
“ , - ”

“ ”
01.05.03. –

: . . . II .

:

1. . . . I .
2. .

, 2003 .

“ ” “ ” “ ”

2000 . 2003 . “ ” -

” (**-605 -1213**).
BMBF-Germany (**BUL 006 99**) DAAD-Germany (**”Stability Pact for South Eastern Europe”**),
().

57 10 : 187 39
192 8

111, - , “ ”, .9, 9 2003 . 14

α - . : (ω)
 (2ω) .

- (linker), -
 , - : “push-pull” .
 , , .
p, **E**
 \check{S} ,
 :

$$p_i = \sum_j r_{ij}(-\check{S};\check{S})E_j(\check{S}_2) + \sum_{jk} s_{ijk}(-\check{S}_1;\check{S}_2,\check{S}_3)E_j(\check{S}_2)E_k(\check{S}_3) +$$

$$+ \sum_{jkl} x_{ijkl}(\check{S};\check{S}_2,\check{S}_3,\check{S}_4)E_j(\check{S}_2)E_k(\check{S}_3)E_l(\check{S}_4) + \dots$$

:
 $\mathbf{p_i}(\check{S_i}) - \check{S_i}$, i ,
 r -
 S -
 X -
 $\mathbf{E_j} - j$
 (S)

, , S
 .
 $(EFISH)$ (HRS)
).

, - , - :
 *
 *
 *
 *
 * “ ”
 *
 * ()
 *
 *
 *

1 (-)

-

.

,

2 (2-{5,5- -3-[(2-

)]- -2- })

“ ”

.

-

2

“ ”,

.

- () - () 3- 4- .

2-{5,5- -3-[(2-)]- -2- } .

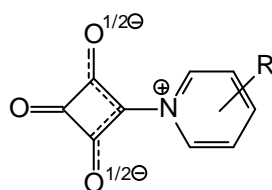
:

1. .
2. , .
3. .
4. .
5. , .
6. - RHF DFT - , - , 4- , 2-{5,5- -3-[(2- 4-)] -2- } - 2-{5,5- -3-[2-(4-)] -2- }).

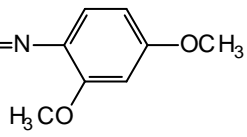
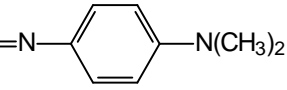
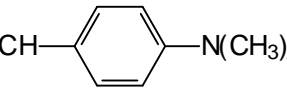
.

III. .

3- 4-



- I – ,
 - II – -CH=N- (
- 1,
- :
- 1.**
- :

<i>I</i>		<i>II</i>	
1a	R = H	1h	R = 4-CH=N-N(CH ₃) ₂
1b	R = 4-CH ₃	1i	R = 3-CH=N-N(CH ₃) ₂
1c	R = 4-N(CH ₃) ₂	1j	R = 4-CH=N- 
1d	R = 4-CN	1k	R = 4-CH=N- 
1e	R = 3-CN	1l	R = 3-N=CH- 
1f	R = 4-COPh		
1g	R = 3-COPh		

III. 1.

, λ_{\max} .

, , , 1- -2-).

1- -2- (NMP) – $10^{-4} \text{ mol.l}^{-1}$.

NMP

2:

2.

NMP

	[mol.l ⁻¹]		
		λ_{\max} [nm]	ϵ [l.mol ⁻¹ .cm ⁻¹]
1a	5.14×10^{-4}	303 367 382 s 496	3 890 11 290 10 500 430
1b	4.23×10^{-4}	305 s 368 486 592	2 130 10 165 2 010 3 070
1c	3.30×10^{-4}	281 s 370 389 452	4 240 30 610 24 850 680
1d	3.40×10^{-4}	295 425 599 s	7 060 14 120 360
1f	3.04×10^{-4}	297 400 532 s	14 470 13 160 330
1j	3.69×10^{-4}	280 380 s 480	3 660 12 060 4 610
1k	3.21×10^{-4}	278 407 580	7 790 6 230 20 090

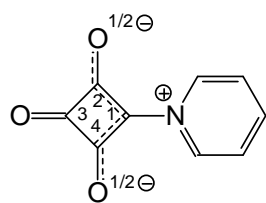
I :
 - I
 280 – 310 nm. 370 – 425 nm,
 -
 280 – 310 nm
 ,
1d – g
 -
 367 nm **1a**,
 - 2.
 (**1b** **1c**)
 ,
 25 – 60 nm.
 -
1a 500 nm $\varepsilon = 430 \text{ l.mol}^{-1}.\text{cm}^{-1}$.
 (4-CH₃ 4-N(CH₃)₂) **1b** **1c**
 486 nm 452 nm ,
1b NMP ,
 – 590 nm – 2.
 ,
 -
 (-CN –COPh) 4-
1d **1f**
 100 40 nm ,
 m- **1e** **1g**
 -
 CT .
II :
 .
 :
 280 – 300 nm
 ,
 (2),
 ,
1a.
 - 370 – 410 nm, (-)
 : 460 – 580 nm.
 - **1k**,
 580 nm (
 $\varepsilon = 20\,090 \text{ l.mol}^{-1}.\text{cm}^{-1}$),
 NMP,
1l. , π -

- CH=N- p- ,
 - D-A- .
1h
 467 nm NMP, - CH=N- p-
 3 ,
 :
3. (λ_1 λ_2
 nm)
 Reihardt E_T^N

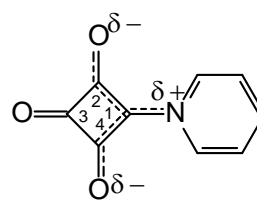
	(E_T^N)	DCE^a (0.269)	NMP (0.355)	CH_3CN (0.460)	C_2H_5OH (0.654)	H_2O (1.00)	$U\}^b$
1a	λ_1	515	496	496	476	443	$\Delta\lambda_1 = 72$
	λ_2	374	367	362	353	339	$\Delta\lambda_2 = 34$
1c	λ_1	446	452	440	422	400	$\Delta\lambda_1 = 52$
	λ_2	369	370	364	357	352	$\Delta\lambda_2 = 18$
1d	λ_1	600	599	580	540	493	$\Delta\lambda_1 = 107$
	λ_2	441	425	422	396	380	$\Delta\lambda_2 = 61$
1k	λ_1	582	580	579	-	-	$\Delta\lambda_1 = 3$
	λ_2	445	407	397	-	-	$\Delta\lambda_2 = 48$

^a DCE = 1,2- , NMP = 1- -2- ;

^b $\Delta\lambda_1$ $\Delta\lambda_2$

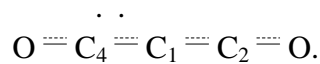


()



()

4-
 - 4- -
 C- ,



3 - CT

1,2-

> NMP >

1c

>

CT

NMP,

>

1e

NMP

• a -

E_T^N ,

λ_{\max}

CT

N-

Reichardt

$E_T^N(30)$,

•

1a-l

•

(CT),

III. 2.

CS₂

PBSQ

III.A.1., 4- {[(4-)] }-
(1k), NMP.

RHF (*Restricted Hartree-Fock*) DFT (*Density Functional Theory*)
6-31G*.

. 2. 1.

(1a)

(PBSQ)

2000 –

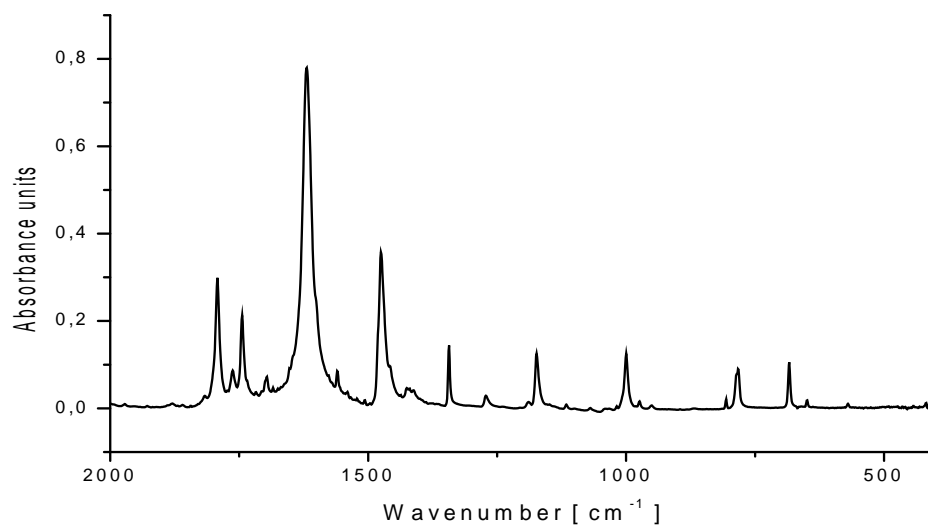
400 cm^{-1} ,
 cm^{-1} ,

KBr,
 CsI.

