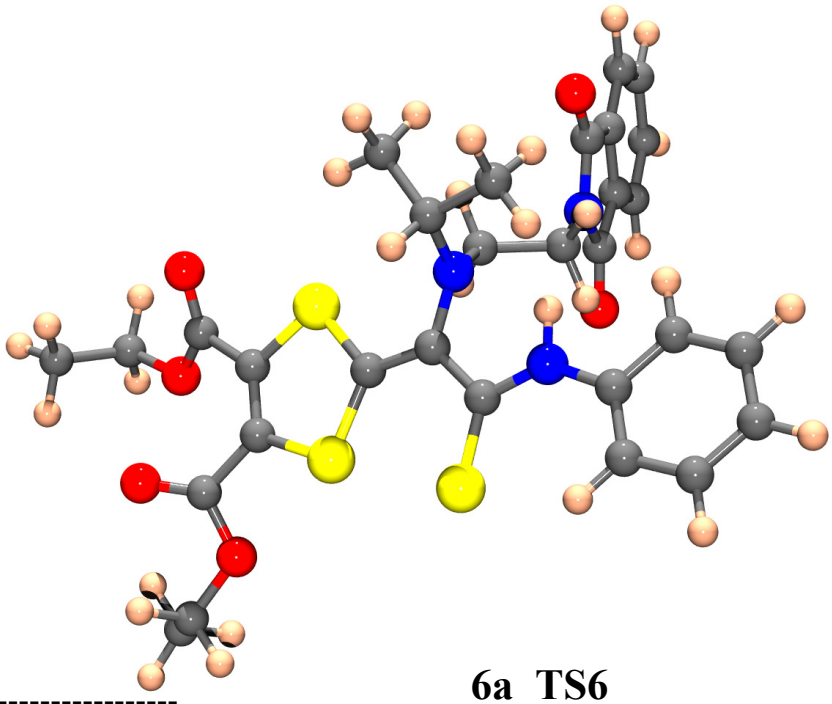
4	6	0	-5.815819	-4.871406	-2.483599
5	6	0	-6.026309	-5.340182	-1.180554
6	6	0	-5.567895	-4.619410	-0.069603
7	6	0	-4.301255	-2.447638	0.639096
8	6	0	-3.951777	-1.665368	-1.531747
9	1	0	-4.972033	-3.293408	-3.724427
10	1	0	-6.183095	-5.452865	-3.324468
11	1	0	-6.553480	-6.278079	-1.030692
12	1	0	-5.725493	-4.973300	0.944520
13	8	0	-4.266369	-2.480820	1.854576
14	8	0	-3.575347	-0.936797	-2.426872
15	7	0	-3.762785	-1.425192	-0.158203
16	6	0	-3.075374	-0.262883	0.381981
17	1	0	-3.510021	-0.063278	1.364786
18	6	0	-1.553417	-0.494191	0.506078
19	1	0	-1.392033	-1.476622	0.962161
20	1	0	-1.123795	-0.532925	-0.498888
21	7	0	-0.872796	0.571640	1.254090
22	6	0	-0.787321	0.532839	2.752017
23	6	0	-1.150578	-0.828874	3.358914
24	6	0	-1.623248	1.650916	3.397275
25	1	0	0.262776	0.728066	3.003422
26	1	0	-0.487367	-1.625326	3.008747
27	1	0	-1.037093	-0.764431	4.446244
28	1	0	-2.185027	-1.125658	3.153488
29	1	0	-1.333683	2.637275	3.021862
30	1	0	-2.694505	1.505181	3.207626
31	1	0	-1.477531	1.654269	4.483890
32	6	0	0.135496	1.335036	0.565286
33	6	0	1.385098	0.774644	0.402350
34	16	0	2.812914	1.486916	-0.368591

35	16	0	1.644029	-0.862354	1.016711
36	6	0	3.312999	-1.019096	0.490848
37	6	0	3.859087	0.063132	-0.106821
38	6	0	-0.231216	2.661458	0.044184
39	16	0	0.883024	3.648917	-0.744395
40	7	0	-1.536412	2.970814	0.270859
41	1	0	-1.993303	2.233484	0.803934
42	6	0	-2.358858	4.076604	-0.016794
43	6	0	-3.639650	4.050836	0.569489
44	6	0	-2.009224	5.158263	-0.840109
45	6	0	-4.546368	5.079624	0.344231
46	1	0	-3.918726	3.216898	1.210126
47	6	0	-2.930918	6.184035	-1.055169
48	1	0	-1.033420	5.191510	-1.301545
49	6	0	-4.196789	6.158607	-0.471441
50	1	0	-5.527635	5.037499	0.809171
51	1	0	-2.645377	7.014697	-1.695165
52	1	0	-4.902416	6.965115	-0.648827
53	6	0	5.298956	0.225094	-0.474771
54	8	0	6.230077	-0.275463	0.117780
55	8	0	5.415257	1.067961	-1.520262
56	6	0	3.908866	-2.355206	0.787060
57	8	0	3.532931	-3.035251	1.722697
58	8	0	4.819021	-2.720751	-0.121613
59	6	0	6.761792	1.405961	-1.942411
60	6	0	7.305980	0.374488	-2.918147
61	1	0	7.393864	1.491126	-1.055260
62	1	0	6.653509	2.386916	-2.409996
63	1	0	8.290675	0.692358	-3.279487
64	1	0	7.415809	-0.598106	-2.430418
65	1	0	6.640749	0.266436	-3.780671
66	6	0	5.533746	-3.959211	0.131971
67	6	0	6.692601	-3.736251	1.091012
68	1	0	5.880384	-4.265486	-0.857444
69	1	0	4.826004	-4.698493	0.514869
70	1	0	7.281279	-4.656931	1.176721
71	1	0	7.341215	-2.932923	0.730639
72	1	0	6.325639	-3.469470	2.086035
73	1	0	-3.282417	0.581021	-0.281907



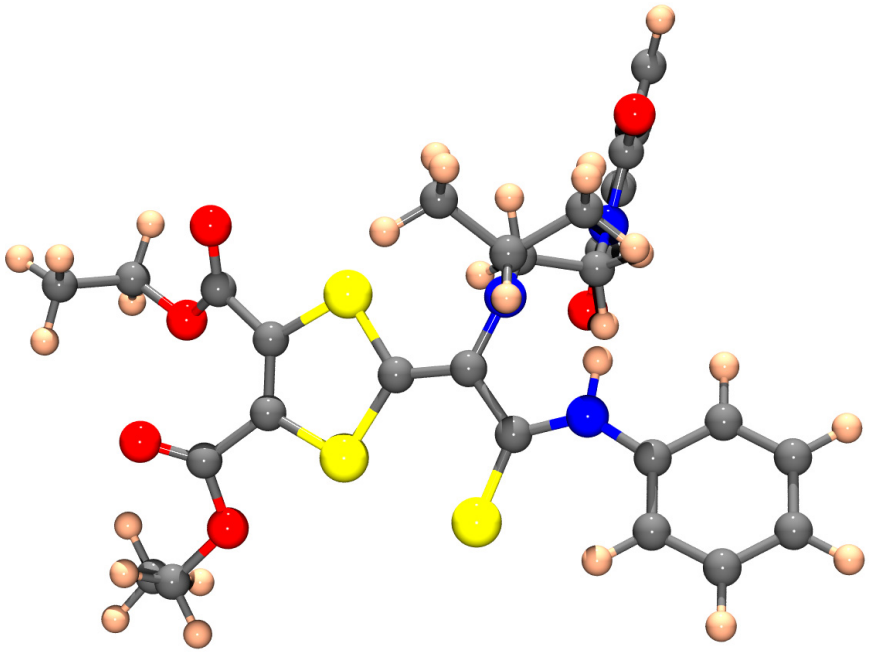
6a_TS6

6a_TS6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.740029	-3.485955	-0.331410
2	6	0	-4.254578	-3.324234	-1.631478
3	6	0	-4.522194	-4.252882	-2.626095
4	6	0	-5.300465	-5.364985	-2.277357
5	6	0	-5.787035	-5.527170	-0.974000
6	6	0	-5.511142	-4.582769	0.023868
7	6	0	-4.277795	-2.326351	0.486773
8	6	0	-3.470040	-2.054139	-1.686219
9	1	0	-4.140353	-4.116987	-3.633205
10	1	0	-5.531370	-6.114531	-3.028961
11	1	0	-6.387631	-6.400087	-0.734515
12	1	0	-5.883176	-4.698734	1.037141
13	8	0	-4.473514	-2.085268	1.663172
14	8	0	-2.885031	-1.552047	-2.623678
15	7	0	-3.537945	-1.515594	-0.387958
16	6	0	-2.896729	-0.278732	0.029062
17	1	0	-3.573429	0.215975	0.731360
18	6	0	-1.530934	-0.548008	0.701450
19	1	0	-1.668373	-1.343296	1.439037
20	1	0	-0.846943	-0.936944	-0.060134
21	7	0	-0.937645	0.624931	1.347992
22	6	0	-1.069744	0.821649	2.826129
23	6	0	-0.876212	-0.456512	3.662352
24	6	0	-2.405493	1.475283	3.230207
25	1	0	-0.261049	1.514791	3.081829
26	1	0	0.041466	-0.990305	3.406691
27	1	0	-0.818094	-0.179499	4.720727
28	1	0	-1.723382	-1.144192	3.559060
29	1	0	-2.548930	2.454900	2.764003
30	1	0	-3.252640	0.828576	2.971389
31	1	0	-2.434355	1.626838	4.315526
32	6	0	0.056200	1.381346	0.633479

33	6	0	1.324136	0.851119	0.495103
34	16	0	2.710655	1.547345	-0.365182
35	16	0	1.657998	-0.726594	1.217751
36	6	0	3.300067	-0.891546	0.617463
37	6	0	3.794103	0.157417	-0.076109
38	6	0	-0.333079	2.681045	0.059449
39	16	0	0.770555	3.680818	-0.727651
40	7	0	-1.655689	2.956333	0.224884
41	1	0	-2.129249	2.193084	0.700389
42	6	0	-2.496763	4.033045	-0.118329
43	6	0	-3.872600	3.824934	0.102490
44	6	0	-2.069599	5.270199	-0.625329
45	6	0	-4.798004	4.823147	-0.178357
46	1	0	-4.214343	2.868996	0.493333
47	6	0	-3.011677	6.261829	-0.902975
48	1	0	-1.018869	5.448194	-0.799081
49	6	0	-4.373044	6.053044	-0.686406
50	1	0	-5.853737	4.636919	-0.000816
51	1	0	-2.664628	7.213965	-1.295592
52	1	0	-5.093520	6.834773	-0.909147
53	6	0	5.211031	0.317087	-0.524221
54	8	0	6.177968	-0.141364	0.044915
55	8	0	5.262841	1.103271	-1.617940
56	6	0	3.939203	-2.191593	0.978650
57	8	0	3.638295	-2.798566	1.988619
58	8	0	4.793896	-2.617018	0.042734
59	6	0	6.581392	1.429050	-2.128462
60	6	0	7.083102	0.352024	-3.077506
61	1	0	7.258909	1.564811	-1.282140
62	1	0	6.438427	2.383438	-2.639681
63	1	0	8.043237	0.658264	-3.508294
64	1	0	7.229815	-0.592699	-2.546553
65	1	0	6.373143	0.193372	-3.895375
66	6	0	5.549698	-3.819276	0.346961
67	6	0	6.770084	-3.497351	1.195309
68	1	0	5.829990	-4.204969	-0.635695
69	1	0	4.886830	-4.532521	0.842736
70	1	0	7.383321	-4.398119	1.313957
71	1	0	7.372515	-2.717397	0.721652
72	1	0	6.470700	-3.152221	2.188913
73	1	0	-2.779475	0.344447	-0.861185



