***Supporting Information for**:*

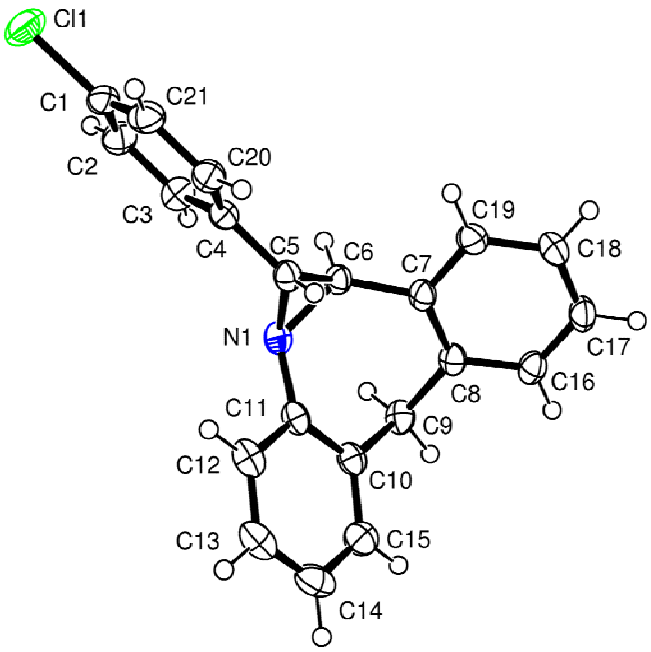
New approach to azepino-fused heterocycles. Conformations of dibenzo[*c*,*f*]pyrrolo[1,2-*a*]-azepine systems

Alexander F. Khlebnikov,*[a] Mikhail S. Novikov [a] Maria V. Golovkina,[a] Petr P. Petrovskii,[a] Alexander S. Konev,[a] Dmitry S. Yufit,[b] and Helen Stoeckli-Evans[c]

[a] *Universitetskii pr. 26 , 198504 St. Petersburg, Russia. Fax: +7 812 4286939; Tel: +7 812 4284021; alexander.khlebnikov@pobox.spbu.ru*

[b] *Department of Chemistry, University of Durham, Durham, South Rd., DH1 3L (UK) . Fax: +44 191-334-2051; Tel: +44 191-334-2004; E-mail: d.s.yufit@durham.ac.uk*

[c] *Institute of Physics, University of Neuchâtel, rue Emile-Argand 11, CH-2000 Neuchâtel, Switzerland. Fax: +41 32 7182511; Tel: +41 32 7182426; E-mail: helen.stoeckli-evans@unine.ch*



X-Ray crystal structure of **2b.**

Table S1 - Crystal Data and Details of the Structure Determination
for: 2b P 21/n R = 0.04

Crystal Data

Formula			**C21 H16 Cl N**
Formula Weight			**317.80**
Crystal System			**Monoclinic**
Space group		**P21/n**	**(No. 14)**
a, b, c [Angstrom]	**11.5596(6)**	**9.9041(5)**	**13.9757(7)**
alpha, beta, gamma [deg]	**90**	**91.254(4)**	**90**
V [Ang3]**			**1599.66(14)**
Z			**4**
D(calc) [g/cm3]**			**1.320**
Mu(MoKa) [/mm]			**0.237**
F(000)			**664**
Crystal Size [mm]		**0.40 x**	**0.40 x 0.45**

Data Collection

Temperature (K)			**173**
Radiation [Angstrom]		**MoKa**	**0.71073**
Theta Min-Max [Deg]			**2.3, 26.7**
Dataset	**-14: 14 ; -12: 12 ; -16: 17**		
Tot., Uniq. Data, R(int)		**16074,**	**3392, 0.051**
Observed data [I > 2.0 sigma(I)]			**2979**

Refinement

Nref, Npar	3392, 209
R, wR2, S	0.0383, 0.0957, 1.05
w = 1/[\s^2^(Fo^2^)+(0.0383P)^2^+0.6473P] where P=(Fo^2^+2Fc^2^)/3	
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.24, 0.26

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: 2b P 21/n R = 0.04

Atom	x	y	z	U(eq) [Ang^2]
Cl1	0.02583(4)	0.76754(4)	0.42065(4)	0.0508(2)
N1	0.37957(10)	0.24743(12)	0.56555(8)	0.0280(3)
C1	0.11285(13)	0.64848(14)	0.47976(12)	0.0332(4)
C2	0.20466(13)	0.59323(15)	0.43182(12)	0.0354(5)
C3	0.27303(13)	0.49776(16)	0.47803(11)	0.0325(4)
C4	0.25086(12)	0.45781(14)	0.57157(10)	0.0267(4)
C5	0.32319(11)	0.35476(14)	0.62198(10)	0.0262(4)
C6	0.45214(11)	0.34985(14)	0.61288(10)	0.0251(4)
C7	0.52974(11)	0.32295(14)	0.69633(10)	0.0262(4)
C8	0.60182(11)	0.20952(15)	0.69835(10)	0.0262(4)
C9	0.59224(12)	0.10497(15)	0.61952(10)	0.0304(4)
C10	0.47544(12)	0.03601(15)	0.61922(10)	0.0285(4)
C11	0.37477(12)	0.11030(15)	0.59848(10)	0.0277(4)
C12	0.26691(13)	0.04690(16)	0.60031(11)	0.0338(4)
C13	0.25871(14)	-0.08938(17)	0.62150(11)	0.0385(5)
C14	0.35753(16)	-0.16373(17)	0.64188(11)	0.0402(5)
C15	0.46493(14)	-0.10055(16)	0.64132(11)	0.0355(5)
C16	0.68129(12)	0.19478(16)	0.77436(10)	0.0300(4)
C17	0.68883(13)	0.28983(16)	0.84679(11)	0.0340(4)
C18	0.61733(13)	0.40156(16)	0.84488(11)	0.0348(5)
C19	0.53790(12)	0.41851(15)	0.76941(11)	0.0315(4)
C20	0.15814(12)	0.51655(15)	0.61807(11)	0.0301(4)
C21	0.08817(13)	0.61173(15)	0.57247(12)	0.0343(4)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters
for: 2b P 21/n R = 0.04

Atom	x	y	z	U(iso) [Ang^2]
H2	0.22060	0.62030	0.36820	0.0420
H3	0.33610	0.45880	0.44550	0.0390
H5	0.29380	0.32520	0.68540	0.0310
H6	0.48300	0.41900	0.56800	0.0300
H9A	0.60350	0.14920	0.55690	0.0360
H9B	0.65390	0.03660	0.62870	0.0360
H12	0.19870	0.09760	0.58690	0.0410
H13	0.18500	-0.13190	0.62200	0.0460
H14	0.35200	-0.25730	0.65620	0.0480
H15	0.53250	-0.15150	0.65630	0.0430
H16	0.73090	0.11830	0.77640	0.0360
H17	0.74340	0.27820	0.89800	0.0410
H18	0.62230	0.46650	0.89480	0.0420
H19	0.48900	0.49560	0.76770	0.0380
H20	0.14250	0.49110	0.68200	0.0360
H21	0.02460	0.65080	0.60440	0.0410

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters
for: 2b P 21/n R = 0.04

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Cl1	0.0450(3)	0.0352(2)	0.0717(3)	0.0184(2)	-0.0113(2)	0.0047(2)
N1	0.0228(6)	0.0327(6)	0.0284(6)	-0.0012(5)	-0.0018(4)	-0.0010(5)
C1	0.0302(7)	0.0226(7)	0.0464(9)	0.0052(6)	-0.0078(6)	-0.0037(6)
C2	0.0392(8)	0.0317(8)	0.0351(8)	0.0088(6)	-0.0003(6)	-0.0045(6)
C3	0.0299(7)	0.0340(8)	0.0336(7)	0.0028(6)	0.0034(6)	0.0008(6)
C4	0.0252(7)	0.0246(7)	0.0301(7)	-0.0004(5)	-0.0016(5)	-0.0038(5)
C5	0.0239(6)	0.0284(7)	0.0262(6)	-0.0002(5)	-0.0012(5)	-0.0024(5)
C6	0.0210(6)	0.0277(7)	0.0264(7)	0.0030(5)	-0.0019(5)	-0.0029(5)
C7	0.0202(6)	0.0304(7)	0.0279(7)	0.0034(5)	-0.0020(5)	-0.0050(5)
C8	0.0201(6)	0.0323(7)	0.0261(7)	0.0018(6)	0.0002(5)	-0.0028(5)

C9	0.0237(7)	0.0380(8)	0.0294(7)	-0.0028(6)	0.0010(5)	0.0041(6)
C10	0.0295(7)	0.0333(7)	0.0226(6)	-0.0065(6)	0.0018(5)	-0.0004(6)
C11	0.0273(7)	0.0333(7)	0.0226(6)	-0.0056(6)	0.0000(5)	-0.0026(6)
C12	0.0282(7)	0.0421(9)	0.0312(7)	-0.0081(6)	0.0016(6)	-0.0055(6)
C13	0.0395(9)	0.0432(9)	0.0329(8)	-0.0100(7)	0.0054(6)	-0.0140(7)
C14	0.0555(10)	0.0321(8)	0.0334(8)	-0.0074(6)	0.0080(7)	-0.0096(7)
C15	0.0427(9)	0.0343(8)	0.0296(7)	-0.0065(6)	0.0028(6)	0.0040(7)
C16	0.0238(7)	0.0350(8)	0.0312(7)	0.0046(6)	-0.0023(5)	0.0004(6)
C17	0.0302(7)	0.0402(8)	0.0311(7)	0.0036(6)	-0.0104(6)	-0.0059(6)
C18	0.0357(8)	0.0336(8)	0.0347(8)	-0.0051(6)	-0.0076(6)	-0.0071(6)
C19	0.0280(7)	0.0278(7)	0.0386(8)	-0.0008(6)	-0.0042(6)	-0.0026(6)
C20	0.0285(7)	0.0294(7)	0.0323(7)	0.0018(6)	0.0012(6)	-0.0030(6)
C21	0.0278(7)	0.0278(7)	0.0472(9)	-0.0004(6)	0.0016(6)	0.0005(6)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom)
for: 2b P 21/n R = 0.04

Cl1	-C1	1.7460(16)	C14	-C15	1.391(2)
N1	-C5	1.4830(18)	C16	-C17	1.384(2)
N1	-C6	1.4649(18)	C17	-C18	1.381(2)
N1	-C11	1.4355(19)	C18	-C19	1.393(2)
C1	-C2	1.381(2)	C20	-C21	1.388(2)
C1	-C21	1.382(2)	C2	-H2	0.9500
C2	-C3	1.383(2)	C3	-H3	0.9500
C3	-C4	1.395(2)	C5	-H5	1.0000
C4	-C5	1.4870(19)	C6	-H6	1.0000
C4	-C20	1.393(2)	C9	-H9A	0.9900
C5	-C6	1.4996(18)	C9	-H9B	0.9900
C6	-C7	1.4799(19)	C12	-H12	0.9500
C7	-C8	1.399(2)	C13	-H13	0.9500
C7	-C19	1.394(2)	C14	-H14	0.9500
C8	-C9	1.514(2)	C15	-H15	0.9500

C8	-C16	1.3968(19)	C16	-H16	0.9500
C9	-C10	1.513(2)	C17	-H17	0.9500
C10	-C11	1.402(2)	C18	-H18	0.9500
C10	-C15	1.393(2)	C19	-H19	0.9500
C11	-C12	1.397(2)	C20	-H20	0.9500
C12	-C13	1.386(2)	C21	-H21	0.9500
C13	-C14	1.384(2)			

Table S6 - Bond Angles (Degrees)
for: 2b P 21/n R = 0.04

C5	-N1	-C6	61.15(9)	N1	-C11	-C12	118.16(13)
C5	-N1	-C11	119.16(11)	C10	-C11	-C12	119.84(14)
C6	-N1	-C11	122.42(11)	C11	-C12	-C13	120.47(14)
Cl1	-C1	-C2	118.63(13)	C12	-C13	-C14	120.16(15)
Cl1	-C1	-C21	119.54(12)	C13	-C14	-C15	119.51(15)
C2	-C1	-C21	121.83(14)	C10	-C15	-C14	121.35(15)
C1	-C2	-C3	118.80(15)	C8	-C16	-C17	121.01(14)
C2	-C3	-C4	121.11(14)	C16	-C17	-C18	120.19(14)
C3	-C4	-C5	121.72(13)	C17	-C18	-C19	119.69(14)
C3	-C4	-C20	118.54(13)	C7	-C19	-C18	120.38(13)
C5	-C4	-C20	119.74(13)	C4	-C20	-C21	121.07(14)
N1	-C5	-C4	119.28(12)	C1	-C21	-C20	118.64(14)
N1	-C5	-C6	58.83(9)	C1	-C2	-H2	121.00
C4	-C5	-C6	122.12(12)	C3	-C2	-H2	121.00
N1	-C6	-C5	60.02(9)	C2	-C3	-H3	119.00
N1	-C6	-C7	124.23(12)	C4	-C3	-H3	119.00
C5	-C6	-C7	121.70(12)	N1	-C5	-H5	115.00
C6	-C7	-C8	120.74(12)	C4	-C5	-H5	115.00
C6	-C7	-C19	119.03(12)	C6	-C5	-H5	115.00
C8	-C7	-C19	119.99(13)	N1	-C6	-H6	114.00
C7	-C8	-C9	120.04(12)	C5	-C6	-H6	114.00
C7	-C8	-C16	118.75(13)	C7	-C6	-H6	114.00
C9	-C8	-C16	121.22(13)	C8	-C9	-H9A	109.00
C8	-C9	-C10	111.21(11)	C8	-C9	-H9B	109.00
C9	-C10	-C11	120.03(13)	C10	-C9	-H9A	109.00
C9	-C10	-C15	121.32(13)	C10	-C9	-H9B	109.00

C11	-C10	-C15	118.65(13)	H9A	-C9	-H9B	108.00
N1	-C11	-C10	121.68(12)	C11	-C12	-H12	120.00
C13	-C12	-H12	120.00	C18	-C17	-H17	120.00
C12	-C13	-H13	120.00	C17	-C18	-H18	120.00
C14	-C13	-H13	120.00	C19	-C18	-H18	120.00
C13	-C14	-H14	120.00	C7	-C19	-H19	120.00
C15	-C14	-H14	120.00	C18	-C19	-H19	120.00
C10	-C15	-H15	119.00	C4	-C20	-H20	120.00
C14	-C15	-H15	119.00	C21	-C20	-H20	119.00
C8	-C16	-H16	120.00	C1	-C21	-H21	121.00
C17	-C16	-H16	119.00	C20	-C21	-H21	121.00
C16	-C17	-H17	120.00				

Table S7 - Torsion Angles (Degrees)
for: 2b P 21/n R = 0.04

C6	-N1	-C5	-C4	111.92(14)
C11	-N1	-C5	-C4	-134.90(13)
C11	-N1	-C5	-C6	113.18(13)
C5	-N1	-C6	-C7	109.96(15)
C11	-N1	-C6	-C5	-108.00(13)
C11	-N1	-C6	-C7	1.96(19)
C5	-N1	-C11	-C10	-121.02(14)
C5	-N1	-C11	-C12	65.42(17)
C6	-N1	-C11	-C10	-48.49(19)
C6	-N1	-C11	-C12	137.95(14)
Cl1	-C1	-C2	-C3	-179.29(12)
C21	-C1	-C2	-C3	0.5(2)
Cl1	-C1	-C21	-C20	179.77(12)
C2	-C1	-C21	-C20	0.0(2)
C1	-C2	-C3	-C4	-0.4(2)
C2	-C3	-C4	-C5	179.66(14)
C2	-C3	-C4	-C20	-0.2(2)
C3	-C4	-C5	-N1	-29.76(19)
C3	-C4	-C5	-C6	39.8(2)
C20	-C4	-C5	-N1	150.10(13)
C20	-C4	-C5	-C6	-140.30(14)

C3	-C4	-C20	-C21	0.7(2)
C5	-C4	-C20	-C21	-179.17(13)
N1	-C5	-C6	-C7	-114.01(14)
C4	-C5	-C6	-N1	-107.17(14)
C4	-C5	-C6	-C7	138.82(14)
N1	-C6	-C7	-C8	45.34(19)
N1	-C6	-C7	-C19	-140.38(14)
C5	-C6	-C7	-C8	118.47(15)
C5	-C6	-C7	-C19	-67.25(18)
C6	-C7	-C8	-C9	-6.4(2)
C6	-C7	-C8	-C16	174.10(13)
C19	-C7	-C8	-C9	179.41(13)
C19	-C7	-C8	-C16	-0.1(2)
C6	-C7	-C19	-C18	-174.55(13)
C8	-C7	-C19	-C18	-0.2(2)
C7	-C8	-C9	-C10	-64.32(17)
C16	-C8	-C9	-C10	115.20(14)
C7	-C8	-C16	-C17	0.3(2)
C9	-C8	-C16	-C17	-179.27(13)
C8	-C9	-C10	-C11	64.90(17)
C8	-C9	-C10	-C15	-113.68(15)
C9	-C10	-C11	-N1	7.9(2)
C9	-C10	-C11	-C12	-178.62(13)
C15	-C10	-C11	-N1	-173.46(13)
C15	-C10	-C11	-C12	0.0(2)
C9	-C10	-C15	-C14	179.43(14)
C11	-C10	-C15	-C14	0.8(2)
N1	-C11	-C12	-C13	173.00(13)
C10	-C11	-C12	-C13	-0.7(2)
C11	-C12	-C13	-C14	0.6(2)
C12	-C13	-C14	-C15	0.3(2)
C13	-C14	-C15	-C10	-1.0(2)
C8	-C16	-C17	-C18	0.0(2)
C16	-C17	-C18	-C19	-0.3(2)
C17	-C18	-C19	-C7	0.4(2)

C4	-C20	-C21	-C1	-0.6(2)

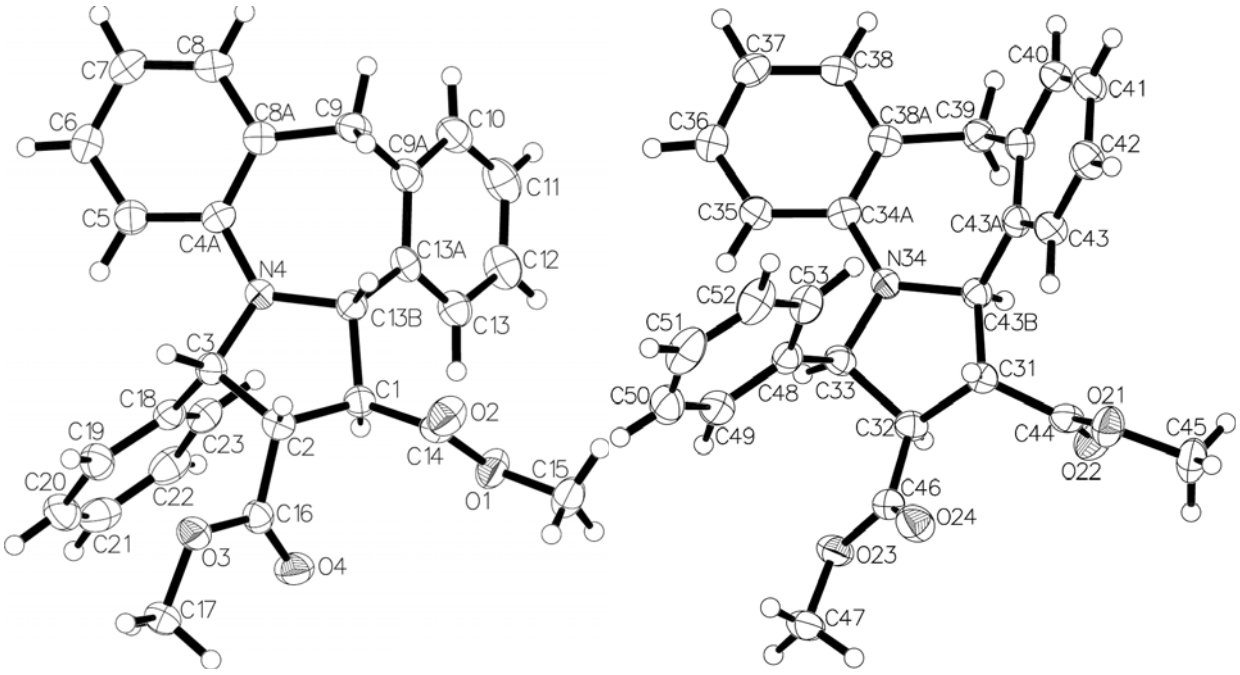
Table S8 - Contact Distances(Angstrom)
for: 2b P 21/n R = 0.04

Cl1	.C20_a	3.5611(15)	C7	.H2_e	3.0900
Cl1	.C18_b	3.6097(16)	C8	.H2_e	2.8300
Cl1	.H12_a	2.9200	C12	.H5	3.0200
Cl1	.H18_b	2.8900	C13	.H9A_f	3.0500
N1	.H3	2.7200	C13	.H5_g	2.9000
N1	.H9A	2.7700	C13	.H20_g	3.0600
N1	.H17_c	2.8000	C14	.H20_g	2.9000
C1	.C21_a	3.536(2)	C14	.H5_g	3.0100
C2	.C8_e	3.508(2)	C14	.H9A_f	2.8300
C3	.C17_c	3.514(2)	C15	.H20_g	2.9300
C3	.C16_c	3.568(2)	C15	.H9A_f	2.9000
C8	.C2_e	3.508(2)	C16	.H21_g	2.9800
C10	.C10_f	3.467(2)	C16	.H2_e	2.9500
C16	.C3_h	3.568(2)	C17	.H21_g	2.9200
C17	.C3_h	3.514(2)	C17	.H9B_i	3.0600
C18	.Cl1_j	3.6097(16)	C18	.H9B_i	2.9800
C20	.Cl1_a	3.5611(15)	C18	.H21_g	3.0700
C21	.C1_a	3.536(2)	C19	.H13_k	3.0600
C1	.H13_d	3.0500	C21	.H13_d	2.8500
C2	.H16_c	3.0400	H2	.C7_e	3.0900
C3	.H17_c	2.9700	H2	.C8_e	2.8300
C3	.H6_e	3.0200	H2	.C16_e	2.9500
C3	.H6	2.8200	H3	.N1	2.7200
C3	.H16_c	3.0700	H3	.C6	2.8800
C5	.H19	3.1000	H3	.H6	2.4200
C5	.H12	2.9600	H3	.H6_e	2.4300
C6	.H9A	2.7700	H5	.C12	3.0200
C6	.H3	2.8800	H5	.H20	2.4000

H5	.C13_k	2.9000	H13	.C1_m	3.0500
H5	.C14_k	3.0100	H13	.C21_m	2.8500
H6	.C3	2.8200	H13	.C19_g	3.0600
H6	.H3	2.4200	H15	.H9B	2.3700
H6	.C3_e	3.0200	H16	.H9B	2.3700
H6	.H3_e	2.4300	H16	.C2_h	3.0400
H6	.H6_e	2.5200	H16	.C3_h	3.0700
H9A	.N1	2.7700	H17	.N1_h	2.8000
H9A	.C6	2.7700	H17	.C3_h	2.9700
H9A	.C13_f	3.0500	H18	.Cl1_j	2.8900
H9A	.C14_f	2.8300	H19	.C5	3.1000
H9A	.C15_f	2.9000	H20	.H5	2.4000
H9B	.H15	2.3700	H20	.C13_k	3.0600
H9B	.H16	2.3700	H20	.C14_k	2.9000
H9B	.C17_l	3.0600	H20	.C15_k	2.9300
H9B	.C18_l	2.9800	H21	.C16_k	2.9800
H12	.C5	2.9600	H21	.C17_k	2.9200
H12	.Cl1_a	2.9200	H21	.C18_k	3.0700

Translation of Symmetry Code to Equiv.Pos

```
a =[  3566.00 ]  = -x,1-y,1-z
b =[  4464.00 ]  = -1/2+x,3/2-y,-1/2+z
c =[  4454.00 ]  = -1/2+x,1/2-y,-1/2+z
d =[  1565.00 ]  = x,1+y,z
e =[  3666.00 ]  = 1-x,1-y,1-z
f =[  3656.00 ]  = 1-x,-y,1-z
g =[  2546.00 ]  = 1/2-x,-1/2+y,3/2-z
h =[  4555.00 ]  = 1/2+x,1/2-y,1/2+z
i =[  2656.00 ]  = 3/2-x,1/2+y,3/2-z
j =[  4565.00 ]  = 1/2+x,3/2-y,1/2+z
k =[  2556.00 ]  = 1/2-x,1/2+y,3/2-z
l =[  2646.00 ]  = 3/2-x,-1/2+y,3/2-z
m =[  1545.00 ]  = x,-1+
```



X-Ray crystal structures of **13.**

Table 1: Crystal data and structure refinement for **13**

Identification code	dax16
Empirical formula	$C_{27}H_{25}NO_4$
Formula weight	427.48
Temperature / K	120.0
Crystal system	Monoclinic
Space group	$P2_1/n$
a / Å, b / Å, c / Å	10.0710(2), 25.9843(5), 17.0032(3)
α/°, β/°, γ/°	90.00, 104.460(10), 90.00
Volume / $Å^3$	4308.58(14)
Z	8
ρ_{calc} / mg mm^{-3}	1.318
μ / mm^{-1}	0.088
F(000)	1808
Crystal size / mm^3	0.3 × 0.28 × 0.14
Theta range for data collection	1.57 to 29.00°
Index ranges	-13 ≤ h ≤ 13, -35 ≤ k ≤ 35, -23 ≤ l ≤ 23
Reflections collected	52462

Independent reflections	11451[R(int) = 0.0702]
Data/restraints/parameters	11451/0/777
Goodness-of-fit on F^2	0.988
Final R indexes [I>2σ (I)]	R_1 = 0.0458, wR_2 = 0.0851
Final R indexes [all data]	R_1 = 0.0965, wR_2 = 0.0949
Largest diff. peak/hole / e $Å^{-3}$	0.265/-0.222

Table 2 Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **13**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
O1	5406.6(11)	5601.7(4)	3550.3(7)	38.2(3)
O2	6539.1(12)	4908.8(4)	4152.1(7)	39.2(3)
O3	10595.5(10)	5564.9(4)	4130.2(6)	32.5(3)
O4	8746.7(11)	6078.3(4)	3755.7(7)	37.7(3)
N4	7986.2(12)	4781.2(5)	2027.8(7)	28.0(3)
C1	7086.6(15)	5251.3(6)	2957.5(9)	25.8(3)
C2	8621.9(15)	5198.7(6)	3293.7(9)	26.6(3)
C3	9144.7(16)	5066.6(6)	2533.4(9)	27.1(4)
C4A	8224.5(15)	4422.1(6)	1463.7(9)	26.0(3)
C5	9433.0(17)	4465.5(6)	1197.6(10)	30.2(4)
C6	9708.2(17)	4138.9(6)	616.4(10)	32.7(4)
C7	8790.6(17)	3756.2(6)	279.5(10)	32.3(4)
C8	7609.9(17)	3705.7(6)	545.5(10)	30.6(4)
C8A	7298.8(15)	4023.3(6)	1130.3(9)	27.1(3)
C9	5972.7(17)	3924.0(6)	1368.2(10)	30.6(4)
C9A	5045.3(16)	4387.1(6)	1228.5(9)	29.8(4)
C10	3840.7(17)	4395.7(7)	610(1)	35.6(4)
C11	3013.3(19)	4828.2(8)	488.2(11)	41.6(5)
C12	3374.1(18)	5252.6(7)	984.9(11)	40.0(4)
C13	4579.9(16)	5251.1(6)	1592.9(10)	32.4(4)
C13A	5434.9(15)	4822.2(6)	1717.0(9)	27.3(3)
C13B	6764.7(15)	4794.4(6)	2368.7(9)	25.1(3)
C14	6332.2(16)	5226.7(6)	3620.3(10)	29.2(4)
C15	4641(2)	5607.5(9)	4169.6(14)	45.5(5)
C16	9295.5(16)	5668.2(6)	3742.6(9)	27.8(4)
C17	11390.1(19)	6000.1(7)	4510.4(12)	37.0(4)
C18	9548.5(16)	5544.9(6)	2135.1(9)	27.8(3)
C19	10892.8(18)	5722.2(7)	2379.9(10)	35.2(4)
C20	11268(2)	6187.9(7)	2101.5(11)	43.2(5)
C21	10302(2)	6474.5(7)	1563.5(11)	44.5(5)
C22	8968(2)	6295.8(7)	1283.5(11)	39.7(4)
C23	8592.3(18)	5831.2(6)	1570.8(10)	32.0(4)
O21	4291.5(11)	2308.7(4)	875.6(7)	36.8(3)
O22	3258.8(12)	3003.6(4)	216.0(7)	40.5(3)
O23	-890.1(11)	2314.0(4)	246.4(7)	37.4(3)