2 –

PBSQ

400 – 100

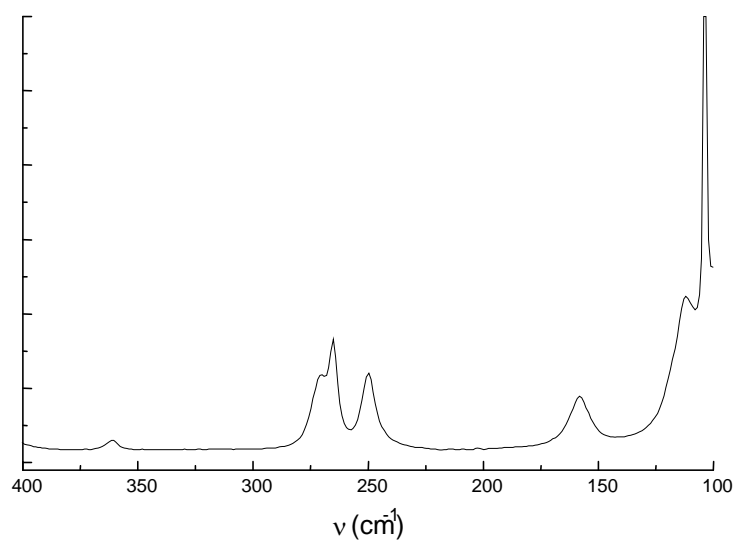


cm^{-1} .

1.

PBSQ (1 mg 200 mg KBr)

2000-400



2.

PBSQ (6 mg 200 mg CsI)

400-100 cm^{-1} .

,

Sq.

Py,

4,

B3LYP

RHF

14

25

cm^{-1} .
 RHF,

DFT

B3LYP.

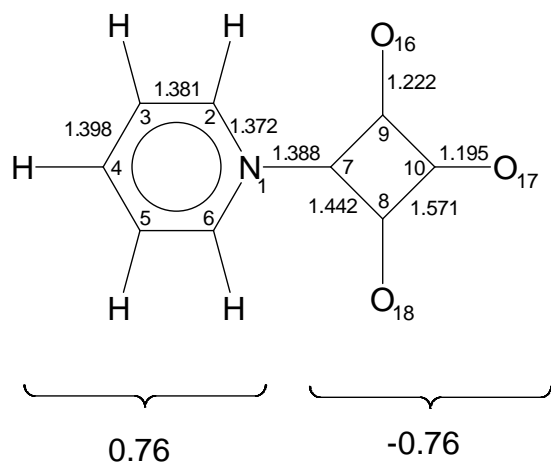
4.
(ϵ cm^{-1}) (A km.mol^{-1}) -

No	RHF	B3LYP				b
ν_i	ϵ^a	ϵ^a	A	ϵ		
6.	1868	1804	404.3	1792	$\nu(\text{C}=\text{O})$	
7.	1796	1774	363	$\begin{cases} 1762 \\ 1743 \end{cases}$	$\nu^s(\text{C}\equiv\text{O})$	
8.	1676	1673	648.5	1697	$\nu^{as}(\text{C}\equiv\text{O})$	
9.	1643	1617	35.7	1615	$\nu_{\text{Py}}(\text{CC}), \delta_{\text{Py}}(\text{CCH})$	8a
10.	1581	1540	2.1	1559	$\nu_{\text{Py}}(\text{CC}), \delta_{\text{Py}}(\text{CCH})$	8b
11.	1493	1476	115.4	1473	$\delta_{\text{Py}}(\text{CCH}), \nu_{\text{Py}}(\text{CC})$	19a
12.	1477	1474	54.5	1466	$\delta_{\text{Py}}(\text{CCH}), \nu_{\text{Py}}(\text{CC})$	19b
13.	1406	1391	200.6	$\begin{cases} 1422 \\ 1417 \end{cases}$	$\nu(\text{C-N}), \nu_{\text{Sq}}(\text{CC})$	

^a 0.8953 (RHF/6-31G*) 0.9614 (B3LYP/6-31G*).

^b B3LYP . : ν , ; δ γ ,
; τ , .
Wilson.

C-C
B3LYP/6-31G*
- **8a, 8b, 19a 19b** -
(8 cm^{-1}).
1615 cm^{-1} (PBSQ **8a.**
B3LYP/6-31G* (1617 cm^{-1}).
1792 cm^{-1}
- $\nu(\text{C}_{10}=\text{C}_{17})$. B3LYP/6-31G*
1804 cm^{-1} . 1762 1697 cm^{-1}
($\text{C}\equiv\text{O}$).
1422 cm^{-1} 1391 (B3LYP) 1406 cm^{-1}
(RHF) . C-N ,
Szafran Koput, -
-
N- C_{Sq} .
B3LYP , 1 -
:



1. PBSQ (Å) GAP T Py- Sq-
B3LYP/6-31G*

“ ” C=O , 1, C₁₀O₁₇ = 1.195 Å
C₉O₁₆ C₈O₁₈

O₁₆C₉C₇C₈O₁₈ “ ” CC . N-C₇ = 1.388 Å
1422 cm⁻¹. v(CN)

- - (CT)

4- - , (0.76)
(-0.76): 1. , p- (p-NA)
“push-pull” “ ” (- CT)
p-NA (7.856 Debye).
11.16 Debye (B3LYP/3-61G*) 12.56
Debye (RHF/6-31G*) – ,
p-NA.

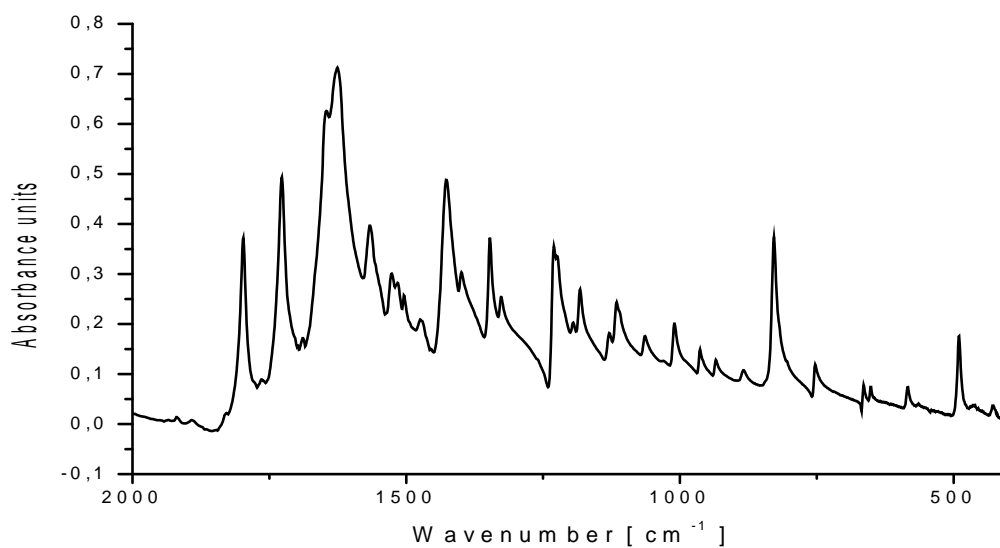
Champagne , p-NA , Del Zoppo .
265 cm⁻¹, 272 250 cm⁻¹