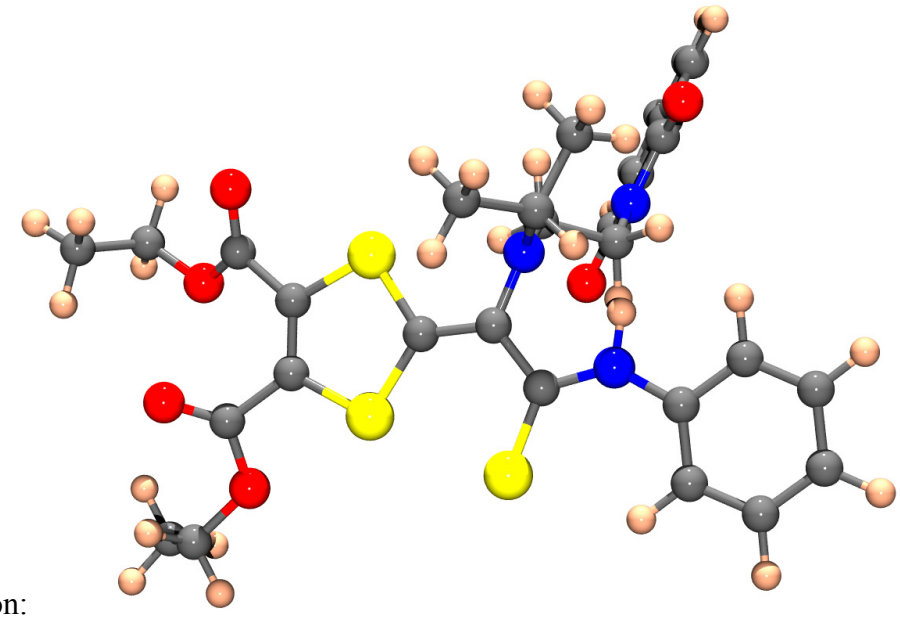
6a_rot7

6a_rot7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.388449	-3.802741	-0.323244
2	6	0	-3.791387	-3.686215	-1.580833
3	6	0	-3.889987	-4.695741	-2.526659
4	6	0	-4.613567	-5.842498	-2.172560
5	6	0	-5.212199	-5.959337	-0.911633
6	6	0	-5.106644	-4.933287	0.037033
7	6	0	-4.097348	-2.558861	0.448507
8	6	0	-3.103253	-2.362687	-1.653520
9	1	0	-3.422537	-4.594495	-3.501232
10	1	0	-4.712998	-6.655134	-2.886547
11	1	0	-5.766668	-6.860785	-0.666737
12	1	0	-5.566566	-5.013418	1.017138
13	8	0	-4.428185	-2.261919	1.581390
14	8	0	-2.470708	-1.875170	-2.567426
15	7	0	-3.336865	-1.748847	-0.408103
16	6	0	-2.841488	-0.433267	-0.032256
17	1	0	-3.638734	0.075443	0.516022
18	6	0	-1.566763	-0.530547	0.833665
19	1	0	-1.762692	-1.203235	1.675313
20	1	0	-0.788130	-1.004577	0.229429
21	7	0	-1.110729	0.767568	1.335056
22	6	0	-1.415487	1.153848	2.743065
23	6	0	-0.593153	0.391064	3.795534
24	6	0	-2.917990	1.051343	3.050586
25	1	0	-1.134990	2.211548	2.807117
26	1	0	0.478263	0.563005	3.666552
27	1	0	-0.869537	0.727171	4.801805
28	1	0	-0.776340	-0.688714	3.746804
29	1	0	-3.512477	1.694400	2.390978
30	1	0	-3.292391	0.026210	2.956487

31	1	0	-3.104902	1.377775	4.079129
32	6	0	-0.072082	1.482436	0.648306
33	6	0	1.199666	0.950047	0.545483
34	16	0	2.582583	1.634368	-0.336668
35	16	0	1.560330	-0.603280	1.315961
36	6	0	3.188751	-0.783060	0.684996
37	6	0	3.666938	0.247948	-0.045313
38	6	0	-0.446023	2.781869	0.055228
39	16	0	0.676190	3.803619	-0.671443
40	7	0	-1.780342	3.036588	0.152031
41	1	0	-2.274890	2.242281	0.552500
42	6	0	-2.608494	4.106394	-0.240718
43	6	0	-3.989481	3.834293	-0.269819
44	6	0	-2.162616	5.400055	-0.552204
45	6	0	-4.903319	4.826547	-0.606234
46	1	0	-4.342717	2.832134	-0.035658
47	6	0	-3.091819	6.384824	-0.889981
48	1	0	-1.106863	5.626763	-0.532081
49	6	0	-4.459116	6.112617	-0.922226
50	1	0	-5.964062	4.591492	-0.624467
51	1	0	-2.731399	7.381802	-1.129201
52	1	0	-5.169764	6.889544	-1.189044
53	6	0	5.075869	0.398805	-0.521291
54	8	0	6.052888	-0.049163	0.038973
55	8	0	5.108500	1.164652	-1.630057
56	6	0	3.836358	-2.072352	1.068319
57	8	0	3.557785	-2.651515	2.100759
58	8	0	4.671234	-2.523053	0.126275
59	6	0	6.417942	1.483083	-2.167637
60	6	0	6.906211	0.390121	-3.105409
61	1	0	7.108963	1.634946	-1.335073
62	1	0	6.265060	2.427996	-2.693404
63	1	0	7.858901	0.689985	-3.556741
64	1	0	7.062847	-0.544846	-2.560221
65	1	0	6.183595	0.216105	-3.908944
66	6	0	5.434670	-3.715900	0.447554
67	6	0	6.670136	-3.370913	1.264443
68	1	0	5.697297	-4.126603	-0.529837
69	1	0	4.782348	-4.416932	0.973877
70	1	0	7.287150	-4.267553	1.394283
71	1	0	7.262089	-2.602354	0.759954
72	1	0	6.388730	-3.001142	2.254406
73	1	0	-2.634058	0.110721	-0.957490



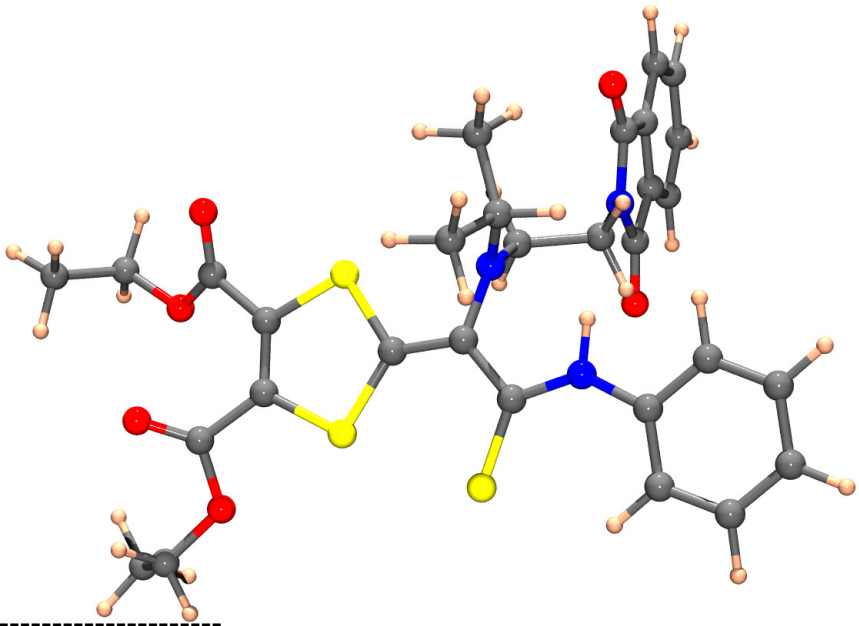
6a_TS7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.659408	-3.546457	-0.366527
2	6	0	-3.894910	-3.570640	-1.535544
3	6	0	-3.990929	-4.614918	-2.443057
4	6	0	-4.886466	-5.650167	-2.142444
5	6	0	-5.652538	-5.626174	-0.970134
6	6	0	-5.548515	-4.565869	-0.059750
7	6	0	-4.325111	-2.300687	0.384236
8	6	0	-3.048470	-2.340361	-1.569134
9	1	0	-3.392828	-4.623147	-3.349015
10	1	0	-4.989578	-6.485843	-2.828779
11	1	0	-6.337809	-6.443661	-0.764814
12	1	0	-6.137761	-4.536938	0.851586
13	8	0	-4.764995	-1.900618	1.445623
14	8	0	-2.246408	-1.981822	-2.406722
15	7	0	-3.366679	-1.633506	-0.394715
16	6	0	-2.766053	-0.366526	-0.008500
17	1	0	-3.532378	0.195139	0.534008
18	6	0	-1.512417	-0.574790	0.873497
19	1	0	-1.766419	-1.266132	1.679843
20	1	0	-0.754784	-1.075434	0.261889
21	7	0	-0.951005	0.654030	1.436196
22	6	0	-1.284587	1.151850	2.805849
23	6	0	-0.050081	1.266704	3.712494
24	6	0	-2.366979	0.314569	3.497693
25	1	0	-1.684592	2.172409	2.696273
26	1	0	0.739951	1.858835	3.241446
27	1	0	-0.326385	1.766388	4.648536
28	1	0	0.355166	0.279430	3.957672
29	1	0	-3.264691	0.168515	2.889179
30	1	0	-1.990018	-0.672747	3.786760
31	1	0	-2.666987	0.828402	4.416793

6a_TS7

32	6	0	-0.022465	1.412482	0.648941
33	6	0	1.261036	0.917505	0.514522
34	16	0	2.594476	1.585520	-0.440553
35	16	0	1.664700	-0.586513	1.351102
36	6	0	3.284559	-0.755963	0.695040
37	6	0	3.721648	0.244615	-0.101959
38	6	0	-0.477530	2.656643	0.007633
39	16	0	0.576555	3.679348	-0.815085
40	7	0	-1.816550	2.870017	0.156639
41	1	0	-2.257607	2.123203	0.683094
42	6	0	-2.710874	3.890414	-0.224402
43	6	0	-4.015740	3.776142	0.294143
44	6	0	-2.407325	4.968142	-1.070633
45	6	0	-4.992193	4.713386	-0.020560
46	1	0	-4.260024	2.945225	0.953624
47	6	0	-3.398722	5.902572	-1.374639
48	1	0	-1.413605	5.068527	-1.480972
49	6	0	-4.689017	5.788811	-0.859258
50	1	0	-5.990867	4.603027	0.393154
51	1	0	-3.148055	6.731744	-2.030958
52	1	0	-5.448830	6.524545	-1.106569
53	6	0	5.114055	0.399313	-0.621059
54	8	0	6.113380	-0.011222	-0.071406
55	8	0	5.103927	1.120199	-1.760408
56	6	0	3.976858	-2.006146	1.129646
57	8	0	3.753767	-2.524946	2.206526
58	8	0	4.780271	-2.499829	0.181873
59	6	0	6.392486	1.433537	-2.348575
60	6	0	6.868478	0.309734	-3.255781
61	1	0	7.105281	1.627833	-1.543659
62	1	0	6.211473	2.354375	-2.907147
63	1	0	7.804568	0.602112	-3.745168
64	1	0	7.051747	-0.600831	-2.678533
65	1	0	6.126258	0.095415	-4.031224
66	6	0	5.573175	-3.662453	0.540368
67	6	0	6.830110	-3.258332	1.294976
68	1	0	5.809007	-4.121644	-0.422152
69	1	0	4.949759	-4.343038	1.125448
70	1	0	7.464278	-4.138822	1.450274
71	1	0	7.393564	-2.510137	0.730707
72	1	0	6.576843	-2.840342	2.273205
73	1	0	-2.508705	0.170400	-0.925135