O24	1006.6(11)	1837.8(4)	712.8(7)	40.0(3)
N34	1604.0(12)	3249.2(5)	2207.4(7)	27.4(3)
C31	2582.6(15)	2703.9(6)	1397.0(9)	24.7(3)
C32	1043.6(15)	2736.9(6)	1040.8(9)	26.5(3)
C33	508.2(16)	2908.2(6)	1779.6(9)	26.2(3)
C34A	1379.7(15)	3590.9(5)	2793.0(9)	25.6(3)
C35	158.2(16)	3551.0(6)	3051.7(9)	28.6(4)
C36	-77.2(17)	3855.6(6)	3665.7(10)	31.7(4)
C37	877.5(17)	4210.4(6)	4056.8(10)	31.7(4)
C38	2052.7(17)	4271.8(6)	3780.3(9)	29.4(4)
C38A	2310.9(15)	3982.8(6)	3146.4(9)	26.0(3)
C39	3606.7(17)	4090.3(6)	2877(1)	29.2(4)
C39A	4559.8(15)	3636.6(6)	3044.8(9)	27.6(4)
C40	5747.7(16)	3645.6(7)	3666.2(10)	31.2(4)
C41	6577.8(17)	3212.3(7)	3844.5(10)	34.8(4)
C42	6226.9(17)	2769.5(7)	3397.2(11)	35.4(4)
C43	5028.4(16)	2752.7(6)	2773.6(10)	30.6(4)
C43A	4179.8(15)	3181.8(6)	2598.1(9)	25.7(3)
C43B	2874.7(15)	3194.7(6)	1920.7(9)	24.8(3)
C44	3392.8(16)	2697.9(6)	758.9(10)	28.3(4)
C45	5175(2)	2287.4(8)	319.8(14)	41.8(5)
C46	413.6(16)	2244.2(6)	657.2(9)	29.9(4)
C47	-1613(2)	1852.2(9)	-106.1(14)	47.1(5)
C48	214.9(16)	2465.7(6)	2300.3(9)	27.7(3)
C49	-1082.3(18)	2243.5(7)	2123.4(11)	36.5(4)
C50	-1375(2)	1847.2(7)	2604.3(13)	46.4(5)
C51	-386(2)	1677.3(7)	3268.0(13)	47.6(5)
C52	903(2)	1893.0(7)	3443.8(12)	44.6(5)
C53	1208.0(18)	2285.0(6)	2965.7(10)	34.2(4)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **13**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka\times b\times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	36.0(7)	37.0(7)	46.0(7)	0.4(6)	18.4(6)	8.1(5)
O2	49.5(8)	34.3(7)	38.6(7)	4.9(6)	19.8(6)	4.6(6)
O3	26.4(6)	34.7(6)	33.4(6)	-5.4(5)	2.0(5)	-1.3(5)
O4	36.4(7)	29.7(6)	43.7(7)	-7.2(5)	4.0(6)	3.0(5)
N4	24.4(7)	29.0(7)	31.6(7)	-6.5(6)	9.0(6)	-4.1(6)
C1	26.5(9)	22.2(8)	28.9(8)	1.1(7)	7.2(7)	0.5(7)
C2	27.2(9)	25.5(8)	26.2(8)	0.7(7)	4.8(7)	-0.5(7)
C3	24.2(9)	27.1(8)	29.1(9)	-0.5(7)	4.7(7)	1.2(7)
C4A	29.6(9)	23.8(8)	23.9(8)	2.2(7)	5.6(7)	3.9(7)
C5	30.7(9)	27.3(9)	33.1(9)	1.9(7)	8.7(8)	1.0(7)
C6	30.9(10)	36(1)	33.7(9)	4.2(8)	12.7(8)	6.0(8)
C7	38.4(10)	31.3(9)	27.3(9)	-0.8(8)	8.2(8)	7.9(8)
C8	37.1(10)	27.0(9)	26.3(8)	0.4(7)	5.2(8)	1.4(7)
C8A	30.4(9)	25.7(8)	24.6(8)	3.2(7)	5.5(7)	0.9(7)
C9	36.2(10)	29.2(9)	27.2(9)	-4.6(7)	9.5(8)	-8.9(7)
C9A	28.7(9)	34.1(9)	28.1(8)	0.2(7)	9.8(7)	-6.7(7)

C10	35.5(10)	41.9(11)	30.0(9)	-2.7(8)	9.1(8)	-10.6(8)
C11	30(1)	56.2(12)	33.6(10)	9.2(9)	-1.6(8)	-6.2(9)
C12	33(1)	41.0(11)	43.4(11)	11.1(9)	5.0(9)	1.5(9)
C13	29.9(9)	31.6(9)	35.6(9)	3.9(8)	8.1(8)	-2.1(7)
C13A	23.7(8)	31.3(9)	26.7(8)	4.1(7)	6.2(7)	-4.1(7)
C13B	26.4(8)	23.4(8)	26.2(8)	0.9(7)	7.7(7)	-0.9(6)
C14	28.6(9)	24.5(8)	34.0(9)	-6.1(7)	6.9(7)	-3.2(7)
C15	43.1(12)	43.5(12)	58.8(14)	-7.7(11)	29.5(11)	2.1(10)
C16	26.3(9)	32.3(9)	25.5(8)	-0.2(7)	7.7(7)	-1.6(7)
C17	30.7(10)	41.8(11)	36.2(10)	-10.6(9)	3.9(9)	-6.9(8)
C18	31.5(9)	28.0(8)	26.1(8)	-4.3(7)	11.1(7)	-1.9(7)
C19	33.9(10)	41(1)	32.1(9)	-2.3(8)	10.9(8)	-5.8(8)
C20	46.6(12)	47.2(11)	40.5(11)	-8.9(9)	19.7(10)	-18(1)
C21	70.5(15)	30.3(10)	41.7(11)	-4.9(9)	31.0(11)	-8.8(10)
C22	56.6(13)	34.5(10)	32.8(10)	2.0(8)	20.2(10)	6.7(9)
C23	36.2(10)	33.2(9)	29.1(9)	-1.4(7)	12.6(8)	3.2(8)
O21	35.4(7)	34.2(6)	45.5(7)	-0.3(6)	19.1(6)	4.9(5)
O22	49.2(8)	41.6(7)	33.9(7)	6.0(6)	16.3(6)	6.4(6)
O23	28.0(6)	43.1(7)	37.6(7)	-12.2(6)	1.6(5)	-2.0(5)
O24	35.1(7)	31.8(7)	52.1(8)	-8.7(6)	8.6(6)	-0.4(5)
N34	23.5(7)	28.9(7)	30.5(7)	-5.8(6)	8.1(6)	-3.1(5)
C31	25.4(8)	23.4(8)	25.2(8)	0.9(7)	5.8(7)	-0.2(6)
C32	26.6(8)	26.6(8)	24.5(8)	0.4(7)	3.1(7)	1.3(7)
C33	22.1(8)	27.0(8)	27.4(8)	-1.3(7)	2.3(7)	1.1(7)
C34A	29.2(9)	22.6(8)	24.4(8)	2.9(7)	5.7(7)	1.8(6)
C35	28.6(9)	25.7(9)	30.6(9)	-0.1(7)	5.7(7)	1.0(7)
C36	31.7(9)	31.5(9)	33.9(9)	3.3(7)	11.8(8)	3.1(7)
C37	39.2(10)	28.6(9)	28.0(9)	-0.6(7)	9.3(8)	6.6(7)
C38	32.4(9)	24.7(8)	27.8(9)	-0.8(7)	1.3(8)	-0.2(7)
C38A	26.9(8)	23.4(8)	26.2(8)	2.9(7)	3.6(7)	3.0(6)
C39	32.6(9)	24.8(9)	30.7(9)	-1.3(7)	9.1(8)	-4.3(7)
C39A	27.2(9)	29.1(9)	28.3(8)	1.0(7)	10.3(7)	-4.5(7)
C40	29.8(9)	33.6(9)	30.5(9)	-6.2(8)	7.9(8)	-9.1(7)
C41	24.6(9)	41.8(10)	34.6(10)	0.3(8)	1.1(8)	-4.9(8)
C42	27.5(9)	35.4(10)	41.1(10)	2.3(8)	4.9(8)	2.9(8)
C43	28.1(9)	30.0(9)	33.0(9)	-0.7(8)	6.6(8)	-2.2(7)
C43A	24.1(8)	28.2(8)	26.0(8)	1.9(7)	8.6(7)	-3.8(6)
C43B	24.9(8)	24.3(8)	25.6(8)	0.5(7)	7.0(7)	-1.1(6)
C44	30.2(9)	24.9(8)	28.4(8)	-5.3(7)	4.6(7)	-2.3(7)
C45	38.8(11)	40.0(11)	55.0(13)	-2(1)	27.1(11)	0.4(9)
C46	26.8(9)	35.4(9)	27.2(8)	-4.9(7)	6.0(7)	-1.1(7)
C47	31.2(11)	56.6(13)	50.9(13)	-29.7(11)	5.4(10)	-7.4(10)
C48	30.0(9)	25.7(8)	29.9(9)	-2.6(7)	12.0(7)	0.3(7)
C49	38.3(11)	36.9(10)	36.1(10)	-4.8(8)	12.2(9)	-6.3(8)
C50	49.8(13)	40.2(11)	57.6(13)	-13(1)	29.3(11)	-17.1(10)
C51	71.0(15)	30.3(10)	52.9(12)	4.5(9)	36.9(12)	3.1(10)
C52	51.5(13)	45.8(12)	41.9(11)	12.3(9)	21.9(10)	17.5(10)
C53	34(1)	35.8(10)	35.4(10)	3.7(8)	13.3(8)	5.4(8)

Table 4 Bond Lengths for **13**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C14	1.3332(18)	O21	C44	1.3384(18)
O1	C15	1.452(2)	O21	C45	1.453(2)
O2	C14	1.2038(18)	O22	C44	1.1996(17)
O3	C16	1.3378(17)	O23	C46	1.3367(18)
O3	C17	1.4418(19)	O23	C47	1.453(2)
O4	C16	1.2032(17)	O24	C46	1.2052(18)
N4	C3	1.4661(19)	N34	C33	1.4598(18)
N4	C4A	1.4011(18)	N34	C34A	1.3941(18)
N4	C13B	1.4854(18)	N34	C43B	1.4854(18)
C1	C2	1.515(2)	C31	C32	1.519(2)
C1	C13B	1.535(2)	C31	C43B	1.541(2)
C1	C14	1.510(2)	C31	C44	1.512(2)
C2	C3	1.551(2)	C32	C33	1.551(2)
C2	C16	1.507(2)	C32	C46	1.503(2)
C3	C18	1.518(2)	C33	C48	1.525(2)
C4A	C5	1.405(2)	C34A	C35	1.410(2)
C4A	C8A	1.414(2)	C34A	C38A	1.413(2)
C5	C6	1.382(2)	C35	C36	1.377(2)
C6	C7	1.381(2)	C36	C37	1.377(2)
C7	C8	1.380(2)	C37	C38	1.387(2)
C8	C8A	1.387(2)	C38	C38A	1.390(2)
C8A	C9	1.511(2)	C38A	C39	1.513(2)
C9	C9A	1.505(2)	C39	C39A	1.502(2)
C9A	C10	1.393(2)	C39A	C40	1.384(2)
C9A	C13A	1.400(2)	C39A	C43A	1.405(2)
C10	C11	1.383(2)	C40	C41	1.390(2)
C11	C12	1.381(3)	C41	C42	1.376(2)
C12	C13	1.384(2)	C42	C43	1.394(2)
C13	C13A	1.392(2)	C43	C43A	1.391(2)
C13A	C13B	1.512(2)	C43A	C43B	1.516(2)
C18	C19	1.392(2)	C48	C49	1.391(2)
C18	C23	1.393(2)	C48	C53	1.391(2)
C19	C20	1.386(2)	C49	C50	1.392(2)
C20	C21	1.376(3)	C50	C51	1.378(3)
C21	C22	1.389(3)	C51	C52	1.377(3)
C22	C23	1.390(2)	C52	C53	1.384(2)

Table 5 Bond Angles for **13**.

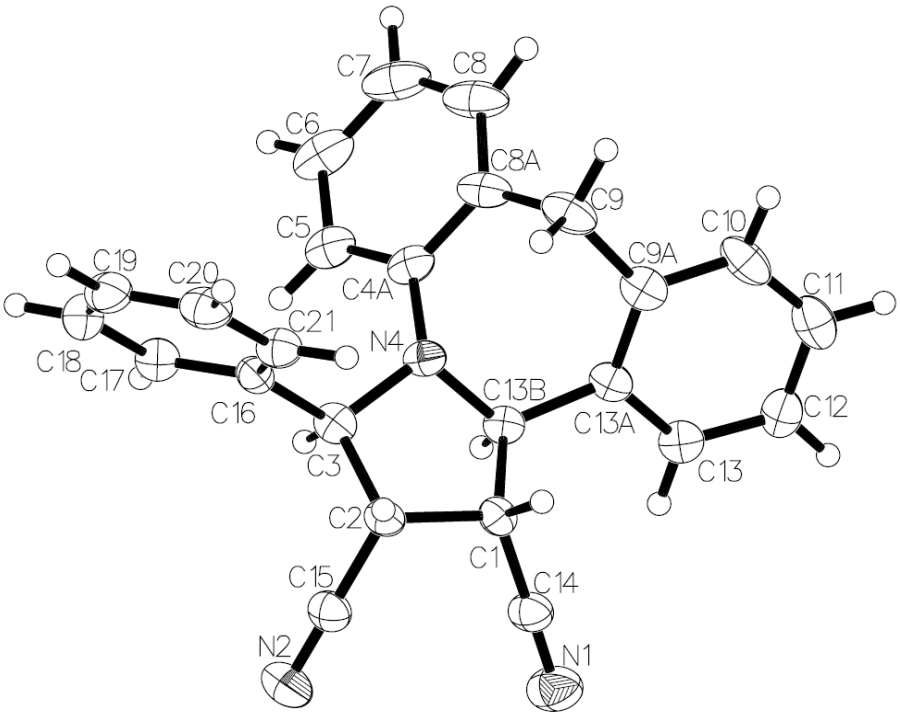
Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1	C14	C1	111.93(14)	O21	C44	C31	111.57(13)
O2	C14	O1	123.68(15)	O22	C44	O21	123.80(14)
O2	C14	C1	124.39(14)	O22	C44	C31	124.62(14)
O3	C16	C2	110.39(13)	O23	C46	C32	111.36(13)
O4	C16	O3	124.48(14)	O24	C46	O23	124.24(15)
O4	C16	C2	125.13(14)	O24	C46	C32	124.40(15)
N4	C3	C2	102.39(12)	N34	C33	C32	101.84(12)
N4	C3	C18	114.52(13)	N34	C33	C48	113.60(12)

N4	C4A	C5	118.51(14)	N34	C34A	C35	119.06(14)
N4	C4A	C8A	123.63(13)	N34	C34A	C38A	123.64(13)
N4	C13B	C1	102.23(12)	N34	C43B	C31	102.28(11)
N4	C13B	C13A	112.54(12)	N34	C43B	C43A	114.03(12)
C1	C2	C3	103.43(12)	C31	C32	C33	102.70(12)
C2	C1	C13B	101.88(12)	C32	C31	C43B	102.25(12)
C3	N4	C13B	112.01(11)	C33	N34	C43B	112.63(11)
C4A	N4	C3	119.41(12)	C34A	N34	C33	120.35(12)
C4A	N4	C13B	125.63(12)	C34A	N34	C43B	126.99(12)
C4A	C8A	C9	123.77(14)	C34A	C38A	C39	122.37(14)
C5	C4A	C8A	117.84(14)	C35	C34A	C38A	117.29(14)
C6	C5	C4A	121.70(16)	C35	C36	C37	121.28(16)
C7	C6	C5	120.39(16)	C36	C35	C34A	121.54(15)
C7	C8	C8A	123.09(16)	C36	C37	C38	117.71(15)
C8	C7	C6	118.33(16)	C37	C38	C38A	122.76(15)
C8	C8A	C4A	118.62(14)	C38	C38A	C34A	119.08(14)
C8	C8A	C9	117.60(14)	C38	C38A	C39	118.52(14)
C9A	C9	C8A	112.11(13)	C39A	C39	C38A	110.87(13)
C9A	C13A	C13B	117.52(14)	C39A	C40	C41	120.73(16)
C10	C9A	C9	121.40(15)	C39A	C43A	C43B	117.35(13)
C10	C9A	C13A	119.81(15)	C40	C39A	C39	121.42(15)
C11	C10	C9A	120.29(17)	C40	C39A	C43A	119.56(15)
C11	C12	C13	120.14(18)	C41	C42	C43	120.05(16)
C12	C11	C10	120.02(17)	C42	C41	C40	119.95(16)
C12	C13	C13A	120.63(17)	C43	C43A	C39A	119.24(14)
C13	C13A	C9A	119.06(15)	C43	C43A	C43B	123.37(14)
C13	C13A	C13B	123.41(14)	C43A	C39A	C39	118.85(14)
C13A	C9A	C9	118.76(14)	C43A	C43	C42	120.44(15)
C13A	C13B	C1	116.44(13)	C43A	C43B	C31	115.14(13)
C14	O1	C15	115.39(14)	C44	O21	C45	115.74(14)
C14	C1	C2	111.78(13)	C44	C31	C32	113.22(12)
C14	C1	C13B	112.99(12)	C44	C31	C43B	111.35(12)
C16	O3	C17	115.40(13)	C46	O23	C47	115.42(14)
C16	C2	C1	113.95(13)	C46	C32	C31	113.76(13)
C16	C2	C3	113.42(13)	C46	C32	C33	113.66(13)
C18	C3	C2	112.03(12)	C48	C33	C32	114.27(12)
C19	C18	C3	119.11(14)	C48	C49	C50	120.37(18)
C19	C18	C23	118.86(15)	C49	C48	C33	119.68(14)
C20	C19	C18	120.99(17)	C49	C48	C53	118.79(16)
C20	C21	C22	120.66(18)	C51	C50	C49	120.15(19)
C21	C20	C19	119.47(18)	C51	C52	C53	120.47(19)
C21	C22	C23	119.67(18)	C52	C51	C50	119.80(18)
C22	C23	C18	120.27(17)	C52	C53	C48	120.40(17)
C23	C18	C3	121.89(14)	C53	C48	C33	121.51(14)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **13**.

Atom	x	y	z	U(eq)
H1	6883(13)	5566(5)	2676(8)	19(4)
H2	8816(14)	4904(5)	3673(8)	23(4)
H3	9966(14)	4849(5)	2693(8)	19(4)

H5	10109(14)	4742(5)	1414(8)	24(4)
H6	10562(15)	4180(5)	463(9)	29(4)
H7	8943(16)	3524(6)	-128(9)	38(5)
H8	6945(15)	3432(6)	325(9)	35(4)
H9A	5498(15)	3632(6)	1022(9)	36(4)
H9B	6180(14)	3802(5)	1933(9)	28(4)
H10	3625(14)	4112(5)	267(9)	21(4)
H11	2207(17)	4836(6)	59(10)	45(5)
H12	2807(17)	5542(7)	932(10)	48(5)
H13	4828(15)	5552(6)	1955(9)	35(5)
H13A	6733(13)	4486(5)	2713(8)	21(4)
H15A	4079(19)	5294(7)	4123(11)	60(6)
H15B	5300.0(2)	5632(8)	4703(14)	84(8)
H15C	4170.0(2)	5928(8)	4066(12)	66(6)
H17A	12243(18)	5840(6)	4877(10)	49(5)
H17B	10870(18)	6201(7)	4846(11)	57(6)
H17C	11585(16)	6219(6)	4069(10)	46(5)
H19	11585(16)	5508(6)	2766(10)	41(5)
H20	12191(18)	6297(6)	2309(10)	49(5)
H21	10580(17)	6808(7)	1358(10)	49(5)
H22	8248(17)	6488(6)	877(10)	43(5)
H23	7640(16)	5696(6)	1374(9)	37(5)
H31	2792(13)	2388(5)	1736(8)	21(4)
H32	808(15)	3009(6)	637(9)	30(4)
H33	-360(14)	3106(5)	1576(8)	19(4)
H35	-529(14)	3300(5)	2803(8)	19(4)
H36	-947(16)	3817(6)	3795(9)	33(4)
H37	749(15)	4426(6)	4506(9)	34(4)
H38	2721(14)	4524(5)	4026(8)	24(4)
H39A	3403(14)	4191(5)	2316(9)	24(4)
H39B	4068(15)	4405(6)	3170(9)	29(4)
H40	5975(15)	3951(6)	3968(9)	33(4)
H41	7374(16)	3219(5)	4278(9)	32(4)
H42	6823(15)	2456(6)	3522(9)	34(4)
H43	4779(16)	2427(6)	245(1)	39(5)
H43A	2910(14)	3482(5)	1540(9)	28(4)
H45A	5733(19)	1966(7)	476(11)	61(6)
H45B	4627(19)	2302(7)	-243(12)	58(6)
H45C	5737(17)	2600(7)	378(10)	49(5)
H47A	-1081(18)	1685(7)	-442(11)	55(6)
H47B	-1719(19)	1626(8)	356(12)	67(7)
H47C	-2503(19)	1983(7)	-443(11)	54(6)
H49	-1781(16)	2382(6)	1655(10)	39(5)
H50	-2250(18)	1718(6)	2481(10)	49(5)
H51	-613(17)	1404(7)	3612(10)	54(6)
H52	1607(18)	1779(7)	3910(11)	53(6)
H53	2111(16)	2452(6)	3114(9)	33(4)



X-Ray crystal structures of **16**.

Table 1: Crystal data and structure refinement for **16**

Identification code	dax17
Empirical formula	$C_{25}H_{19}N_3$ x 0.125 CH_2Cl_2
Formula weight	366.74
Temperature / K	-153
Crystal system	Monoclinic
Space group	C2/c
a / Å, b / Å, c / Å	36.9379(14), 28.7704(11), 15.8020(6)
α/°, β/°, γ/°	90.00, 113.740(10), 90.00
Volume / $Å^3$	15372.1(10)
Z	32
ρ_{calc} / mg mm^{-3}	1.268
μ / mm^{-1}	0.092
F(000)	6164
Crystal size / mm^3	0.24 × 0.16 × 0.14
Theta range for data collection	1.42 to 27.00°
Index ranges	-47 ≤ h ≤ 47, -36 ≤ k ≤ 36, -20 ≤ l ≤ 20
Reflections collected	69184

Independent reflections	16751[R(int) = 0.1100]
Data/restraints/parameters	16751/0/1021
Goodness-of-fit on F^2	0.950
Final R indexes [I>2σ (I)]	R_1 = 0.0606, wR_2 = 0.1357
Final R indexes [all data]	R_1 = 0.1394, wR_2 = 0.1546
Largest diff. peak/hole / e $Å^{-3}$	0.876/-0.242

Table 2 Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **16**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
N1	7189.5(8)	3494.1(10)	6528(2)	49.8(8)
N2	6157.4(8)	3630.8(9)	6141.8(19)	43.5(7)
N4	6713.4(6)	5026.2(7)	5715.9(16)	26.6(5)
C1	6987.9(8)	4360.2(9)	6568.8(19)	26.9(6)
C2	6552.1(8)	4410.5(9)	6463.2(19)	26.6(6)
C3	6363.1(8)	4771(1)	5678(2)	28.9(7)
C4A	6662.8(8)	5369.9(10)	5017(2)	29.6(7)
C5	6346.1(9)	5370.5(10)	4158(2)	34.9(7)
C6	6322(1)	5716.5(12)	3521(2)	46.8(9)
C7	6610.8(11)	6052.3(12)	3734(3)	49.5(9)
C8	6922.9(11)	6046.3(11)	4583(3)	47.2(9)
C8A	6954.6(9)	5712.6(10)	5240(2)	33.3(7)
C9	7288.6(9)	5693.5(10)	6172(2)	38.9(8)
C9A	7567.0(8)	5295.3(10)	6230.9(19)	31.4(7)
C10	7962.9(9)	5389.7(11)	6423(2)	38.5(8)
C11	8220.0(9)	5047.0(12)	6405(2)	38.7(8)
C12	8083.7(8)	4598.1(11)	6159(2)	35.4(7)
C13	7693.1(8)	4496.5(10)	5958.8(19)	29.9(7)
C13A	7429.3(8)	4836.2(10)	6005.4(19)	27.4(6)
C13B	7012.1(7)	4667.5(9)	5789.9(19)	26.9(6)
C14	7105.2(8)	3878.6(11)	6543(2)	32.9(7)
C15	6330.0(8)	3974.2(10)	6274(2)	31.7(7)
C16	6062.3(8)	5078.9(9)	5830(2)	27.3(6)
C17	5681.5(9)	5111.8(10)	5165(2)	37.1(7)
C18	5401.1(9)	5389.6(11)	5323(3)	46.4(9)
C19	5510.2(10)	5621.6(10)	6159(3)	44.6(9)
C20	5890.1(9)	5586.9(10)	6817(2)	40.3(8)
C21	6165.2(8)	5322.3(10)	6657(2)	31.8(7)
N21	5482.3(9)	4068.6(10)	3563(2)	59.9(9)
N22	6529.5(9)	3856.8(10)	4083(2)	53.8(8)
N34	5871.4(6)	2516.2(7)	4372.5(15)	25.3(5)
C31	5654.7(8)	3192.0(9)	3514(2)	30.8(7)
C32	6098.9(8)	3106.4(9)	3706(2)	29.4(7)
C33	6244.4(8)	2750.9(9)	4516(2)	28.1(6)
C34A	5883.4(8)	2162.5(9)	5016(2)	26.2(6)
C35	6187.5(8)	2116.4(10)	5883(2)	28.8(7)
C36	6182.5(9)	1752.8(10)	6458(2)	33.1(7)
C37	5866.6(9)	1445.8(10)	6177(2)	34.7(7)
C38	5560.5(9)	1494.9(9)	5315(2)	32.4(7)

C38A	5565.5(8)	1845.0(9)	4717(2)	28.2(6)
C39	5247.2(8)	1908.1(9)	3757(2)	30.7(7)
C39A	4993.2(8)	2323.5(10)	3721.6(19)	27.4(6)
C40	4591.3(8)	2261.6(10)	3519.6(19)	32.0(7)
C41	4354.3(8)	2621.8(11)	3565(2)	32.4(7)
C42	4513.0(8)	3060.2(11)	3829(2)	33.6(7)
C43	4912.4(8)	3128.3(10)	4046.9(19)	30.0(7)
C43A	5155.7(8)	2768.2(9)	3991.7(19)	26.3(6)
C43B	5587.4(8)	2894.5(9)	4257.8(19)	25.6(6)
C44	5553.7(9)	3685.0(11)	3531(2)	39.1(8)
C45	6340.9(9)	3529.0(11)	3922(2)	36.3(7)
C46	6564.3(8)	2433.1(9)	4495(2)	29.2(7)
C47	6510.7(9)	2163.2(10)	3725(2)	35.3(7)
C48	6814.7(10)	1879.0(11)	3713(3)	46.9(9)
C49	7169.2(10)	1859.6(11)	4471(3)	50.2(10)
C50	7226.3(9)	2125.6(11)	5245(3)	45.3(9)
C51	6925.0(8)	2413.7(10)	5250(2)	36.1(7)
Cl1A	5395(1)	5406.1(13)	2316(3)	40.1(10)
Cl1B	5350.5(10)	5341.9(13)	2552(3)	35.9(9)
C1SB	5067(3)	5076(3)	2421(9)	21(2)
N31	5230.9(9)	1227.1(10)	8757(2)	55.7(8)
N32	6193.0(8)	960.1(9)	8634(2)	48.8(7)
N64	6061.8(6)	2518.8(7)	9268.8(16)	25.7(5)
C61	5590.5(8)	1952.3(9)	8469.7(19)	27.1(6)
C62	5995.7(8)	1836.1(9)	8427(2)	28.3(6)
C63	6304.5(8)	2132.5(9)	9197(2)	26.6(6)
C64A	6251.3(8)	2838.4(9)	10016.3(19)	25.7(6)
C65	6569.3(8)	2728.2(10)	10818(2)	34.5(7)
C66	6725.7(9)	3061.5(11)	11510(2)	43.0(8)
C67	6559.4(10)	3496.6(12)	11399(2)	45.2(9)
C68	6245.5(9)	3612.7(11)	10586(2)	38.2(8)
C68A	6086.8(8)	3288.6(10)	9877(2)	29.9(7)
C69	5746.3(8)	3394.3(10)	8979(2)	34.1(7)
C69A	5366.4(8)	3147.3(10)	8864(2)	30.9(7)
C70	5023.8(9)	3413.0(11)	8631(2)	40.6(8)
C71	4669.3(9)	3222.2(12)	8535(2)	43.1(8)
C72	4649.1(9)	2753.2(12)	8698(2)	40.3(8)
C73	4987.2(8)	2481.2(11)	8940(2)	33.8(7)
C73A	5346.8(8)	2671.4(10)	9012.7(18)	27.0(6)
C73B	5687.7(7)	2326.3(9)	9236.4(19)	26.9(6)
C74	5389.8(9)	1543.9(11)	8635(2)	35.7(7)
C75	6102.6(9)	1346.5(11)	8539(2)	36.2(7)
C76	6637.8(8)	2286.0(9)	8930(2)	28.4(6)
C77	6994.9(9)	2054.9(12)	9263(2)	46.1(9)
C78	7291.9(10)	2179.7(13)	8978(3)	59.2(11)
C79	7227.3(9)	2535.3(12)	8347(3)	49.0(9)
C80	6870.6(9)	2766.6(10)	8004(2)	39.6(8)
C81	6574.4(9)	2640.2(10)	8294(2)	35.4(7)
N41	7086.5(9)	-1402.9(10)	6223(2)	57.3(8)
N42	6121.3(8)	-1580.7(9)	6304(2)	53.4(8)
N94	6356.1(6)	-33.3(7)	5739.5(15)	24.2(5)
C91	6778.5(7)	-641.5(9)	6536.0(19)	25.6(6)
C92	6359.3(7)	-718.0(9)	6524(2)	26.2(6)
C93	6079.3(7)	-400.6(9)	5739.8(19)	23.8(6)
C94A	6212.1(7)	315.7(9)	5033.2(19)	23.8(6)