. 2. 3. 4-

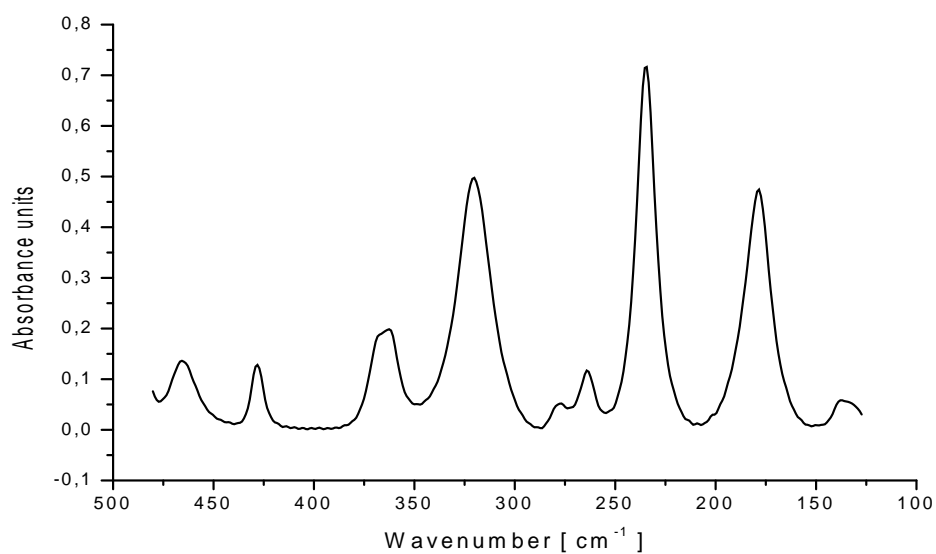
-

(1c)

o 1c (2000 – 400 cm^{-1}) 3 4. (400 – 100 cm^{-1})



3. 4- (1 mg 200 mg KBr) 2000 – 400 cm^{-1} -



4. 4- (6 mg 200 mg CsI) 400-100 cm^{-1} . -

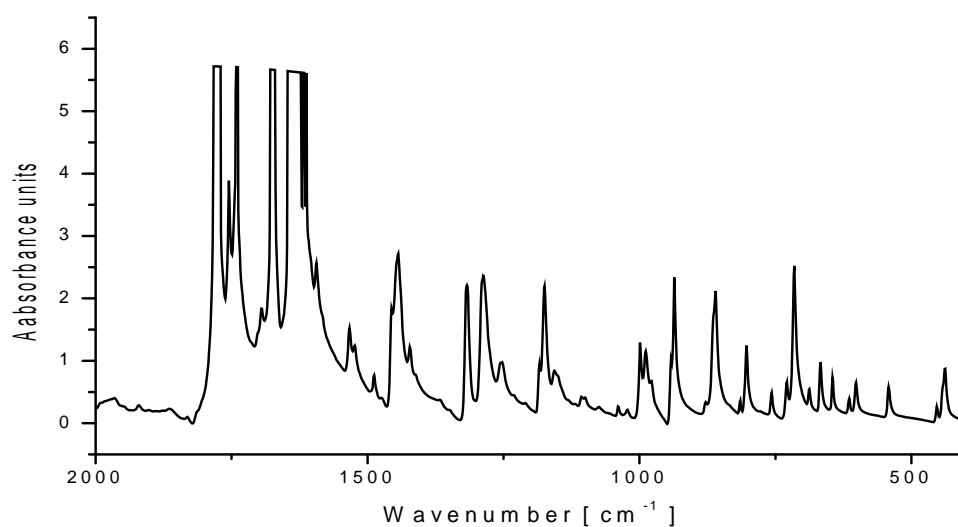
B3LYP RHF

5. 16.5 20.4 cm^{-1} .
RHF,

DFT

B3LYP.

5.						(€
cm ⁻¹)		(A	km.mol ⁻¹)	4-	-	
No	RHF	B3LYP				^b
€ _i	€ ^a	€ ^a	A	€		
11.	1796	1865	610.6	1798	v(C = O)	
12.	1770	1805	252.7	1729	v ^s (C ≡ O)	
13.	1664	1672	734.3	1649	v ^{as} (C ≡ O)	
14.	1642	1648	324.7	1635	v _{Py} (CC), δ _{Py} (CCH)	8a
15.	1525	1537	591.3	1568	v _{Py} (CC), δ _{Py} (CCH)	8b
16.	1501	1527	3.5	1528	δ _{Py} (CCH), v(C ⁴ -N ¹³)	
17.	1494	1498	27.6	1517	δ _{Me} (HCH), δ _{Py} (CCH), δ _{Py} (CCC)	19a
18.	1492	1492	2.8	1505	δ _{Py} (CCC), δ _{Py} (CCH), δ _{sq} (CCO)	
19.	1472	1475	0.1	1474	δ _{Me} (HCH), δ _{Py} (CCC)	19b^c
20.	1464	1472	15.3	1470	δ _{Me} (HCH), δ _{Py} (CCC)	
^a	0.8953 (RHF/6-31G*) 0.9614 (B3LYP/6-31G*).					
^b	B3LYP . : v, ; δ γ, ; τ, .					
^c	Wilson.					
1798 cm ⁻¹	v(C = O)					1792 cm ⁻¹
PBSQ,	PBSQ.					1762 cm ⁻¹
1729 cm ⁻¹ ,	v ^s (C ≡ O),					1697 cm ⁻¹
“	1649 cm ⁻¹ .					“
Debye,	4- - 18.0					- 392 – 395 °C.
. 2. 6. 4-	(1f)					
	(2000 – 400 cm ⁻¹) o 4- 5.					-
	1f					
6,	4-					.



5. 4-
(1 mg 200 mg KBr) 2000 – 400 cm⁻¹ -

6. 4- 4-
(4-BP) (4B-PBSQ)

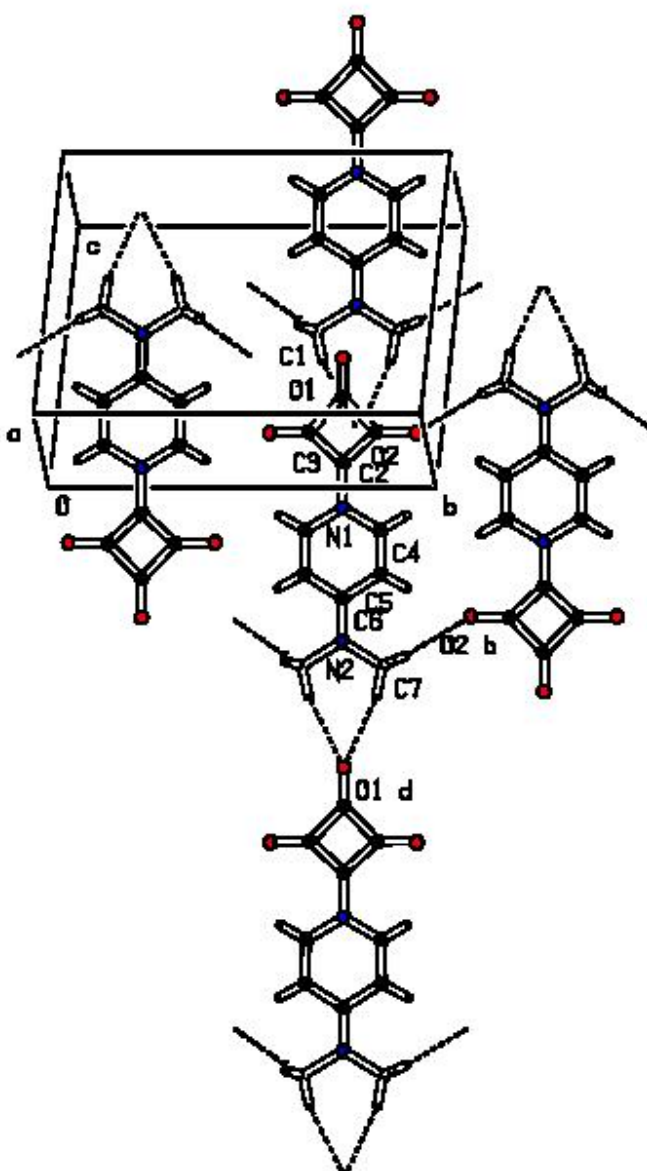
No	<u>4-BP</u>		<u>4B-PBSQ</u>	
v _i	()	()	()	
10.			1778	v(C=O)
11.			1740	v ^{as} (C≡O)
12.			1695	v ^s (C≡O)
13.	1657	1662	1675	v _{Bz} (C=O)
14.	1597	1596	1624	8a
15.	1597	1598	1594	8a*
16.	1576	1570	1524	8b*
17.	1549	1551	1533	8b
18.	1491	1490	1488	19a*
19.	1491	1488	1474	19a
20.	1446	1449	{1444 1456	19b*
21.	1409	1412		19b