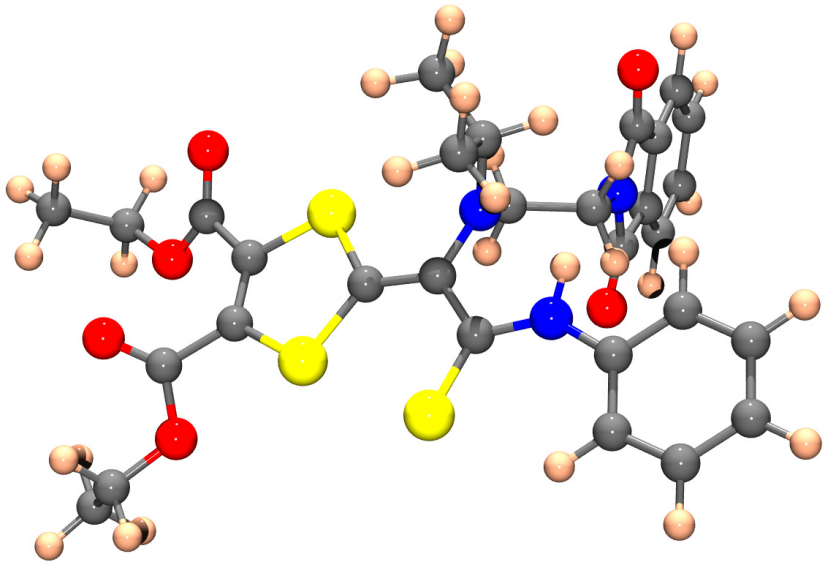
6a_rot8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.856321	-3.460410	-0.275952
2	6	0	-4.602672	-3.078128	-1.595448
3	6	0	-5.023196	-3.850448	-2.667838
4	6	0	-5.715058	-5.034141	-2.377584
5	6	0	-5.969619	-5.417270	-1.054601
6	6	0	-5.540314	-4.629605	0.022062
7	6	0	-4.277619	-2.425015	0.629871
8	6	0	-3.856792	-1.784652	-1.574495
9	1	0	-4.820766	-3.543595	-3.689296
10	1	0	-6.060513	-5.666121	-3.190782
11	1	0	-6.508457	-6.340596	-0.861888
12	1	0	-5.732007	-4.917206	1.051173
13	8	0	-4.277143	-2.381997	1.845884
14	8	0	-3.447887	-1.117548	-2.502386
15	7	0	-3.708778	-1.458031	-0.213172
16	6	0	-3.023940	-0.270671	0.273004
17	1	0	-3.543624	0.047748	1.181816
18	6	0	-1.533876	-0.554792	0.573312
19	1	0	-1.474634	-1.488697	1.143260
20	1	0	-1.013496	-0.724974	-0.372967
21	7	0	-0.838499	0.520273	1.284207
22	6	0	-1.209320	0.820075	2.695554
23	6	0	-0.184718	1.747529	3.358046
24	6	0	-1.387060	-0.460955	3.525412
25	1	0	-2.182508	1.347745	2.722138
26	1	0	-0.074899	2.696417	2.826176
27	1	0	-0.516655	1.973084	4.376799
28	1	0	0.798381	1.269220	3.419161
29	1	0	-2.204873	-1.091242	3.163604
30	1	0	-0.463923	-1.051078	3.533426
31	1	0	-1.624776	-0.185705	4.558742
32	6	0	0.093815	1.328890	0.552253

6a_rot8

33	6	0	1.357340	0.797187	0.394091
34	16	0	2.733944	1.462770	-0.491132
35	16	0	1.666717	-0.767827	1.153771
36	6	0	3.313809	-0.946238	0.566519
37	6	0	3.814840	0.080536	-0.156477
38	6	0	-0.320439	2.620211	-0.005727
39	16	0	0.742989	3.602631	-0.866301
40	7	0	-1.624736	2.920866	0.263428
41	1	0	-2.076962	2.197741	0.810144
42	6	0	-2.469596	4.014286	-0.016695
43	6	0	-3.728565	3.985215	0.614416
44	6	0	-2.160330	5.085706	-0.868539
45	6	0	-4.654113	5.000422	0.405046
46	1	0	-3.976593	3.159037	1.278448
47	6	0	-3.100168	6.098538	-1.066663
48	1	0	-1.201803	5.121410	-1.364438
49	6	0	-4.344711	6.069602	-0.439188
50	1	0	-5.617865	4.955440	0.904910
51	1	0	-2.845731	6.921711	-1.729006
52	1	0	-5.064729	6.865818	-0.604635
53	6	0	5.233678	0.219564	-0.600103
54	8	0	6.190822	-0.273888	-0.042980
55	8	0	5.304181	1.029172	-1.676228
56	6	0	3.959772	-2.233634	0.966219
57	8	0	3.708572	-2.780667	2.022259
58	8	0	4.754716	-2.722222	0.008254
59	6	0	6.629931	1.340824	-2.175969
60	6	0	7.115455	0.275854	-3.146743
61	1	0	7.307017	1.445592	-1.324833
62	1	0	6.506683	2.308685	-2.666643
63	1	0	8.082530	0.574064	-3.567565
64	1	0	7.243201	-0.682726	-2.636180
65	1	0	6.405853	0.147986	-3.970332
66	6	0	5.504751	-3.922524	0.334297
67	6	0	6.767144	-3.586602	1.112853
68	1	0	5.734154	-4.357393	-0.641028
69	1	0	4.853243	-4.600515	0.891083
70	1	0	7.367871	-4.493632	1.247071
71	1	0	7.362762	-2.841899	0.577953
72	1	0	6.517968	-3.189588	2.100744
73	1	0	-3.127883	0.501427	-0.493728



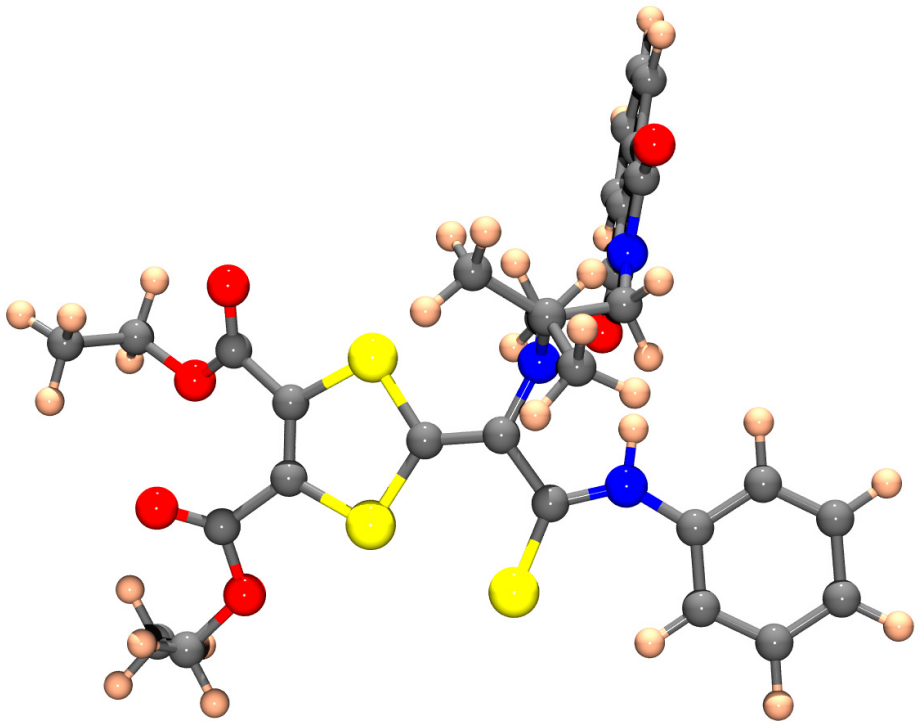
6a_TS8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.786961	-3.553277	-0.266517
2	6	0	-4.348530	-3.254791	-1.558826
3	6	0	-4.610234	-4.100304	-2.626693
4	6	0	-5.333614	-5.270574	-2.360173
5	6	0	-5.772817	-5.570016	-1.064248
6	6	0	-5.503451	-4.708680	0.007844
7	6	0	-4.351430	-2.451877	0.642202
8	6	0	-3.615973	-1.954062	-1.516901
9	1	0	-4.265307	-3.858258	-3.627188
10	1	0	-5.558190	-5.958090	-3.170696
11	1	0	-6.331264	-6.485220	-0.889373
12	1	0	-5.839545	-4.930479	1.016014
13	8	0	-4.529246	-2.325238	1.837719
14	8	0	-3.075371	-1.345907	-2.418368
15	7	0	-3.668424	-1.535201	-0.175459
16	6	0	-3.060936	-0.309977	0.318673
17	1	0	-3.621936	-0.020617	1.211567
18	6	0	-1.565368	-0.505505	0.653903
19	1	0	-1.469775	-1.412240	1.263936
20	1	0	-1.023872	-0.688791	-0.277645
21	7	0	-0.966397	0.651643	1.325068
22	6	0	-1.242282	0.823273	2.784269
23	6	0	-0.702093	2.155428	3.315635
24	6	0	-0.743195	-0.332195	3.671689
25	1	0	-2.338265	0.847270	2.887668
26	1	0	-1.105425	3.018275	2.779317
27	1	0	-0.979524	2.255693	4.370023
28	1	0	0.390244	2.194043	3.252407
29	1	0	-1.072633	-1.311348	3.311367
30	1	0	0.348464	-0.340941	3.742403
31	1	0	-1.148637	-0.209144	4.682734

