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Table S1 Crystallographic data for compounds **1-4**

	1	**2-I**	**2-II**	**2-III**	**3**	**4**
Molecular formula	$C_{20}N_2H_{12}$	$C_{20}N_2H_{12}$	$C_{20}N_2H_{12}$	$C_{20}N_2H_{12}$	$C_{20}N_2H_{12}$	$C_{20}N_2H_{12}$
Temperature (K)	293(2)	293(2)	293(2)	293(2)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
space group	Pbca	$P2_1/c$	C2/c	Pbcn	$P2_1/n$	$P2_1/c$
Unit cell dimensions:						
a (Å)	15.7823(7)	18.418(2)	20.3520(6)	16.062(1)	13.933(2)	9.957(3)
b (Å)	8.7508(4)	13.829(1)	9.0912(3)	7.8336(5)	5.869(1)	22.606(6)
c (Å)	19.8826(9)	11.274(1)	7.5400(2)	21.484(1)	17.354(2)	6.205(2)
α (°)	90	90	90	90	90	90
β (°)	90	107.010(2)	92.280(1)	90	104.734(3)	104.21(1)
γ (°)	90	90	90	90	90	90
Volume ($Å^3$)	2745.9(2)	2745.9(5)	1393.99(7)	2703.3(3)	1372.5(3)	1354.0(6)
Z	8	8	4	8	4	4
absorption coeff. (mm^{-1})	0.08	0.08	0.08	0.08	0.08	0.08
F(000)	1168	1168	584	1168	584	584
Crystal size (mm)	0.25 x 0.1 x 0.1	0.2 x 0.2 x 0.1	0.3 x 0.1 x 0.1	0.3 x 0.3 x 0.1	0.2 x 0.2 x 0.1	0.3 x 0.2 x 0.2
θ range (°)	2.0 - 23.25	1.1 - 32.0	2.0 - 32.8	2.3 - 29.9	2.0 - 23.28	1.8 – 23.25
Reflections collected (unique)	24627 (1965)	30420(8931)	14182 (2434)	23933 (3731)	8304(1986)	10773 (1942)
Rint	0.0525	0.0352	0.0606	0.0258	0.0339	0.1487
Data/restraints/parameters	1965 / 12 / 247	8931/0/493	2434/ 0 / 100	3731 / 0 / 247	1986 / 0 / 200	1942 / 0 /200
Goodness-of-fit on F^2	1.298	1.029	1.01	1.017	1.131	0.933
Final R_1 wR_2 [I>2σ(I)]	0.0806, 0.1721	0.0486, 0.1217	0.0553, 0.1256	0.0391, 0.1028	0.0532, 0.1353	0.0630, 0.1430
Final R_1 wR_2 (all data)	0.0833, 0.1736	0.1075,0.1489	0.1510, 0.1768	0.0583, 0.1172	0.0763, 0.1515	0.1428, 0.1845
Largest diff. peak and hole ($eÅ^{-3}$)	0.20, -0.27	0.22, -0.17	0.31, -0.20	0.20, -0.17	0.15, -0.14	0.26, -0.21

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Table S2 The shorter C-H---N intermolecular distances for the mono-aza and diaza[5]helicenes characterized in this work or known from the literature

[5]helicene	label	C---N distances (Å)	Reference in the paper
carbo	**8a-I**	-	14, 15
	8a-II	-	15
1-aza	**9**	3.958(2)	*unpubl.*
4-aza	**10**	3.47(3), 3.52(2)	2
5-aza	**11**	3.787(1)	2
6-aza	**12**	3.516(2), 3.544(2)	2
7-aza	**13**	3.583(5)	*unpubl.*
1,7-diaza	**3**	3.557(5)	this work
1,12-diaza	**4**	3.663(6), 3.669(6), 3.714(7)	this work
1,14-diaza	**14**	3.800	5
4,11-diaza	**1**	3.314(5), 3.420(5), 3.667(5), 3.835(5)	this work
5,10-diaza	**2-I**	3.546(2), 3.603(2), 3.612(2), 3.625(2), 3.641(2), 3.670(3), 3.689(2)	this work
	2-II	3.468(3), 3.784(3)	this work
	2-III	3.374(2), 3.796(2), 3.818(2)	this work