* “ ”

4- - 4-

v(C=O)

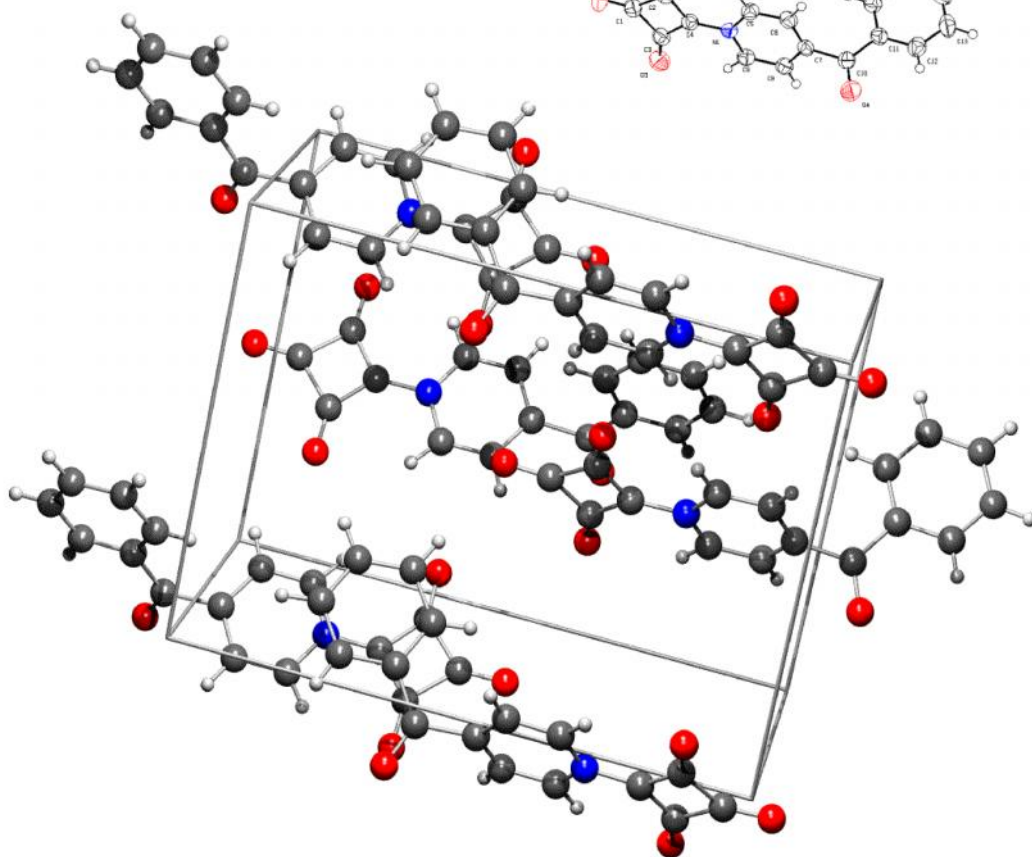
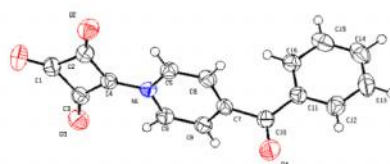
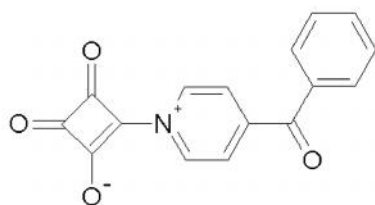
O2 O2 e C-H .
 .
 2 2 -
 .
 ,
 6.
 . 3. 2. 4- -
 (1f)
 4- -
 . , -
 , Λ -
 .
 ,
 ,
 - 30 GW/cm².
 . 4-
 :
 — π - ; —
 (),
 ;
 —
 . 100 C, 7
 , 1f.



—

4-Benzoylpyridinium betaine of squaric acid

Pna2₁

$$a = 14.6707(14)$$
$$b = 8.1155(9)$$
$$c = 10.4940(10)$$


7.

(1f)

4-

-

III. B.

2-(5,5-

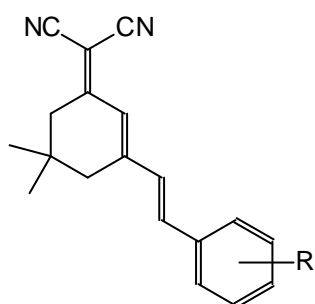
-3-

-2-

}

EFISH

7,



7.

2	R = H	2j	R = 4- H-3-OCH ₃
2b	R = 4-CH ₃	2k	R = 2- H-5- NO ₂
2c	R = 3-OH	2l	R = 2- OCH ₃ -4- OCH ₃
2d	R = 4-OH	2m	R = 3- OC ₂ H ₅ -4- OCH ₃
2e	R = 2-OCH ₃	2n	R = 2- OCH ₃ -4-OCH ₃ -6-OCH ₃
2f	R = 4-CN	2o	R = 3- H-4- OCH ₃ -5-I
2g	R = 4-N(CH ₃) ₂	2p	R = 3-OCH ₃ -4-OH-5-NO ₂
2h	R = 4-NO ₂	2q	N-
2i	R = 2- H-3-OCH ₃	2r	1H-

III. B. 1.

III.A.1. o

λ_{\max}

(III. .1.),
CT - 1.

8
2 (λ_{max} λ_{max} , c $\log \nu$):

8.

	λ_{max} [nm]	c [$\times 10^{-4}$ mol.l ⁻¹]	$\log \nu$
2	394 (CHCl ₃)		
2d	414 (CH ₂ Cl ₂)	3.1864	4.723
	418 (CH ₃ CN)	2.7765	4.751
	426 (CH ₃ OH)	3.7171	4.664
	445 (CHCl ₃)		4.517
2e	401 (CH ₃ OH)		4.441
	404 (C ₂ H ₅ OH)	3.7123	4.427
	414 (CHCl ₃)		4.574
2g	483 ()	3.1173	4.515
	500 (C ₂ H ₅ OH)	2.8105	4.204
	504 (CHCl ₃)	3.1202	4.504
2l	430 (CH ₃ OH)		4.401
	431 (C ₂ H ₅ OH)	4.2431	4.403
	436 (CHCl ₃)		4.473

2n	440 (CH ₂ Cl ₂)	3.8963	4.351
	440 (CH ₃ CN)	3.9595	4.414
	443 (CH ₃ OH)		4.333
	451 (CHCl ₃)		4.489
2q	457 (CH ₃ OH)	2.4848	4.363
2r	476 (CH ₃ OH)	3.2991	4.592

, **2**, 394 nm

p- λ_{\max} - 8. - **2d** - λ_{\max} 445 nm (CHCl₃). 2- 20 nm

394 nm, **2**, 414 nm.

4- λ_{\max} - λ_{\max} 504 nm ($\Delta\lambda_{\max} = 110$ nm) CHCl₃. 2, 4 6 56

nm. λ_{\max} , σ -

4- λ_{\max} 436 nm (). **2n** λ_{\max} 451 nm . .

N- **2q**, λ_{\max} **2q** 470 nm.

2r $\lambda_{\max} = 476$ nm. 1H-

383 nm (), **2h** - 389 nm (). λ_{\max} - **2f** λ_{\max} (nm), 4-NO₂ - 4-CN - 8.

λ_{\max} - $\Delta\lambda_{\max} = 110$ nm. 90 nm, a N- 75 nm.