6a_TS8

32	6	0	0.048684	1.400579	0.637973
33	6	0	1.304292	0.846022	0.490146
34	16	0	2.701202	1.523268	-0.366746
35	16	0	1.600461	-0.752323	1.184135
36	6	0	3.234195	-0.946180	0.569572
37	6	0	3.751026	0.101969	-0.109029
38	6	0	-0.332179	2.694339	0.043763
39	16	0	0.784992	3.695729	-0.719876
40	7	0	-1.659113	2.965279	0.186017
41	1	0	-2.126071	2.220406	0.697783
42	6	0	-2.499397	4.039440	-0.164601
43	6	0	-3.809397	3.978158	0.350086
44	6	0	-2.138825	5.123632	-0.979706
45	6	0	-4.734381	4.974898	0.063711
46	1	0	-4.097871	3.140675	0.982574
47	6	0	-3.078945	6.117606	-1.256001
48	1	0	-1.140665	5.182915	-1.387567
49	6	0	-4.373847	6.057151	-0.742871
50	1	0	-5.738221	4.905368	0.473881
51	1	0	-2.784556	6.950979	-1.888400
52	1	0	-5.093585	6.838883	-0.967940
53	6	0	5.170040	0.236340	-0.557519
54	8	0	6.126095	-0.264869	-0.006114
55	8	0	5.240430	1.054530	-1.626631
56	6	0	3.847075	-2.265584	0.907060
57	8	0	3.547931	-2.875832	1.915375
58	8	0	4.675719	-2.701462	-0.047358
59	6	0	6.566425	1.365988	-2.126618
60	6	0	7.048210	0.305674	-3.104269
61	1	0	7.244971	1.464500	-1.275886
62	1	0	6.444319	2.336903	-2.611456
63	1	0	8.015299	0.604374	-3.524692
64	1	0	7.174672	-0.656142	-2.599538
65	1	0	6.337188	0.184182	-3.927596
66	6	0	5.406485	-3.924983	0.232787
67	6	0	6.642999	-3.643733	1.072191
68	1	0	5.667039	-4.303820	-0.757927
69	1	0	4.732163	-4.629074	0.726274
70	1	0	7.234561	-4.560922	1.174062
71	1	0	7.260212	-2.873433	0.601807
72	1	0	6.361943	-3.303184	2.072645
73	1	0	-3.182597	0.456068	-0.452302



6a_rot9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.760897	-3.581611	-0.209126
2	6	0	-4.204500	-3.417369	-1.480020
3	6	0	-4.377649	-4.367399	-2.475603
4	6	0	-5.134435	-5.503339	-2.158181
5	6	0	-5.692509	-5.667750	-0.884014
6	6	0	-5.511872	-4.701725	0.114936
7	6	0	-4.394802	-2.395263	0.619606
8	6	0	-3.464560	-2.120406	-1.504110
9	1	0	-3.941214	-4.229634	-3.460036
10	1	0	-5.292021	-6.270009	-2.911465
11	1	0	-6.274271	-6.559447	-0.668466
12	1	0	-5.939778	-4.818987	1.105741
13	8	0	-4.676327	-2.147079	1.775439
14	8	0	-2.840217	-1.606658	-2.410393
15	7	0	-3.630195	-1.568373	-0.221694
16	6	0	-3.056125	-0.301375	0.200556
17	1	0	-3.678077	0.067348	1.020759
18	6	0	-1.588972	-0.449861	0.656715
19	1	0	-1.522545	-1.305134	1.342838
20	1	0	-0.979007	-0.688904	-0.217380
21	7	0	-1.085292	0.777647	1.285092
22	6	0	-1.391059	0.923608	2.741101
23	6	0	-1.381898	2.387020	3.199721
24	6	0	-0.505808	0.077316	3.672398
25	1	0	-2.418554	0.550162	2.843996
26	1	0	-2.116571	2.998140	2.668505
27	1	0	-1.620800	2.429978	4.267482

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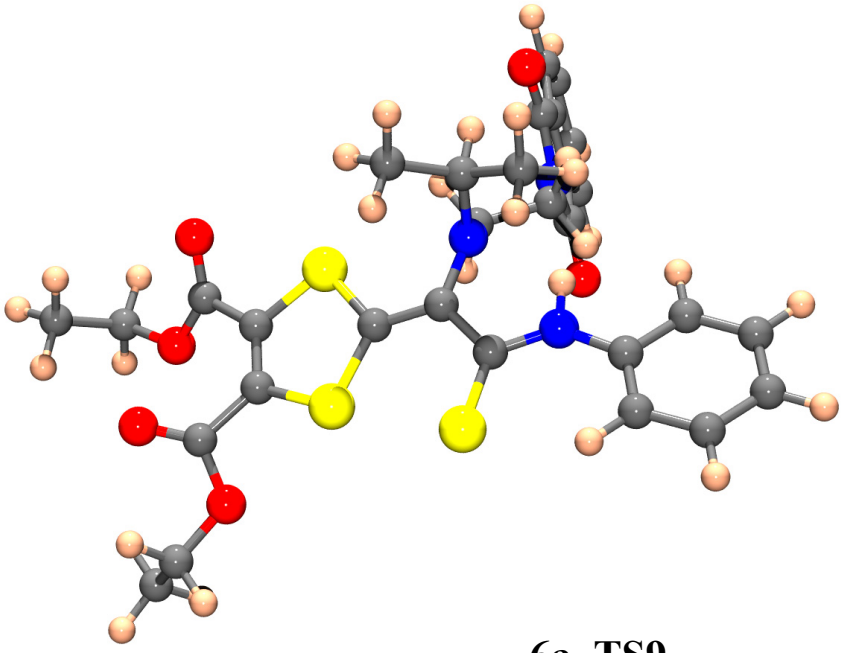
28	1	0	-0.395349	2.842799	3.062350
29	1	0	-0.492323	-0.978198	3.384252
30	1	0	0.525376	0.444586	3.684530
31	1	0	-0.894495	0.133049	4.696012
32	6	0	0.032491	1.468802	0.696542
33	6	0	1.269754	0.862522	0.589420
34	16	0	2.731953	1.536386	-0.168344
35	16	0	1.493972	-0.789979	1.184903
36	6	0	3.120608	-1.024032	0.567867
37	6	0	3.698770	0.044395	-0.022497
38	6	0	-0.248301	2.801781	0.118566
39	16	0	0.973585	3.834224	-0.403744
40	7	0	-1.579533	3.067597	0.050409
41	1	0	-2.113539	2.294174	0.443876
42	6	0	-2.358726	4.166282	-0.355484
43	6	0	-3.747473	4.028696	-0.158619
44	6	0	-1.867737	5.350884	-0.926919
45	6	0	-4.622359	5.047087	-0.516999
46	1	0	-4.138142	3.111870	0.278670
47	6	0	-2.759762	6.364662	-1.279882
48	1	0	-0.807113	5.470763	-1.090598
49	6	0	-4.132944	6.227774	-1.081156
50	1	0	-5.688776	4.916495	-0.354212
51	1	0	-2.363889	7.275914	-1.720412
52	1	0	-4.813583	7.026170	-1.362373
53	6	0	5.129338	0.140310	-0.445178
54	8	0	6.052959	-0.438359	0.084950
55	8	0	5.252678	1.019812	-1.459252
56	6	0	3.654400	-2.397289	0.806184
57	8	0	3.289824	-3.076081	1.747220
58	8	0	4.493950	-2.792004	-0.156541
59	6	0	6.598846	1.300197	-1.922340
60	6	0	7.050478	0.278096	-2.953591
61	1	0	7.267370	1.319897	-1.058235
62	1	0	6.526620	2.301848	-2.351455
63	1	0	8.036863	0.557326	-3.341324
64	1	0	7.125958	-0.716145	-2.504671
65	1	0	6.349394	0.236662	-3.793244
66	6	0	5.149043	-4.073951	0.034588
67	6	0	6.366678	-3.938167	0.935355
68	1	0	5.425820	-4.376996	-0.977568
69	1	0	4.420907	-4.780635	0.440127
70	1	0	6.902274	-4.893713	0.975951
71	1	0	7.043489	-3.168227	0.554683
72	1	0	6.067153	-3.668772	1.952022
73	1	0	-3.119247	0.392993	-0.642443



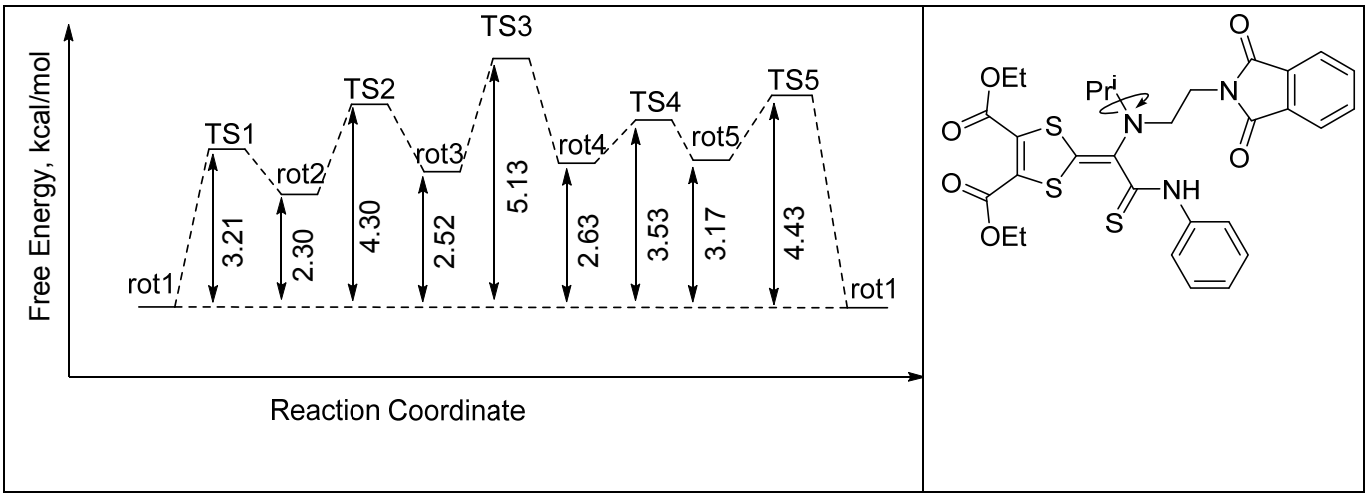
6a_TS9

6a_TS9

Standard orientation:

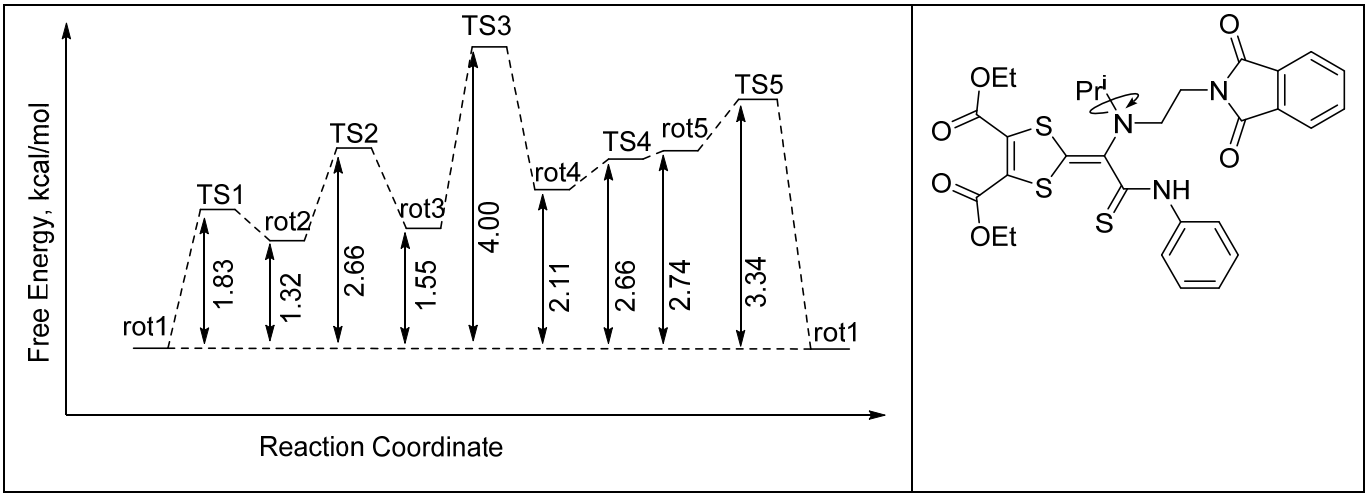
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.606425	-3.706289	-0.117628
2	6	0	-4.385269	-3.356800	-1.452174
3	6	0	-4.722091	-4.211767	-2.491015
4	6	0	-5.294105	-5.445183	-2.151259
5	6	0	-5.515423	-5.795680	-0.813327
6	6	0	-5.172007	-4.924310	0.229097
7	6	0	-4.140563	-2.580025	0.744156
8	6	0	-3.771408	-1.995817	-1.486097
9	1	0	-4.546400	-3.929769	-3.524534
10	1	0	-5.570882	-6.142207	-2.937123
11	1	0	-5.960288	-6.759272	-0.581814
12	1	0	-5.339177	-5.185913	1.269359
13	8	0	-4.151886	-2.479374	1.955519
14	8	0	-3.426505	-1.330679	-2.441731
15	7	0	-3.664162	-1.598576	-0.141245
16	6	0	-3.102116	-0.331781	0.296793
17	1	0	-3.644821	-0.031391	1.197368
18	6	0	-1.591432	-0.441501	0.592206
19	1	0	-1.427653	-1.335878	1.209886
20	1	0	-1.062172	-0.594121	-0.351912
21	7	0	-1.070833	0.766089	1.242942
22	6	0	-1.371593	0.903613	2.705226
23	6	0	-2.150336	2.187328	3.037602
24	6	0	-0.142192	0.787670	3.618416
25	1	0	-2.030800	0.055617	2.926620
26	1	0	-3.070710	2.270014	2.448953
27	1	0	-2.434795	2.182435	4.095795
28	1	0	-1.547623	3.083956	2.859241
29	1	0	0.341452	-0.188025	3.534102
30	1	0	0.597098	1.561990	3.386613
31	1	0	-0.448191	0.920723	4.661960
32	6	0	0.044519	1.463560	0.660616
33	6	0	1.270788	0.838364	0.534184

34	16	0	2.752503	1.507622	-0.185410
35	16	0	1.452803	-0.837108	1.076401
36	6	0	3.096230	-1.072257	0.506900
37	6	0	3.700228	0.002698	-0.044873
38	6	0	-0.211685	2.818307	0.128355
39	16	0	1.029430	3.842286	-0.366743
40	7	0	-1.537552	3.109829	0.061229
41	1	0	-2.094764	2.326250	0.395050
42	6	0	-2.290100	4.229763	-0.338846
43	6	0	-3.684155	4.035511	-0.398316
44	6	0	-1.766610	5.494757	-0.649217
45	6	0	-4.533671	5.074642	-0.758678
46	1	0	-4.098664	3.056634	-0.165888
47	6	0	-2.632992	6.527725	-1.009940
48	1	0	-0.700470	5.661851	-0.610202
49	6	0	-4.012274	6.332960	-1.069212
50	1	0	-5.605129	4.898345	-0.799263
51	1	0	-2.212052	7.501229	-1.247168
52	1	0	-4.672784	7.146964	-1.353690
53	6	0	5.142983	0.093075	-0.425392
54	8	0	6.045858	-0.504251	0.119513
55	8	0	5.302825	0.990076	-1.418738
56	6	0	3.611508	-2.455254	0.730164
57	8	0	3.215662	-3.150299	1.646269
58	8	0	4.473521	-2.837336	-0.217842
59	6	0	6.664186	1.266801	-1.837761
60	6	0	7.136332	0.260304	-2.875127
61	1	0	7.307762	1.263750	-0.954721
62	1	0	6.613064	2.277078	-2.249305
63	1	0	8.136001	0.537484	-3.228817
64	1	0	7.189924	-0.742941	-2.443420
65	1	0	6.459588	0.241501	-3.735307
66	6	0	5.113369	-4.128298	-0.035475
67	6	0	6.311327	-4.019026	0.894810
68	1	0	5.410590	-4.415580	-1.046447
69	1	0	4.370482	-4.835768	0.340777
70	1	0	6.836466	-4.980489	0.932177
71	1	0	7.004184	-3.249979	0.542307
72	1	0	5.991273	-3.762876	1.908666
73	1	0	-3.284383	0.398561	-0.496772



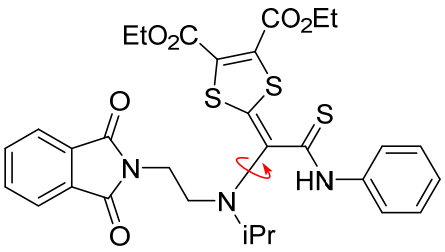
Calculated free energy values for the rotation of the isopropyl group in compound **6a**, level of theory: B3LYP/6-31G(d) (kcal/mol):

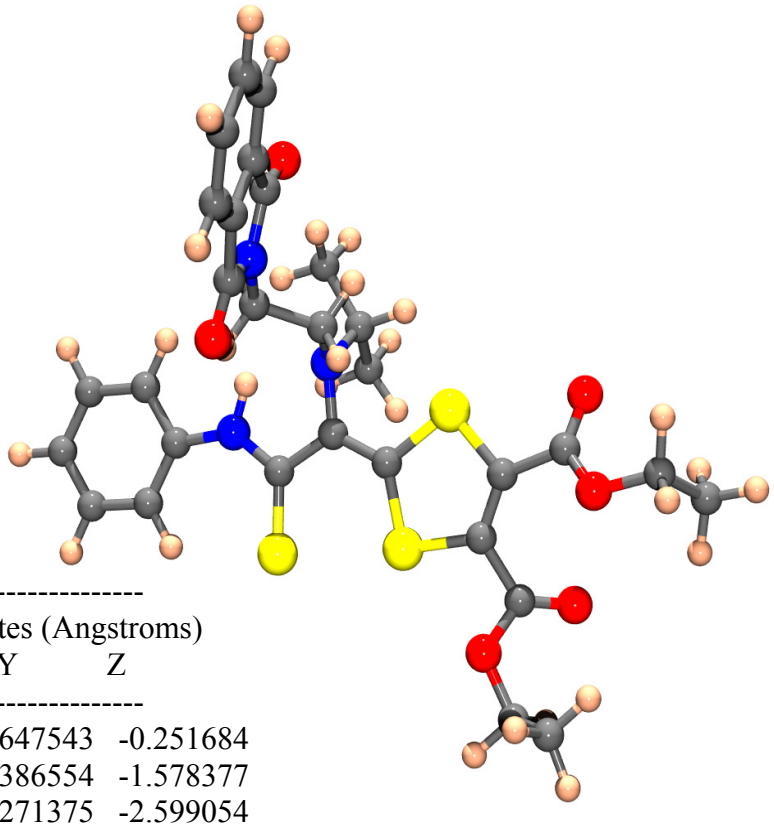
	6a_rot5	6a_TS5	6a_rot6	6a_TS6	6a_rot7	6a_TS7	6a_rot8	6a_TS8	6a_rot9	6a_TS9
G	0	3,21	2,30	4,30	2,52	5,13	2,63	3,53	3,17	4,43



Calculated free energy values for the rotation of the isopropyl group in compound **6a** with solvation, level of theory: PCM/B3LYP/6-311++G(2d,p) (kcal/mol):

	6a_rot5	6a_TS5	6a_rot6	6a_TS6	6a_rot7	6a_TS7	6a_rot8	6a_TS8	6a_rot9	6a_TS9
G	0	1,83	1,32	2,66	1,55	4,00	2,11	2,66	2,74	3,34





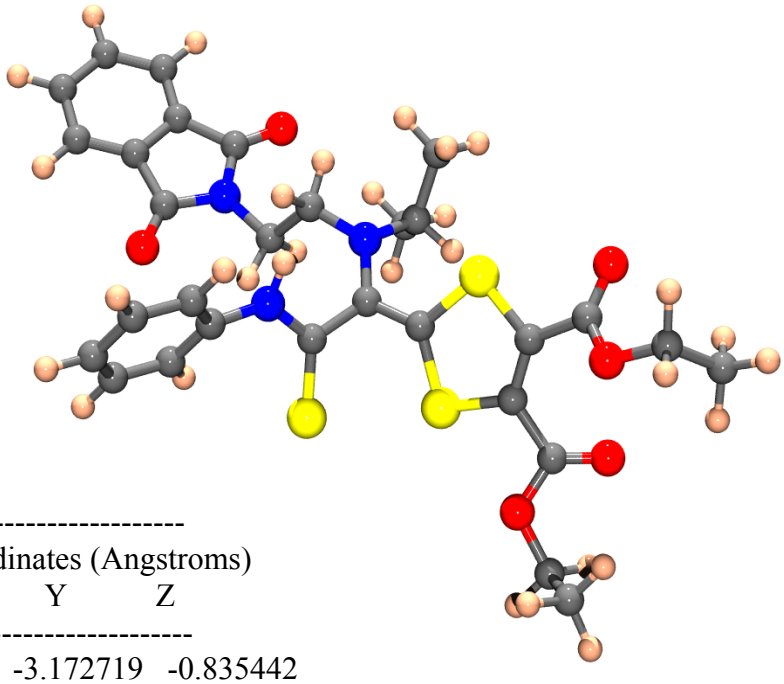
6a_rot1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.636555	-3.647543	-0.251684
2	6	0	-4.285772	-3.386554	-1.578377
3	6	0	-4.600001	-4.271375	-2.599054
4	6	0	-5.284895	-5.442713	-2.248560
5	6	0	-5.635964	-5.704750	-0.918119
6	6	0	-5.314105	-4.803812	0.105823
7	6	0	-4.160230	-2.510173	0.589091
8	6	0	-3.576093	-2.073267	-1.627086
9	1	0	-4.323379	-4.058012	-3.626911
10	1	0	-5.548810	-6.160501	-3.020036
11	1	0	-6.166494	-6.621778	-0.678030
12	1	0	-5.581968	-4.996612	1.140060
13	8	0	-4.262530	-2.348569	1.791154
14	8	0	-3.111982	-1.486672	-2.582630
15	7	0	-3.545144	-1.613225	-0.296465
16	6	0	-2.945520	-0.356404	0.126986
17	1	0	-3.607403	0.095595	0.870643
18	6	0	-1.539737	-0.566781	0.724009
19	1	0	-1.592774	-1.354510	1.483447
20	1	0	-0.878523	-0.931453	-0.068827
21	7	0	-0.988525	0.660507	1.326679
22	6	0	-0.905060	0.662007	2.821000
23	6	0	-2.309055	0.560769	3.435904
24	6	0	-0.183605	1.905163	3.346992
25	1	0	-0.338301	-0.223652	3.151765
26	1	0	-2.860075	-0.320858	3.094768
27	1	0	-2.226406	0.492694	4.526555
28	1	0	-2.903733	1.453255	3.201302
29	1	0	0.851529	1.963359	3.001484
30	1	0	-0.698774	2.823833	3.044589
31	1	0	-0.169695	1.871924	4.441344
32	6	0	0.003484	1.359598	0.544802
33	6	0	1.265735	0.824353	0.400757
34	16	0	2.621218	1.476252	-0.541163