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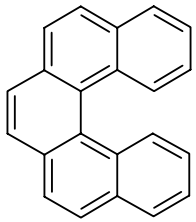

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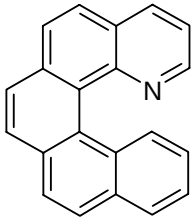

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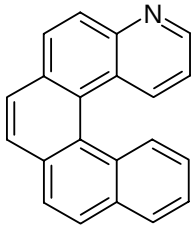

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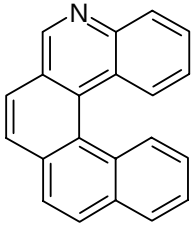

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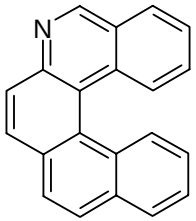

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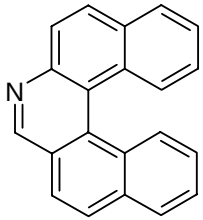

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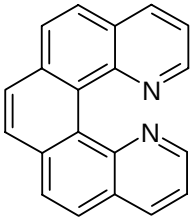

14

Scheme S1

Chemical Structures of compounds **6-14**

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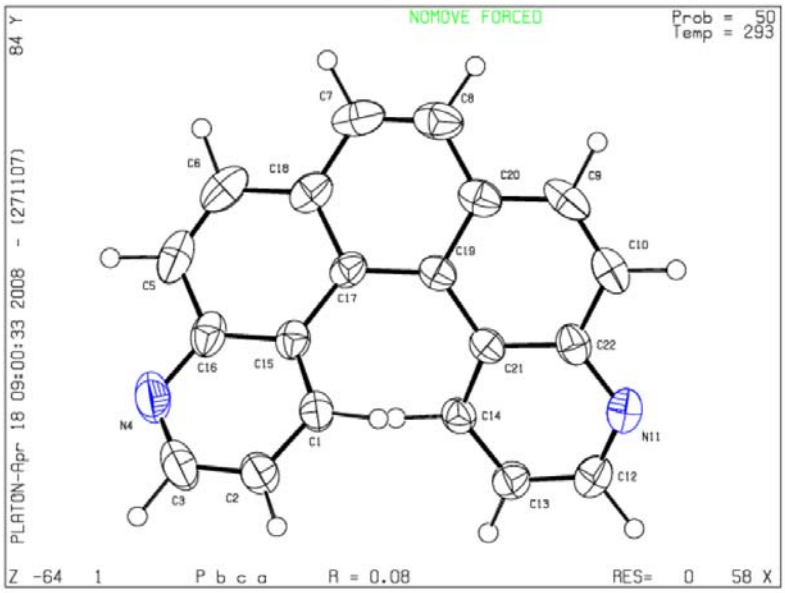
Labeling scheme for the crystallographic structures deposited