III. B. 2.

(Gaussian, Gamess .) ,
 (Density
Functional Theory – DFT) ,
 DFT, *ab initio* ,
 DFT
 HF MP2 (Møller-Plesset,
 : *Second-order Møller-Plesset perturbation theory*)
 DFT
 , 2-{5,5- -3-[(2-)] -
 2-{5,5- -3-[(4-)] -
 2- }
 B3LYP/6-31G*.
 push-pull ,
 (o
 ;
).
 8 2-{5,5- -3-[(2-)] -2- } -
 ,
 ,
 Wortmann .
 ,
 394 nm () ,
 f = 0.92.
 ,
 DFT.
 2-{5,5- -3-[(4-)] -2- } ,

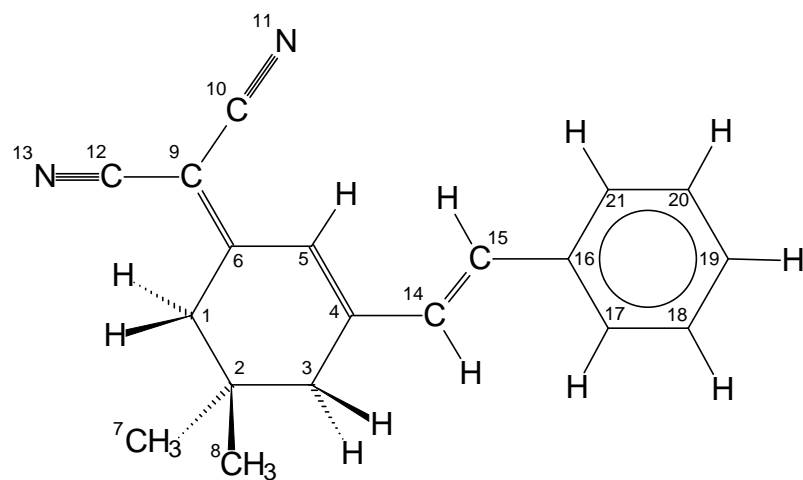
DFT

(EFISHG).

DCPM p- (**2g**) $\lambda_{\max} = 519 \text{ nm}$ (NMP);
 $\beta = 246 \times 10^{-30} \text{ esu}$ (μ) 8.7 Debye.
 1907 nm),

B. 2. 1. 2-{5,5- **-3-[(2-**)] **-2-** }-
(2a)

3
 - 2-{5,5- -3-[(2-)] -2- }-
 (DCPM).



3. DCPM,

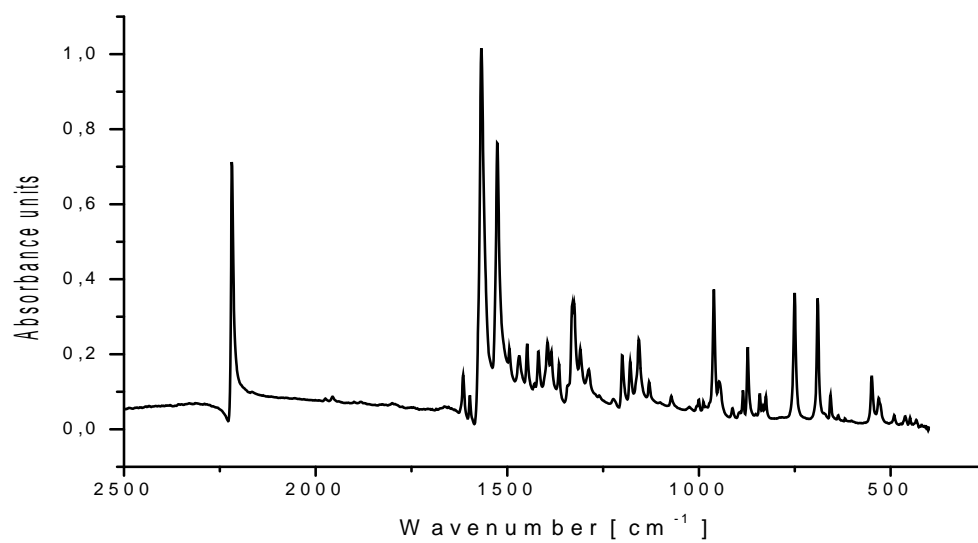
2 $2500 - 400 \text{ cm}^{-1}$,
 8. (**9.**

KBr,
 CsI)
 DPCM

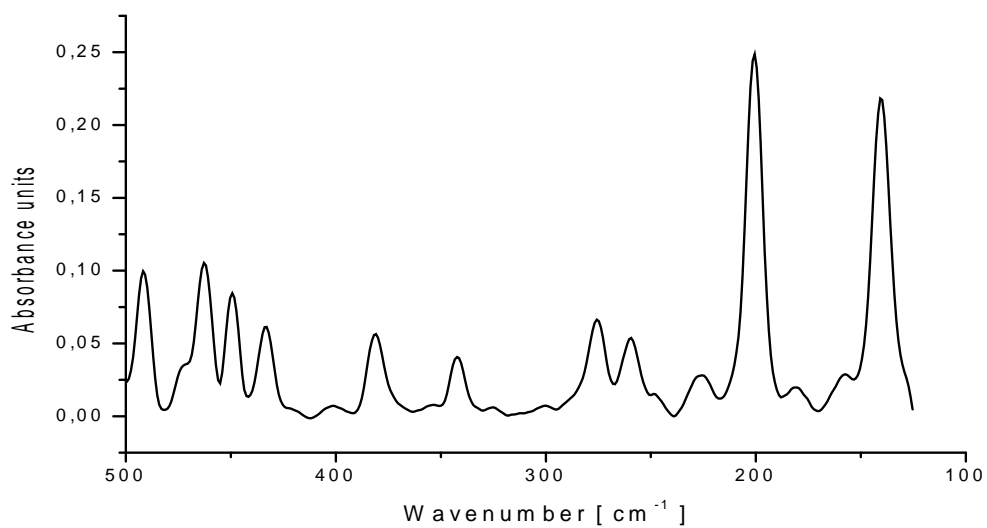
10.

9.