6a, rot1 (0 kcal mol^{-1})

35	16	0	1.641092	-0.691670	1.232113
36	6	0	3.284175	-0.859103	0.632552
37	6	0	3.744077	0.145934	-0.144341
38	6	0	-0.420288	2.623056	-0.083400
39	16	0	0.613623	3.524415	-1.060832
40	7	0	-1.703964	2.950012	0.224220
41	1	0	-2.108363	2.243560	0.840529
42	6	0	-2.562765	4.017058	-0.096742
43	6	0	-3.830775	3.980333	0.516756
44	6	0	-2.257141	5.078885	-0.962741
45	6	0	-4.768188	4.977014	0.274803
46	1	0	-4.076294	3.160731	1.189365
47	6	0	-3.209697	6.072331	-1.194734
48	1	0	-1.290958	5.121690	-1.443320
49	6	0	-4.463164	6.034801	-0.585618
50	1	0	-5.738829	4.926304	0.760715
51	1	0	-2.958018	6.887682	-1.867810
52	1	0	-5.193259	6.815909	-0.777139
53	6	0	5.152997	0.311879	-0.618551
54	8	0	6.139266	-0.023192	0.000417
55	8	0	5.167289	0.954121	-1.803072
56	6	0	3.958258	-2.110516	1.085338
57	8	0	3.645510	-2.672764	2.117597
58	8	0	4.864010	-2.550543	0.205577
59	6	0	6.469150	1.279748	-2.355674
60	6	0	7.032446	0.116758	-3.157073
61	1	0	7.134580	1.561657	-1.536177
62	1	0	6.277568	2.150059	-2.986911
63	1	0	7.979149	0.414281	-3.622320
64	1	0	7.223000	-0.742876	-2.508586
65	1	0	6.338474	-0.182461	-3.948962
66	6	0	5.658463	-3.698726	0.605274
67	6	0	6.834513	-3.272957	1.470303
68	1	0	5.988050	-4.129392	-0.342764
69	1	0	5.009648	-4.409571	1.122510
70	1	0	7.478720	-4.137646	1.667227
71	1	0	7.422007	-2.500122	0.966915
72	1	0	6.486474	-2.878659	2.429218
73	1	0	-2.899286	0.291434	-0.751750



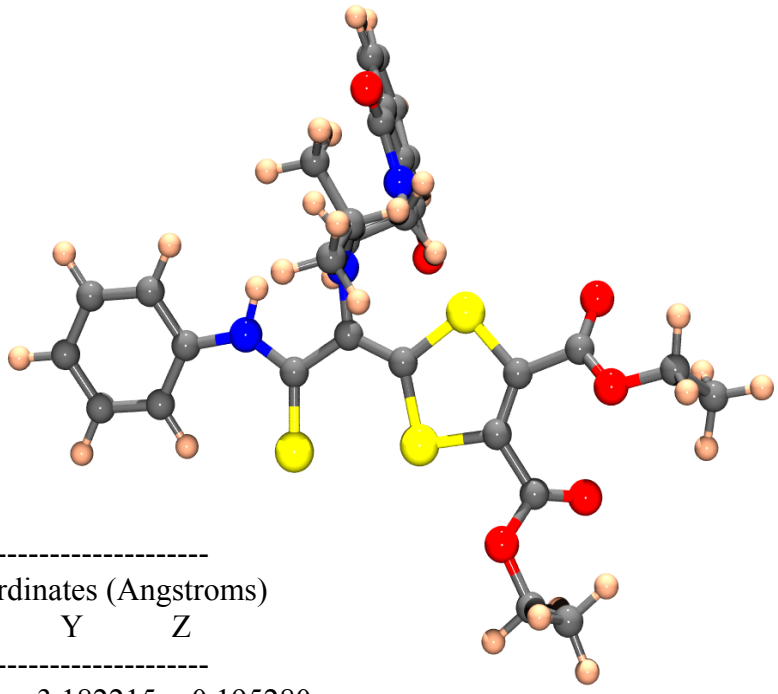
6a, $TS_{C-N}1$ (32 kcal mol^{-1})

6a_$TS_{C-N}1$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.815667	-3.172719	-0.835442
2	6	0	-5.106554	-2.126716	0.043502
3	6	0	-6.404140	-1.671647	0.223915
4	6	0	-7.416840	-2.301029	-0.512540
5	6	0	-7.124756	-3.349309	-1.394307
6	6	0	-5.810255	-3.802695	-1.568586
7	6	0	-3.344068	-3.417361	-0.796905
8	6	0	-3.830587	-1.673406	0.673909
9	1	0	-6.620239	-0.858901	0.910386
10	1	0	-8.445764	-1.971798	-0.398949
11	1	0	-7.931521	-3.817299	-1.951145
12	1	0	-5.572761	-4.614782	-2.248768
13	8	0	-2.682818	-4.236829	-1.405920
14	8	0	-3.652016	-0.801332	1.500767
15	7	0	-2.826743	-2.486709	0.118294
16	6	0	-1.411248	-2.401664	0.449551
17	1	0	-1.037087	-3.421142	0.580912
18	6	0	-0.608778	-1.678209	-0.644628
19	1	0	-0.852109	-2.117384	-1.619290
20	1	0	-0.931626	-0.644398	-0.698961
21	7	0	0.844667	-1.786729	-0.393173
22	6	0	1.324878	-3.075679	-1.046904
23	6	0	1.991859	-4.108635	-0.115515
24	6	0	2.095936	-2.879091	-2.358737
25	1	0	0.383832	-3.553611	-1.325905
26	1	0	1.542476	-4.081049	0.884062
27	1	0	1.810624	-5.108999	-0.525742
28	1	0	3.072478	-3.991858	-0.022340
29	1	0	1.563345	-2.199018	-3.032074
30	1	0	3.104029	-2.487629	-2.207654
31	1	0	2.188491	-3.848997	-2.860887
32	6	0	1.609745	-0.576824	-0.489896
33	6	0	1.102579	0.697685	-0.234556
34	16	0	1.793888	2.187425	-0.948547

35	16	0	-0.296528	1.019078	0.818347
36	6	0	-0.329868	2.768146	0.588548
37	6	0	0.615034	3.280006	-0.228050
38	6	0	3.085668	-0.665877	-0.471984
39	16	0	4.131588	0.437445	-1.180400
40	7	0	3.512883	-1.641974	0.393907
41	1	0	2.779747	-2.019326	0.982940
42	6	0	4.807873	-2.077471	0.755059
43	6	0	4.960984	-2.599013	2.050194
44	6	0	5.901908	-2.090376	-0.123020
45	6	0	6.186445	-3.113016	2.466264
46	1	0	4.115552	-2.588453	2.734864
47	6	0	7.124510	-2.602903	0.307975
48	1	0	5.798103	-1.698889	-1.125497
49	6	0	7.278963	-3.113783	1.598003
50	1	0	6.285235	-3.507263	3.473965
51	1	0	7.965053	-2.603674	-0.380723
52	1	0	8.237895	-3.507828	1.921943
53	6	0	0.798829	4.740246	-0.544427
54	8	0	1.768749	5.374208	-0.194655
55	8	0	-0.207239	5.194002	-1.302881
56	6	0	-1.342015	3.561134	1.325059
57	8	0	-1.393455	4.774225	1.350876
58	8	0	-2.191907	2.742915	1.976099
59	6	0	-0.193393	6.614129	-1.606749
60	6	0	0.645637	6.906856	-2.840800
61	1	0	0.176173	7.152693	-0.731407
62	1	0	-1.246076	6.858932	-1.764273
63	1	0	0.573287	7.971293	-3.092542
64	1	0	1.696959	6.667800	-2.658777
65	1	0	0.292749	6.325962	-3.699220
66	6	0	-3.251245	3.368255	2.738915
67	6	0	-3.945620	2.272127	3.524827
68	1	0	-3.928692	3.866820	2.037211
69	1	0	-2.812715	4.135929	3.383340
70	1	0	-4.801452	2.691721	4.065295
71	1	0	-4.297980	1.478208	2.859655
72	1	0	-3.262863	1.825037	4.254306
73	1	0	-1.329341	-1.871857	1.401311



6a_rot1b

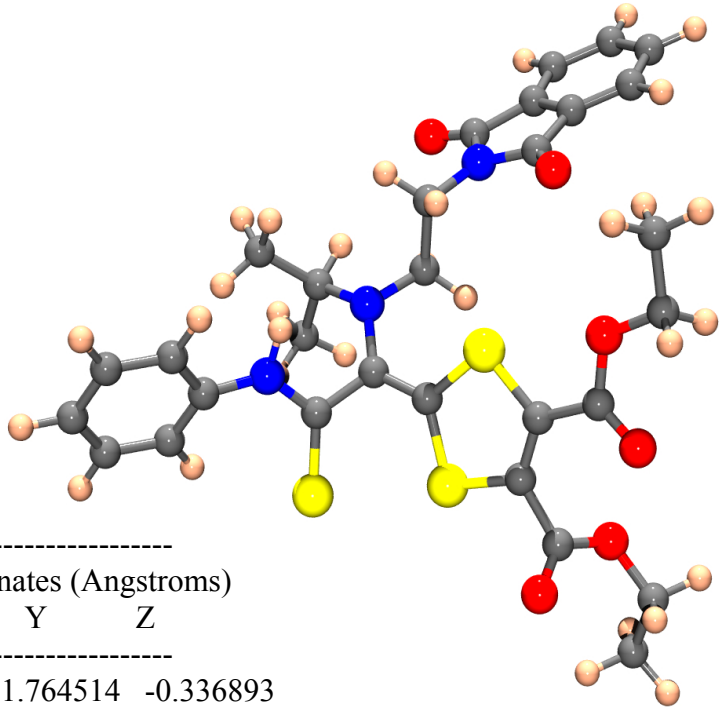
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.133581	-3.182215	-0.195280
2	6	0	4.559973	-3.267309	-1.465962
3	6	0	5.227494	-3.864816	-2.524609
4	6	0	6.505060	-4.382309	-2.271416
5	6	0	7.080364	-4.296790	-0.997213
6	6	0	6.397251	-3.690775	0.065801
7	6	0	4.167445	-2.489638	0.707333
8	6	0	3.207705	-2.635657	-1.413425
9	1	0	4.771584	-3.925969	-3.507936
10	1	0	7.059602	-4.858111	-3.075241
11	1	0	8.072405	-4.707490	-0.832086
12	1	0	6.833617	-3.619869	1.057346
13	8	0	4.284943	-2.213413	1.887348
14	8	0	2.386883	-2.505054	-2.297529
15	7	0	3.046781	-2.200076	-0.083512
16	6	0	1.852448	-1.535382	0.419586
17	1	0	1.646069	-1.935444	1.416076
18	6	0	2.050385	-0.003563	0.477569
19	1	0	3.022456	0.189306	0.944054
20	1	0	2.104583	0.381394	-0.545089
21	7	0	1.009245	0.754965	1.184835
22	6	0	0.847369	0.567405	2.653330
23	6	0	-0.046740	1.662022	3.246634
24	6	0	2.210507	0.559355	3.363012
25	1	0	0.368888	-0.401391	2.868448
26	1	0	-1.050343	1.659063	2.814184
27	1	0	-0.147532	1.499187	4.324616
28	1	0	0.389285	2.655770	3.091688
29	1	0	2.848539	-0.275522	3.059581
30	1	0	2.753910	1.497102	3.186671
31	1	0	2.047913	0.467808	4.442268