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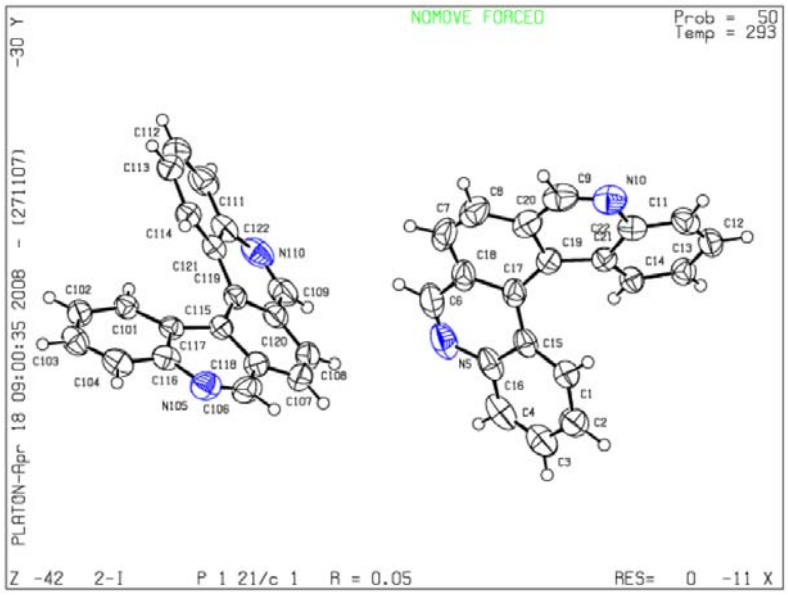
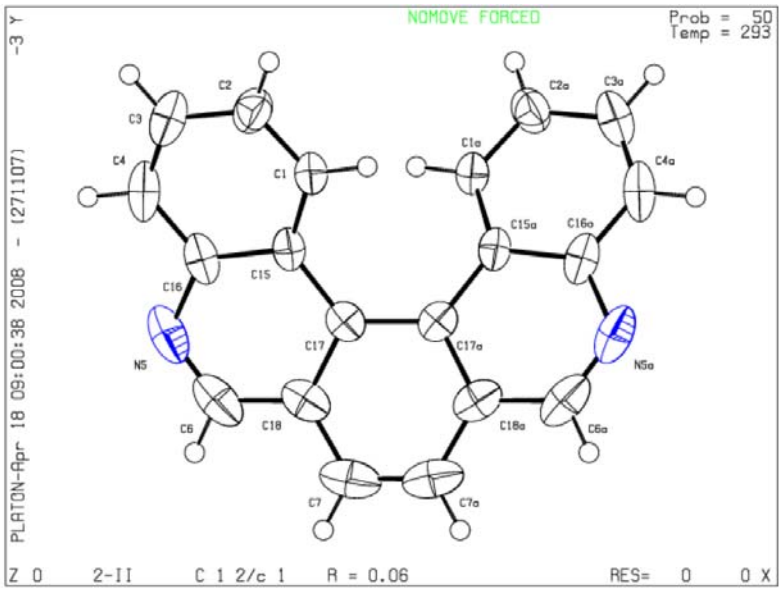


2-I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C4
C1
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C3a
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C4a
C15a
C16a
C15
C16
N5
C17
C17a
N5a
C6
C18
C18a
C6a
C7
C7a
Z 0
2-II
C 1 2/c 1
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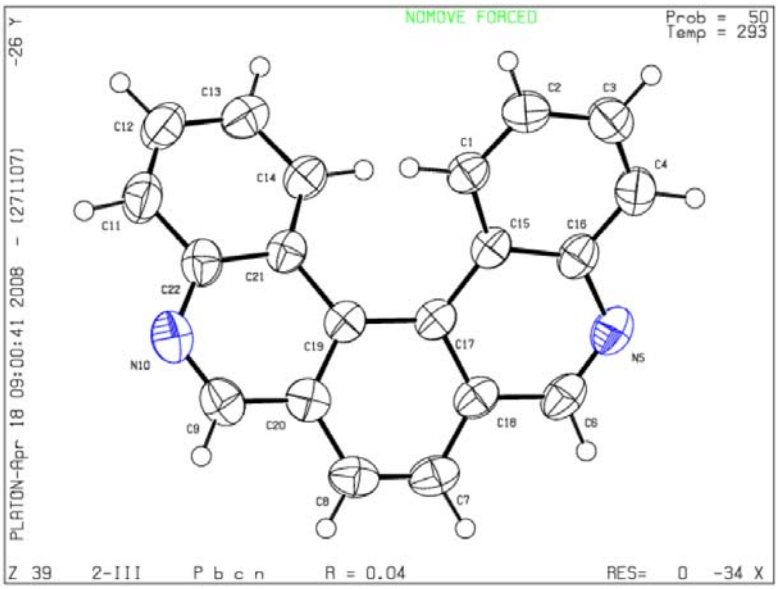
RES= 0 0 X