C95	5912.2(8)	243(1)	4167(2)	29.6(7)
C96	5802.5(8)	604.4(10)	3517(2)	31.5(7)
C97	5987.0(8)	1029.5(10)	3741(2)	32.8(7)
C98	6286.5(8)	1100.1(10)	4605(2)	30.1(7)
C98A	6401.3(8)	750.4(9)	5260.6(19)	26.5(6)
C99	6737.9(8)	801.9(9)	6189.2(19)	28.3(7)
C99A	7096.4(8)	525.2(10)	6238.5(19)	26.9(6)
C100	7450.5(8)	761.7(10)	6441(2)	32.8(7)
C101	7786.0(8)	540.1(11)	6455(2)	34.6(7)
C102	7772.5(8)	71.6(11)	6261(2)	32.7(7)
C103	7421.6(7)	-168.5(10)	6045.5(19)	28.1(6)
C104	7081.7(7)	50.0(9)	6040.6(18)	25.4(6)
C105	6719.7(7)	-263.2(9)	5796.8(19)	24.4(6)
C106	6955.5(8)	-1065.2(11)	6368(2)	35.1(7)
C107	6223.7(8)	-1203.0(11)	6407(2)	36.1(7)
C108	5740.9(7)	-229.5(9)	5949.8(19)	24.3(6)
C109	5395.1(8)	-493.1(10)	5684(2)	29.7(7)
C110	5093.0(8)	-357.2(10)	5938(2)	31.6(7)
C111	5128.3(8)	42.2(10)	6448.7(19)	30.0(7)
C112	5468.7(8)	306.7(10)	6713(2)	30.9(7)
C113	5775.6(8)	170.7(9)	6475.4(19)	28.4(6)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **16**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	59.8(19)	40.5(18)	64(2)	10.3(15)	40.0(16)	7.4(14)
N2	46.9(17)	37.3(16)	51.3(18)	-5.3(14)	25.0(14)	-12.2(13)
N4	34.5(14)	23.8(13)	28.4(13)	2.4(11)	19.9(11)	3.3(10)
C1	26.6(16)	28.3(16)	27.2(16)	-0.2(13)	12.2(13)	-2.7(11)
C2	30.5(16)	23.9(15)	29.3(16)	-1.3(13)	16.0(13)	-2.3(11)
C3	33.3(17)	29.0(16)	27.8(16)	-5.5(13)	15.9(13)	-2.5(12)
C4A	40.8(18)	26.3(16)	29.8(17)	0.8(13)	22.7(14)	9.4(13)
C5	47.9(19)	31.8(17)	37.1(18)	3.1(15)	29.6(16)	10.8(14)
C6	69(2)	47(2)	37(2)	11.0(17)	34.9(18)	26.4(18)
C7	89(3)	30.2(19)	50(2)	10.5(17)	50(2)	16.5(18)
C8	82(3)	24.3(17)	57(2)	-0.2(17)	51(2)	1.6(16)
C8A	56(2)	20.1(15)	39.7(19)	-3.7(14)	36.6(16)	-0.4(13)
C9	55(2)	32.0(18)	41(2)	-7.6(15)	31.7(17)	-12.2(14)
C9A	40.2(18)	35.1(17)	24.6(16)	-4.1(14)	18.9(14)	-4.3(13)
C10	45(2)	46(2)	32.2(18)	-7.7(16)	24.3(15)	-18.9(15)
C11	35.3(18)	59(2)	26.1(17)	-0.5(16)	17.1(14)	-11.3(15)
C12	32.1(17)	51(2)	27.6(17)	9.2(15)	16.9(14)	6.0(14)
C13	37.1(18)	32.9(17)	23.6(15)	-1.2(13)	16.2(13)	0.5(13)
C13A	34.2(17)	29.7(16)	23.0(15)	-0.4(13)	16.3(13)	-2.9(12)
C13B	31.0(16)	25.9(15)	25.0(15)	-1.9(13)	12.6(13)	-0.6(12)
C14	37.8(18)	29.0(17)	37.9(18)	1.9(14)	21.7(15)	0.3(13)
C15	34.7(17)	31.3(17)	35.3(18)	-0.2(14)	20.6(14)	-1.5(13)
C16	25.7(16)	25.2(15)	32.8(17)	-0.8(13)	13.6(13)	-2.5(11)
C17	36.6(18)	33.6(17)	40.4(19)	0.4(15)	14.6(15)	-0.2(13)
C18	30.9(18)	42(2)	65(3)	9.5(19)	17.7(17)	2.6(14)
C19	45(2)	30.0(18)	72(3)	5.2(18)	37.6(19)	6.8(14)
C20	51(2)	29.4(18)	50(2)	-4.4(16)	30.9(18)	-0.8(14)
C21	38.5(17)	27.9(16)	33.7(17)	-1.6(14)	19.4(14)	1.3(13)
N21	70(2)	33.6(17)	92(3)	18.7(17)	48.8(19)	6.6(14)
N22	65(2)	46.4(18)	50.0(19)	1.0(15)	23.2(16)	-25.5(15)
N34	27.6(13)	23.2(12)	28.9(13)	1.3(10)	15.4(11)	-2.4(9)
C31	32.4(17)	28.4(16)	32.8(17)	1.5(14)	14.4(14)	-4.1(12)

C32	34.9(17)	27.0(16)	30.8(17)	-3.4(13)	17.9(14)	-7.4(12)
C33	33.6(16)	25.7(15)	30.2(16)	-7.6(13)	18.2(13)	-4.9(12)
C34A	33.0(16)	21.4(15)	32.9(17)	-2.9(13)	22.5(14)	1.0(11)
C35	33.8(17)	28.1(16)	31.2(17)	-0.8(13)	20.1(14)	2.4(12)
C36	45.3(19)	31.0(17)	30.9(17)	1.0(14)	23.6(15)	10.5(14)
C37	54(2)	21.7(16)	39.4(19)	4.1(14)	30.5(17)	6.0(14)
C38	46.6(19)	20.8(15)	40.9(19)	-4.5(14)	29.0(16)	-2.8(13)
C38A	34.1(17)	22.6(15)	35.7(17)	-2.0(13)	22.1(14)	0.1(12)
C39	37.8(17)	26.3(16)	33.1(17)	-6.7(14)	19.6(14)	-8.2(12)
C39A	34.2(17)	28.4(16)	23.5(15)	-1.7(13)	15.5(13)	-0.4(12)
C40	33.4(17)	39.7(18)	25.1(16)	-2.6(14)	14.0(13)	-8.0(13)
C41	29.8(16)	45.5(19)	26.6(16)	3.2(15)	16.2(13)	-0.4(14)
C42	36.1(18)	41.2(19)	30.6(17)	8.3(15)	20.8(14)	8.4(14)
C43	38.1(18)	30.8(16)	26.1(16)	0.6(13)	18.1(14)	-0.1(13)
C43A	27.8(15)	29.0(16)	25.4(15)	2.0(13)	14.1(13)	-1.0(12)
C43B	34.5(16)	21.9(15)	23.4(15)	-2.4(12)	14.7(13)	-3.4(12)
C44	45(2)	31.7(19)	49(2)	10.2(16)	27.5(17)	0.7(14)
C45	36.5(18)	38.9(19)	35.6(19)	1.6(15)	16.6(15)	-6.9(14)
C46	32.4(17)	23.0(15)	39.0(18)	-0.1(14)	21.5(14)	-5.1(12)
C47	46.2(19)	26.8(16)	41.9(19)	-6.6(15)	26.9(16)	-7.7(13)
C48	64(2)	30.2(18)	66(3)	-13.6(17)	46(2)	-6.0(16)
C49	53(2)	29.9(19)	85(3)	-6.3(19)	46(2)	0.9(15)
C50	38.0(19)	36.3(19)	67(3)	1.0(18)	26.1(18)	-1.6(14)
C51	39.9(19)	27.0(17)	49(2)	-4.2(15)	25.8(16)	-2.6(13)
N31	71(2)	42.5(18)	59(2)	-4.3(16)	32.1(17)	-23.8(15)
N32	52.5(18)	29.1(16)	60(2)	-4.1(14)	17.2(15)	-0.3(13)
N64	27.6(13)	23.7(12)	30.8(13)	-4.1(11)	17.0(11)	-4.0(9)
C61	33.2(16)	25.1(15)	24.1(15)	2.4(13)	12.7(13)	-2.7(12)
C62	38.6(17)	23.7(15)	26.6(16)	0.7(13)	17.5(13)	-3.8(12)
C63	35.1(16)	20.3(14)	28.6(16)	-0.6(13)	17.3(13)	0.1(11)
C64A	29.0(16)	26.3(15)	28.2(16)	-6.3(13)	18.2(13)	-7.3(11)
C65	35.0(18)	31.9(17)	39.4(19)	-8.0(15)	17.8(15)	-4.2(13)
C66	38.4(19)	49(2)	41(2)	-10.3(17)	15.7(16)	-9.4(15)
C67	49(2)	43(2)	51(2)	-24.6(18)	28.3(19)	-20.4(16)
C68	46(2)	28.9(17)	51(2)	-9.1(15)	30.9(18)	-8.2(14)
C68A	34.0(17)	25.6(16)	39.1(18)	-3.8(14)	24.1(14)	-7.2(12)
C69	42.7(19)	24.1(16)	44(2)	5.0(14)	26.2(16)	-0.3(13)
C69A	38.9(18)	33.9(17)	27.5(16)	2.1(14)	21.5(14)	0.9(13)
C70	48(2)	43(2)	38.7(19)	9.8(16)	26.5(16)	10.6(15)
C71	36.1(19)	67(2)	30.8(18)	9.2(17)	18.2(15)	18.6(16)
C72	30.3(18)	68(2)	26.5(17)	-4.0(17)	15.2(14)	-4.2(15)
C73	35.0(18)	42.2(19)	27.4(16)	-4.0(14)	15.8(14)	-5.6(14)
C73A	27.5(16)	36.1(17)	19.1(15)	-0.5(13)	11.0(12)	-1.7(12)
C73B	31.0(16)	28.8(16)	22.7(15)	-1.3(13)	12.8(12)	-8.2(12)
C74	42.4(19)	33.0(18)	33.3(18)	-4.7(14)	17.0(15)	-11.5(14)
C75	39.8(19)	31.2(18)	37.9(19)	-4.8(15)	16.1(15)	-6.2(14)
C76	32.5(17)	24.7(15)	32.3(17)	-2.3(13)	17.5(13)	-1.9(12)
C77	44(2)	48(2)	54(2)	16.9(18)	27.7(18)	7.0(15)
C78	41(2)	68(3)	80(3)	19(2)	36(2)	12.9(18)
C79	46(2)	50(2)	67(3)	2(2)	39.4(19)	-5.1(16)
C80	49(2)	29.2(17)	54(2)	4.8(16)	33.8(17)	-2.7(14)
C81	42.0(18)	26.9(16)	47(2)	-0.6(15)	28.5(16)	1.5(13)
N41	69(2)	43.8(18)	71(2)	7.9(17)	41.2(18)	21.4(15)
N42	50.7(18)	31.2(17)	77(2)	8.4(16)	24.6(16)	-4.6(13)
N94	27.3(13)	22.2(12)	27.7(13)	3.3(10)	15.8(11)	0.3(9)
C91	26.1(15)	26.7(15)	25.2(15)	-0.9(13)	11.5(12)	0.0(11)
C92	31.2(16)	23.3(15)	29.7(16)	-3.8(13)	18.0(13)	-2.0(11)
C93	25.9(15)	23.5(15)	24.1(15)	-2.3(12)	12.2(12)	-3.0(11)
C94A	22.5(14)	25.7(15)	26.5(15)	3.6(13)	13.3(12)	2.5(11)
C95	30.1(16)	26.2(16)	36.0(17)	-2.1(14)	17.1(14)	-3.2(12)
C96	34.4(17)	31.5(17)	29.9(17)	4.4(14)	14.2(14)	8.2(13)

C97	40.7(18)	29.2(17)	33.8(18)	7.2(14)	20.5(15)	10.3(13)
C98	35.5(17)	25.9(16)	35.8(18)	0.2(14)	21.6(14)	-1.0(12)
C98A	29.8(16)	27.5(16)	29.8(16)	-3.3(13)	20.0(13)	0.8(12)
C99	33.7(17)	25.6(16)	30.9(17)	-5.1(13)	18.4(14)	-1.8(12)
C99A	28.6(16)	33.1(16)	21.1(15)	-0.2(13)	12.3(12)	-1.1(12)
C100	38.3(18)	34.4(17)	27.7(17)	-3.9(14)	15.5(14)	-4.9(13)
C101	30.4(17)	48(2)	27.2(17)	0.2(15)	13.2(14)	-9.4(14)
C102	28.7(17)	46.1(19)	28.1(17)	2.0(15)	16.3(13)	1.5(13)
C103	26.0(16)	31.7(16)	28.6(16)	2.4(13)	13.1(13)	1.6(12)
C104	25.5(15)	32.2(16)	20.9(15)	-2.7(13)	11.8(12)	-1.3(12)
C105	25.2(15)	25.5(15)	25.4(15)	0.0(13)	13.3(12)	1.7(11)
C106	37.1(18)	33.1(18)	38.7(19)	4.1(15)	19.1(15)	7.0(14)
C107	33.6(18)	30.8(18)	46(2)	6.8(16)	18.5(15)	2.3(13)
C108	27.0(15)	22.0(14)	26.2(15)	0.3(12)	13.2(12)	-0.7(11)
C109	31.8(17)	25.8(16)	32.2(17)	-6.1(13)	13.6(13)	-4.1(12)
C110	28.1(16)	33.7(17)	36.7(18)	-3.0(14)	16.8(14)	-6.2(12)
C111	25.5(16)	34.2(17)	32.7(17)	-1.2(14)	14.2(13)	2.2(12)
C112	31.8(17)	26.3(16)	37.4(18)	-3.1(14)	16.7(14)	0.7(12)
C113	28.2(16)	24.9(15)	32.6(17)	-4.4(13)	12.7(13)	-2.7(11)

Table 4 Bond Lengths for **16**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C14	1.152(4)	N31	C74	1.141(4)
N2	C15	1.149(3)	N32	C75	1.153(4)
N4	C3	1.468(3)	N64	C63	1.460(3)
N4	C4A	1.438(3)	N64	C64A	1.437(3)
N4	C13B	1.481(3)	N64	C73B	1.470(3)
C1	C2	1.557(3)	C61	C62	1.562(4)
C1	C13B	1.547(4)	C61	C73B	1.551(4)
C1	C14	1.457(4)	C61	C74	1.468(4)
C2	C3	1.551(4)	C62	C63	1.547(4)
C2	C15	1.463(4)	C62	C75	1.454(4)
C3	C16	1.514(4)	C63	C76	1.519(4)
C4A	C5	1.390(4)	C64A	C65	1.374(4)
C4A	C8A	1.397(4)	C64A	C68A	1.410(4)
C5	C6	1.393(4)	C65	C66	1.393(4)
C6	C7	1.377(5)	C66	C67	1.374(4)
C7	C8	1.372(5)	C67	C68	1.381(4)
C8	C8A	1.385(4)	C68	C68A	1.392(4)
C8A	C9	1.493(4)	C68A	C69	1.500(4)
C9	C9A	1.517(4)	C69	C69A	1.517(4)
C9A	C10	1.396(4)	C69A	C70	1.395(4)
C9A	C13A	1.409(4)	C69A	C73A	1.396(4)
C10	C11	1.377(4)	C70	C71	1.371(4)
C11	C12	1.384(4)	C71	C72	1.381(4)
C12	C13	1.378(4)	C72	C73	1.391(4)
C13	C13A	1.403(4)	C73	C73A	1.398(4)
C13A	C13B	1.518(4)	C73A	C73B	1.529(4)
C16	C17	1.379(4)	C76	C77	1.378(4)
C16	C21	1.394(4)	C76	C81	1.384(4)
C17	C18	1.408(4)	C77	C78	1.390(4)
C18	C19	1.387(5)	C78	C79	1.381(5)
C19	C20	1.373(4)	C79	C80	1.378(4)
C20	C21	1.372(4)	C80	C81	1.394(4)
N21	C44	1.140(4)	N41	C106	1.149(4)

N22	C45	1.139(4)	N42	C107	1.141(4)
N34	C33	1.467(3)	N94	C93	1.471(3)
N34	C34A	1.427(3)	N94	C94A	1.435(3)
N34	C43B	1.471(3)	N94	C105	1.467(3)
C31	C32	1.563(4)	C91	C92	1.556(3)
C31	C43B	1.553(4)	C91	C105	1.547(4)
C31	C44	1.470(4)	C91	C106	1.457(4)
C32	C33	1.554(4)	C92	C93	1.551(4)
C32	C45	1.466(4)	C92	C107	1.469(4)
C33	C46	1.505(4)	C93	C108	1.500(3)
C34A	C35	1.385(4)	C94A	C95	1.387(4)
C34A	C38A	1.411(4)	C94A	C98A	1.407(4)
C35	C36	1.390(4)	C95	C96	1.401(4)
C36	C37	1.386(4)	C96	C97	1.375(4)
C37	C38	1.383(4)	C97	C98	1.383(4)
C38	C38A	1.386(4)	C98	C98A	1.382(4)
C38A	C39	1.510(4)	C98A	C99	1.501(4)
C39	C39A	1.506(4)	C99	C99A	1.520(4)
C39A	C40	1.399(4)	C99A	C100	1.393(4)
C39A	C43A	1.405(4)	C99A	C104	1.399(4)
C40	C41	1.377(4)	C100	C101	1.386(4)
C41	C42	1.383(4)	C101	C102	1.379(4)
C42	C43	1.387(4)	C102	C103	1.385(4)
C43	C43A	1.397(4)	C103	C104	1.401(4)
C43A	C43B	1.520(4)	C104	C105	1.528(4)
C46	C47	1.389(4)	C108	C109	1.397(4)
C46	C51	1.386(4)	C108	C113	1.395(4)
C47	C48	1.396(4)	C109	C110	1.385(4)
C48	C49	1.374(5)	C110	C111	1.380(4)
C49	C50	1.386(5)	C111	C112	1.383(4)
C50	C51	1.390(4)	C112	C113	1.386(4)

Table 5 Bond Angles for **16**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
N1	C14	C1	178.1(3)	N31	C74	C61	179.4(4)
N2	C15	C2	179.0(3)	N32	C75	C62	179.0(4)
N4	C3	C2	101.3(2)	N64	C63	C62	101.5(2)
N4	C3	C16	113.1(2)	N64	C63	C76	113.1(2)
N4	C13B	C1	100.44(19)	N64	C73B	C61	102.0(2)
N4	C13B	C13A	116.9(2)	N64	C73B	C73A	116.0(2)
C3	N4	C13B	105.7(2)	C63	N64	C73B	108.0(2)
C3	C2	C1	105.1(2)	C63	C62	C61	105.3(2)
C4A	N4	C3	118.2(2)	C64A	N64	C63	116.1(2)
C4A	N4	C13B	113.7(2)	C64A	N64	C73B	114.2(2)
C4A	C5	C6	119.4(3)	C64A	C65	C66	119.7(3)
C4A	C8A	C9	118.1(3)	C64A	C68A	C69	118.6(3)
C5	C4A	N4	123.3(3)	C65	C64A	N64	124.3(2)
C5	C4A	C8A	120.4(3)	C65	C64A	C68A	120.7(3)
C7	C6	C5	120.5(3)	C66	C67	C68	120.3(3)
C7	C8	C8A	121.7(3)	C67	C66	C65	120.2(3)
C8	C7	C6	119.6(3)	C67	C68	C68A	120.7(3)
C8	C8A	C4A	118.4(3)	C68	C68A	C64A	118.3(3)
C8	C8A	C9	123.5(3)	C68	C68A	C69	123.1(3)

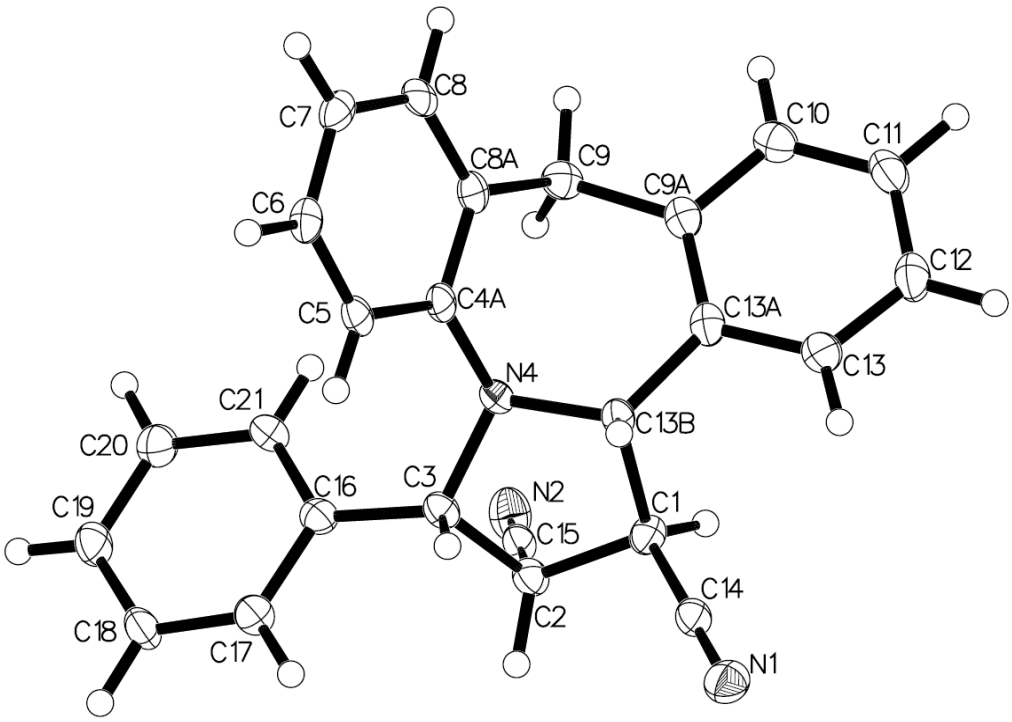
C8A	C4A	N4	116.3(3)	C68A	C64A	N64	115.0(2)
C8A	C9	C9A	111.1(2)	C68A	C69	C69A	113.6(2)
C9A	C13A	C13B	126.0(2)	C69A	C73A	C73	118.8(3)
C10	C9A	C9	119.4(3)	C69A	C73A	C73B	125.6(2)
C10	C9A	C13A	118.5(3)	C70	C69A	C69	118.2(3)
C10	C11	C12	119.9(3)	C70	C69A	C73A	118.6(3)
C11	C10	C9A	121.8(3)	C70	C71	C72	119.4(3)
C12	C13	C13A	121.7(3)	C71	C70	C69A	122.3(3)
C13	C12	C11	119.4(3)	C71	C72	C73	119.4(3)
C13	C13A	C9A	118.6(3)	C72	C73	C73A	121.4(3)
C13	C13A	C13B	115.4(2)	C73	C73A	C73B	115.6(3)
C13A	C9A	C9	121.7(3)	C73A	C69A	C69	123.2(2)
C13A	C13B	C1	112.5(2)	C73A	C73B	C61	111.1(2)
C13B	C1	C2	104.5(2)	C73B	C61	C62	104.9(2)
C14	C1	C2	113.1(2)	C74	C61	C62	113.5(2)
C14	C1	C13B	114.1(2)	C74	C61	C73B	113.0(2)
C15	C2	C1	114.4(2)	C75	C62	C61	114.8(2)
C15	C2	C3	112.1(2)	C75	C62	C63	111.1(2)
C16	C3	C2	112.8(2)	C76	C63	C62	111.4(2)
C16	C17	C18	120.1(3)	C76	C77	C78	120.7(3)
C17	C16	C3	120.5(3)	C76	C81	C80	120.4(3)
C17	C16	C21	119.3(3)	C77	C76	C63	120.8(3)
C19	C18	C17	119.3(3)	C77	C76	C81	119.3(3)
C20	C19	C18	120.2(3)	C79	C78	C77	119.7(3)
C20	C21	C16	120.6(3)	C79	C80	C81	119.8(3)
C21	C16	C3	120.1(2)	C80	C79	C78	120.2(3)
C21	C20	C19	120.5(3)	C81	C76	C63	119.8(2)
N21	C44	C31	178.5(4)	N41	C106	C91	178.4(4)
N22	C45	C32	179.5(4)	N42	C107	C92	178.8(4)
N34	C33	C32	100.6(2)	N94	C93	C92	100.5(2)
N34	C33	C46	114.4(2)	N94	C93	C108	113.9(2)
N34	C43B	C31	100.2(2)	N94	C105	C91	102.17(19)
N34	C43B	C43A	118.3(2)	N94	C105	C104	115.9(2)
C33	N34	C43B	104.9(2)	C93	C92	C91	105.5(2)
C33	C32	C31	104.6(2)	C94A	N94	C93	117.6(2)
C34A	N34	C33	117.4(2)	C94A	N94	C105	114.04(19)
C34A	N34	C43B	115.5(2)	C94A	C95	C96	119.5(3)
C34A	C35	C36	120.0(3)	C94A	C98A	C99	117.9(2)
C34A	C38A	C39	117.7(2)	C95	C94A	N94	124.1(2)
C35	C34A	N34	123.6(2)	C95	C94A	C98A	120.2(3)
C35	C34A	C38A	120.2(3)	C96	C97	C98	120.1(3)
C37	C36	C35	120.0(3)	C97	C96	C95	120.3(3)
C37	C38	C38A	121.0(3)	C98	C98A	C94A	119.0(3)
C38	C37	C36	120.0(3)	C98	C98A	C99	123.0(2)
C38	C38A	C34A	118.7(3)	C98A	C94A	N94	115.6(2)
C38	C38A	C39	123.6(3)	C98A	C98	C97	121.0(3)
C38A	C34A	N34	116.1(3)	C98A	C99	C99A	111.1(2)
C39A	C39	C38A	110.7(2)	C99A	C104	C103	118.9(2)
C39A	C43A	C43B	125.0(2)	C99A	C104	C105	125.7(2)
C40	C39A	C39	119.7(2)	C100	C99A	C99	118.3(2)
C40	C39A	C43A	118.0(2)	C100	C99A	C104	118.5(2)
C40	C41	C42	120.1(3)	C101	C100	C99A	122.0(3)
C41	C40	C39A	122.1(3)	C101	C102	C103	119.3(3)
C41	C42	C43	118.9(3)	C102	C101	C100	119.6(3)
C42	C43	C43A	121.8(3)	C102	C103	C104	121.7(3)

C43	C43A	C39A	119.2(2)	C103	C104	C105	115.4(2)
C43	C43A	C43B	115.8(2)	C104	C99A	C99	123.1(2)
C43A	C39A	C39	121.9(2)	C104	C105	C91	112.5(2)
C43A	C43B	C31	113.1(2)	C105	N94	C93	107.18(19)
C43B	C31	C32	103.9(2)	C105	C91	C92	104.7(2)
C44	C31	C32	113.7(2)	C106	C91	C92	113.4(2)
C44	C31	C43B	113.5(2)	C106	C91	C105	112.8(2)
C45	C32	C31	114.1(2)	C107	C92	C91	115.0(2)
C45	C32	C33	112.3(2)	C107	C92	C93	112.0(2)
C46	C33	C32	113.4(2)	C108	C93	C92	111.3(2)
C46	C47	C48	120.5(3)	C109	C108	C93	119.9(2)
C46	C51	C50	120.9(3)	C110	C109	C108	120.3(3)
C47	C46	C33	121.5(3)	C110	C111	C112	119.7(2)
C48	C49	C50	120.0(3)	C111	C110	C109	120.5(3)
C49	C48	C47	120.1(3)	C111	C112	C113	120.4(3)
C49	C50	C51	119.8(3)	C112	C113	C108	120.3(3)
C51	C46	C33	119.8(3)	C113	C108	C93	121.2(2)
C51	C46	C47	118.7(3)	C113	C108	C109	118.8(2)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **16**.