6a, rot1b (2 kcal mol^{-1})

32	6	0	-0.024977	1.338595	0.373238
33	6	0	-1.221971	0.682279	0.174109
34	16	0	-2.621220	1.244988	-0.764833
35	16	0	-1.477146	-0.888760	0.946897
36	6	0	-3.137300	-1.119065	0.422785
37	6	0	-3.651262	-0.160996	-0.378915
38	6	0	0.276927	2.661174	-0.209563
39	16	0	-0.771311	3.436469	-1.274499
40	7	0	1.467643	3.157879	0.223477
41	1	0	1.891387	2.525166	0.901461
42	6	0	2.207948	4.328078	-0.025604
43	6	0	3.402819	4.456119	0.710237
44	6	0	1.858090	5.339952	-0.933759
45	6	0	4.225584	5.563768	0.546836
46	1	0	3.683139	3.675804	1.415387
47	6	0	2.695892	6.445867	-1.086693
48	1	0	0.945805	5.259613	-1.505952
49	6	0	3.876660	6.571196	-0.356256
50	1	0	5.141236	5.638731	1.127174
51	1	0	2.410870	7.220485	-1.793757
52	1	0	4.516779	7.438990	-0.486665
53	6	0	-4.969114	-0.227065	-1.081752
54	8	0	-5.511398	-1.245336	-1.452451
55	8	0	-5.435979	1.018192	-1.302734
56	6	0	-3.756658	-2.372629	0.946388
57	8	0	-3.093961	-3.359807	1.201710
58	8	0	-5.069539	-2.241498	1.161899
59	6	0	-6.670922	1.130199	-2.056251
60	6	0	-7.881438	1.020463	-1.142477
61	1	0	-6.679783	0.356961	-2.827959
62	1	0	-6.606428	2.114431	-2.525101
63	1	0	-8.797276	1.181503	-1.722603
64	1	0	-7.932931	0.027449	-0.687108
65	1	0	-7.839192	1.773357	-0.349051
66	6	0	-5.786246	-3.435886	1.573241
67	6	0	-6.158110	-4.291301	0.372187
68	1	0	-6.670723	-3.045435	2.081361
69	1	0	-5.168340	-3.985173	2.287633
70	1	0	-6.792460	-5.124261	0.696667
71	1	0	-6.701993	-3.698668	-0.368542
72	1	0	-5.262920	-4.705136	-0.100418
73	1	0	1.030832	-1.803302	-0.246367

6a_TS$_{C-N}$2



6a, TS$_{C-N}$2 (29 kcal mol^{-1})

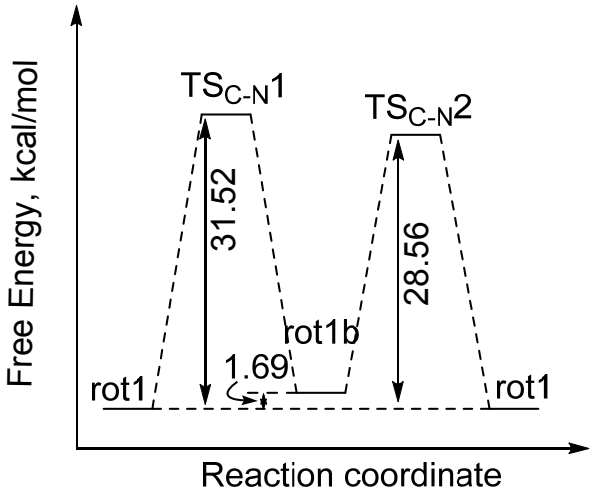
Standard orientation:

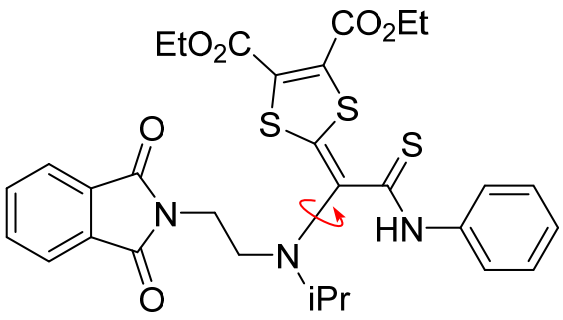
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.429639	-1.764514	-0.336893
2	6	0	6.584336	-0.382780	-0.202141
3	6	0	7.824279	0.187779	0.043545
4	6	0	8.920930	-0.677689	0.154689
5	6	0	8.765743	-2.063326	0.019797
6	6	0	7.508511	-2.629608	-0.230144
7	6	0	4.988174	-2.048653	-0.596939
8	6	0	5.247545	0.257314	-0.377974
9	1	0	7.933341	1.263168	0.144371
10	1	0	9.908743	-0.268908	0.347473
11	1	0	9.635494	-2.707845	0.110108
12	1	0	7.377176	-3.701811	-0.338303
13	8	0	4.446568	-3.123088	-0.785633
14	8	0	4.958775	1.435434	-0.364343
15	7	0	4.342054	-0.804116	-0.587485
16	6	0	2.917651	-0.622172	-0.847041
17	1	0	2.663868	-1.144265	-1.770404
18	6	0	2.070599	-1.161091	0.335437
19	1	0	2.421243	-2.170352	0.552817
20	1	0	2.305346	-0.566265	1.222397
21	7	0	0.623596	-1.267972	0.117500
22	6	0	0.198467	-2.616230	-0.386652
23	6	0	0.306627	-3.683941	0.711357
24	6	0	0.909772	-3.064566	-1.675044
25	1	0	-0.853185	-2.523025	-0.644753
26	1	0	-0.149288	-4.617083	0.363063
27	1	0	1.348142	-3.910139	0.966473
28	1	0	-0.211357	-3.370013	1.622484
29	1	0	0.802442	-2.313703	-2.465563
30	1	0	1.972134	-3.277813	-1.522006
31	1	0	0.437844	-3.988052	-2.030940
32	6	0	-0.201710	-0.156847	-0.193129
33	6	0	-1.590158	-0.256792	-0.116256
34	16	0	-2.709805	0.609396	-1.196955

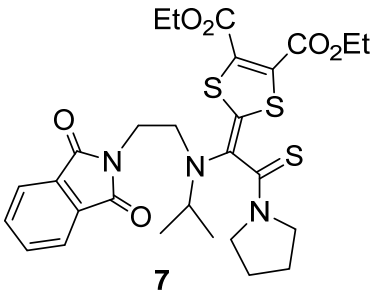
35	16	0	-2.401891	-1.443942	0.935171
36	6	0	-4.042909	-0.970244	0.520758
37	6	0	-4.184574	-0.067097	-0.477385
38	6	0	0.313883	1.227095	-0.321523
39	16	0	-0.294090	2.377068	-1.375343
40	7	0	1.174165	1.563151	0.706614
41	1	0	1.107633	0.960507	1.516740
42	6	0	1.783902	2.811319	1.001312
43	6	0	2.423481	3.591698	0.030651
44	6	0	1.796519	3.223902	2.340320
45	6	0	3.048070	4.778620	0.405426
46	1	0	2.441150	3.267449	-1.001166
47	6	0	2.432977	4.408864	2.706395
48	1	0	1.295617	2.619766	3.094221
49	6	0	3.056571	5.196011	1.738499
50	1	0	3.543180	5.376486	-0.354654
51	1	0	2.432085	4.716672	3.748534
52	1	0	3.548416	6.122998	2.019456
53	6	0	-5.480177	0.321030	-1.108092
54	8	0	-6.469921	-0.378692	-1.149856
55	8	0	-5.373363	1.533750	-1.688416
56	6	0	-5.087765	-1.659629	1.335161
57	8	0	-4.945636	-2.796613	1.741736
58	8	0	-6.121862	-0.858809	1.617460
59	6	0	-6.529100	2.011126	-2.422468
60	6	0	-7.512296	2.716586	-1.501554
61	1	0	-6.994303	1.163102	-2.930809
62	1	0	-6.108073	2.695209	-3.162518
63	1	0	-8.335960	3.134109	-2.091971
64	1	0	-7.931255	2.015930	-0.773836
65	1	0	-7.022889	3.535544	-0.964939
66	6	0	-7.234282	-1.460080	2.330672
67	6	0	-8.166079	-2.195022	1.379786
68	1	0	-7.728812	-0.609125	2.804516
69	1	0	-6.836251	-2.124732	3.101401
70	1	0	-9.046619	-2.548190	1.929023
71	1	0	-8.493088	-1.534685	0.571963
72	1	0	-7.664361	-3.061338	0.939952
73	1	0	2.767239	0.446378	-0.996503

Calculated free energy values for the rotation of the N-C bond in compound **6a**, level of theory: B3LYP/6-31G(d) (kcal/mol):

	6a_rot1	6a_$TS_{C-N}1$	6a_rot1b	6a_$TS_{C-N}2$
ΔG	0	31,52	1,69	28,56







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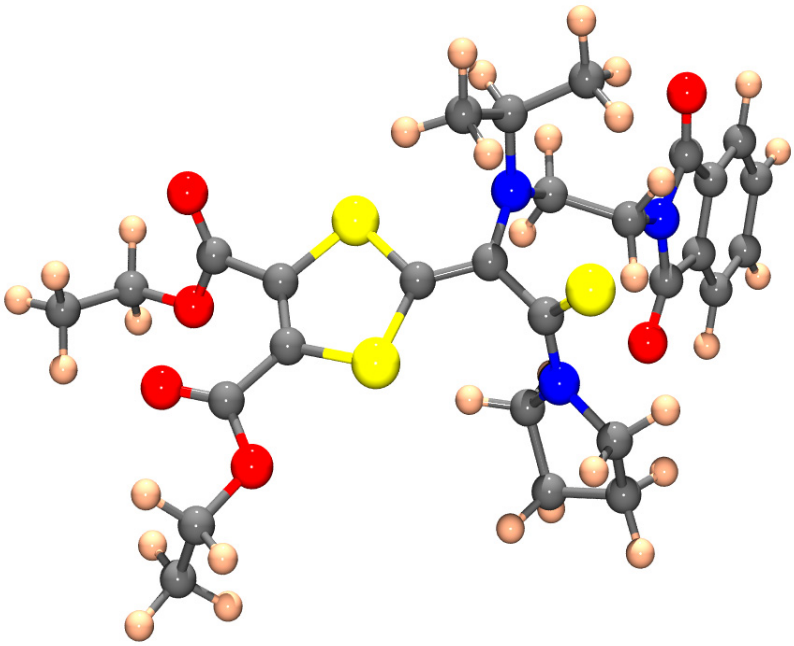