2-II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C12
C14
C11
C2
C3
C1
C4
C15
C16
C22
C21
N10
C19
C17
N5
C9
C20
C18
C6
C8
C7
Z 39
2-III
P b c n
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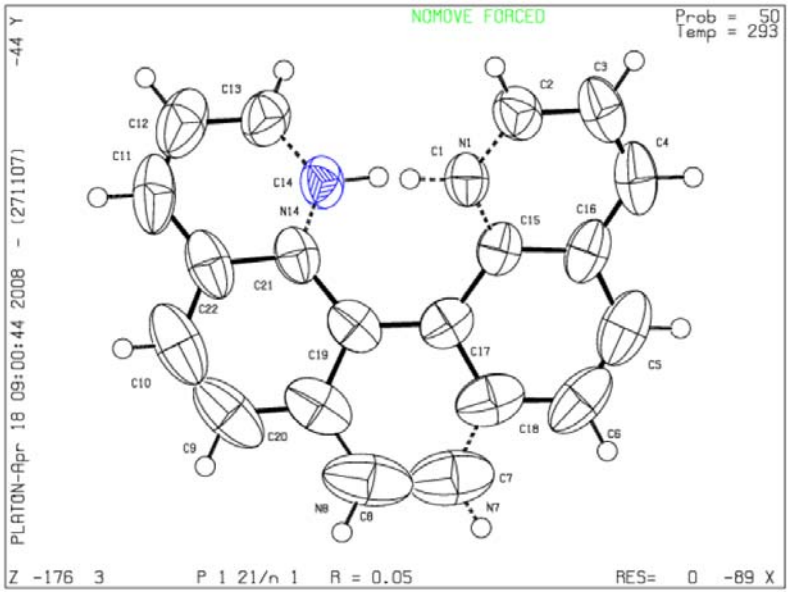
RES= 0 -34 X

2-III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C14
N14
C21
C22
C10
C9
C20
C19
C1
N1
C2
C3
C4
C15
C16
C17
C5
C18
C6
C7
N8
C8
N7
Z -176 3
P 1 21/n 1
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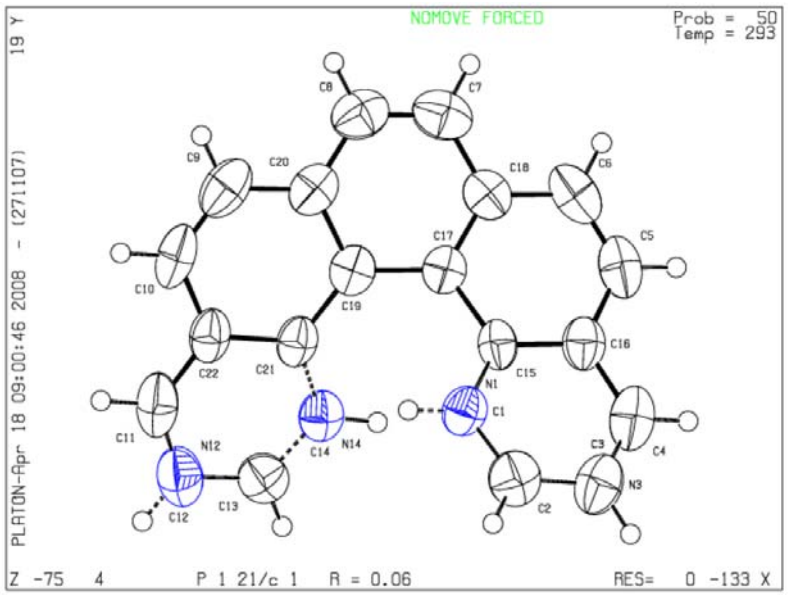
RES= 0 -89 X

3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C17
C5
C19
C22
C21
C16
C15
N1
C1
C11
N12
C14
N14
C3
C4
C13
C2
N3
C12
Z -75 4
P 1 21/c 1
R = 0.06
RES= 0 -133 X

4