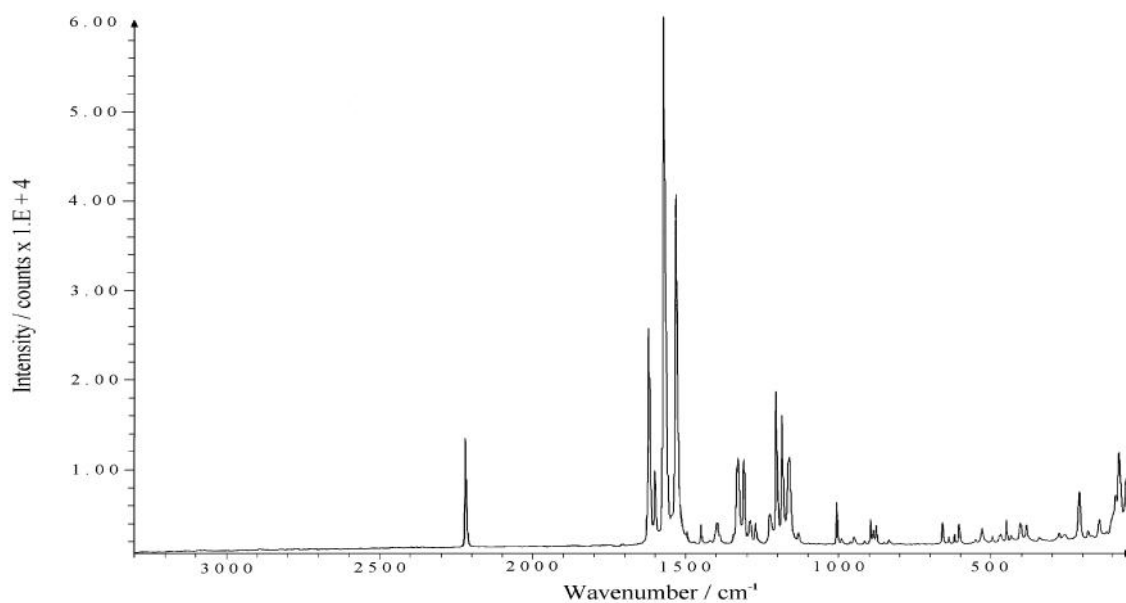
Wilson,



cm⁻¹ **8.** DPCM (1 mg 200 mg KBr) 2500 – 400



– 100 cm⁻¹ **9.** DPCM (6 mg 250 mg CsI) 500



10. DPCM 4000 – 30 cm^{-1}

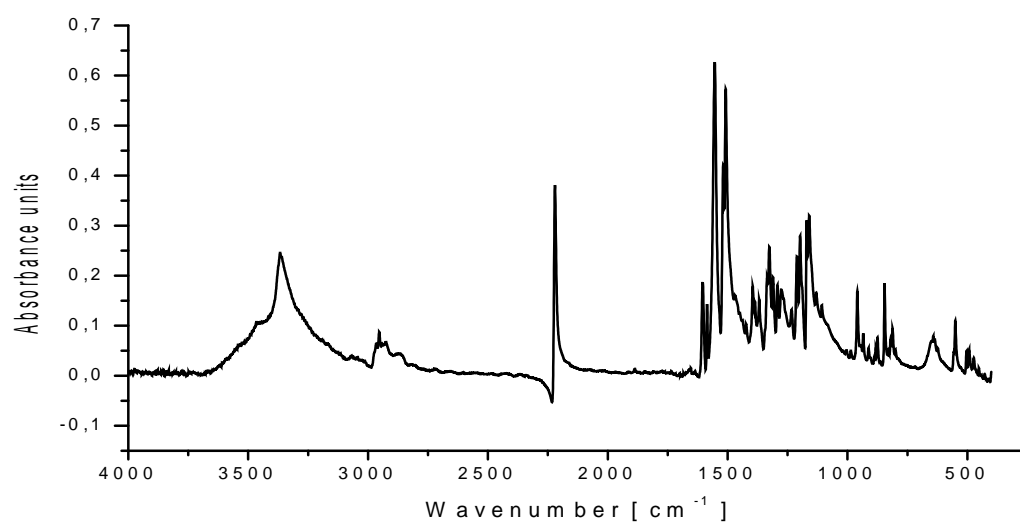
(9) . 8.5 cm^{-1} .
9. (v cm^{-1}) (A km.mol^{-1}) DCPM.

No.	<u>B3LYP</u>						^b
ν_i	ϵ	ϵ^a	A	()	()		
19.	2337	2247	107.9			$\nu^{\text{as}}(\text{CN})$	
20.	2322	2232	28.2	2218	2218	$\nu^{\text{s}}(\text{CN})$	
21.	1687	1622	43.4	1615	1617	$\nu(\text{C}^{14}=\text{C}^{15})$	
22.	1659	1595	5.6	1598	1599	8a	
23.	1633	1570	19.0			8b	
24.	1607	1545	468.8	1567	1566	$\nu(\text{C}^4=\text{C}^5)$	
25.	1566	1506	283.9	1525	1527	$\nu(\text{C}^6=\text{C}^9)$	
26.	1545	1485	3.1	1494	1496	19a	
27.	1541	1482	3.2	1468		$\delta(\text{CH}_3)$	
31.	1498	1440	29.3	1448	1449	19b	

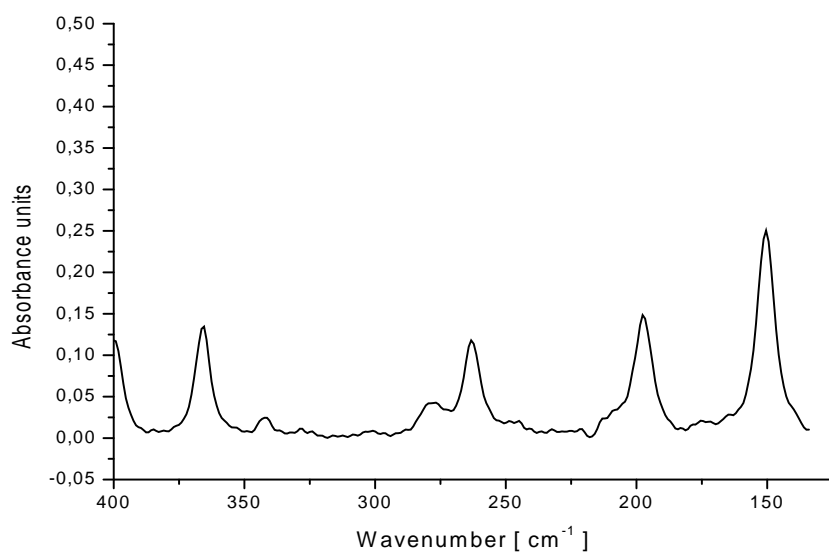
^a 0.9614 (B3LYP/6-31G*).

^b B3LYP . : ν , ; δ γ ,
; τ ,
Wilson.

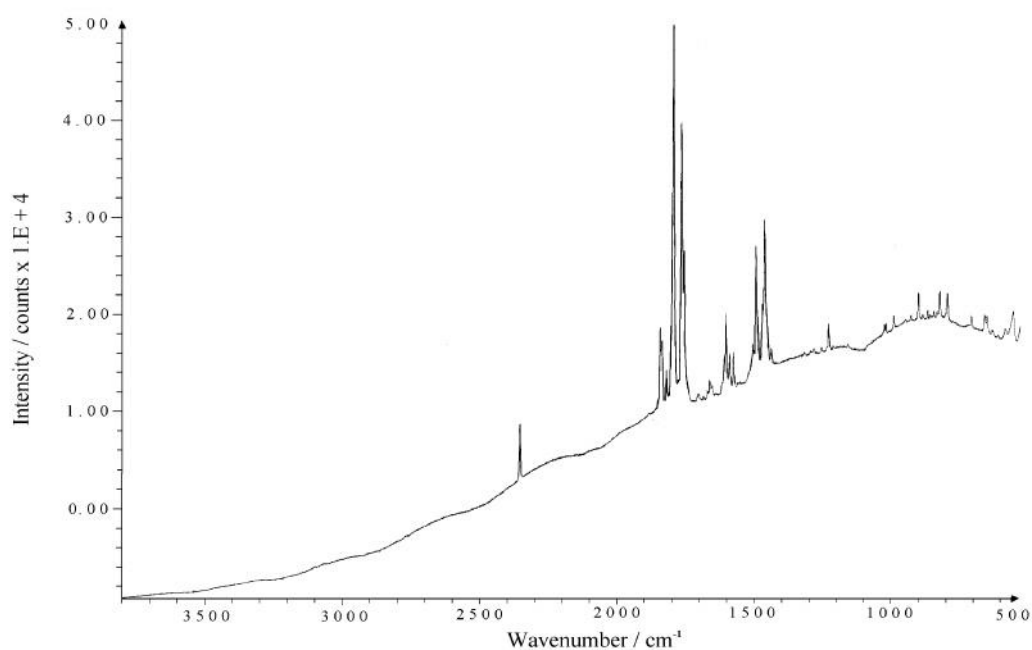
C_1 DPCM
 $v(C^4=C^5) \quad v(C^6=C^9)$ CC : $v(C^{14}=C^{15})$,
 $1622 - 1506 \text{ cm}^{-1}$ (B3LYP/6-31G*).
 $1615 - 1525 \text{ cm}^{-1}$ ().
 $(1617 - 1527 \text{ cm}^{-1})$.
 1545 cm^{-1} ($\nu = 468 \text{ km.mol}^{-1}$)
 1567 () 1566 cm^{-1} ().
 15 cm^{-1}
 $\nu^s(CN) \quad \nu^{as}(CN)$,
 2218 cm^{-1} .
19b **14** CC **8a, 8b, 19a,**
 cm^{-1} . B3LYP/6-31G*, **8**
8b -
 1566 cm^{-1} **8b**
19a **19b** - 9.
 $1567 \quad 1525 \text{ cm}^{-1}$ () $1615 \quad 2218 \text{ cm}^{-1}$
 $1617 \quad 2218 \text{ cm}^{-1}$, $1566, 1527$
DPCM
8.80 Debye, - p-NA.
(CT),
B. 2. 3. 2-{5,5- **-3**-[2-(4-)] **-2-**
(2d)
(KBr) (11 12.
CsI) **2d** 13.
B3LYP
10,



11. **2d** (1 mg 200 mg KBr) 4000 – 400 cm⁻¹



12. **2d** (6 mg 250 mg CsI) 400 – 100 cm⁻¹



13. 2d 4000 – 30 cm⁻¹

10.