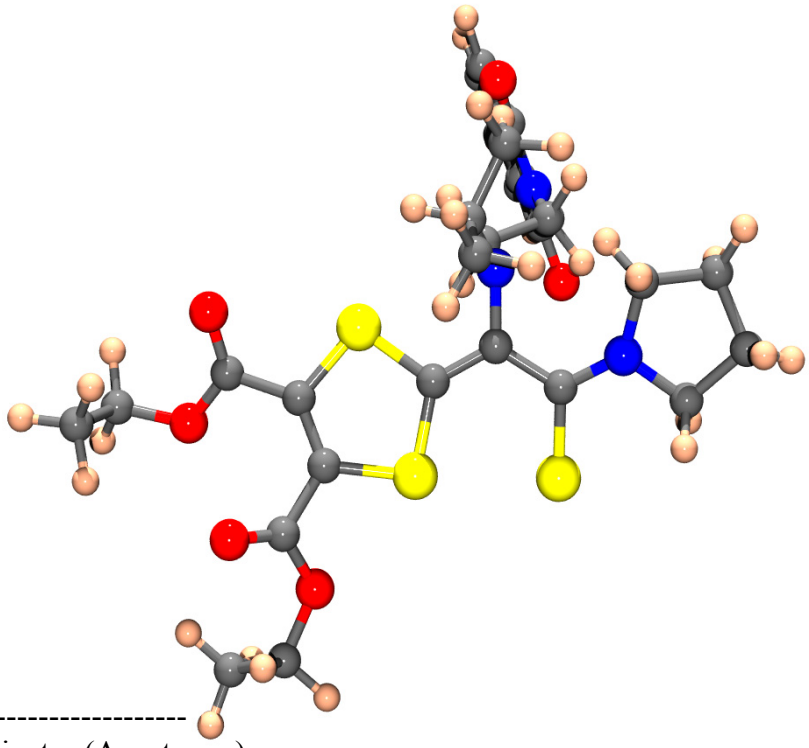
7_rot1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.380161	-0.915458	-0.791063
2	6	0	-5.930929	0.144387	-1.582379
3	6	0	-6.656567	0.590492	-2.676847
4	6	0	-7.862936	-0.064056	-2.960875
5	6	0	-8.313161	-1.126601	-2.167335
6	6	0	-7.571821	-1.569970	-1.063469
7	6	0	-5.378326	-1.144156	0.292483
8	6	0	-4.630253	0.622982	-1.026777
9	1	0	-6.298865	1.415364	-3.285315
10	1	0	-8.459832	0.256921	-3.809851
11	1	0	-9.252483	-1.613828	-2.412874
12	1	0	-7.911506	-2.392403	-0.441578
13	8	0	-5.384316	-1.970541	1.183034
14	8	0	-3.914473	1.522727	-1.431238
15	7	0	-4.372546	-0.182458	0.089253
16	6	0	-3.195419	-0.056633	0.941070
17	1	0	-3.502034	-0.260940	1.967063
18	6	0	-2.083177	-1.036959	0.486343
19	1	0	-2.507726	-2.045368	0.494858
20	1	0	-1.834880	-0.810805	-0.558271
21	7	0	-0.852661	-1.061857	1.266025
22	6	0	-0.755596	-1.988504	2.431355
23	6	0	-0.795777	-3.460758	1.990166
24	6	0	-1.803034	-1.735217	3.528377
25	1	0	0.231702	-1.786840	2.858215
26	1	0	-0.055707	-3.673936	1.214058
27	1	0	-0.586740	-4.107408	2.849795
28	1	0	-1.784302	-3.744425	1.609928
29	1	0	-1.785028	-0.691712	3.852797

7, rot1 (0 kcal mol^{-1})

30	1	0	-2.811871	-1.993785	3.184334
31	1	0	-1.584796	-2.369050	4.396482
32	6	0	0.037536	0.034004	1.155754
33	6	0	1.330455	-0.186302	0.816880
34	16	0	2.608311	1.057013	0.880731
35	16	0	1.924167	-1.799449	0.342123
36	6	0	3.522415	-1.246096	-0.136429
37	6	0	3.846928	0.043255	0.111249
38	6	0	-0.395078	1.436091	1.530495
39	16	0	-0.586008	1.839444	3.151267
40	6	0	5.198299	0.616701	-0.096943
41	8	0	6.195165	-0.027189	-0.357051
42	8	0	5.177869	1.955256	0.082294
43	6	0	4.397227	-2.305905	-0.747356
44	8	0	4.620891	-3.362309	-0.197223
45	8	0	4.790521	-1.964829	-1.980110
46	6	0	6.447659	2.647218	-0.020647
47	6	0	6.761114	3.012300	-1.463188
48	1	0	7.225822	2.011925	0.408861
49	1	0	6.317257	3.535510	0.601472
50	1	0	7.686792	3.597840	-1.502868
51	1	0	6.897998	2.111628	-2.068097
52	1	0	5.955136	3.612717	-1.897236
53	6	0	5.670443	-2.900677	-2.660125
54	6	0	7.119207	-2.703714	-2.243072
55	1	0	5.519539	-2.676094	-3.718514
56	1	0	5.325606	-3.916457	-2.451414
57	1	0	7.762078	-3.363957	-2.836983
58	1	0	7.432144	-1.668311	-2.402186
59	1	0	7.253987	-2.946173	-1.185980
60	1	0	-2.865498	0.979903	0.875732
61	6	0	-0.454976	2.037784	-0.922711
62	6	0	-1.016459	3.703257	0.774167
63	6	0	-0.421005	3.438571	-1.543409
64	1	0	-1.332764	1.484150	-1.274728
65	1	0	0.444675	1.455409	-1.121770
66	6	0	-1.349024	4.244073	-0.622098
67	1	0	-0.192177	4.244947	1.255730
68	1	0	-1.857998	3.716582	1.472042
69	1	0	0.599192	3.839792	-1.507879
70	1	0	-0.747725	3.429196	-2.587184
71	1	0	-1.197816	5.325268	-0.690629
72	1	0	-2.394413	4.027055	-0.868347
73	7	0	-0.595085	2.309970	0.529730



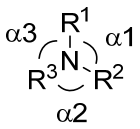
7_rot2

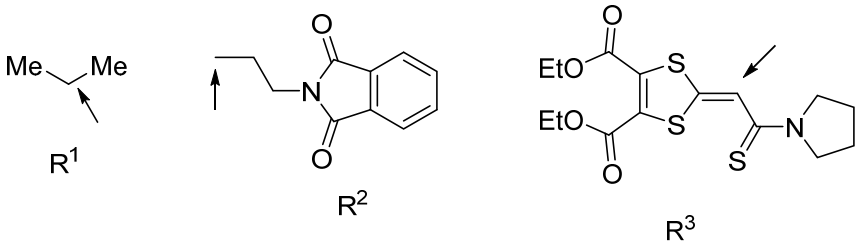
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.200293	-2.720134	-0.196722
2	6	0	-4.942286	-2.398585	-1.531231
3	6	0	-5.424725	-3.178146	-2.571741
4	6	0	-6.183188	-4.307012	-2.233497
5	6	0	-6.442062	-4.629627	-0.895258
6	6	0	-5.950692	-3.834329	0.148756
7	6	0	-4.545351	-1.691908	0.665232
8	6	0	-4.118798	-1.152855	-1.563584
9	1	0	-5.217999	-2.918084	-3.605288
10	1	0	-6.577676	-4.943339	-3.020626
11	1	0	-7.033301	-5.511349	-0.664796
12	1	0	-6.145445	-4.075268	1.189251
13	8	0	-4.531410	-1.604128	1.879097
14	8	0	-3.695269	-0.539268	-2.521404
15	7	0	-3.921896	-0.796858	-0.216141
16	6	0	-3.158898	0.361740	0.227316
17	1	0	-3.718328	0.837781	1.036573
18	6	0	-1.749450	-0.038894	0.709327
19	1	0	-1.851567	-0.826883	1.464246
20	1	0	-1.213234	-0.479471	-0.138843
21	7	0	-0.981519	1.084382	1.269144
22	6	0	-0.785194	1.049049	2.751065
23	6	0	-2.127636	1.106372	3.501161
24	6	0	0.147782	2.160377	3.237352
25	1	0	-0.322574	0.090013	3.033892
26	1	0	-2.823815	0.326942	3.176023
27	1	0	-1.945246	0.949179	4.570568
28	1	0	-2.618489	2.079439	3.389598
29	1	0	1.142726	2.091807	2.790543
30	1	0	-0.256817	3.153999	3.018073

7, rot2 (8 kcal mol^{-1})

31	1	0	0.262350	2.077388	4.323336
32	6	0	0.020377	1.637923	0.390067
33	6	0	1.197591	0.918736	0.230877
34	16	0	2.587963	1.270262	-0.818480
35	16	0	1.390204	-0.573970	1.164319
36	6	0	3.013808	-0.968929	0.625300
37	6	0	3.585854	-0.095395	-0.230798
38	6	0	-0.257257	2.848957	-0.406477
39	16	0	0.773306	3.233890	-1.708614
40	6	0	5.007544	-0.117263	-0.690201
41	8	0	5.956242	-0.425781	-0.001838
42	8	0	5.091287	0.330231	-1.959503
43	6	0	3.543838	-2.236907	1.200358
44	8	0	3.129917	-2.696299	2.248262
45	8	0	4.456159	-2.815419	0.409393
46	6	0	6.423043	0.462989	-2.518455
47	6	0	6.903607	-0.851812	-3.112358
48	1	0	7.096662	0.817900	-1.734712
49	1	0	6.313197	1.235112	-3.283073
50	1	0	7.877669	-0.705646	-3.593197
51	1	0	7.014894	-1.609576	-2.331837
52	1	0	6.198993	-1.218765	-3.865469
53	6	0	5.129342	-3.986993	0.938679
54	6	0	6.280478	-3.588061	1.849205
55	1	0	5.481563	-4.510334	0.046994
56	1	0	4.395560	-4.607224	1.459099
57	1	0	6.843798	-4.480491	2.145500
58	1	0	6.954447	-2.897269	1.334710
59	1	0	5.905574	-3.102265	2.754495
60	1	0	-3.096454	1.049224	-0.619618
61	6	0	-2.244331	3.728624	0.971703
62	6	0	-1.570672	4.820643	-1.078307
63	6	0	-3.429637	4.534030	0.441190
64	1	0	-1.760574	4.261653	1.803987
65	1	0	-2.498871	2.733888	1.311363
66	6	0	-2.748292	5.580946	-0.447876
67	1	0	-1.796835	4.443896	-2.082207
68	1	0	-0.667624	5.431054	-1.167778
69	1	0	-4.083012	3.886276	-0.156274
70	1	0	-4.028844	4.967438	1.248002
71	1	0	-3.411917	6.004054	-1.207422
72	1	0	-2.378351	6.410017	0.166952
73	7	0	-1.320364	3.666775	-0.179608





Experimental and calculated values of the angles surrounding the amine nitrogen atom in compound **7**

	Exp1	Exp2	Exp3	7 Rot1	7 Rot2
α1	115.80	110.53	115.83	118.92	115.31
α2	116.50	113.54	117.54	118.43	115.05
α3	119.72	117.70	119.18	120.03	121.44
Sum	352.02	341.77	352.55	357.38	351.8