Atom	x	y	z	U(eq)
H1	7161	4494	7165	32
H2	6554	4542	7037	32
H3	6239	4610	5083	35
H5	6152	5142	4011	42
H6	6109	5721	2948	56
H7	6594	6282	3305	59
H8	7118	6272	4720	57
H9A	7184	5654	6641	47
H9B	7433	5984	6292	47
H10F	8056	5692	6567	46
H11D	8485	5117	6559	46
H12	8254	4367	6129	43
H13	7602	4195	5788	36
H13A	6919	4487	5215	32
H17	5610	4950	4612	45
H18	5145	5417	4872	56
H19	5326	5801	6274	54
H20	5962	5744	7375	48
H21	6423	5305	7104	38
H31	5491	3065	2903	37
H32	6113	2960	3161	35
H33	6341	2918	5106	34
H35	6395	2329	6081	35
H36	6391	1715	7032	40
H37	5860	1207	6567	42
H38	5348	1290	5134	39
H39B	5369	1950	3320	37
H39A	5083	1631	3580	37
H40	4481	1968	3349	38
H41	4087	2570	3419	39
H42	4355	3305	3860	40
H43	5021	3421	4235	36
H43A	5679	3074	4834	31
H47	6270	2172	3214	42
H48	6777	1702	3192	56
H49	7371	1668	4463	60
H50	7465	2111	5760	54

H51	6966	2596	5767	43
H1SB	5210	4881	2972	25
H1SA	4933	4929	1807	25
H61	5418	2092	7879	33
H62	5987	1941	7829	34
H63	6411	1958	9779	32
H65	6680	2432	10899	41
H66	6943	2989	12050	52
H67	6659	3714	11873	54
H68	6139	3910	10511	46
H69A	5818	3306	8474	41
H69B	5699	3727	8937	41
H70	5036	3731	8538	49
H71	4444	3407	8362	52
H72	4412	2621	8646	48
H73	4974	2166	9055	41
H73A	5736	2174	9826	32
H77	7038	1813	9683	55
H78	7533	2024	9212	71
H79	7425	2619	8154	59
H80	6827	3006	7579	48
H81	6333	2795	8059	42
H91	6952	-517	7142	31
H92	6362	-604	7111	31
H93	5980	-567	5149	29
H95	5785	-43	4018	35
H96	5604	557	2932	38
H97	5910	1270	3311	39
H98	6412	1387	4747	36
H99A	6656	694	6666	34
H99B	6809	1128	6303	34
H10	7462	1078	6571	39
H10A	8019	706	6596	42
H10B	7997	-81	6275	39
H10C	7411	-483	5900	34
H10D	6668	-416	5205	29
H10E	5368	-761	5335	36
H11	4865	-536	5762	38
H11A	4924	133	6615	36
H11B	5492	578	7052	37
H11C	6006	347	6667	34



X-Ray crystal structures of **18.**

Table 1: Crystal data and structure refinement for **18.**

Identification code	dax18
Empirical formula	$C_{25}H_{19}N_3$
Formula weight	361.43
Temperature / K	119.88
Crystal system	Monoclinic
Space group	$P2_1$
a / Å, b / Å, c / Å	12.6196(2), 5.85170(10), 12.6336(2)
α/°, β/°, γ/°	90.00, 99.2900(10), 90.00
Volume / Å^3	920.71(3)
Z	2
ρ_{calc} / mg mm^{-3}	1.304
μ / mm^{-1}	0.604
F(000)	380
Crystal size / mm^3	0.18 × 0.02 × 0.01
Theta range for data collection	3.54 to 55.92°
Index ranges	-13 ≤ h ≤ 13, -6 ≤ k ≤ 6, -13 ≤ l ≤ 11

Reflections collected	3871
Independent reflections	2041[R(int) = 0.0249]
Data/restraints/parameters	2041/1/329
Goodness-of-fit on F^2	1.066
Final R indexes [I>2σ (I)]	R_1 = 0.0331, wR_2 = 0.0805
Final R indexes [all data]	R_1 = 0.0355, wR_2 = 0.0822
Largest diff. peak/hole / e $Å^{-3}$	0.120/-0.150

Table 2 Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$×10^3) for **18**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
N1	1038.7(16)	784(4)	4953.4(17)	29.3(5)
N2	279.1(18)	9060(4)	7233.9(17)	31.3(6)
N4	2749.5(14)	5760(3)	7344.4(15)	18.9(5)
C1	1413.1(18)	4788(4)	5853(2)	20.6(6)
C2	950.7(18)	4906(4)	6916.8(19)	20.0(6)
C3	1943.9(18)	4366(4)	7761.5(19)	18.6(5)
C4A	3828.3(18)	5835(4)	7910.1(18)	18.7(6)
C5	4275.0(18)	4187(4)	8639.8(18)	19.9(6)
C6	5315.9(18)	4422(5)	9169.0(19)	22.5(6)
C7	5917.5(19)	6307(4)	8984.3(19)	22.6(6)
C8	5470.7(19)	7967(4)	8268(2)	20.8(6)
C8A	4429.5(19)	7759(4)	7719.2(18)	19.3(6)
C9	3920.3(19)	9531(4)	6941(2)	21.7(6)
C9A	3688.2(18)	8762(4)	5786.8(19)	20.0(6)
C10	4048.6(19)	10124(5)	5004(2)	24.3(6)
C11	3836(2)	9554(5)	3928(2)	27.9(6)
C12	3284(2)	7584(5)	3609(2)	27.1(6)
C13	2939.3(19)	6190(5)	4375(2)	24.2(6)
C13A	3121.3(18)	6776(4)	5459(2)	20.1(6)
C13B	2654.7(17)	5139(4)	6198.2(18)	18.0(5)
C14	1192.5(18)	2566(5)	5336(2)	22.1(6)
C15	559.4(18)	7236(5)	7091.5(19)	22.2(6)
C16	1786.0(17)	4818(4)	8902.9(19)	19.4(6)
C17	1253.3(18)	3140(4)	9407(2)	23.6(6)
C18	1041.8(19)	3483(4)	10438(2)	25.0(6)
C19	1366.7(18)	5462(4)	10980(2)	25.9(6)
C20	1892.3(18)	7145(5)	10485(2)	26.5(6)
C21	2092.5(19)	6814(4)	9448(2)	22.9(6)

Table 3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **18**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	22.3(11)	37.2(15)	28.7(13)	-4.3(12)	4.5(10)	-0.9(10)
N2	38.8(13)	31.6(14)	24.9(12)	-0.9(11)	9.6(10)	5.3(11)
N4	17.1(9)	23.3(11)	17.2(11)	1.1(8)	5.8(9)	-2.6(8)
C1	19.7(12)	23.5(14)	17.9(14)	-0.8(12)	0.5(11)	0.8(10)
C2	20.1(12)	22.1(14)	19.1(14)	-0.1(11)	6.4(12)	-0.3(11)
C3	19.0(11)	19.3(14)	18.7(13)	0.1(10)	6.9(10)	0.6(10)
C4A	20.0(12)	24.2(14)	13.0(12)	-2.1(10)	6.1(11)	0.3(11)
C5	23.3(13)	23.1(15)	15.1(13)	-0.5(11)	8.7(11)	0.4(11)
C6	25.4(13)	27.5(15)	14.9(13)	-1.4(11)	3.9(11)	2.9(11)
C7	18.8(13)	31.8(15)	17.3(14)	-7.2(11)	3.4(12)	1.4(11)
C8	22.3(13)	23.9(15)	19.0(14)	-4.3(11)	12.1(11)	-2.5(11)
C8A	23.5(12)	22.0(13)	14.2(13)	-3.1(10)	8.3(11)	2.6(10)
C9	20.8(12)	21.2(15)	24.5(15)	-2.8(11)	7.5(12)	-0.4(12)
C9A	18.6(11)	22.1(14)	19.4(14)	3.9(11)	3.5(11)	5.7(11)
C10	22.6(12)	22.2(15)	28.2(15)	4.0(12)	4.0(12)	1.1(12)
C11	24.8(12)	37.2(17)	23.5(15)	7.8(13)	9.3(12)	1.0(12)
C12	26.5(13)	37.8(17)	17.8(14)	0.7(13)	5.9(12)	3.9(13)
C13	23.8(13)	26.8(16)	22.8(15)	-1.2(12)	6.3(12)	-1.4(12)
C13A	18.7(12)	24.6(15)	17.2(13)	2.3(10)	3.4(10)	6.1(11)
C13B	20.6(11)	18.9(14)	15.2(13)	-0.1(10)	4.8(10)	0.5(10)
C14	17.3(12)	31.5(16)	18.2(13)	-0.5(13)	5.3(10)	-1.1(11)
C15	19.4(12)	31.7(17)	16.1(13)	2.2(11)	5.0(11)	-3.4(12)
C16	15.9(11)	21.3(14)	20.7(14)	2.9(10)	2.2(10)	0.7(10)
C17	23.8(13)	24.7(16)	22.7(15)	1.7(11)	4.4(12)	-1.2(11)
C18	25.5(13)	30.9(16)	20.2(15)	5.1(11)	8.5(12)	-2.0(12)
C19	22.7(12)	36.8(17)	19.8(15)	-1.8(12)	8.3(12)	1.1(12)
C20	25.9(14)	30.8(16)	23.4(15)	-3.3(12)	5.4(12)	-1.8(12)
C21	21.5(13)	26.5(16)	21.9(14)	2.2(11)	7.2(12)	-3.9(11)

Table 4 Bond Lengths for **18**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C14	1.153(3)	C8	C8A	1.389(3)
N2	C15	1.148(3)	C8A	C9	1.501(3)
N4	C3	1.466(3)	C9	C9A	1.509(3)
N4	C4A	1.432(3)	C9A	C10	1.401(3)
N4	C13B	1.479(3)	C9A	C13A	1.392(3)
C1	C2	1.551(3)	C10	C11	1.385(4)
C1	C13B	1.571(3)	C11	C12	1.372(4)
C1	C14	1.461(4)	C12	C13	1.389(4)
C2	C3	1.542(3)	C13	C13A	1.394(4)
C2	C15	1.479(4)	C13A	C13B	1.522(3)
C3	C16	1.510(3)	C16	C17	1.400(3)
C4A	C5	1.389(3)	C16	C21	1.379(3)
C4A	C8A	1.400(4)	C17	C18	1.386(4)
C5	C6	1.381(3)	C18	C19	1.374(4)
C6	C7	1.380(4)	C19	C20	1.391(4)
C7	C8	1.384(4)	C20	C21	1.388(4)

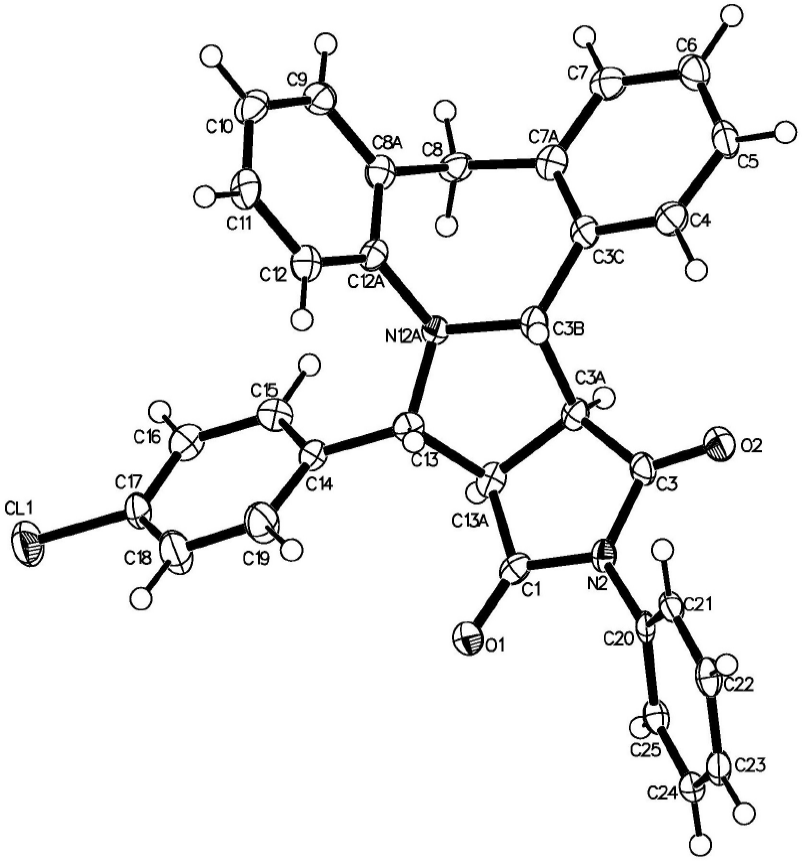
Table 5 Bond Angles for **18**.

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
N1	C14	C1	178.0(3)	C9A	C13A	C13B	125.0(2)
N2	C15	C2	178.5(3)	C10	C9A	C9	118.5(2)
N4	C3	C2	99.82(18)	C11	C10	C9A	121.5(3)
N4	C3	C16	116.87(19)	C11	C12	C13	119.4(2)
N4	C13B	C1	102.92(17)	C12	C11	C10	120.0(3)
N4	C13B	C13A	117.91(19)	C12	C13	C13A	121.3(3)
C2	C1	C13B	104.55(17)	C13	C13A	C13B	115.4(2)
C3	N4	C13B	105.31(17)	C13A	C9A	C9	123.2(2)
C3	C2	C1	102.32(18)	C13A	C9A	C10	118.3(2)
C4A	N4	C3	119.74(18)	C13A	C13B	C1	112.28(19)
C4A	N4	C13B	114.59(18)	C14	C1	C2	110.8(2)
C4A	C8A	C9	118.8(2)	C14	C1	C13B	110.5(2)
C5	C4A	N4	124.1(2)	C15	C2	C1	110.61(19)
C5	C4A	C8A	120.0(2)	C15	C2	C3	109.83(19)
C6	C5	C4A	120.3(2)	C16	C3	C2	114.03(18)
C6	C7	C8	119.6(2)	C16	C21	C20	120.7(2)
C7	C6	C5	120.2(2)	C17	C16	C3	117.3(2)
C7	C8	C8A	121.2(2)	C18	C17	C16	120.3(2)
C8	C8A	C4A	118.7(2)	C18	C19	C20	119.9(2)
C8	C8A	C9	122.5(2)	C19	C18	C17	120.2(2)
C8A	C4A	N4	115.88(19)	C21	C16	C3	123.7(2)
C8A	C9	C9A	115.0(2)	C21	C16	C17	118.9(2)
C9A	C13A	C13	119.5(2)	C21	C20	C19	119.9(3)

Table 6 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **18**.

Atom	x	y	z	U(eq)
H1	1118(17)	5970.0(4)	5354(18)	14(6)

H2	320.0(2)	3840.0(5)	6980.0(2)	36(7)
H3	2089(18)	2720.0(5)	7651(17)	17(6)
H5	3862(18)	2920.0(4)	8769(18)	14(6)
H6	5605(16)	3250.0(4)	9674(19)	9(6)
H7	6632(18)	6480.0(4)	9393(17)	17(6)
H8	5880(18)	9350.0(4)	8147(17)	12(5)
H9A	3257(18)	10020.0(4)	7178(18)	10(5)
H9B	4364(18)	10960.0(5)	6974(17)	18(6)
H10	4460(19)	11400.0(5)	5209(19)	23(7)
H11	4090.0(2)	10590.0(5)	3370.0(2)	37(7)
H12	3109(19)	7110.0(4)	2830.0(2)	27(7)
H13	2600.0(2)	4810.0(5)	4143(19)	23(7)
H13A	2987(16)	3610.0(4)	6145(17)	10(6)
H17	1034(19)	1730.0(5)	9007(19)	26(7)
H18	620.0(2)	2270.0(5)	10760.0(2)	37(7)
H19	1240.0(2)	5710.0(5)	11680.0(2)	30(7)
H20	2110.0(2)	8600.0(5)	10850.0(2)	28(7)
H21	2431(18)	7970.0(4)	9133(18)	15(6)



X-Ray crystal structures of **20**.

Table 1 Crystal data and structure refinement for **20**.

Identification code	dax12
Empirical formula	$C_{31}H_{23}N_2ClO_2$

Formula weight	490.96
Temperature/K	100.0
Crystal system	Monoclinic
Space group	$P2_1/n$
a/Å, b/Å, c/Å	10.6905(2), 7.6706(1), 29.1159(4)
α/°, β/°, γ/°	90.00, 90.142(1), 90.00
Volume/Å^3	2387.57(6)
Z	4
ρ_{calc}mg/mm^3	1.366
m/mm^{-1}	1.675
F(000)	1024
Crystal size/mm^3	0.05 × 0.03 × 0.04
Theta range for data collection	3.04 to 52.50°
Index ranges	-11 ≤ h ≤ 11, -7 ≤ k ≤ 7, -29 ≤ l ≤ 27
Reflections collected	8647
Independent reflections	2697[R(int) = 0.0909]
Data/restraints/parameters	2697/0/417
Goodness-of-fit on F^2	1.042
Final R indexes [I>2σ (I)]	R_1 = 0.0426, wR_2 = 0.1130
Final R indexes [all data]	R_1 = 0.0525, wR_2 = 0.1178
Largest diff. peak/hole / e Å^{-3}	0.383/-0.451

Table 2 Atomic Coordinates (Å×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **20**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
Cl1	4891.2(7)	13708.1(11)	4572.5(3)	38.9(3)
O1	4972.1(19)	6737(3)	3140.5(7)	24.3(5)
O2	8090.9(18)	2875(3)	2817.2(7)	30.4(6)
N2	6346(2)	4545(3)	2937.6(7)	17.2(6)
N12A	8508(2)	6894(3)	3928.3(8)	18.4(6)
C1	6026(3)	6188(4)	3119.8(9)	18.7(7)
C3	7618(3)	4207(4)	2960.9(9)	19.7(7)
C3A	8257(3)	5738(4)	3191.2(10)	17.8(7)
C3B	8879(3)	5337(4)	3664.7(9)	18.8(7)
C3C	10259(3)	4897(4)	3651(9)	18.9(7)
C4	10564(3)	3244(4)	3482(10)	23.5(8)
C5	11796(3)	2708(5)	3441.3(10)	24.9(8)
C6	12743(3)	3817(4)	3572.3(10)	27.8(8)
C7	12461(3)	5443(5)	3746.4(10)	25.2(8)
C7A	11226(3)	6018(4)	3792.6(9)	20(7)
C8	10976(3)	7751(4)	4017.3(11)	21.9(8)
C8A	10197(3)	7535(4)	4445.4(10)	20.7(7)
C9	10673(3)	7784(4)	4883.8(10)	23.6(8)
C10	9910(3)	7549(4)	5264.5(11)	27.1(8)
C11	8682(3)	7063(4)	5207.3(11)	24.9(8)
C12	8191(3)	6793(4)	4773.7(10)	21.8(8)
C12A	8950(3)	7029(4)	4392.4(10)	18.9(7)
C13	7187(3)	7132(4)	3832.6(10)	19(7)
C13A	7201(3)	7011(4)	3300.6(10)	18.8(7)
C14	6630(3)	8799(4)	4017.6(9)	20.7(8)
C15	7337(3)	10296(4)	4064(10)	22.5(7)
C16	6789(3)	11797(5)	4240(11)	24.5(8)
C17	5550(3)	11806(4)	4354.9(10)	26.4(8)
C18	4833(3)	10331(5)	4304.1(13)	40.6(10)
C19	5385(3)	8835(5)	4145.4(12)	33.8(9)
C20	5420(3)	3399(4)	2749.7(9)	16.8(7)
C21	5290(3)	1727(4)	2921.6(11)	18.2(7)
C22	4367(3)	661(4)	2747.4(10)	20.6(8)
C23	3568(3)	1271(4)	2408.9(11)	22.2(8)
C24	3701(3)	2940(4)	2242.9(11)	20.3(8)
C25	4633(3)	4004(5)	2410.1(10)	18.2(8)

Table 3 Anisotropic Displacement Parameters ($Å^2×10^3$) for **20**. The Anisotropic displacement factor exponent takes the form: $-2π^2[h^2a^{*2}U_{11}+...+2hka×b×U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl1	37.5(5)	31.8(6)	47.5(6)	-15.6(4)	3.5(4)	6.8(4)
O1	24.3(13)	22.2(12)	26.4(12)	-5(10)	-1.7(9)	4.2(10)
O2	21.6(12)	35.7(15)	33.9(13)	-13.6(12)	-1(10)	3.6(11)
N2	20.3(14)	13.8(14)	17.6(13)	-3.1(11)	2.7(10)	-1.1(11)
N12A	19.4(14)	19.9(14)	15.8(14)	-1.9(11)	-1.1(10)	3.4(11)
C1	22.2(19)	21.8(19)	12.1(15)	2.7(14)	0.3(13)	-4.3(15)
C3	19.9(17)	24(2)	15.5(16)	-0.5(15)	5(13)	3.4(15)
C3A	19.3(16)	20.9(18)	13.2(16)	0.3(14)	4.3(14)	-3.1(14)
C3B	20.8(16)	17.1(17)	18.5(16)	-1.9(14)	2.4(13)	-1.8(14)
C3C	22.7(16)	21.5(18)	12.5(15)	3.8(14)	4.2(12)	1.9(14)
C4	26.5(19)	26.4(19)	17.6(17)	2.1(15)	0.7(14)	1(16)
C5	30(2)	25(2)	20.5(18)	-1.4(16)	5.6(14)	9.4(17)
C6	27(2)	36(2)	20.1(17)	0.3(16)	4.5(15)	8.5(17)
C7	22.9(19)	34(2)	18.4(17)	3.7(16)	0.5(14)	-3(17)
C7A	25.5(18)	20.5(18)	13.9(15)	5.1(14)	4.1(13)	-2.5(14)
C8	17.3(18)	27(2)	21.1(18)	-1.7(16)	-1.4(14)	-5(16)
C8A	25.2(18)	16.3(16)	20.6(18)	0.1(14)	1(14)	0.1(14)
C9	24.3(19)	22(19)	25(2)	-0.6(15)	-2.7(15)	2.7(15)
C10	37(2)	25.7(19)	18.3(19)	0.5(15)	-6.3(17)	3.6(16)
C11	36(2)	25(2)	14(19)	4.9(15)	7.3(16)	3.4(15)
C12	27(2)	15.7(17)	22(2)	1(14)	2.5(16)	0(15)
C12A	26.3(18)	15.1(17)	15.3(17)	0.1(13)	-2.2(14)	0.8(14)
C13	19.2(17)	18.3(18)	19.6(17)	0.7(14)	-0.4(13)	-1.3(14)
C13A	27.2(18)	14(18)	15.1(16)	2.1(14)	1.5(13)	-3(14)
C14	21.8(18)	25(2)	15(16)	-2.7(14)	-0.8(13)	2.1(15)
C15	22.3(18)	21.4(19)	24(18)	3.7(15)	-0.2(14)	-0.7(16)
C16	30(2)	19.2(19)	24.2(18)	1.4(15)	-1.5(15)	-4.3(17)
C17	31(2)	22.7(19)	25.4(18)	-7.8(15)	-0.6(14)	9.7(16)
C18	24(2)	37(2)	60(3)	-24(2)	8.3(17)	-2.2(18)
C19	26(2)	27(2)	48(2)	-13.6(18)	3.2(16)	-3.4(17)
C20	19.3(16)	17.2(18)	14(15)	-5.4(14)	3.9(13)	3.8(14)
C21	21.4(17)	17(19)	16.1(17)	0.1(15)	2.7(15)	7.2(15)
C22	26.7(19)	12.5(19)	22.7(18)	-1(15)	7.8(15)	-0.1(15)
C23	19.2(18)	23(2)	24.7(18)	-10.6(16)	6.1(15)	-2.9(16)
C24	20.1(17)	24(2)	17(17)	-4.1(16)	0.1(15)	6.4(15)
C25	24.9(19)	12(2)	17.5(17)	1.9(16)	5.1(14)	3.1(16)

Table 4 Bond Lengths for **20**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C17	1.740(3)	C8	C8A	1.510(4)
O1	C1	1.204(3)	C8A	C9	1.386(4)
O2	C3	1.214(3)	C8A	C12A	1.397(4)
N2	C1	1.410(4)	C9	C10	1.389(5)
N2	C3	1.386(4)	C10	C11	1.375(5)
N2	C20	1.431(4)	C11	C12	1.382(4)
N12A	C3B	1.475(4)	C12	C12A	1.388(4)
N12A	C12A	1.434(4)	C13	C13A	1.552(4)
N12A	C13	1.450(4)	C13	C14	1.511(4)
C1	C13A	1.501(4)	C14	C15	1.381(4)
C3	C3A	1.514(4)	C14	C19	1.383(4)
C3A	C3B	1.560(4)	C15	C16	1.390(4)
C3A	C13A	1.527(4)	C16	C17	1.368(4)
C3B	C3C	1.514(4)	C17	C18	1.375(5)
C3C	C4	1.399(4)	C18	C19	1.371(5)
C3C	C7A	1.405(4)	C20	C21	1.384(4)
C4	C5	1.385(4)	C20	C25	1.377(4)
C5	C6	1.376(5)	C21	C22	1.377(4)
C6	C7	1.380(5)	C22	C23	1.384(4)
C7	C7A	1.399(4)	C23	C24	1.376(5)
C7A	C8	1.506(4)	C24	C25	1.377(4)

Table 5 Bond Angles for **20**.

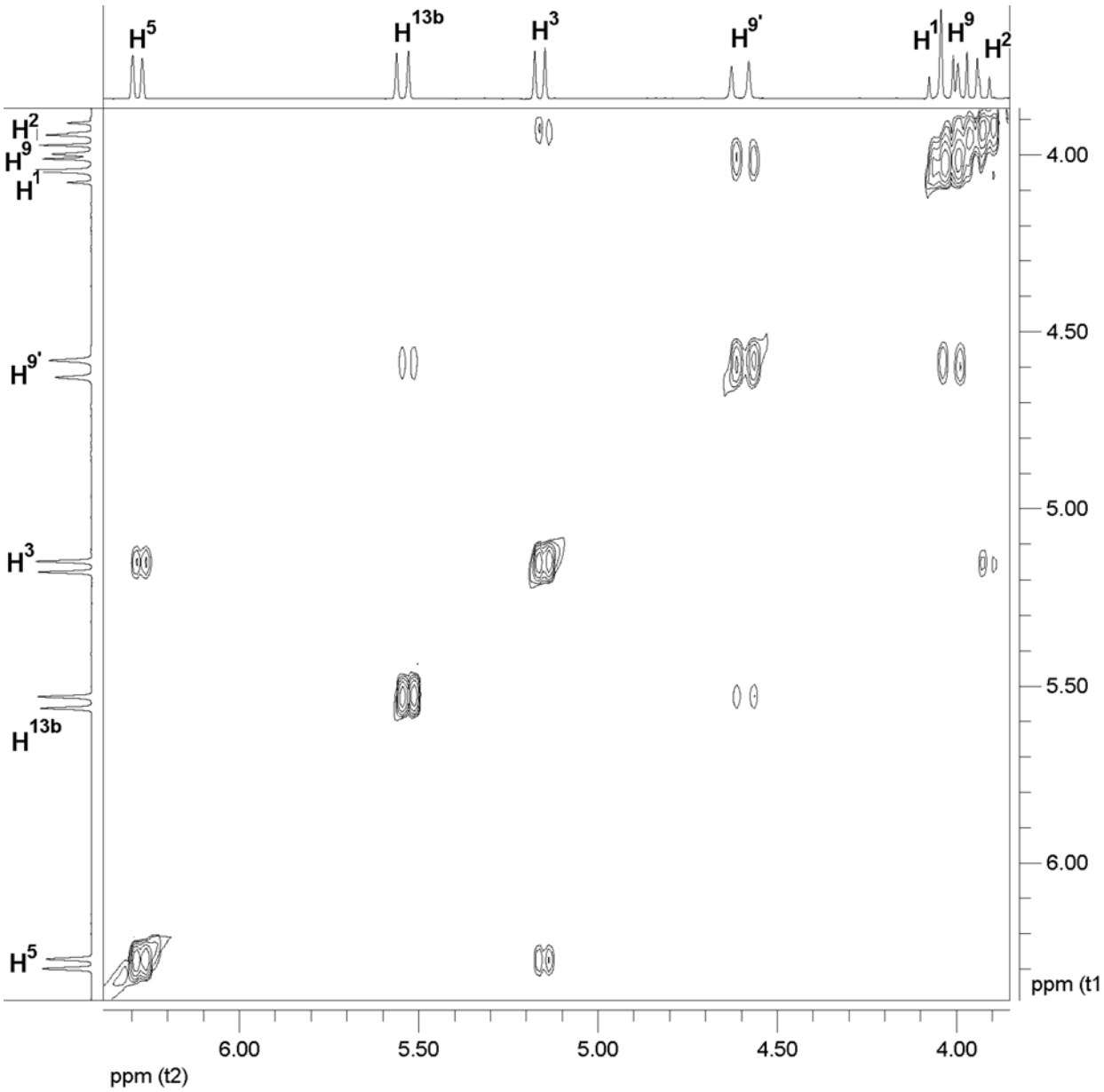
Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
O1	C1	N2	124.0(3)	C9	C8A	C8	122.9(3)
O1	C1	C13A	128.1(3)	C9	C8A	C12A	119.2(3)
O2	C3	N2	123.3(3)	C10	C11	C12	120.8(3)
O2	C3	C3A	128.1(3)	C11	C10	C9	120.0(3)
N2	C1	C13A	107.7(2)	C11	C12	C12A	119.3(3)
N2	C3	C3A	108.5(2)	C12	C12A	N12A	123.5(3)
N12A	C3B	C3A	100.7(2)	C12	C12A	C8A	120.5(3)
N12A	C3B	C3C	117.3(2)	C12A	N12A	C3B	117.4(2)
N12A	C13	C13A	99.9(2)	C12A	N12A	C13	119.4(2)
N12A	C13	C14	115.0(2)	C12A	C8A	C8	117.9(3)
C1	N2	C20	121.6(2)	C13	N12A	C3B	105.4(2)
C1	C13A	C3A	106.0(2)	C13A	C3A	C3B	104.8(2)
C1	C13A	C13	111.4(2)	C14	C13	C13A	114.3(2)
C3	N2	C1	112.8(2)	C14	C15	C16	119.6(3)
C3	N2	C20	125.6(2)	C15	C14	C13	121.5(3)
C3	C3A	C3B	115.4(2)	C15	C14	C19	119.0(3)
C3	C3A	C13A	104.8(2)	C16	C17	Cl1	119.1(3)
C3A	C13A	C13	104.8(2)	C16	C17	C18	120.7(3)
C3C	C3B	C3A	115.7(2)	C17	C16	C15	120.3(3)
C3C	C7A	C8	122.5(3)	C18	C17	Cl1	120.2(2)
C4	C3C	C3B	116.0(3)	C18	C19	C14	121.5(3)
C4	C3C	C7A	119.1(3)	C19	C14	C13	119.5(3)
C5	C4	C3C	121.4(3)	C19	C18	C17	119.0(3)
C5	C6	C7	119.9(3)	C21	C20	N2	120.1(3)
C6	C5	C4	119.5(3)	C21	C22	C23	120.1(3)
C6	C7	C7A	121.8(3)	C22	C21	C20	119.3(3)
C7	C7A	C3C	118.2(3)	C23	C24	C25	120.2(3)
C7	C7A	C8	119.2(3)	C24	C23	C22	120.0(3)
C7A	C3C	C3B	124.9(3)	C24	C25	C20	119.7(3)
C7A	C8	C8A	111.1(2)	C25	C20	N2	119.2(3)
C8A	C9	C10	120.2(3)	C25	C20	C21	120.7(3)
C8A	C12A	N12A	115.9(2)				

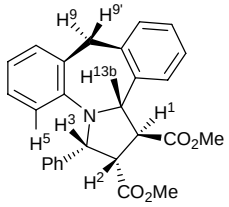
Table 6 Torsion Angles for **20**.