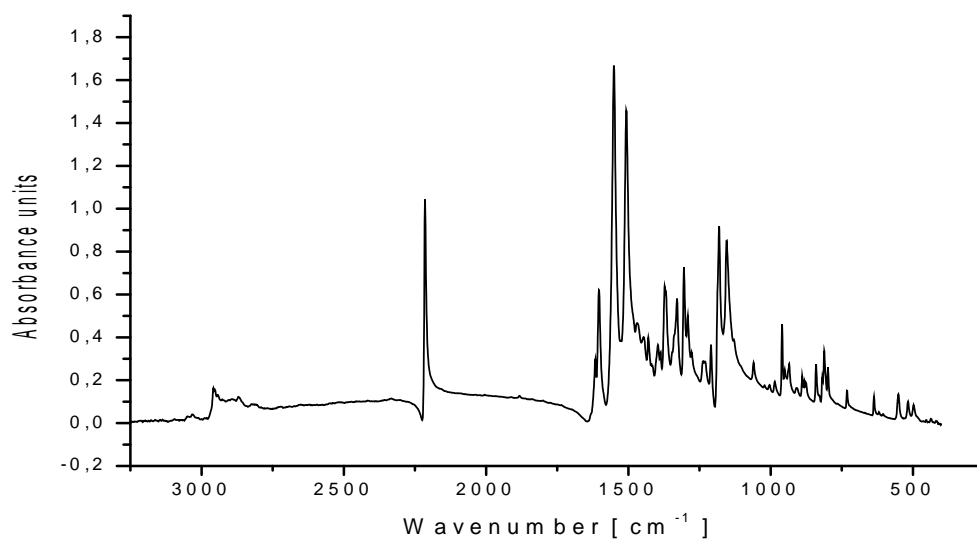
(v cm⁻¹) (A km.mol⁻¹) 2-{5,5- -3-[2-(4- -

No.	B3LYP						b
v _i	€	€ ^a	A	()	()		
1.	3745	3600	112.2	3364		v(O-H)	
19.	2335	2245	130.1	2220		v ^{as} (CN)	
20.	2320	2230	32.7		2222	v ^s (CN)	
21.	1685	1620	18.0		1614	v(C ¹⁴ =C ¹⁵)	
22.	1669	1605	179.6	1603	1605	v(Ph)	
23.	1635	1572	1.2	1586	1587	v(Ph)	
24.	1599	1537	930.5	1554	1554	v(C ⁴ =C ⁵)	
25.	1565	1505	24.3	1539	1537	v(Ph)	
26.	1560	1500	497.8	1518	1520	v(C ⁶ =C ⁹)	
27.	1541	1482	1.9	1506	1510	δ(CH ₃)	

^a 0.9614 (B3LYP/6-31G*).

^b B3LYP . ; v, ; δ γ, ; τ, .
Wilson.

3745 cm^{-1} , (= 112.2 km.mol^{-1}).
3364 cm^{-1} .
,
,
,
,
,
v(O-H)
,
(
.
III.B.3.)
v(O-H),
:
9.2 cm^{-1} .
15 cm^{-1} , 2220 cm^{-1} ,
2222 cm^{-1} .
- , 2 cm^{-1}
.
, 1620 cm^{-1} ,
1614 cm^{-1} . -
1603 cm^{-1} .
- 1554 cm^{-1} . 1500
 cm^{-1} 1518 cm^{-1} ().
,
.
,
,
.
() CC ,
0.017 Å. C-O - 0.004
1.367 Å. 1.361 Å,
2-{5,5- -3-[2-(4-
)]- -2- } 8.90 Debye.
-
,
(
).
B. 2. 5. 2-{5,5- -3-[2-(4-)] -2-
}
(2g)
(3200 – 400 cm^{-1}) 2-{5,5- -3-[2-(4-
)] -2- }
14.



14.

2g (1 mg 200 mg KBr)

3200 – 400 cm⁻¹

2g

11.

11.

2-{5,5-

-3-[2-(4-

)]

-2-

}

No. v _i	() [cm ⁻¹]	
20.	2214	v ^{as} (CN)
21.	1616	v(C ¹⁴ =C ¹⁵)
22.	1604	v _{Ph} (C-C)
23.	1551	v(C ⁴ =C ⁵)
24.	1507	v(C ⁶ =C ⁹)
25.	1482	v _{Ph} (C-C)
26.	1469	δ(CH ₃)
27.	1446	δ(CH ₃) // v _{Ph} (C-C)
28.	1429	δ(CH ₃)
29.	1418	δ(C ¹ H ₂), δ(C ³ H ₂)

p-

v(C-H)

11.

-

,

.

-

– 2214 cm⁻¹.

.

1616 1604

cm⁻¹.

,

11,

1616 cm⁻¹

1551 cm⁻¹,

1507 cm⁻¹,

p-

B. 3.

B. 3. 2.

2-{5,5-
-3-[2-(4-
(2d)
-2-
}
- 205 – 207 °C,
615 nm (CH₃COCH₃)
490 (H₂O)

{5,5-
-3-[2-(4-
Pna2₁.
)]
C-
-2-
C(CH₃)₂,
} 0.624 (2) Å

CN [O-H...N: O...N 2.958 (3) Å O-H...N 173°]
[013].

15

2d.

B. 3. 5.

-4-
)]
-2-
2-{5,5-
-3-[2-(4-
)]
-2-
}
(2m)

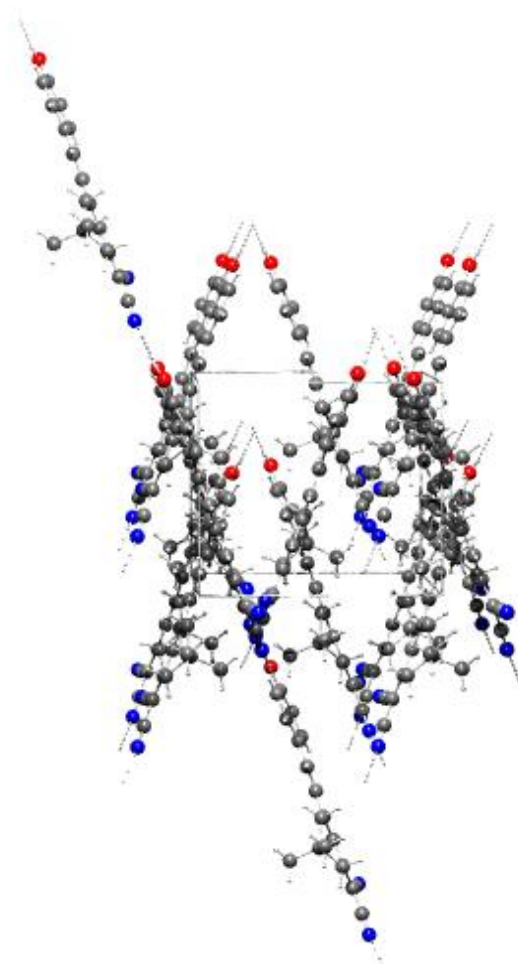
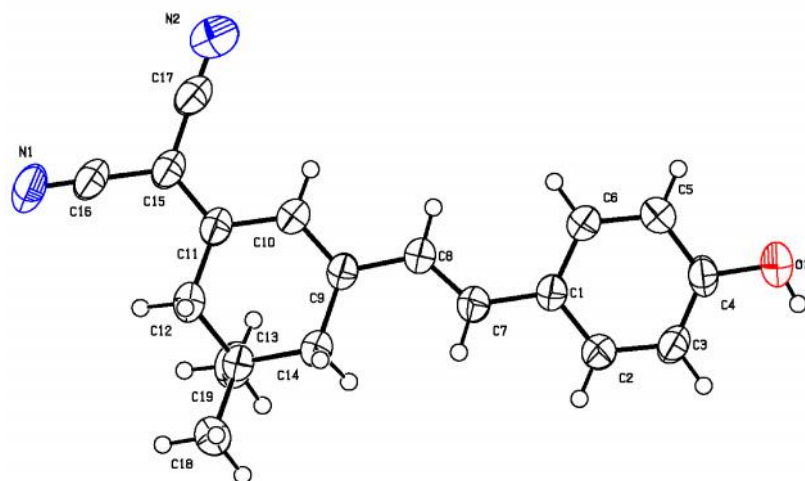
194 – 195 °C.

180 °C

(disorder).

P12₁/n1.