A	B	C	D	Angle/˚
O1	C1	C13A	C3A	178.6(3)
O1	C1	C13A	C13	65.2(4)
O2	C3	C3A	C3B	-64.8(4)
O2	C3	C3A	C13A	-179.5(3)
N2	C1	C13A	C3A	2.3(3)
N2	C1	C13A	C13	-111.2(3)
N2	C3	C3A	C3B	114.8(3)
N2	C3	C3A	C13A	0.1(3)
N2	C20	C21	C22	177.9(2)
N2	C20	C25	C24	-176.9(2)
N12A	C3B	C3C	C4	167.4(2)
N12A	C3B	C3C	C7A	-12.8(4)
N12A	C13	C13A	C1	146.6(2)
N12A	C13	C13A	C3A	32.4(3)
N12A	C13	C14	C15	30.3(4)
N12A	C13	C14	C19	-149.5(3)
C1	N2	C3	O2	-179.0(3)
C1	N2	C3	C3A	1.4(3)
C1	N2	C20	C21	-123.3(3)
C1	N2	C20	C25	54.1(3)
C3	N2	C1	O1	-178.9(3)
C3	N2	C1	C13A	-2.3(3)
C3	N2	C20	C21	57.1(4)
C3	N2	C20	C25	-125.5(3)
C3	C3A	C3B	N12A	-137.8(2)
C3	C3A	C3B	C3C	94.8(3)
C3	C3A	C13A	C1	-1.4(3)
C3	C3A	C13A	C13	116.5(2)
C3A	C3B	C3C	C4	-74.0(3)
C3A	C3B	C3C	C7A	105.9(3)
C3B	N12A	C12A	C8A	77.2(3)
C3B	N12A	C12A	C12	-106.9(3)
C3B	N12A	C13	C13A	-49.5(3)
C3B	N12A	C13	C14	-172.3(2)
C3B	C3A	C13A	C1	-123.4(2)
C3B	C3A	C13A	C13	-5.4(3)
C3C	C7A	C8	C8A	57.3(4)
C7	C7A	C8	C8A	-118.8(3)
C7A	C8	C8A	C9	109.5(3)
C7A	C8	C8A	C12A	-69.3(4)
C12A	N12A	C3B	C3A	-178.2(2)
C12A	N12A	C3B	C3C	-51.7(3)
C12A	N12A	C13	C13A	175.9(2)
C12A	N12A	C13	C14	53.0(3)
C13	N12A	C3B	C3A	46.1(3)
C13	N12A	C3B	C3C	172.6(2)
C13	N12A	C12A	C8A	-153.4(3)
C13	N12A	C12A	C12	22.5(4)
C13A	C3A	C3B	N12A	-23.0(3)
C13A	C3A	C3B	C3C	-150.5(3)
C13A	C13	C14	C15	-84.5(3)
C13A	C13	C14	C19	95.7(3)
C14	C13	C13A	C1	-90.1(3)
C14	C13	C13A	C3A	155.7(2)
C20	N2	C1	O1	1.5(4)
C20	N2	C1	C13A	178.0(2)
C20	N2	C3	O2	0.6(4)
C20	N2	C3	C3A	-179.0(2)

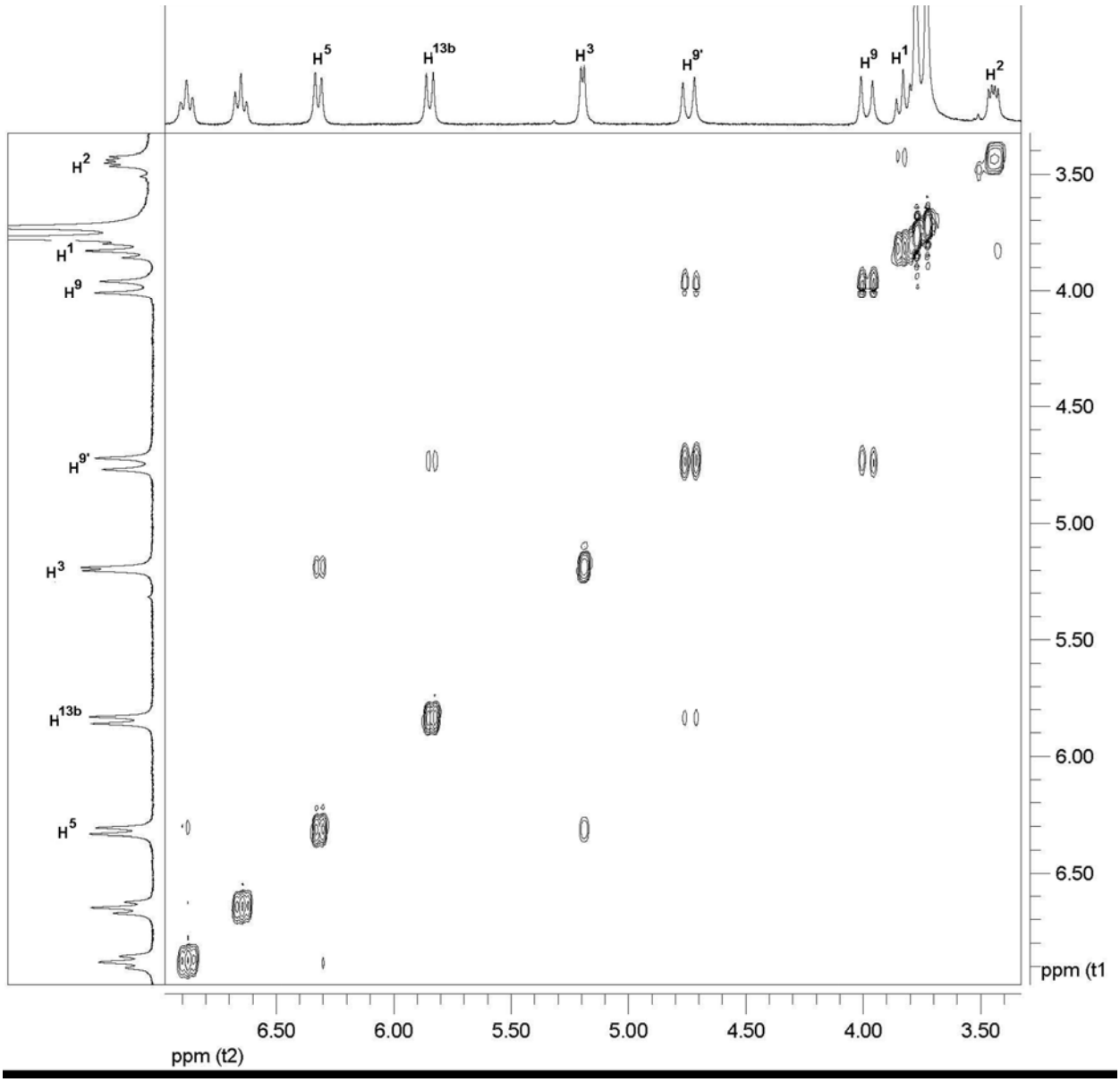
Table 7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **20**.

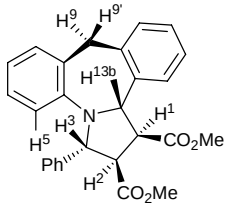
Atom	x	y	z	U(eq)
H3A	8860(3)	6180(4)	3001(10)	15(8)
H3B	8400(2)	4280(4)	3792(9)	16(7)
H4	9870(3)	2470(4)	3366(10)	28(8)
H5	11990(3)	1570(4)	3318(10)	26(8)
H6	13630(3)	3450(4)	3546(10)	34(9)
H7	13110(3)	6220(4)	3844(10)	27(9)
H8A	10460(3)	8520(4)	3823(10)	23(8)
H8B	11760(2)	8280(3)	4107(8)	1(6)
H9	11510(3)	8120(4)	4910(11)	34(9)
H10	10250(3)	7730(4)	5559(13)	43(10)
H11	8180(3)	6870(4)	5442(11)	22(8)
H12	7350(3)	6450(4)	4734(10)	25(9)
H13	6670(2)	6060(4)	3947(9)	18(7)
H13A	7330(2)	8150(4)	3169(9)	13(7)
H15	8230(3)	10290(4)	3985(9)	21(8)
H16	7280(3)	12750(4)	4294(9)	12(7)
H18	3950(4)	10280(5)	4403(13)	62(11)
H19	4900(3)	7720(5)	4110(13)	56(11)
H21	5780(3)	1370(4)	3144(10)	18(9)
H22	4280(3)	-420(4)	2851(10)	20(8)
H23	2980(3)	590(4)	2287(10)	29(9)
H24	3210(3)	3340(4)	2015(10)	11(8)
H25	4710(2)	4970(4)	2317(9)	3(8)



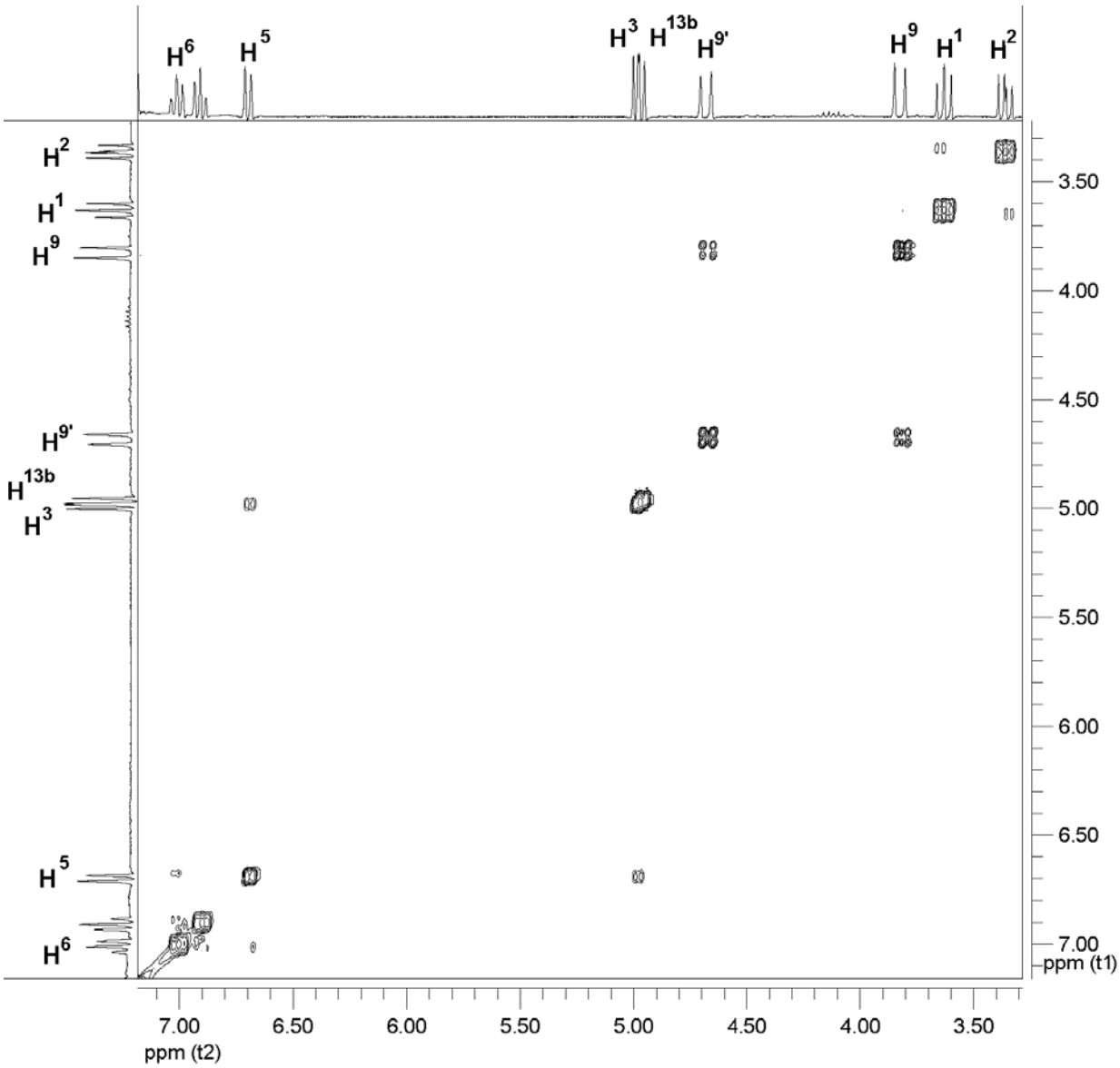


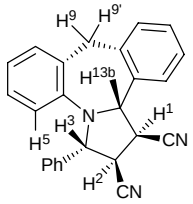
2D ^{1}H NOESY spectrum of compound **13.**



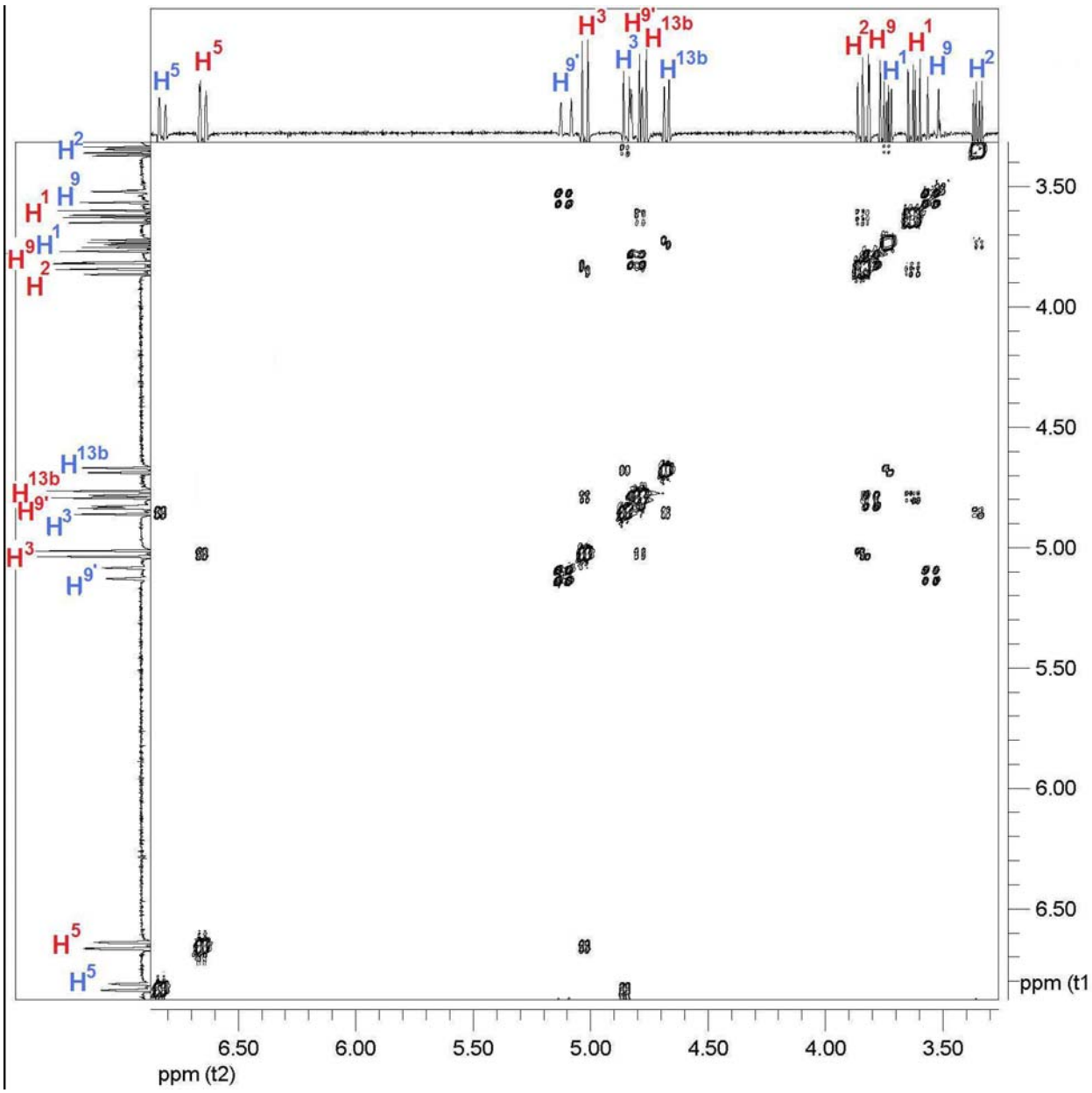


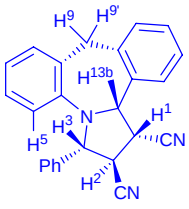
2D ^{1}H NOESY spectrum of compound **15**.

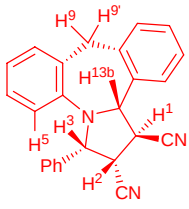




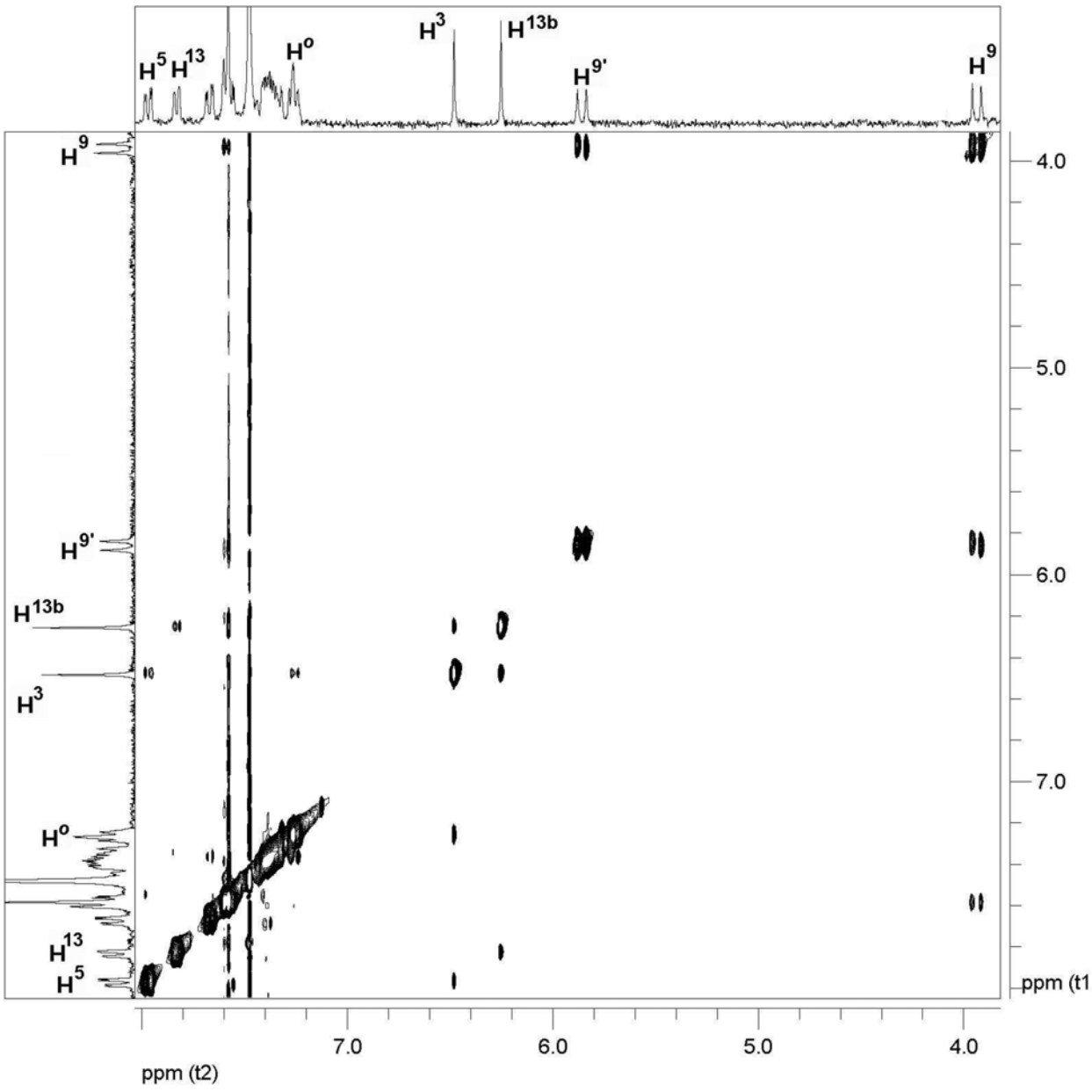
2D ^{1}H NOESY spectrum of compound **16**.

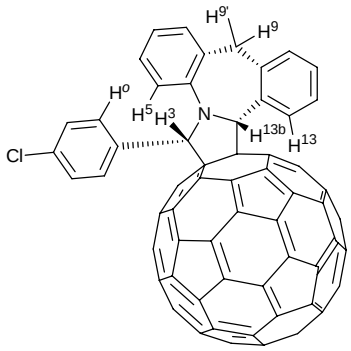






2D ^{1}H NOESY spectrum of compound **18**. and **19**





2D ^{1}H NOESY spectrum of compound **29**

Computational Details

All calculations were performed with the B3LYP density functional method[1] by using the Gaussian suite of quantum chemical programs. Geometry optimizations of intermediates, transition states, reactants, and products in the gas phase were performed at the B3LYP/6-31G(d) level using Gaussian 03.[2] Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequencies for transition states was carried out to check whether the frequency indeed pertains to the desired reaction coordinate. Intrinsic reaction coordinates (IRC) were calculated to authenticate all transition states.

[1] (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Becke, A. D. *Phys. Rev. A* **1998**, *38*, 3098. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1998**, *37*, 785.

[2] Frisch, M.J.; Trucks, G.W. Schlegel, H.B.; Scuseria, G.E.; Robb, M.A.; Cheeseman, J.R.; Montgomery, J.A. Jr.; Vreven, T.; Kudin, K.N.; Burant, J.C.; Millam, J.M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G.A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J.E.; Hratchian, H.P.; Cross, J.B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R.E.; Yazyev, O.; Austin ,A.J.; Cammi, R.; Pomelli, C.; Ochterski, J.W.; Ayala, P.Y.; Morokuma, K.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Zakrzewski, V.G.; Dapprich, S.; Daniels,A.D.; Strain, M.C.; Farkas, O.; Malick , D.K.; Rabuck, A.D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J.V.; Cui, Q.; Baboul, A.G.; Clifford, S.; Cioslowski, J.; Stefanov, B.B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R.L.; Fox, D.J.; Keith, T.; Al-Laham, M. A.; Peng, C.Y.; Nanayakkara, A.; Challacombe, M.; Gill, P.M.W.; Johnson, B.; Chen, W.; Wong, M.W.; Gonzalez, C.; Pople , J.A. Gaussian 03, Revision B.05, Gaussian, Inc., Pittsburgh PA, **2003**.

Table. B3LYP/6-31G(d) Absolute Energies (au), Cartesian Coordinates of stationary points of compounds and transition states of isomerizations and cycloadditions

Compound *trans*-**2a**

E = -865.199625436, **H (0K)** = -864.878436,
H (298K) = -864.861317, **G (298K)** = -864.923123 au.
Imaginary frequency = 0.

C	-2.0676550	1.3856970	0.5392460
C	-0.7283300	1.5243230	0.1238180
N	0.2846970	0.6665370	0.6165310
C	0.1725060	-0.7884850	0.6827750
C	-1.0450590	-1.5424360	0.2387550
C	-2.3265430	-1.1098600	0.6295060
C	-0.9052250	-2.7256150	-0.4942510
C	-2.0221990	-3.4838750	-0.8466110
C	-3.2932730	-3.0562460	-0.4637220
C	-3.4385410	-1.8750050	0.2658150
C	-3.0028850	2.3294610	0.1079620
C	-2.6404310	3.3948510	-0.7179920
C	-1.3129150	3.5191500	-1.1282680
C	-0.3622820	2.5914350	-0.7074640
C	1.1125560	-0.1218380	-0.2948550
C	2.5956250	-0.1140690	-0.1260250
C	3.1949680	0.3800430	1.0400350
C	3.4106950	-0.6331470	-1.1405620
C	4.7971540	-0.6685600	-0.9902770
C	5.3868650	-0.1808860	0.1773620
C	4.5809830	0.3454870	1.1896960
H	0.6447260	-1.1887770	1.5834230
H	0.0894680	-3.0537170	-0.7867900
H	-1.8992360	-4.4006340	-1.4168160
H	-4.1711570	-3.6369230	-0.7344110
H	-4.4312500	-1.5393680	0.5572080
H	-4.0386730	2.2194840	0.4223290
H	-3.3878420	4.1144610	-1.0397780
H	-1.0121170	4.3404080	-1.7734630
H	0.6773100	2.6900340	-1.0078350
H	0.7697670	-0.1549310	-1.3303320
H	2.5631600	0.8064840	1.8138500
H	2.9553220	-1.0108090	-2.0538920
H	5.4162430	-1.0728430	-1.7869530
H	6.4669210	-0.2052970	0.2951950
H	5.0340370	0.7360890	2.0973470
C	-2.4830370	0.1969220	1.3880040
H	-3.5254140	0.3183720	1.6998030
H	-1.8819970	0.1681250	2.3077120

TS of izomerization of compound *trans*-**2a -** *trans*-**2a'**

E = -865.18142747, **H (0K)** = -864.860987,
H (298K) = -864.844338, **G (298K)** = -864.904832 au.
Imaginary frequency = 1.

N	0.2287100	0.6594740	-0.6831340
C	-2.0000060	1.5654150	0.1125260
C	-0.6662090	1.6959120	-0.3050930
C	0.0379930	-0.7671890	-0.7463150
C	-1.1531150	-1.5940620	-0.3937110
C	-2.3827870	-1.1323070	0.0956120
C	-2.7115260	2.7527810	0.3845250
C	-2.1423560	4.0139620	0.2888120
C	-0.8050030	4.1284660	-0.1030480
C	-0.0914100	2.9802210	-0.4053170
C	-0.9749400	-2.9784280	-0.6017150
C	-1.9682430	-3.9018640	-0.3157140
C	-3.1924860	-3.4473230	0.1829790
C	-3.3819030	-2.0865750	0.3762020
C	0.9491320	-0.1468820	0.3029880
C	2.4362910	-0.2244240	0.2472630
C	3.1443000	0.1641330	-0.8984310
C	4.5332350	0.0519620	-0.9421770
C	5.2353670	-0.4478440	0.1574960
C	4.5378260	-0.8317300	1.3041800
C	3.1479890	-0.7191420	1.3481930
H	0.5743110	-1.1864370	-1.5998370
H	-3.7503930	2.6643270	0.6978200
H	-2.7334670	4.8973500	0.5138690
H	-0.3330340	5.1032410	-0.1906300
H	0.9381130	3.0371600	-0.7449390
H	-0.0213560	-3.3215640	-0.9968750
H	-1.7957080	-4.9612370	-0.4841960
H	-3.9926310	-4.1466940	0.4095540
H	-4.3396920	-1.7330340	0.7535940
H	0.5248040	-0.1583930	1.3089270
H	2.5930230	0.5689880	-1.7423420
H	5.0703870	0.3604650	-1.8355430
H	6.3182630	-0.5324680	0.1225960
H	5.0755480	-1.2155590	2.1673140
H	2.6084410	-1.0174330	2.2446690
C	-2.8034830	0.3006240	0.3824100
H	-3.0609440	0.3317390	1.4521370
H	-3.7686230	0.4389930	-0.1241590

Compound *trans*-**2a'**

E = -865.19074519, **H (0K)** = -864.869430,
H (298K) = -864.852323, **G (298K)** = -864.914022 au.
Imaginary frequency = 0.

N	0.3199310	0.6847720	-0.6310490
C	-1.7910430	1.3575160	0.6106450
C	-0.7353510	1.5947600	-0.2956390
C	0.1820690	-0.7749510	-0.6915090
C	-1.0606580	-1.5536450	-0.4076020
C	-2.0502670	-1.1907570	0.5315110
C	-2.7382940	2.3722940	0.8010840
C	-2.6589160	3.5946050	0.1355310
C	-1.6123770	3.8215790	-0.7563280

TS of izomerization of compound *trans*-**2a' –** ylide **22**

E = -865.12709372, **H (0K)** = -864.809585,
H (298K) = -864.844338, **G (298K)** = -864.904832 au.
Imaginary frequency = 1.

N	-0.0083040	-0.8577040	-0.4632930
C	2.2050830	-0.9252260	0.5291830
C	1.2271500	-1.5601090	-0.2614150
C	0.0213900	0.3789440	-1.1428960
C	0.5666580	1.5874460	-0.5976480
C	1.5113180	1.6101330	0.4758210
C	3.4335210	-1.5744720	0.6853600
C	3.6814530	-2.8081350	0.0768660
C	2.6943820	-3.4245720	-0.6915690

C	-0.6655770	2.8221200	-0.9673720	C	1.4573510	-2.7979390	-0.8568210
C	-1.2386080	-2.7278900	-1.1555350	C	0.2949610	2.8076850	-1.2681350
C	-2.3517440	-3.5474630	-0.9836990	C	0.8925490	4.0014250	-0.8917080
C	-3.3269040	-3.1896580	-0.0556440	C	1.7927220	4.0222830	0.1769340
C	-3.1685000	-2.0182210	0.6844940	C	2.0896330	2.8278060	0.8375480
C	1.0543400	-0.1104430	0.3524840	C	-0.9465800	-0.7367440	0.5259310
C	2.5459870	-0.1313200	0.2731000	C	-2.3671330	-0.5738490	0.3293410
C	3.2248260	0.3228210	-0.8651340	C	-3.0222460	-0.7137270	-0.9191480
C	4.6164050	0.2610250	-0.9286720	C	-4.4035520	-0.6508590	-1.0051750
C	5.3495280	-0.2540970	0.1430670	C	-5.1859150	-0.4271280	0.1382600
C	4.6803810	-0.7040410	1.2826770	C	-4.5579820	-0.2811270	1.3749090
C	3.2882550	-0.6412810	1.3464050	C	-3.1705820	-0.3567570	1.4716200
H	0.7301150	-1.1822860	-1.5416700	H	-0.2182430	0.3601160	-2.2047230
H	-3.5577080	2.1948070	1.4943160	H	4.2067150	-1.1094850	1.2924630
H	-3.4109330	4.3587300	0.3125290	H	4.6476630	-3.2878370	0.2082350
H	-1.5329960	4.7662610	-1.2873410	H	2.8842910	-4.3859060	-1.1607220
H	0.1567040	2.9674010	-1.6607420	H	0.6704160	-3.2517110	-1.4519110
H	-0.4823100	-3.0005670	-1.8878170	H	-0.4093370	2.7917770	-2.0966060
H	-2.4564410	-4.4522550	-1.5761110	H	0.6541150	4.9173920	-1.4265290
H	-4.2068990	-3.8102460	0.0897610	H	2.2700210	4.9487210	0.4831970
H	-3.9329450	-1.7342660	1.4042450	H	2.8128270	2.8384070	1.6511410
H	0.6720360	-0.1411450	1.3698160	H	-0.6225510	-0.8888580	1.5589620
H	2.6477190	0.7398050	-1.6850660	H	-2.4305280	-0.8776910	-1.8139630
H	5.1311530	0.6210900	-1.8159510	H	-4.8837610	-0.7738310	-1.9727460
H	6.4341600	-0.2999730	0.0923750	H	-6.2675560	-0.3664150	0.0588760
H	5.2418080	-1.1008380	2.1246260	H	-5.1490310	-0.1081560	2.2705350
H	2.7712460	-0.9919830	2.2374030	H	-2.6903980	-0.2464790	2.4411590
C	-1.9505350	0.0609190	1.3863680	C	1.9033840	0.3716630	1.2682110
H	-1.1394190	-0.0474750	2.1189630	H	1.0994540	0.1609960	1.9963420
H	-2.8629090	0.1363100	1.9866020	H	2.7786350	0.6224520	1.8765100

Ylide **22**

E = -865.14222285, **H (0K)** = -864.822991,
H (298K) = -864.805497, **G (298K)** = -864.867509 au.
Imaginary frequency = 0.

N	0.3744300	-0.8829440	-0.6342660	C	-1.3723040	1.7388510	0.4178950
C	2.3446850	-0.3358350	0.5803300	C	-0.1603230	1.2358270	-0.0970020
C	1.7630030	-1.1979820	-0.3703690	N	0.2285700	-0.1114760	0.0941420
C	0.2465120	0.2796370	-1.3870340	C	-0.4983310	-1.2036350	0.5066110
C	0.0948770	1.5454190	-0.6757230	C	-1.9162870	-1.4043060	0.2189780
C	0.7025260	1.7345480	0.6013160	C	-2.8331180	-0.3611560	0.4924050
C	3.7033950	-0.5024190	0.8453030	C	-2.3947280	-2.6301950	-0.2743280
C	4.4508600	-1.4818870	0.1766930	C	-3.7485910	-2.8054750	-0.5521730
C	3.8439100	-2.3224600	-0.7542760	C	-4.6443250	-1.7576110	-0.3296660
C	2.4779700	-2.1881000	-1.0302110	C	-4.1847580	-0.5492860	0.1994370
C	-0.5169260	2.6543580	-1.2963920	C	-1.6829650	3.0828560	0.1809080
C	-0.5713200	3.9005800	-0.6817890	C	-0.8323180	3.9255040	-0.5312660
C	-0.0177220	4.0703370	0.5886240	C	0.3600410	3.4096530	-1.0425150
C	0.6145290	2.9919120	1.2084900	C	0.6851190	2.0736290	-0.8408650
C	-0.5457950	-1.4380090	0.1671350	C	1.2304610	-0.7956370	-0.6022560
C	-1.9706150	-1.2587380	0.1692080	C	2.6129630	-0.7835820	-0.2104640
C	-2.6933730	-0.3352200	-0.6254830	C	3.0625070	-0.1153310	0.9528680
C	-4.0865950	-0.3637350	-0.6433500	C	3.5738540	-1.4688450	-0.9923800
C	-4.7984310	-1.2532250	0.1620070	C	4.9181030	-1.4619700	-0.6419900
C	-4.0996530	-2.1447330	0.9868390	C	5.3486660	-0.7792940	0.5013870
C	-2.7139340	-2.1506110	0.9872460	C	4.4111590	-0.1081310	1.2927770
H	0.8993950	0.2836450	-2.2565570	H	0.0429180	-1.9272150	1.1045120
H	4.1867220	0.1368470	1.5802380	H	-1.6892840	-3.4360020	-0.4608030
H	5.5108620	-1.5865090	0.3910500	H	-4.1026920	-3.7535540	-0.9478910
H	4.4263230	-3.0827020	-1.2671090	H	-5.7010730	-1.8860920	-0.5477980

TS of izomerization of compound *trans*-**2a –** ylide **21**

E = -865.150978123, **H (0K)** = -864.832530,
H (298K) = -864.815359, **G (298K)** = -864.876971 au.
Imaginary frequency = 1.

H	1.9801130	-2.8262800	-1.7540750	H	-4.8908800	0.2500960	0.4130020
H	-0.9538470	2.5130180	-2.2822830	H	-2.6203260	3.4717630	0.5726350
H	-1.0528920	4.7343070	-1.1866950	H	-1.1020530	4.9649310	-0.6941820
H	-0.0607670	5.0351200	1.0866320	H	1.0334750	4.0426390	-1.6139800
H	1.0789330	3.1374770	2.1824660	H	1.5932570	1.6579220	-1.2639820
H	-0.1422550	-2.1900100	0.8378580	H	0.9132230	-1.3926680	-1.4513850
H	-2.1578400	0.3930120	-1.2169090	H	2.3374230	0.3921640	1.5823490
H	-4.6211880	0.3436990	-1.2720540	H	3.2465510	-2.0003140	-1.8833310
H	-5.8848990	-1.2424910	0.1648300	H	5.6375350	-1.9921770	-1.2610980
H	-4.6417590	-2.8378590	1.6246960	H	6.3999010	-0.7776940	0.7756190
H	-2.1787920	-2.8618740	1.6126100	H	4.7345270	0.4163120	2.1886240
C	1.4667000	0.6414750	1.3529940	C	-2.3346570	0.8759230	1.2135840
H	0.7340040	0.0317860	1.9145430	H	-3.1888900	1.4921280	1.5126340
H	2.0892560	1.1275500	2.1112720	H	-1.8446200	0.5513690	2.1444110

Ylide **21**

E = -865.171796466, **H (0K)** = -864.852018,
H (298K) = -864.834471, **G (298K)** = -864.896597 au.
Imaginary frequency = 0.

C	0.7558110	1.3503840	-0.4596990	C	-1.7710160	1.3393430	0.7426070
C	-0.0351010	0.5584560	0.3803340	C	-0.7075940	1.4795130	-0.1576750
N	-0.0963110	-0.8909430	0.2188980	N	0.3364820	0.4637930	-0.2305880
C	1.0732070	-1.5936190	0.2763930	C	-0.0150570	-0.8185650	-0.5455760
C	2.4157130	-1.1213620	0.0950230	C	-1.2863610	-1.4578290	-0.3556700
C	2.7648100	-0.0301120	-0.7500890	C	-2.2292050	-1.0836170	0.6426740
C	3.4716420	-1.8590190	0.6874140	C	-1.5842080	-2.5953630	-1.1472050
C	4.7996610	-1.5053800	0.4956080	C	-2.7697770	-3.2996550	-0.9897100
C	5.1267100	-0.4006390	-0.2984390	C	-3.7057100	-2.8979100	-0.0311870
C	4.1036030	0.3222940	-0.9140770	C	-3.4208040	-1.7941200	0.7751500
C	0.7661320	2.7347300	-0.2425470	C	-2.7373950	2.3516740	0.7829090
C	0.0240810	3.3121730	0.7839250	C	-2.6519810	3.4698090	-0.0434900
C	-0.7305090	2.5006550	1.6346800	C	-1.5970710	3.5814950	-0.9503870
C	-0.7602780	1.1248890	1.4332690	C	-0.6260670	2.5843840	-1.0099630
C	-1.3068840	-1.5093180	0.2680230	C	1.6082580	0.9297070	-0.1214710
C	-2.6162570	-0.9957680	-0.0372590	C	2.8424590	0.2018250	-0.0120040
C	-2.9135490	0.2052570	-0.7308910	C	3.0013620	-1.1859460	0.2398910
C	-3.7191920	-1.8117600	0.3293610	C	4.0322510	0.9781930	-0.0796870
C	-5.0272280	-1.4470200	0.0394830	C	5.2868710	0.4121780	0.0855760
C	-5.2980740	-0.2498940	-0.6305560	C	5.4186700	-0.9587240	0.3374110
C	-4.2279870	0.5628600	-1.0139440	C	4.2659810	-1.7402580	0.4244690
H	0.9293960	-2.6529740	0.4655620	H	0.7734660	-1.3866740	-1.0183330
H	3.2239320	-2.7096610	1.3179690	H	-0.8663090	-2.9075530	-1.9022010
H	5.5848350	-2.0861470	0.9728240	H	-2.9695230	-4.1622830	-1.6202910
H	6.1642740	-0.1168930	-0.4493430	H	-4.6364220	-3.4432440	0.0959040
H	4.3494400	1.1629050	-1.5598060	H	-4.1302550	-1.4893530	1.5419390
H	1.3764480	3.3587950	-0.8904530	H	-3.5678390	2.2513860	1.4770960
H	0.0429710	4.3888590	0.9278960	H	-3.4109290	4.2451330	0.0120690
H	-1.2959370	2.9356710	2.4534080	H	-1.5300600	4.4368470	-1.6162640
H	-1.3470890	0.4812050	2.0784910	H	0.1886100	2.6504430	-1.7235030
H	-1.2332330	-2.5727960	0.4719130	H	1.6734780	2.0074950	-0.0816270
H	-2.1120400	0.8502440	-1.0708010	H	2.1361260	-1.8290690	0.3357050
H	-3.5273200	-2.7450350	0.8543230	H	3.9473840	2.0468100	-0.2645020
H	-5.8426220	-2.1000260	0.3411790	H	6.1706390	1.0418940	0.0189230
H	-6.3205280	0.0388070	-0.8566690	H	6.4008000	-1.4060530	0.4606300
H	-4.4167560	1.4883530	-1.5528800	H	4.3474490	-2.8046920	0.6311100
C	1.6572330	0.6988130	-1.4782030	C	-1.8969630	0.0762480	1.5577500
H	2.0714110	1.4523600	-2.1550520	H	-2.6715580	0.1960250	2.3216940
H	1.0857460	-0.0167760	-2.0877010	H	-0.9502880	-0.1279470	2.0792850

Ylide **23**

E = -865.176344605, **H (0K)** = -864.855851,
H (298K) = -864.838437, **G (298K)** = -864.900468 au.
Imaginary frequency = 0.

TS of izomerization of compound ylide **23 –** *cis*-**2a'**

Compound *cis*-**2a'**

E = -865.14126062, **H (0K)** = -864.823295,
H (298K) = -864.806016, **G (298K)** = -864.868107 au.
Imaginary frequency = 1.

C	2.1475750	-0.7785630	0.6209230
C	1.3351190	-1.4989890	-0.2754320
N	0.1462840	-0.8462840	-0.6764170
C	0.0647640	0.3624020	-1.3394460
C	0.4613570	1.6202820	-0.7492800
C	1.2366280	1.6886290	0.4427920
C	0.1708210	2.8127760	-1.4470110
C	0.6090870	4.0479050	-0.9893140
C	1.3670950	4.1159810	0.1820170
C	1.6758180	2.9433870	0.8743750
C	3.3819900	-1.3259580	0.9764530
C	3.7812850	-2.5754160	0.4931520
C	2.9372450	-3.2983090	-0.3503220
C	1.7110960	-2.7582210	-0.7432450
C	-1.1334230	-1.2627010	-0.9983040
C	-2.3349160	-0.8999700	-0.2687500
C	-2.3509350	-0.0959740	0.8931640
C	-3.5674940	-1.4195870	-0.7218890
C	-4.7564770	-1.1503730	-0.0498520
C	-4.7542010	-0.3518180	1.0952860
C	-3.5409660	0.1712970	1.5580770
H	-0.0897530	0.3370190	-2.4163830
H	-0.4145100	2.7461530	-2.3611780
H	0.3650990	4.9519310	-1.5405760
H	1.7234470	5.0733530	0.5521810
H	2.2792350	3.0043110	1.7775420
H	4.0243180	-0.7843680	1.6672720
H	4.7405030	-2.9895410	0.7909850
H	3.2369270	-4.2765660	-0.7165530
H	1.0553350	-3.3032610	-1.4165640
H	-1.2489340	-2.0478680	-1.7530000
H	-1.4219470	0.3252580	1.2617230
H	-3.5809910	-2.0457030	-1.6115620
H	-5.6890350	-1.5665640	-0.4228900
H	-5.6805970	-0.1407810	1.6220330
H	-3.5243170	0.7926180	2.4502330
C	1.5932870	0.4697250	1.2898920
H	2.3044940	0.7933110	2.0574880
H	0.6882010	0.1556610	1.8344590

E = -865.17786150, **H (0K)** = -864.857111,
H (298K) = -864.839875, **G (298K)** = -864.901971 au.
Imaginary frequency = 0.

C	2.6100830	-0.2750630	0.3832130
C	1.6913710	-1.3015440	0.0595480
N	0.3655380	-0.8310030	0.0569030
C	0.0831130	0.1023150	-1.0147830
C	0.0073520	1.5289330	-0.5951700
C	1.0727940	1.9763690	0.2196380
C	-0.9461120	2.4263370	-1.0799910
C	-0.8741080	3.7822490	-0.7604700
C	0.1773220	4.2415650	0.0315030
C	1.1363060	3.3460040	0.5082540
C	3.9679620	-0.5872220	0.3632270
C	4.4091170	-1.8820150	0.0575890
C	3.4835510	-2.8841990	-0.2230460
C	2.1136040	-2.5964230	-0.2272020
C	-0.7638930	-1.1421080	-0.7929730
C	-2.1315650	-1.1585370	-0.1904390
C	-2.3938540	-0.6032990	1.0687460
C	-3.1870590	-1.7272000	-0.9151400
C	-4.4826720	-1.7356780	-0.3978660
C	-4.7372270	-1.1778560	0.8559380
C	-3.6882980	-0.6142940	1.5864940
H	0.7269530	-0.0299350	-1.8920670
H	-1.7483310	2.0529850	-1.7112940
H	-1.6262730	4.4722930	-1.1329640
H	0.2555640	5.2968950	0.2796890
H	1.9484110	3.7190980	1.1292390
H	4.6953010	0.1841270	0.6078950
H	5.4727730	-2.1029490	0.0515010
H	3.8208620	-3.8921280	-0.4500660
H	1.3824780	-3.3664430	-0.4579720
H	-0.6182040	-1.8883550	-1.5794170
H	-1.5733550	-0.1767820	1.6361130
H	-2.9917460	-2.1673730	-1.8909830
H	-5.2902560	-2.1827510	-0.9716930
H	-5.7447820	-1.1859380	1.2631960
H	-3.8783750	-0.1836250	2.5662390
C	2.1091270	1.0699710	0.9177450
H	2.9904160	1.6899540	1.1177990
H	1.6783140	0.8481190	1.9075800

TS of izomerization of compound *cis*-**2a** – *cis*-**2a**

E = -865.17104105, **H (0K)** = -864.850585,
H (298K) = -864.834022, **G (298K)** = -864.894118 au.
Imaginary frequency = 1.

C	2.0121280	-0.8503680	-0.3912180
C	1.9681720	0.0248000	0.7096820
N	0.8970890	0.1532640	1.6174650
C	-0.3507280	-0.5272820	1.7534090
C	-1.0474410	-1.4011040	0.7628820
C	-0.5065590	-1.8933270	-0.4328160
C	-2.3442550	-1.7986100	1.1461200
C	-3.1158830	-2.6463950	0.3666130
C	-2.5842590	-3.1359460	-0.8299450
C	-1.3027550	-2.7610720	-1.2077600
C	3.2368610	-0.9677300	-1.0775550
C	4.3590110	-0.2188670	-0.7474310
C	4.2841090	0.6891870	0.3130280
C	3.1062080	0.7892960	1.0375410

Compound *cis*-**2a**

E = -865.19229437, **H (0K)** = -864.870743,
H (298K) = -864.853817, **G (298K)** = -864.914410 au.
Imaginary frequency = 0.

C	-1.9937780	1.2954070	0.1414990
C	-0.7298730	1.5630640	0.7088540
N	-0.2184020	0.7643150	1.7507990
C	-0.2519390	-0.6898370	1.8129370
C	-0.8094400	-1.5544150	0.7232010
C	-2.0506870	-1.2321300	0.1417790
C	-0.1534850	-2.7337490	0.3530560
C	-0.7110130	-3.5924180	-0.5944060
C	-1.9351410	-3.2708890	-1.1806520
C	-2.5949050	-2.0970870	-0.8129920
C	-2.5087580	2.1895470	-0.8006820
C	-1.8055840	3.3309640	-1.1891020
C	-0.5566900	3.5865090	-0.6219830
C	-0.0239750	2.7123920	0.3223140

C	-0.2810690	1.0023190	1.6397070	C	1.0683360	0.0515160	1.7289280
C	-0.8729470	1.7542720	0.4880570	H	-0.5076100	-1.0487310	2.8143590
C	-0.3203550	1.8152960	-0.7977120	H	0.8033260	-2.9744970	0.8087620
C	-2.0587500	2.4653740	0.7380650	H	-0.1899530	-4.5037070	-0.8748410
C	-2.6886460	3.1920880	-0.2690050	H	-2.3771070	-3.9306510	-1.9226960
C	-2.1351460	3.2352100	-1.5509130	H	-3.5500060	-1.8483190	-1.2701540
C	-0.9487100	2.5492800	-1.8066920	H	-3.4826860	1.9810340	-1.2387570
H	-0.5060480	-0.8924630	2.7730440	H	-2.2284360	4.0092920	-1.9246580
H	-2.7416070	-1.4230970	2.0868630	H	0.0069440	4.4696660	-0.9112010
H	-4.1147370	-2.9289990	0.6874340	H	0.9431180	2.9113680	0.7739630
H	-3.1612010	-3.8107680	-1.4565190	C	-2.7647420	0.0484010	0.5391120
H	-0.8894370	-3.1499490	-2.1364820	H	-3.7546070	0.0726100	0.0720180
H	3.2882720	-1.6547400	-1.9203640	H	-2.9341100	0.0521030	1.6256330
H	5.2800530	-0.3395920	-1.3108110	C	2.0135170	-0.0007300	0.5724630
H	5.1464040	1.2892830	0.5907730	C	3.3858540	-0.0262080	0.8713950
H	3.0384380	1.4427530	1.9022000	C	1.6287480	-0.0236500	-0.7785380
H	-0.3999270	1.5388030	2.5838990	C	4.3458850	-0.0874800	-0.1373110
H	0.6149470	1.3130440	-1.0122700	H	3.7032680	0.0012100	1.9115820
H	-2.4913240	2.4424740	1.7361500	C	2.5901430	-0.0786400	-1.7877850
H	-3.6087510	3.7286610	-0.0523610	H	0.5807740	0.0025220	-1.0494240
H	-2.6206180	3.8049610	-2.3386810	C	3.9499400	-0.1130260	-1.4750310
H	-0.5000500	2.5878640	-2.7960490	H	5.4008460	-0.1100800	0.1230740
C	0.8454230	-1.5697610	-1.0536670	H	2.2698260	-0.0939410	-2.8261580
H	1.2425080	-2.5161630	-1.4417610	H	4.6934020	-0.1561450	-2.2664810
H	0.6170060	-0.9848820	-1.9596620	H	1.5973480	0.1508160	2.6770460

Compound **28**

E = -326.79462920, **H (0K)** = -326.651148, **H (298K)** = -326.642696, **G (298K)** = -326.683402 au. Imaginary frequency = 0.

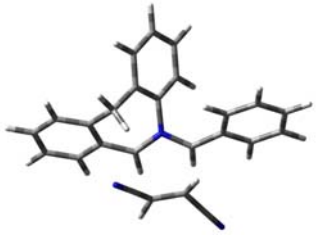
N	1.2909220	0.0546260	0.0000330
C	2.6328380	-0.0736180	-0.0009180
H	3.0733550	-1.0556220	-0.0004210
C	0.6005020	-1.2123400	0.0002470
C	-0.7006640	-1.5076050	0.0001780
C	-1.8622980	0.7900380	-0.0010490
H	-2.8152640	1.3141990	-0.0020970
C	-0.7380360	1.5434510	-0.0000500
H	-0.9031490	2.6207870	-0.0002950
C	0.6561910	1.2524300	0.0015230
H	1.3430910	2.0902500	0.0019630
H	-0.8783750	-2.5832660	-0.0000030
H	1.3081400	-2.0309760	0.0005410
H	3.2372360	0.8209900	-0.0021230
C	-1.9678040	-0.7043070	0.0001610
H	-2.5634590	-1.0442130	-0.8663960
H	-2.5624080	-1.0428260	0.8680500

TS of izomerization of compound **28**

E = -326.74725441, **H (0K)** = -326.605684, **H (298K)** = -326.598008, **G (298K)** = -326.636238 au. Imaginary frequency = 1.

N	1.1653850	0.1203930	-0.0457300
C	2.6001600	0.0987160	0.4002790
H	3.1543170	-0.2778920	-0.4787180
C	0.5827520	-1.0771740	-0.5221940
C	-0.6569280	-1.5180580	-0.2351810
C	-1.8579960	0.6002620	-0.0549000
H	-2.8733050	0.8534680	-0.3538360
C	-0.8674350	1.4890640	-0.2787480
H	-1.1055750	2.4778590	-0.6644340
C	0.5274290	1.2583160	0.0217070
H	1.1908330	2.0726630	0.3072150
H	-0.9725510	-2.4748840	-0.6421580
H	1.2905380	-1.6712150	-1.0893250
H	2.6223950	-0.7256790	1.1349090
C	-1.6148350	-0.7285800	0.6229700
H	-2.5531570	-1.2716600	0.7589590
H	-1.1900770	-0.5606900	1.6238990

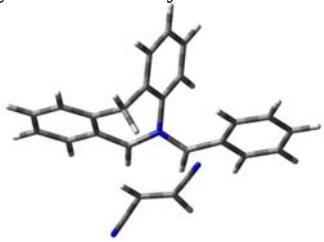
TS-1 of cycloaddition of ylide **21** to fumaronitrile



E = -1128.24793120, **H (0K)** = -1127.875649, **H (298K)** = -1127.852104, **G (298K)** = -1127.928117 au. Imaginary frequency = 1.

C	-0.9959930	1.8582810	0.6138600

TS-2 of cycloaddition of ylide **21** to fumaronitrile

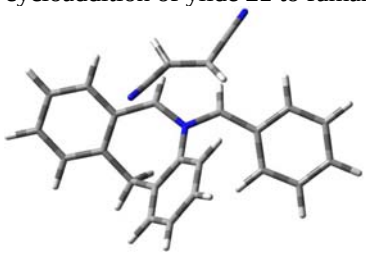


E = -1128.25133291, **H (0K)** = -1127.879111, **H (298K)** = -1127.855563, **G (298K)** = -1127.931238 au. Imaginary frequency = 1.

C	-0.6198620	1.9137540	0.6001470

C	-0.0781660	1.3739440	-0.3276400	C	0.1260550	1.2957550	-0.4105700
N	0.0710930	-0.0473230	-0.6135170	N	0.0543190	-0.1393100	-0.6413910
C	-1.0202290	-0.8286010	-0.8835230	C	-1.1607430	-0.7444420	-0.8541940
C	-2.4151000	-0.4805510	-0.7182790	C	-2.4678440	-0.1887600	-0.5734270
C	-2.9016900	0.3174690	0.3487670	C	-2.7355580	0.6588550	0.5338260
C	-3.3446180	-1.0643920	-1.6069240	C	-3.5514380	-0.6232590	-1.3679680
C	-4.7085070	-0.8408820	-1.4713650	C	-4.8509230	-0.2095260	-1.1017440
C	-5.1786140	-0.0297830	-0.4351250	C	-5.1029340	0.6484360	-0.0283260
C	-4.2740440	0.5408400	0.4611100	C	-4.0451890	1.0730660	0.7774640
C	-0.3461740	-2.7661290	0.6697380	C	0.3008530	4.0575150	-0.0977350
C	-0.3024770	4.1288880	0.0593640	C	-0.5138140	3.3029250	0.7424160
C	1.0256650	-2.5351860	0.6447580	C	1.0090230	3.4286920	-1.1236440
C	0.6870280	2.2592980	-1.0979950	C	0.5417550	-2.4575520	1.0882430
C	1.3235480	-0.6019850	-0.7762970	C	1.1886710	-0.8992530	-0.7433000
C	2.5900590	-0.0404780	-0.3283890	C	2.5721840	-0.5025460	-0.5293240
C	2.7475680	0.7400030	0.8389310	C	3.0093160	0.4318430	0.4360160
C	3.7530270	-0.3978760	-1.0445270	C	3.5555380	-1.1864810	-1.2795020
C	5.0125930	0.0244760	-0.6276740	C	4.9106400	-0.9323800	-1.0954250
C	5.1483400	0.8142490	0.5151600	C	0.9178870	2.0495540	-1.2833960
C	0.5798530	3.6315690	-0.9015570	C	5.3246860	0.0088010	-0.1499500
H	-0.8003420	-1.6504990	-1.5541060	H	-1.1207720	-1.5807370	-1.5417340
H	-2.9775250	-1.6922980	-2.4154120	H	-3.3569270	-1.2948830	-2.1999710
H	-5.4037880	-1.2951700	-2.1715570	H	-5.6663290	-0.5547920	-1.7310150
H	-6.2438460	0.1475100	-0.3175990	H	-6.1158210	0.9764550	0.1871650
H	-4.6405310	1.1549160	1.2799690	H	-4.2407530	1.7268960	1.6241930
H	-1.7952720	3.6266090	1.5247960	H	-1.0880510	3.7912570	1.5253150
H	-0.3884570	5.1990490	0.2247210	H	0.3723420	5.1328260	0.0383420
H	1.1805430	4.3074430	-1.5027870	H	1.6290710	4.0075920	-1.8015070
H	1.3650570	1.8663620	-1.8464370	H	1.4623660	1.5511340	-2.0773460
H	1.3767390	-1.3269380	-1.5798140	H	1.0416830	-1.7900150	-1.3446800
H	1.8800940	1.0088150	1.4327910	H	2.2913190	0.9416630	1.0657410
H	3.6600530	-1.0231070	-1.9282050	H	3.2426080	-1.9212980	-2.0180290
H	5.8900960	-0.2662620	-1.1987200	H	5.6438020	-1.4687960	-1.6917560
H	6.1302910	1.1460210	0.8403590	H	6.3821650	0.2094080	-0.0026970
H	4.1031020	1.7640950	2.1466830	H	4.6788560	1.3970350	1.3688170
C	-1.9238700	0.9160370	1.3370420	C	-1.5933090	1.1050870	1.4227650
H	-2.4656980	1.4512370	2.1221470	H	-1.9726900	1.7064030	2.2540980
H	-1.3620750	0.1162680	1.8294620	H	-1.0802730	0.2396460	1.8628760
C	-1.0871410	3.2451160	0.7938810	C	-0.8167610	-2.5807320	0.8308530
C	4.0083490	1.1637230	1.2457120	H	-1.5498110	-2.0911830	1.4609800
C	-1.1463900	-2.4357210	1.7939070	C	4.3669670	0.6800660	0.6144050
N	-1.8151330	-2.1873810	2.7179270	H	1.2552210	-3.1615780	0.6749490
C	1.8679680	-3.3138240	-0.2009230	C	0.9928870	-1.6485630	2.1664950
N	2.5495800	-3.9221990	-0.9254420	N	1.3459910	-0.9615750	3.0411010
H	-0.7846480	-3.4764340	-0.0241820	C	-1.3053000	-3.5877200	-0.0462200
H	1.5115260	-2.0302100	1.4730290	N	-1.7038420	-4.3813770	-0.8027330

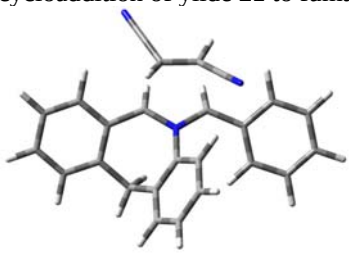
TS-3 of cycloaddition of ylide **21** to fumaronitrile



E = -1128.24456972, **H (0K)** = -1127.872053, **H (298K)** = -1127.848519, **G (298K)** = -1127.924501 au. Imaginary frequency = 1.