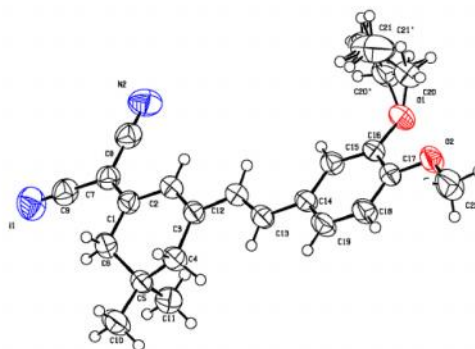
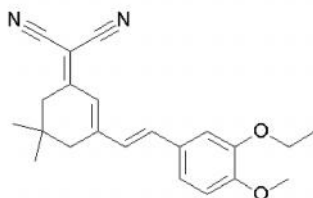
16.



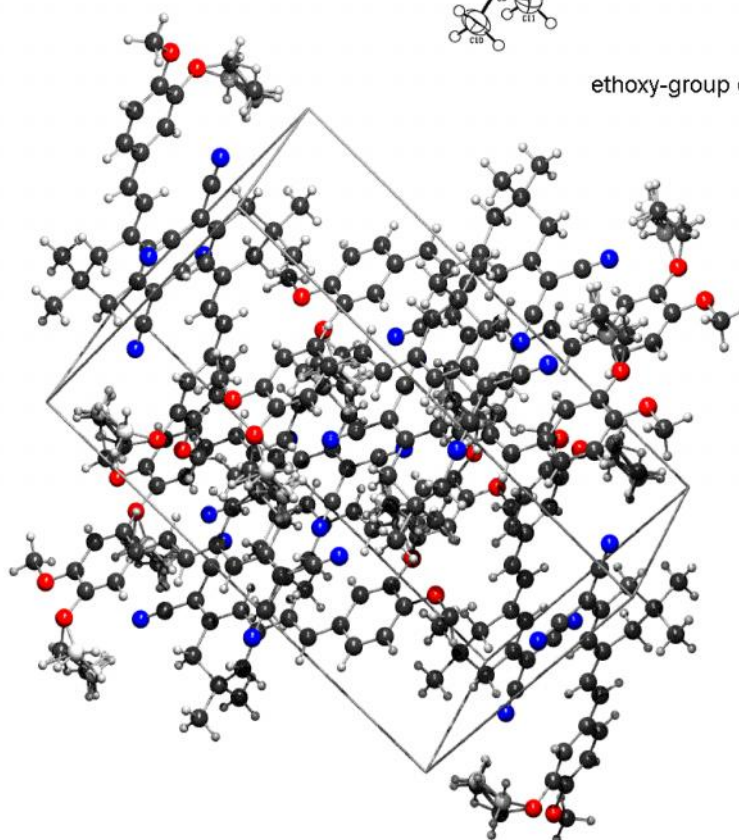
15. $a = 15.4413 (3) \text{ \AA}, b = 10.9988 (3) \text{ \AA}, c = 9.5699 (2) \text{ \AA}, Z = 4$, *Pna*2₁

)] -2- } 2-{5,5- (2d) -3-[2-(4-

2-{3-[2-(3-ethoxy,4-methoxy-phenyl)-vinyl]-
5,5-dimethyl-cyclohex-2-enylidene}-malononitrile



ethoxy-group disordered



P12₁/n1

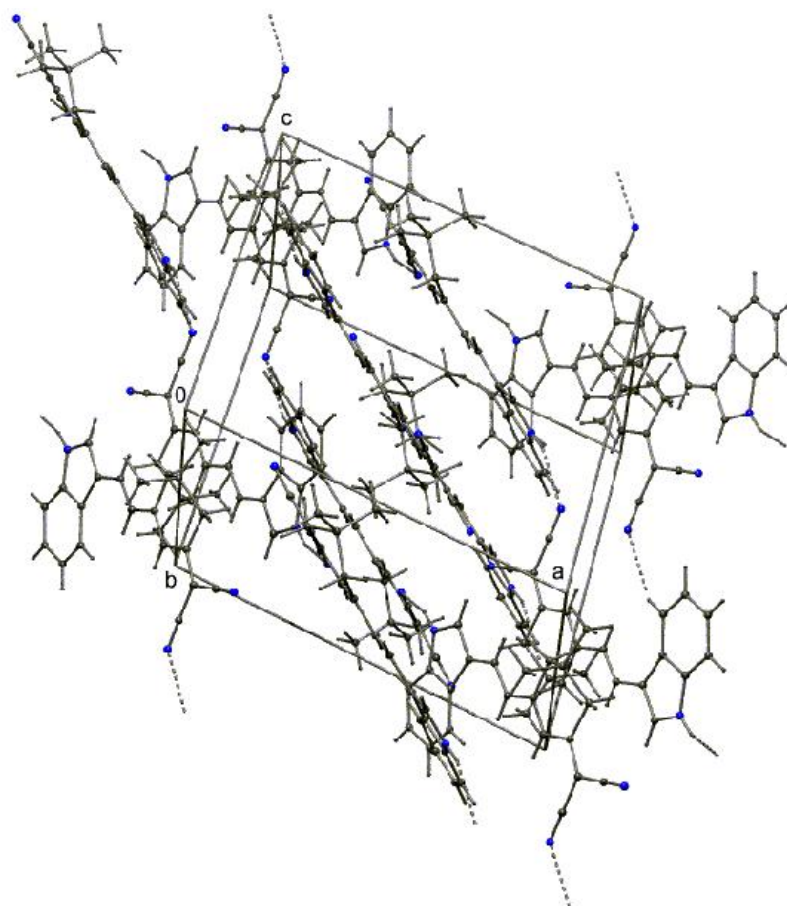
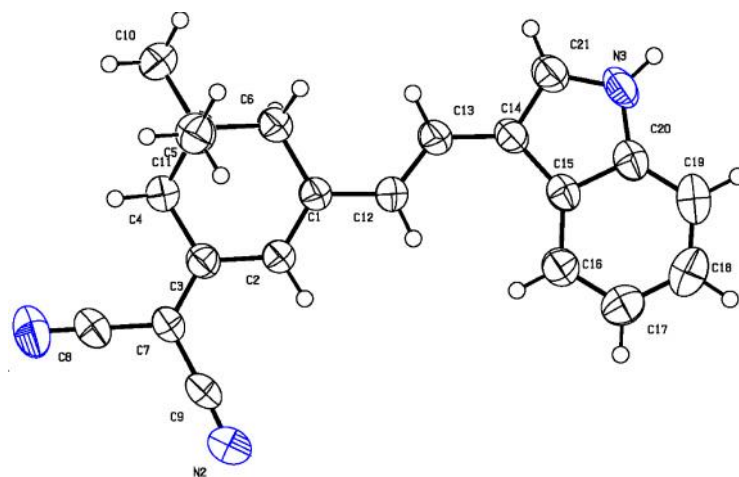
a = 7.559(1)
b = 19.943(2)
c = 12.990(2)
 β = 93.62(2)

16. M)] -2- } 2-{5,5- -3-[2-(3- (2m)

B. 3. 7. **2-{5,5-** **-3-[2-(1H-**
-3-)] **-2-** } **(2r)**

“guest-host”
 $\lambda_{\text{max}} = 476 \text{ nm}$
“guest-host”
“ ”
P2₁/n.
C(CH₃)₂,
C- 0.627 (2) Å
N-H
[N...N 3.168 (3) Å N-H...N 148°],
[10 $\bar{1}$]
 $\nu_{\text{N-H}} = 3390 \text{ cm}^{-1}$
(KBr). C-H
2r 17.

“push-pull” **1 -I** (3- 4-
2a-r (-
2-{5,5- **-3-[(2-**)]- **-2-** }-
).
,
ab initio DFT -
9
:



$a = 15.5033 (3) \text{ \AA}$, $b = 7.5309 (2) \text{ \AA}$, $c = 15.9609 (4) \text{ \AA}$, $S = 110.774 (1)$, $Z = 4$, $P2_1/n$

17. $-3-) [-2- \}$ 2-{5,5- -3-[2-(1H- (2r)

1.

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2b, 2d, 2e, 2l, 2m, 2n 2r
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2n
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2d
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2b
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2m “ ”
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2.

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ab initio DFT
DFT
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RHF
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O-H N-H
2.

3.

- **1a-l**
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CT
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- :
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