C	5.0732700	0.2682800	-0.8154850
C	4.1404490	-1.9529230	-0.7571490
H	1.4729140	1.8290880	1.8390160

TS-4 of cycloaddition of ylide **21** to fumaronitrile

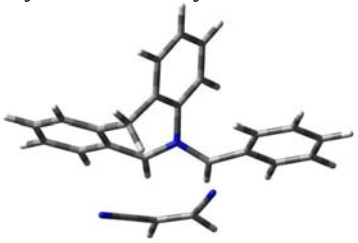


E = -1128.24362738, **H (0K)** = -1127.870878, **H (298K)** = -1127.847436, **G (298K)** = -1127.923242 au. Imaginary frequency = 1.

C	-0.5548020	2.5497890	0.8849460
C	0.8425960	2.5665230	0.7697170
C	-0.7564500	-2.1758730	0.0046520

C	-0.9568490	-2.0444130	-0.1303560	C	0.0334340	-1.0680730	0.3457510
C	-0.0676380	-1.0494300	0.2926780	N	0.0074860	0.1106140	-0.5141300
N	0.1178230	0.1336700	-0.5372970	C	-1.1693800	0.7918410	-0.6955720
C	-0.9581580	0.9815250	-0.7195700	C	-2.5247390	0.2335190	-0.5464400
C	-2.3674160	0.5717340	-0.8032790	C	-2.8291490	-1.1255160	-0.7979080
C	-2.7953090	-0.7346750	-1.1391020	C	-3.5875050	1.1192820	-0.2814430
C	-3.3437930	1.5759430	-0.6528750	C	-4.9017710	0.6679780	-0.2132480
C	-4.6988430	1.2988780	-0.7907080	C	-5.1900300	-0.6813330	-0.4228360
C	-5.1151640	0.0008120	-1.0905410	C	-4.1527850	-1.5641970	-0.7187810
C	-4.1612610	-1.0003240	-1.2643300	C	-0.7008970	-3.3103820	0.8208710
C	-1.1205770	-3.1746270	0.6775240	C	0.1169800	-3.3480620	1.9483290
C	-0.4238380	-3.3095790	1.8765490	C	0.8852690	-2.2325690	2.2800670
C	0.4437730	-2.2988190	2.2919730	C	0.8477270	-1.0919600	1.4804320
C	0.6237570	-1.1680540	1.5003140	C	1.1651520	0.7713600	-0.8283720
C	1.3570510	0.6551040	-0.7361420	C	2.5158750	0.2002830	-0.9138840
C	2.6513490	-0.0258170	-0.7113860	C	2.8084280	-1.1726880	-1.0342010
C	2.8531190	-1.4222000	-0.7127170	C	3.5916600	1.1096010	-0.9744940
C	3.7915930	0.8065130	-0.7822250	C	4.9023550	0.6693790	-1.1268650
C	-0.4790160	2.3629470	1.0702940	C	5.1770870	-0.6958480	-1.2293150
C	5.2573130	-1.1165480	-0.7984550	C	4.1225850	-1.6091430	-1.1884900
C	0.9214300	2.3913040	1.0947350	H	-1.0839690	1.6035170	-1.4079810
H	-0.7022010	1.8324840	-1.3421630	H	-3.3791810	2.1731500	-0.1331320
H	-3.0305860	2.5892230	-0.4175590	H	-5.6993550	1.3730790	0.0028650
H	-5.4276380	2.0932930	-0.6580410	H	-6.2136360	-1.0414850	-0.3701800
H	-6.1716100	-0.2286840	-1.1960630	H	-4.3712250	-2.6125000	-0.9085860
H	-4.4778970	-2.0091980	-1.5183920	H	-1.3153060	-4.1693860	0.5638630
H	-1.8113210	-3.9509220	0.3588670	H	0.1482290	-4.2404570	2.5670180
H	-0.5651670	-4.1953090	2.4891150	H	1.5201330	-2.2398250	3.1607650
H	0.9787560	-2.3839140	3.2327540	H	1.4617800	-0.2411410	1.7405580
H	1.3065420	-0.3886710	1.8126380	H	0.9883830	1.6052880	-1.4957940
H	1.3422870	1.5700340	-1.3130240	H	2.0085680	-1.9034080	-1.0298460
H	2.0078620	-2.0989940	-0.7036170	H	3.3927670	2.1746640	-0.8907890
H	3.6607300	1.8850420	-0.8038040	H	5.7107380	1.3944570	-1.1604820
H	5.9309030	0.9338880	-0.8601160	H	6.1998960	-1.0428940	-1.3452020
H	6.2579660	-1.5383740	-0.8291430	H	4.3198370	-2.6734780	-1.2849720
H	4.2680310	-3.0321650	-0.7662210	C	-1.7147560	-2.0856410	-1.1560590
C	-1.7737190	-1.8278660	-1.3799540	H	-2.1242970	-3.0736560	-1.3855910
H	-2.2775800	-2.7556910	-1.6663680	H	-1.1924960	-1.7336990	-2.0568340
H	-1.1166890	-1.5459270	-2.2150120	H	1.2917580	3.2999520	0.1066210
C	1.6336950	3.4145650	0.4172180	C	1.6914750	2.1297940	1.8242580
N	2.2228580	4.2326120	-0.1726500	N	2.4015330	1.7863220	2.6840780
C	-1.2092420	1.6999690	2.1052690	C	-1.3059590	3.5655590	0.2283730
N	-1.8118360	1.1753040	2.9530670	N	-1.9100990	4.3896210	-0.3353710
H	-1.0030750	3.1899110	0.6016120	H	-1.0294710	2.0601700	1.7287260

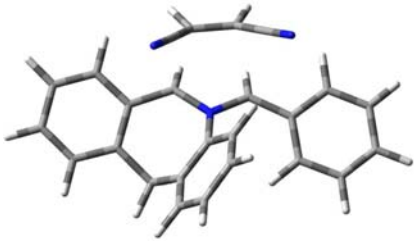
TS-1 of cycloaddition of ylide **21** to malenitrile



E = -1128,24575572, **H (0K)** = -1127,873443, **H (298K)** = -1127,850020, **G (298K)** = -1127,925113 au. Imaginary frequency = 1.

C	-0.6678100	1.6205520	0.8594730
C	0.1479740	1.2764440	-0.2254730
N	0.1187510	-0.0545840	-0.8129840
C	-1.0670290	-0.6026750	-1.2303260
C	-2.3973220	-0.1365950	-0.9101340

TS-2 of cycloaddition of ylide **21** to malenitrile



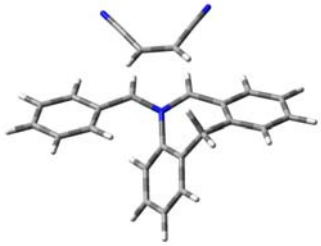
E = -1128,24035926, **H (0K)** = -1127,867760, **H (298K)** = -1127,844329, **G (298K)** = -1127,919796 au. Imaginary frequency = 1.

C	-0.5596570	2.6841810	0.1399260
C	0.8306980	2.7936980	-0.0043430
C	-0.8746670	-1.9611170	0.2958980
C	-0.0241540	-0.8516670	0.3899960
N	0.0452300	0.0749310	-0.7348380

C	-2.7473090	0.4154440	0.3496330
C	-3.4178980	-0.3542220	-1.8616750
C	-4.7349780	-0.0042460	-1.5976980
C	-5.0671340	0.5681510	-0.3664060
C	-4.0744950	0.7725590	0.5912320
C	-0.5936780	2.9308500	1.3494000
C	0.2542730	3.8742390	0.7756480
C	1.0302200	3.5244600	-0.3311400
C	0.9728830	2.2288320	-0.8345170
C	1.2783490	-0.7545110	-1.0483450
C	2.6418020	-0.3895970	-0.6820250
C	3.0119580	0.2458760	0.5236390
C	3.6728870	-0.8027530	-1.5543930
C	5.0114140	-0.5713550	-1.2522930
C	5.3588740	0.0758020	-0.0646210
C	4.3525090	0.4754340	0.8184350
H	-0.9669110	-1.2500280	-2.0935400
H	-3.1577770	-0.7968490	-2.8205550
H	-5.5016320	-0.1743360	-2.3483940
H	-6.0957290	0.8412340	-0.1485640
H	-4.3359130	1.1971000	1.5572090
H	-1.2214240	3.2055110	2.1929600
H	0.2986950	4.8814650	1.1800740
H	1.6763110	4.2565520	-0.8063340
H	1.5683060	1.9492220	-1.6960720
H	1.1933570	-1.4168720	-1.9039240
H	2.2549030	0.5363800	1.2410170
H	3.4118470	-1.3054450	-2.4833470
H	5.7829510	-0.8946970	-1.9459800
H	6.4026000	0.2580280	0.1754920
H	4.6125340	0.9595920	1.7556240
C	-1.6730510	0.6314810	1.3942510
H	-2.1176310	1.0076220	2.3199230
H	-1.1863760	-0.3190860	1.6395940
C	-0.6459360	-2.8889150	-0.1187820
C	0.6964480	-2.7085380	0.2083310
H	1.4595310	-3.2119570	-0.3747640
C	1.0958510	-2.2762990	1.5055820
N	1.4255450	-1.8925200	2.5559520
C	-1.7171650	-2.7778730	0.8041960
N	-2.6195870	-2.7009660	1.5403290
H	-0.8804200	-3.4222310	-1.0354450

C	-1.0828080	0.7915260	-1.0767920
C	-2.4722070	0.3302770	-0.9189470
C	-2.8452920	-1.0335320	-0.8709810
C	-3.4912120	1.3012570	-0.9421660
C	-4.8345310	0.9466880	-0.8842340
C	-5.1941860	-0.3993240	-0.8072700
C	-4.1983330	-1.3746210	-0.8037310
C	-0.9216550	-2.8541230	1.3709710
C	-0.1474050	-2.6469620	2.5111090
C	0.6784940	-1.5259750	2.5934510
C	0.7448120	-0.6244430	1.5334210
C	1.2399030	0.5597430	-1.1650220
C	2.5623050	-0.0502810	-1.0243870
C	2.7991480	-1.4172050	-0.7726960
C	3.6781710	0.7813070	-1.2525840
C	4.9739780	0.2775480	-1.2114600
C	5.1924850	-1.0761510	-0.9483860
C	4.0983610	-1.9172000	-0.7366450
H	-0.9174570	1.4133150	-1.9506550
H	-3.2233030	2.3523640	-0.9968960
H	-5.5969940	1.7202870	-0.8910760
H	-6.2400920	-0.6882480	-0.7563590
H	-4.4725030	-2.4261080	-0.7611880
H	-1.5821650	-3.7151570	1.3087070
H	-0.1977950	-3.3521370	3.3358740
H	1.2726840	-1.3417560	3.4830210
H	1.3933930	0.2391070	1.6030820
H	1.1402890	1.2549420	-1.9879160
H	1.9682570	-2.0969750	-0.6268210
H	3.5201880	1.8382900	-1.4485750
H	5.8143620	0.9453570	-1.3788770
H	6.2034780	-1.4720040	-0.9131510
H	4.2541890	-2.9759330	-0.5475960
C	-1.7786410	-2.1096400	-0.9030470
H	-2.2445330	-3.0995020	-0.9035190
H	-1.1945820	-2.0275520	-1.8308600
H	1.2039540	3.3461900	-0.8613370
C	1.7650860	2.6211860	1.0483970
N	2.5632030	2.4873960	1.8902240
H	-1.1747830	3.2737930	-0.5319860
C	-1.1772810	2.3862450	1.3946310
N	-1.7077300	2.1552790	2.4053960

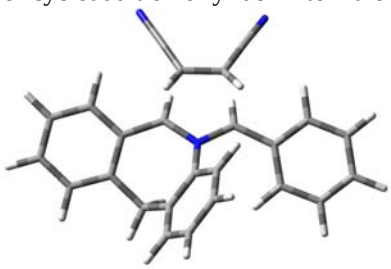
TS-3 of cycloaddition of ylide **21** to malenitrile



E = -1128,24810447, **H (0K)** = -1127,875921, **H (298K)** = -1127,852326, **G (298K)** = -1127,928573 au. Imaginary frequency = 1.

C	0.8383500	-2.0476290	0.6475400
C	0.0171840	-1.4661830	-0.3266180
N	-0.0509700	-0.0258540	-0.5131150
C	1.0955730	0.7107860	-0.6853500
C	2.4574730	0.2726370	-0.4623830
C	2.8312550	-0.6011730	0.5917620
C	3.4754350	0.8550100	-1.2484510

TS-4 of cycloaddition of ylide **21** to malenitrile



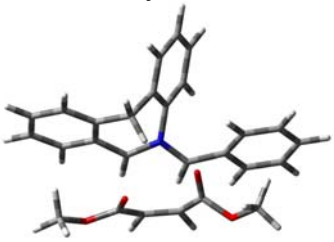
E = -1128,24370860, **H (0K)** = -1127,870898, **H (298K)** = -1127,847447, **G (298K)** = -1127,923490 au. Imaginary frequency = 1.

C	-0.4597030	2.1807470	1.2392400
C	0.9425760	2.1718500	1.1517030
H	1.5080250	1.5523550	1.8372320
C	-0.8728960	-2.2390320	0.0448740
C	-0.0238520	-1.1898100	0.4203660
N	0.0655810	-0.0095500	-0.4291200

C	4.8138820	0.5517600	-1.0294820
C	5.1707080	-0.3381710	-0.0136370
C	4.1779890	-0.9042820	0.7884080
C	0.8626340	-3.4446120	0.7460660
C	0.1001570	-4.2441920	-0.1012040
C	-0.6874210	-3.6498640	-1.0891690
C	-0.7252320	-2.2641750	-1.2047550
C	-1.2594170	0.6154520	-0.6296290
C	-2.5786210	0.0927690	-0.3090430
C	-2.8479170	-0.8498250	0.7094560
C	-3.6795540	0.6603130	-0.9880700
C	-4.9849280	0.2861390	-0.6825290
C	-5.2314170	-0.6630250	0.3108350
C	-4.1548570	-1.2221450	1.0060150
H	0.9615810	1.5792460	-1.3192890
H	3.1996210	1.5534850	-2.0334040
H	5.5784460	1.0097890	-1.6503030
H	6.2149030	-0.5795070	0.1634170
H	4.4547140	-1.5794990	1.5948430
H	1.4986940	-3.9027400	1.4990870
H	0.1304170	-5.3252820	-0.0004100
H	-1.2689560	-4.2610320	-1.7727720
H	-1.3321510	-1.7931600	-1.9695060
H	-1.2322660	1.4738940	-1.2902950
H	-2.0324970	-1.2855890	1.2765940
H	-3.5001950	1.4109230	-1.7525220
H	-5.8113190	0.7407400	-1.2217800
H	-6.2496150	-0.9569260	0.5494570
H	-4.3353480	-1.9490650	1.7936080
C	1.7533640	-1.1832240	1.4806560
H	2.1995200	-1.7728960	2.2869590
H	1.1778450	-0.3737930	1.9508960
C	0.5711240	2.3970230	1.0765290
C	-0.8142880	2.2920400	1.1088790
C	-1.6819110	3.2403670	0.4964730
N	-2.4137470	3.9804530	-0.0287610
H	-1.2747010	1.6387140	1.8425670
C	1.2635490	3.4318900	0.3878670
N	1.8592970	4.2407200	-0.2042740
H	1.1605600	1.8393580	1.7948920

C	-1.0601720	0.7676020	-0.5905870
C	-2.4491280	0.2826370	-0.6034590
C	-2.8140000	-1.0529020	-0.9021020
C	-3.4767100	1.2339940	-0.4372650
C	-4.8166650	0.8681020	-0.5041170
C	-5.1685950	-0.4586370	-0.7572540
C	-4.1648780	-1.4039990	-0.9600790
C	-0.9478710	-3.3662180	0.8705140
C	-0.1992110	-3.4536240	2.0420450
C	0.6345820	-2.3968040	2.4084450
C	0.7240930	-1.2670210	1.5987840
C	1.2727470	0.6015520	-0.6412070
C	2.5919740	-0.0436540	-0.6919660
C	2.8183560	-1.4332160	-0.7709480
C	3.7137450	0.8117110	-0.7548190
C	5.0032470	0.2990630	-0.8558500
C	5.2125450	-1.0806470	-0.9138840
C	4.1123230	-1.9386110	-0.8804170
H	-0.8795130	1.6418340	-1.2055440
H	-3.2179600	2.2703310	-0.2499570
H	-5.5845730	1.6228800	-0.3605620
H	-6.2130950	-0.7522210	-0.8123370
H	-4.4296150	-2.4342000	-1.1866510
H	-1.6076800	-4.1810480	0.5841300
H	-0.2683140	-4.3397200	2.6663870
H	1.2211230	-2.4482970	3.3207920
H	1.3946630	-0.4636930	1.8709740
H	1.1843360	1.4850530	-1.2604420
H	1.9854770	-2.1257370	-0.7720320
H	3.5668140	1.8871230	-0.7196920
H	5.8469050	0.9826740	-0.8943000
H	6.2189490	-1.4813070	-0.9967830
H	4.2572640	-3.0136200	-0.9482120
C	-1.7420430	-2.0862270	-1.1766710
H	-2.1996640	-3.0449250	-1.4375460
H	-1.1318170	-1.7731110	-2.0355790
C	1.6693770	3.2665860	0.5999490
N	2.2934710	4.1283430	0.1226820
C	-1.2143360	3.3325770	0.8717230
N	-1.8485620	4.2616670	0.5645110
H	-0.9377920	1.5162950	1.9515170

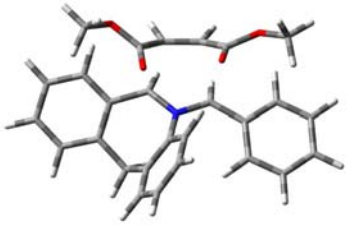
TS-1 of cycloaddition of ylide **21** to dimethyl maleate



E = -1399,51099964, **H (0K)** = -1399,049440, **H (298K)** = -1399,020658, **G (298K)** = -1399,107735 au. Imaginary frequency = 1.

C	-0.4140780	1.9571200	1.0783350
C	0.3143840	1.7794010	-0.1045940
N	0.1653050	0.5895400	-0.9280470
C	-1.0774420	0.2020360	-1.3627430
C	-2.3528790	0.6775730	-0.8674230
C	-2.5922940	0.9993840	0.4947610
C	-3.4381360	0.7074170	-1.7698610
C	-4.7122760	1.0766090	-1.3572260

TS-2 of cycloaddition of ylide **21** to dimethyl maleate

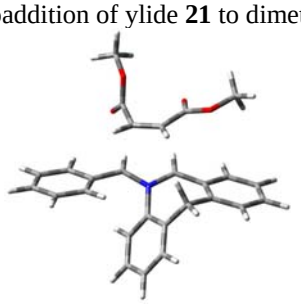


E = -1399,50368831, **H (0K)** = -1399,041894, **H (298K)** = -1399,013025, **G (298K)** = -1399,101258 au. Imaginary frequency = 1.

C	-1.1023280	0.0589370	-1.3290860
C	3.6292660	-0.3246280	-1.5272750
C	-1.0431760	-2.3627050	0.6076260
C	-0.1917520	-1.2531250	0.5253620
N	-0.0301050	-0.6101790	-0.7725840
C	-0.4950350	2.1662630	-0.7232950
C	-2.5154620	-0.3320810	-1.1333610
C	-2.9220290	-1.6547040	-0.8310890
C	-3.5096750	0.6269680	-1.4024400

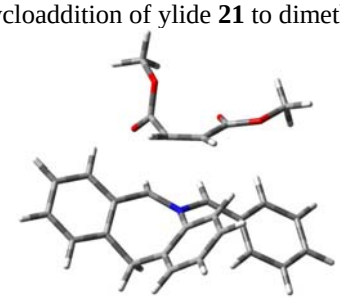
C	-4.9357550	1.4211520	-0.0215290	C	-4.8629950	0.3068730	-1.3406080
C	-3.8762910	1.3812250	0.8871290	C	-5.2576420	-0.9900350	-1.0120190
C	-0.2249030	3.1465660	1.7943530	C	-4.2846330	-1.9566360	-0.7618850
C	0.6482990	4.1349920	1.3484090	C	-1.1601960	-3.0207650	1.8357090
C	1.3331580	3.9593880	0.1444640	C	-0.4532640	-2.5775300	2.9528060
C	1.1609860	2.7863770	-0.5833060	C	0.3577870	-1.4463430	2.8570880
C	1.2609060	-0.1035520	-1.3834770	C	0.4903460	-0.7734160	1.6436490
C	2.6604740	0.1106350	-1.0331580	C	1.2012640	-0.3143680	-1.2694370
C	3.1252680	0.4913760	0.2460870	C	2.4905260	-0.9348650	-0.9549060
C	3.6253860	-0.1770560	-2.0231100	C	2.6855150	-2.1265700	-0.2254200
C	4.9881850	-0.0684920	-1.7611220	C	0.8994910	2.1430470	-0.8559850
C	5.4300980	0.3301100	-0.4982260	C	4.9012030	-0.8607910	-1.3564660
C	4.4894530	0.6030360	0.4994380	C	5.0780910	-2.0331250	-0.6180090
H	-1.0751070	-0.2441420	-2.3496450	C	3.9619660	-2.6613780	-0.0637710
H	-3.2643240	0.4375440	-2.8087380	H	-0.8857090	0.3960130	-2.3378960
H	-5.5284480	1.0987550	-2.0742270	H	-3.2153670	1.6435230	-1.6390760
H	-5.9279820	1.7119010	0.3126060	H	-5.6064890	1.0725500	-1.5448870
H	-4.0507650	1.6344220	1.9302300	H	-6.3112210	-1.2498050	-0.9569030
H	-0.7848500	3.2908820	2.7147420	H	-4.5839640	-2.9740780	-0.5207740
H	0.7815430	5.0443420	1.9279070	H	-1.8198400	-3.8816620	1.9115980
H	1.9966210	4.7324270	-0.2320570	H	-0.5524990	-3.1023770	3.8991840
H	1.6857170	2.6421890	-1.5208590	H	0.8831480	-1.0707050	3.7299390
H	1.0931760	-0.5607700	-2.3525120	H	1.0905820	0.1257330	1.5793040
H	2.4171590	0.6742630	1.0445590	H	1.1536270	0.1189550	-2.2590200
H	3.2930140	-0.4844980	-3.0123240	H	1.8415290	-2.6541420	0.1988150
H	5.7053640	-0.2915050	-2.5467960	H	3.5075020	0.5944610	-2.0918390
H	6.4927650	0.4207670	-0.2909580	H	5.7567390	-0.3623050	-1.8046850
H	4.8212190	0.9024260	1.4904500	H	6.0702390	-2.4552040	-0.4841220
C	-1.4498940	0.9411270	1.4865360	H	4.0800810	-3.5845550	0.4975890
H	-1.8164590	1.1631630	2.4933270	C	-1.8855460	-2.7357730	-0.5875690
H	-1.0118140	-0.0630790	1.5127080	H	-2.3807210	-3.6965820	-0.4172250
C	-0.7438590	-2.2662740	-0.8738960	H	-1.2523150	-2.8522250	-1.4784250
C	0.6075950	-2.2694890	-0.5775800	H	1.2719140	2.3981490	-1.8433490
H	1.2761140	-2.6973080	-1.3174260	H	-1.0219190	2.5872510	-1.5735840
H	-1.0095110	-2.5388090	-1.8912040	C	-1.2580130	2.3305230	0.5406460
C	1.2186060	-2.1583350	0.7660120	O	-1.0410320	1.8444660	1.6282750
O	0.8944690	-1.4198740	1.6767990	O	-2.3377490	3.1373050	0.3024780
O	2.2889430	-2.9917570	0.8458520	C	1.9323540	2.2806760	0.1752060
C	-1.8856940	-2.3530270	0.0491360	O	1.8579100	2.1164130	1.3805710
O	-1.8931780	-2.2856330	1.2641800	O	3.1068420	2.6624730	-0.4243120
O	-3.0245220	-2.5678700	-0.6762880	C	-3.1939240	3.3431580	1.4339540
C	-4.2243700	-2.6733200	0.0982650	H	-2.6415460	3.8037330	2.2575250
H	-5.0198740	-2.8774740	-0.6202530	H	-3.9860980	4.0079440	1.0859690
H	-4.1473260	-3.4874100	0.8247950	H	-3.6133580	2.3935040	1.7777600
H	-4.4239290	-1.7392990	0.6303120	C	4.2146400	2.8233230	0.4684040
C	3.0051300	-2.9543650	2.0877360	H	4.4608230	1.8765390	0.9571940
H	3.7749570	-3.7227640	2.0038680	H	5.0469710	3.1564980	-0.1540400
H	3.4628980	-1.9727390	2.2371910	H	3.9901760	3.5692130	1.2359610
H	2.3366640	-3.1686610	2.9258320				

TS-3 of cycloaddition of ylide **21** to dimethyl maleate



E = -1399,51011569, **H (0K)** = -1399,049047,
H (298K) = -1399,020009, **G (298K)** = -1399,109320

TS-4 of cycloaddition of ylide **21** to dimethyl maleate



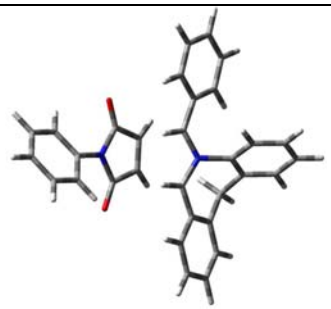
E = -1399,50544492, **H (0K)** = -1399,043621,
H (298K) = -1399,014801, **G (298K)** = -1399,103037

au. Imaginary frequency = 1.			
C	0.5352650	-2.7827310	0.6624190
C	-0.2876230	-2.1544540	-0.2828720
N	-0.2275210	-0.7244950	-0.5315670
C	0.9679980	-0.1049530	-0.7528650
C	2.2941970	-0.6657390	-0.6202420
C	2.6580980	-1.5615890	0.4173680
C	3.3042150	-0.1987400	-1.4906430
C	4.6169720	-0.6392450	-1.3699770
C	4.9582270	-1.5528240	-0.3685960
C	3.9770960	-2.0024460	0.5170140
C	0.4223250	-4.1699250	0.8235310
C	-0.4734750	-4.9194970	0.0664330
C	-1.2600380	-4.2850630	-0.8967310
C	-1.1631150	-2.9090430	-1.0734450
C	-1.3809340	0.0221580	-0.6750860
C	-2.7169800	-0.3708120	-0.2466180
C	-2.9956550	-1.1705570	0.8847800
C	-3.8156800	0.1838810	-0.9407440
C	-5.1245310	-0.0733730	-0.5430640
C	-5.3816910	-0.8885550	0.5618860
C	-4.3071840	-1.4288460	1.2733740
H	0.8788370	0.8204090	-1.3093610
H	3.0371530	0.5087890	-2.2712820
H	5.3735930	-0.2761640	-2.0603160
H	5.9820490	-1.9023250	-0.2691250
H	4.2437900	-2.6931450	1.3138070
H	1.0583100	-4.6608950	1.5559060
H	-0.5475690	-5.9928230	0.2169220
H	-1.9459970	-4.8576870	-1.5138710
H	-1.7673070	-2.4088230	-1.8211150
H	-1.3223590	0.7956250	-1.4290950
H	-2.1801070	-1.5892300	1.4654800
H	-3.6247870	0.8345880	-1.7889890
H	-5.9483350	0.3651650	-1.1005570
H	-6.4032930	-1.0918410	0.8708790
H	-4.4907580	-2.0507730	2.1460340
C	1.5942170	-1.9978710	1.3990680
H	2.0313410	-2.6108450	2.1930900
H	1.1507950	-1.1118770	1.8728880
C	0.4668500	1.6934530	1.1063670
C	-0.8571750	1.8504390	0.7692510
H	-1.6181270	1.4534020	1.4338870
H	0.7399120	1.0781810	1.9559210
C	1.5389840	2.4884820	0.5092370
O	1.4524610	3.1656560	-0.5069460
O	2.6895910	2.3809450	1.2244720
C	-1.3255380	2.9925970	-0.1024500
O	-1.7885640	2.9197240	-1.2233240
O	-1.2302210	4.1538730	0.5759070
C	3.8052430	3.1118520	0.7017810
H	4.6236880	2.9367770	1.4015750
H	4.0735940	2.7483560	-0.2938730
H	3.5755850	4.1793480	0.6401200
C	-1.5958120	5.3280860	-0.1677780
H	-2.6310320	5.2622540	-0.5130860
H	-1.4739110	6.1609380	0.5257340
H	-0.9340870	5.4443630	-1.0298560

TS-1 of cycloaddition of ylide **21** to N-phenylmaleimide

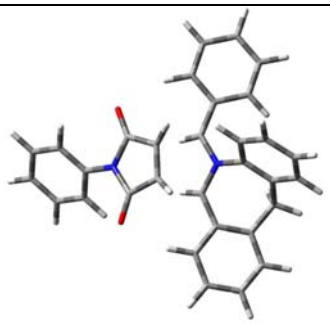
au. Imaginary frequency = 1.			
C	-0.3210280	1.8964720	0.7577790
C	3.3340940	-0.7876380	-1.2630610
H	0.9150040	0.7358290	2.0554520
C	-1.7707780	-2.5458910	0.1918940
C	-0.6509050	-1.7409630	0.4377120
N	-0.3209140	-0.6650370	-0.4833260
C	-1.2142120	0.3782180	-0.6817730
C	-2.6790630	0.2742670	-0.5402640
C	-3.4082680	-0.9308180	-0.6891650
C	-3.4126340	1.4676490	-0.3757070
C	-4.8016660	1.4660010	-0.2984910
C	-5.5068260	0.2658020	-0.3928530
C	-4.8022630	-0.9193810	-0.5951870
C	-2.0600110	-3.5799650	1.0890670
C	-1.2582390	-3.8129920	2.2044710
C	-0.1498000	-2.9984860	2.4405130
C	0.1556860	-1.9650110	1.5585810
C	0.9807050	-0.4163970	-0.7842550
C	2.0805020	-1.3573990	-0.9352670
C	2.0022510	-2.7666080	-0.8673400
C	0.8945050	1.3903210	1.1929700
C	4.4560540	-1.5800910	-1.4748650
C	4.3647670	-2.9714370	-1.3820080
C	3.1298160	-3.5533210	-1.0880410
H	-0.8910030	1.0692260	-1.4510320
H	-2.8806470	2.4105770	-0.3337450
H	-5.3318530	2.4052430	-0.1656290
H	-6.5912880	0.2533680	-0.3283270
H	-5.3422650	-1.8574250	-0.7039660
H	-2.9295370	-4.2053590	0.9034720
H	-1.4981010	-4.6244150	2.8859150
H	0.4823470	-3.1659670	3.3075620
H	1.0302020	-1.3486070	1.7190690
H	1.1236290	0.5348600	-1.2804280
H	1.0572940	-3.2545350	-0.6641350
H	3.4082500	0.2922960	-1.3577190
H	5.4044680	-1.1104790	-1.7226940
H	5.2393610	-3.5934090	-1.5509160
H	3.0377910	-4.6352470	-1.0368420
C	-2.6731520	-2.2239160	-0.9704040
H	-3.3864350	-3.0376320	-1.1327000
H	-2.0796330	-2.1216840	-1.8897420
H	-1.1810970	1.7799380	1.4112790
C	-0.3482580	3.1556600	-0.0820980
O	-0.6839540	3.2509980	-1.2467430
O	-0.0041480	4.2194630	0.6697660
C	2.1842270	1.8838920	0.7309240
O	2.3882790	2.6040720	-0.2401100
O	3.1923150	1.4407650	1.5356330
C	0.0884620	5.4662090	-0.0402940
H	-0.8662710	5.7183410	-0.5094430
H	0.3559460	6.2094020	0.7117060
H	0.8628620	5.3983810	-0.8083950
C	4.4982020	1.9299140	1.2137730
H	5.1573110	1.5366460	1.9893840
H	4.8218870	1.5754760	0.2311750
H	4.5152240	3.0235170	1.2159530

TS-2 of cycloaddition of ylide **21** to N-phenylmaleimide



E = -1455.65688750, **H (0K)** = -1455.185872, **H (298K)** = -1455.157692, **G (298K)** = -1455.245210 au. Imaginary frequency = 1.

C	3.4915630	-0.4387750	-0.3133800
C	2.6216520	0.2529230	0.5382600
N	1.1775720	0.1248850	0.4262160
C	0.5918380	-1.1182760	0.4401420
C	1.2463790	-2.3973110	0.2827160
C	2.3549850	-2.6045530	-0.5802800
C	0.6671120	-3.5206000	0.9128110
C	1.1922320	-4.7946930	0.7369930
C	2.3087100	-4.9833190	-0.0812390
C	2.8773300	-3.8879470	-0.7338890
C	4.8701440	-0.2754250	-0.1270660
C	5.3730540	0.5446130	0.8795270
C	4.4919470	1.2001920	1.7419670
C	3.1190730	1.0511760	1.5745290
C	0.3745520	1.2349740	0.4248590
C	0.7537400	2.6202840	0.2162430
C	1.8633970	3.0563860	-0.5449970
C	-0.1221410	3.6069010	0.7235280
C	0.1139200	4.9607450	0.5074560
C	1.2277490	5.3740510	-0.2255400
C	2.0936120	4.4117970	-0.7540830
H	-0.3956310	-1.1253440	0.8858970
H	-0.2058190	-3.3776060	1.5433240
H	0.7303290	-5.6413160	1.2368830
H	2.7245750	-5.9767090	-0.2234140
H	3.7308270	-4.0344990	-1.3919440
H	5.5514220	-0.8103580	-0.7837560
H	6.4463700	0.6612300	0.9993060
H	4.8694640	1.8244520	2.5462540
H	2.4261130	1.5557570	2.2381630
H	-0.5981810	1.0653350	0.8706860
H	2.5408640	2.3323490	-0.9834760
H	-1.0022510	3.2973390	1.2792910
H	-0.5783600	5.6947110	0.9107000
H	1.4138550	6.4309710	-0.3942670
H	2.9535260	4.7198210	-1.3432900
C	2.9400360	-1.4201940	-1.3185100
H	3.7301600	-1.7465700	-2.0013460
H	2.1615770	-0.9374880	-1.9251880
C	-1.9738930	-1.3205220	-1.0645420
O	-2.2672820	-2.4874080	-0.8758370
C	-2.1367110	1.0003650	-1.1195690
O	-2.5951350	2.1218530	-0.9900760
C	-0.7480600	-0.7678590	-1.6845960
C	-0.8398500	0.5987910	-1.7081720
H	-0.2275540	1.3126650	-2.2404050
H	-0.0634640	-1.4143610	-2.2136960
N	-2.7663390	-0.2006000	-0.6871590
C	-4.0349440	-0.2771210	-0.0444850

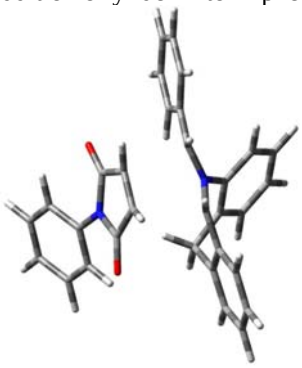


E = -1455.65699289, **H (0K)** = -1455.185277, **H (298K)** = -1455.157308, **G (298K)** = -1455.243805 au. Imaginary frequency = 1.

C	-2.0586150	-1.0946990	1.1425730
O	-2.4347640	-2.2551680	1.1405790
C	-2.1561330	1.2148990	0.9544230
O	-2.6081910	2.3313310	0.7576470
C	-0.7605720	-0.5371230	1.5825460
C	-0.8216400	0.8402820	1.4800670
H	-0.2369300	1.5760790	2.0124260
H	-0.0822190	-1.1301600	2.1796340
C	3.5747290	-0.6450370	-0.2283640
C	2.5165880	0.1149220	0.2875550
N	1.2236630	0.0865370	-0.3834200
C	0.5467530	-1.1042270	-0.4503140
C	1.1464530	-2.4441740	-0.4500420
C	2.4498090	-2.7128720	-0.9346890
C	0.3358490	-3.5302780	-0.0609290
C	0.8128470	-4.8359580	-0.1167780
C	2.1070750	-5.0926420	-0.5729080
C	2.9131440	-4.0295220	-0.9775830
C	4.8119040	-0.5913660	0.4230570
C	4.9957670	0.1939680	1.5590150
C	3.9274240	0.9323230	2.0691130
C	2.6887610	0.8949800	1.4335190
C	0.5107380	1.2439600	-0.5396920
C	1.0693200	2.5964660	-0.6773460
C	2.3930970	2.8756350	-1.0743320
C	0.1918460	3.6844970	-0.4826030
C	0.6306480	4.9943960	-0.6557100
C	1.9487890	5.2570030	-1.0354980
C	2.8226400	4.1895300	-1.2483740
H	-0.4132550	-1.0182970	-0.9453420
H	-0.6663510	-3.3387140	0.3106710
H	0.1711780	-5.6532140	0.2007580
H	2.4842930	-6.1104840	-0.6201630
H	3.9175730	-4.2214360	-1.3482120
H	5.6361670	-1.1803770	0.0292330
H	5.9661350	0.2253550	2.0462150
H	4.0538690	1.5419070	2.9587830
H	1.8658380	1.4840460	1.8145720
H	-0.4421540	1.0853660	-1.0281270
H	3.0869600	2.0660280	-1.2695920
H	-0.8326010	3.4943830	-0.1748370
H	-0.0637530	5.8140480	-0.4910940
H	2.2888180	6.2799500	-1.1719250
H	3.8464180	4.3767430	-1.5620110
C	3.3274090	-1.5678870	-1.3953380
H	4.2760500	-1.9491470	-1.7846690
H	2.8351450	-1.0217250	-2.2124040
N	-2.8442310	0.0041010	0.6995500
C	-4.1581570	-0.1001670	0.1573680

C	-5.0567310	0.6190120	-0.3871790
C	-4.2654410	-1.2518320	0.9362110
C	-6.2904650	0.5414480	0.2578410
H	-4.8774960	1.3768330	-1.1383810
C	-5.5091500	-1.3275880	1.5612330
H	-3.4839080	-1.9572520	1.1884180
C	-6.5258340	-0.4306880	1.2308360
H	-7.0737770	1.2451810	-0.0111450
H	-5.6790150	-2.0924150	2.3145400
H	-7.4917400	-0.4900170	1.7250060

TS-3 of cycloaddition of ylide **21** to N-phenylmaleimide

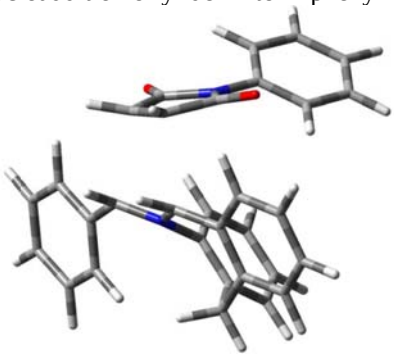


E = -1455.65190529, **H (0K)** = -1455.180439, **H (298K)** = -1455.152466, **G (298K)** = -1455.238747 au. Imaginary frequency = 1.

C	0.3332810	-1.4746430	1.6857830
C	-0.6780090	-1.8451010	0.7906340
N	-0.6225270	-1.5006570	-0.6235700
C	0.4930470	-1.7978140	-1.3677750
C	1.7965840	-2.1869250	-0.8807810
C	2.3692200	-1.6873270	0.3173790
C	2.5803130	-3.0282350	-1.7016080
C	3.8690700	-3.3942420	-1.3376720
C	4.4133510	-2.9235760	-0.1394600
C	3.6596510	-2.0779690	0.6746530
C	0.2159320	-1.8782290	3.0222870
C	-0.8655390	-2.6366630	3.4600660
C	-1.8451970	-3.0316010	2.5469640
C	-1.7486430	-2.6420370	1.2155390
C	-1.7386890	-1.0371610	-1.2807470
C	-2.9812410	-0.5603800	-0.6968890
C	-3.0756970	0.1612410	0.5129890
C	-4.1653290	-0.7562030	-1.4417040
C	-5.3908500	-0.2800580	-0.9874600
C	-5.4692690	0.4084920	0.2252620
C	-4.3050640	0.6277790	0.9658740
H	0.2652660	-2.0491670	-2.3961030
H	2.1558800	-3.3986230	-2.6319650
H	4.4487650	-4.0473390	-1.9839890
H	5.4216760	-3.2027490	0.1526640
H	4.0876260	-1.6953700	1.5981510
H	0.9965580	-1.5897530	3.7213530
H	-0.9370120	-2.9302020	4.5034990
H	-2.6817860	-3.6461190	2.8659130
H	-2.5025420	-2.9498920	0.5008130
H	-1.8018180	-1.3902490	-2.3036490
H	-2.1832560	0.3698540	1.0912860
H	-4.1146910	-1.2959020	-2.3850800
H	-6.2864860	-0.4499880	-1.5791550
H	-6.4247900	0.7813000	0.5833790

C	-5.1412940	0.8361020	0.5024700
C	-4.4675370	-1.1433210	-0.7252650
C	-6.4195150	0.7291520	-0.0444400
H	-4.8991970	1.6460810	1.1780790
C	-5.7538090	-1.2474920	-1.2518240
H	-3.7117050	-1.8754790	-0.9810620
C	-6.7341160	-0.3115220	-0.9191020
H	-7.1740990	1.4637970	0.2236700
H	-5.9858840	-2.0642290	-1.9301040
H	-7.7339010	-0.3932480	-1.3366750

TS-4 of cycloaddition of ylide **21** to N-phenylmaleimide



E = -1455.65050462, **H (0K)** = -1455.178897, **H (298K)** = -1455.150932, **G (298K)** = -1455.237435 au. Imaginary frequency = 1.

C	-0.5284300	0.4722540	-2.6883720
C	0.8396870	0.6079290	-2.5660970
C	-0.5598190	-1.9423280	1.6915630
C	0.1838230	-1.1381810	0.8143450
N	0.2351260	-1.4901630	-0.6013920
C	-0.9155380	-1.6026120	-1.3344490
C	-2.2746170	-1.7927770	-0.8138590
C	-2.5442580	-2.5462450	0.3530740
C	-3.3618130	-1.3270340	-1.5775900
C	-4.6741980	-1.5797430	-1.1891890
C	-4.9321930	-2.3066980	-0.0267950
C	-3.8654290	-2.7825350	0.7356010
C	-0.5720530	-1.6093230	3.0503440
C	0.1389470	-0.5129660	3.5320940
C	0.8730220	0.2753800	2.6463760
C	0.9018630	-0.0369940	1.2893760
C	1.4190000	-1.3947790	-1.2831700
C	2.7558630	-1.5178280	-0.6689930
C	3.0161390	-2.3923450	0.4041440
C	3.8380210	-0.8191270	-1.2339700
C	5.1316670	-0.9894000	-0.7441050
C	5.3747280	-1.8563230	0.3220370
C	4.3096960	-2.5555560	0.8938430
H	-0.7390620	-1.9721610	-2.3360650
H	-3.1742880	-0.7282760	-2.4609300
H	-5.4937690	-1.1948480	-1.7892520
H	-5.9543240	-2.5036750	0.2844840
H	-4.0578580	-3.3614560	1.6359940
H	-1.1523510	-2.2250450	3.7327860
H	0.1167650	-0.2736720	4.5915170
H	1.4251240	1.1395530	3.0020870
H	1.4924440	0.5704020	0.6167760
H	1.3398800	-1.7572690	-2.3000160
H	2.2030820	-2.9582630	0.8477660
H	3.6568150	-0.1076990	-2.0318660
H	5.9494750	-0.4302130	-1.1904530

H	-4.3508200	1.1837090	1.8982670	H	6.3831510	-1.9849230	0.7056930
C	1.5597650	-0.7536470	1.1884190	H	4.4862310	-3.2393620	1.7200390
H	2.1596160	-0.4026620	2.0329360	C	-1.3856060	-3.0889910	1.1607130
H	1.2632450	0.1300200	0.6147000	H	-1.7540020	-3.6997100	1.9904150
C	0.5999190	0.4372700	-2.6298850	H	-0.7659890	-3.7422660	0.5292540
C	-0.6943390	0.8575240	-2.4453140	C	-1.1853810	1.4490300	-1.7993110
C	-0.7057360	1.8988420	-1.3915830	O	-2.3721750	1.6969490	-1.6861800
O	-1.6684070	2.5200250	-0.9767040	C	1.1177490	1.6798620	-1.5836180
C	1.4850790	1.1939160	-1.7280740	O	2.2041000	2.1202870	-1.2389380
O	2.6993550	1.1368490	-1.6496300	H	-1.0728970	0.0387910	-3.5156980
H	-1.5352030	0.7707940	-3.1182050	H	1.5925690	0.3335370	-3.2915200
H	1.0203400	-0.1106020	-3.4613980	N	-0.1377850	2.1151680	-1.0965210
N	0.6395910	2.0497610	-0.9504180	C	-0.3374310	3.1085130	-0.0971450
C	1.0960260	3.0027630	0.0098990	C	-1.4034570	2.9849790	0.8050640
C	0.3370890	4.1504260	0.2934200	C	0.5267570	4.2084700	-0.0085260
C	2.3164910	2.8067780	0.6782590	C	-1.6015310	3.9607470	1.7804550
C	0.7906550	5.0692170	1.2387710	H	-2.0765180	2.1404920	0.7303540
H	-0.6054320	4.3097610	-0.2099620	C	0.3251760	5.1681130	0.9829900
C	2.7583220	3.7421780	1.6131240	H	1.3543710	4.2989630	-0.6996380
H	2.9297270	1.9493790	0.4407650	C	-0.7385690	5.0533900	1.8787410
C	2.0003080	4.8754490	1.9055710	H	-2.4353710	3.8594230	2.4701350
H	0.1873700	5.9491300	1.4471170	H	1.0036660	6.0148070	1.0467500
H	3.7089660	3.5767700	2.1138610	H	-0.8948210	5.8086510	2.6443160
H	2.3487740	5.5987950	2.6377620				

Compound **36-A**

E = -712.79985152, **H (0K)** = -712.499675,
H (298K) = -712.485341, **G (298K)** = -712.539527 au.
Imaginary frequency = 0.

N	0.6538310	1.2609020	0.0919160	N	-0.7934490	1.2058920	0.2666770
C	-1.2158040	2.6901320	0.2111580	C	1.0583770	2.6434950	0.2746970
C	0.0538970	3.5336440	0.3452010	C	-0.2183120	3.4728900	0.5728870
C	1.1237040	2.6075720	-0.2410010	C	-1.3804590	2.5401120	0.1755830
C	1.5009760	0.1641880	-0.0341510	C	-1.5995090	0.0759510	-0.0061000
C	2.6966080	0.3080480	-0.7747480	C	-2.8106170	0.1464030	-0.7085440
C	3.6024190	-0.7401990	-0.9171130	C	-3.5831120	-1.0010170	-0.9028800
C	3.3467880	-1.9780050	-0.3353870	C	-3.1539420	-2.2290510	-0.4044010
C	2.1648540	-2.1352230	0.3896170	C	-1.9552570	-2.2980530	0.3112310
C	1.2439960	-1.1010660	0.5644410	C	-1.1806650	-1.1602310	0.5318180
C	-0.0112630	-1.3730250	1.3785540	C	0.0762640	-1.1896200	1.3711810
C	-1.2690850	-1.1742330	0.5615580	C	1.3414240	-0.9618800	0.5616240
C	-2.0667000	-2.2579990	0.1869490	C	2.3545120	-1.9302940	0.5939710
C	-3.2057500	-2.0732570	-0.5978220	C	3.5221140	-1.7985520	-0.1539660
C	-3.5509730	-0.7902060	-1.0156670	C	3.6854800	-0.6815580	-0.9725010
C	-2.7557580	0.2984000	-0.6496870	C	2.6833760	0.2840350	-1.0181140
C	-1.6097400	0.1239060	0.1324130	C	1.5125430	0.1727530	-0.2525360
C	-0.7417080	1.2820790	0.6043240	C	0.5336790	1.3322250	-0.3669430
H	-1.5463010	2.7018530	-0.8335520	H	1.5953340	2.4050690	1.1975860
H	0.2674930	3.7402450	1.4008650	H	-0.2517250	4.4092840	0.0076760
H	2.1175670	2.7899820	0.1875200	H	-1.7107510	2.7766820	-0.8531850
H	2.9155100	1.2514850	-1.2607430	H	-3.1533250	1.0953390	-1.1084040
H	4.5088860	-0.5792860	-1.4956120	H	-4.5190780	-0.9294880	-1.4510980
H	4.0442140	-2.8037140	-0.4406170	H	-3.7508590	-3.1241600	-0.5559630
H	1.9471160	-3.0958860	0.8522650	H	-1.6275560	-3.2484140	0.7271620
H	0.0261000	-2.4024590	1.7487330	H	-0.0084800	-0.4121150	2.1427220
H	-0.0324750	-0.7317160	2.2713030	H	0.1520120	-2.1524200	1.8873790
H	-1.7912990	-3.2575450	0.5156570	H	2.2154000	-2.8086610	1.2204060
H	-3.8186890	-2.9262420	-0.8770560	H	4.2895830	-2.5665770	-0.1071450
H	-4.4384890	-0.6300760	-1.6220660	H	4.5813520	-0.5645560	-1.5763900
H	-3.0499590	1.2909700	-0.9743420	H	2.8070190	1.1496210	-1.6659830
H	-0.7224800	1.2444270	1.7075870	H	0.3885210	1.5205940	-1.4497580

Compound **36-B**

E = -712.79992176, **H (0K)** = -712.500206,
H (298K) = -712.485736, **G (298K)** = -712.540463 au.
Imaginary frequency = 0.

H	-2.0460120	3.0322180	0.8366870	H	1.7577360	3.1586260	-0.3902680
H	-0.0047980	4.4915170	-0.1805190	H	-0.2731140	3.7285280	1.6350140
H	1.2080340	2.7493800	-1.3313630	H	-2.2532990	2.6157630	0.8314650

TS of isomerization **36-A - 36-B**

E = -712.78662831, **H (0K)** = -712.487217,
H (298K) = -712.473511, **G (298K)** = -712.526094 au.
Imaginary frequency = 1.

N	-0.5495410	0.9812860	0.4649630	N	-0.6774980	1.1743510	-0.2859360
C	0.8214160	2.5570760	-0.7322330	C	1.1369210	2.6214600	0.0988290
C	-0.4157200	3.2622750	-0.1605750	C	-0.1039510	3.5085600	-0.0283660
C	-0.7641090	2.3292390	1.0020180	C	-1.2536700	2.5323300	-0.3311870
C	-1.6067970	0.0820690	0.2471480	C	-1.5946390	0.1215950	-0.1199170
C	-2.9610780	0.4701380	0.3379350	C	-2.9892870	0.3672090	-0.1451070
C	-3.9970110	-0.4214460	0.0851380	C	-3.9401300	-0.6365860	0.0120130
C	-3.7122270	-1.7326780	-0.2938390	C	-3.5374800	-1.9537850	0.2142190
C	-2.3803870	-2.1228540	-0.3845650	C	-2.1774400	-2.2344190	0.2110350
C	-1.3136120	-1.2571270	-0.0997920	C	-1.2173200	-1.2344110	0.0231370
C	0.0625070	-1.9243230	-0.1101970	C	1.2882200	-1.2139180	-0.0497510
C	1.4102470	-1.2232200	0.0227350	C	2.2925840	-2.1732710	-0.2664990
C	2.4856870	-2.0506690	0.3781120	C	3.6329940	-1.8248420	-0.2293770
C	3.7984630	-1.5859230	0.4020710	C	3.9861350	-0.4997050	0.0328910
C	4.0583970	-0.2622020	0.0573950	C	2.9844650	0.4427340	0.2352730
C	2.9968830	0.5787450	-0.2751980	C	1.6115840	0.1280040	0.1898730
C	1.6707900	0.1268270	-0.2777830	C	0.5963530	1.2263430	0.4734280
C	0.4992360	1.0464350	-0.5947380	H	1.8442210	3.0025860	0.8398600
H	1.6867410	2.8252980	-0.1177910	H	-0.3012310	4.0400220	0.9083470
H	-1.2351710	3.2773270	-0.8896970	H	-2.0427550	2.6553980	0.4247890
H	-1.7707900	2.4572460	1.3979690	H	-3.3475840	1.3735770	-0.3106440
H	-3.2148390	1.4942750	0.5862400	H	-4.9944030	-0.3762070	-0.0207800
H	-5.0260350	-0.0799520	0.1645130	H	-4.2613210	-2.7512950	0.3517420
H	-4.5091770	-2.4388170	-0.5083140	H	-1.8096420	-3.2491790	0.3257740
H	-2.1464310	-3.1503020	-0.6592590	H	1.9759800	-3.1937930	-0.4561750
H	0.0346820	-2.6881550	0.6792730	H	4.3943980	-2.5812950	-0.3982220
H	0.1182120	-2.5074170	-1.0426520	H	5.0289480	-0.1994520	0.0753810
H	2.2850540	-3.0907790	0.6283010	H	3.2806270	1.4647770	0.4407740
H	4.6078950	-2.2551770	0.6815950	H	0.3683120	1.2085120	1.5558350
H	5.0754500	0.1206590	0.0550740	H	1.6585900	2.5478670	-0.8607600
H	3.2159810	1.6073770	-0.5409470	H	0.0147210	4.2657820	-0.8086960
H	0.0407280	0.7020320	-1.5339270	H	-1.7145180	2.7013450	-1.3115290
H	1.0504650	2.8309350	-1.7665640	O	0.0445130	-1.7741120	-0.0846390
H	-0.2124720	4.2924480	0.1507970				
H	-0.0696130	2.4998420	1.8388390				

Compound **37-A**

E = -748.69671681, **H (0K)** = -748.421731,
H (298K) = -748.407499, **G (298K)** = -748.461532 au.
Imaginary frequency = 0.

N	0.6287940	1.2621120	-0.0533650	O	0.0643130	-1.3317360	-1.0574280
C	-1.2021450	2.6981730	0.2591870	N	-0.7601250	1.2180840	-0.2707990
C	0.0786680	3.5346210	0.3399240	C	-1.3403860	2.5572990	-0.2195740
C	1.1332150	2.6172770	-0.2957520	H	-1.7236610	2.8017680	0.7887850
C	1.4849370	0.1713240	-0.0895870	C	-0.1550820	3.4784150	-0.5640020
C	2.7464630	0.2798550	-0.7177170	H	-0.1522440	3.7204180	-1.6305310
C	3.6477540	-0.7822620	-0.7540980	C	1.1007900	2.6485430	-0.1917140
C	3.3260200	-2.0064650	-0.1735710	H	1.7511680	3.1619360	0.5221340
C	2.0760440	-2.1476930	0.4304340	C	0.5430590	1.3276660	0.4030180
C	1.1736830	-1.0921740	0.4732960	H	0.3698490	1.4844610	1.4865610
C	-1.1977160	-1.1575700	0.4533780	C	-1.5864400	0.1108390	-0.0095850

C	-1.9770410	-2.2700970	0.1499270	C	-1.1380900	-1.1684480	-0.3907020
C	-3.1966640	-2.0909470	-0.5046280	C	-1.9328440	-2.2958530	-0.2178090
C	-3.6192440	-0.8066350	-0.8470020	H	-1.5413940	-3.2553050	-0.5415050
C	-2.8270960	0.2998740	-0.5290500	C	-3.2112670	-2.1756300	0.3312180
C	-1.6029090	0.1428700	0.1274920	H	-3.8329890	-3.0570880	0.4579800
C	-0.7089110	1.2812630	0.5814850	C	-3.6796160	-0.9168890	0.7027380
H	-1.6012070	2.7350640	-0.7609710	H	-4.6743170	-0.8059400	1.1259030
H	0.3352950	3.7330620	1.3872430	C	-2.8752110	0.2127380	0.5388620
H	2.1242940	2.7561670	0.1564540	H	-3.2570280	1.1847450	0.8320750
H	3.0209530	1.2153750	-1.1915110	C	1.5049220	0.1607890	0.2658050
H	4.6072020	-0.6418500	-1.2450600	C	1.2567930	-1.0320920	-0.4260310
H	4.0232050	-2.8384220	-0.1940310	C	2.2507180	-2.0094490	-0.5553660
H	1.7739450	-3.0816830	0.8947090	H	2.0061770	-2.9093580	-1.1107980
H	-1.6198010	-3.2554840	0.4319270	C	3.5016600	-1.8289420	0.0225290
H	-3.8119540	-2.9533300	-0.7462860	H	4.2633530	-2.5965490	-0.0824520
H	-4.5685100	-0.6609250	-1.3548620	C	3.7589710	-0.6668140	0.7535680
H	-3.1817390	1.2934410	-0.7844530	H	4.7241920	-0.5146030	1.2279720
H	-0.5990480	1.1900460	1.6757170	C	2.7675500	0.3022800	0.8673530
H	-1.9870180	3.0275440	0.9466400	H	2.9737810	1.2089070	1.4315850
H	-0.0015250	4.4978120	-0.1727740	H	-0.2142490	4.4219470	-0.0131810
H	1.2368890	2.8132840	-1.3743330	H	1.6971320	2.4218710	-1.0798060
O	-0.0203590	-1.3366710	1.1603560	H	-2.1765610	2.6333620	-0.9215500