First Synthesis of Dendritic Polyphenylazomethines and the Structural Studies

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Supporting Information

X-ray crystallographic data file (CIF) for DPA G2

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Department of Chemistry
Faculty of Science and Technology
Keio University
Hiyoshi 3-14-1, Kohoku-ku
Yokohama 223-8522
Japan
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#           Data items needed for deposition
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This CIF is aimed for Cambridge Structural Database.
The original paper has been submitted.

Journal:
Journal of the American Chemical Society

Title:
First Synthesis of Phenylazomethine Dendrimer Ligands and Structural Studies

Authors:
Masayoshi Higuchi, Satoshi Shiki, Katsuhiko Ariga, Kimihisa Yamamoto

;
# TITLE

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Supplementary Information of X-ray Crystal Analysis of DPA G2
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;
Department of Chemistry
Faculty of Science and Technology
Keio University
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Yokohama 223-8522
Japan
;

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The crystals were grown by slow diffusion of methanol vapor into a chlorobenzene solution of the compound. The crystal was sealed in a capillary with mother liquor to avoid efflorescence.
;

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X-ray intensities were measured for +h, -k, +-l (\q<69.1\%) and +-h, +k, +-l (\q<30.0\%) reflections. All H-atom positions attached to carbon atoms were calcurated geometrically, with U~iso~(H) = 1.2U~eq~(parent atom). There exists a positional disorder on the oxygen and carbon atoms in methanol of crystallization. The site occupancy factors of each set of the disordered oxygen and carbon atoms (O46, C48 and O47, C49) were assumed to be 0.3 and 0.2, respectively.
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_publ_section_references
;
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O47   O  0.0372(7)  0.428(3)   0.550(2)   0.17(1)    Uani 0.20 d P . .
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N2    N  0.2306(1)  0.2446(4)  1.5341(2)  0.0804(9)  Uani 1.00 d . . .
N3    N  0.1488(1)  -0.1239(4) 0.9483(2)  0.0833(10) Uani 1.00 d . . .
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C9    C  0.1339(2)  0.4023(5)  1.3370(2)  0.085(1)   Uani 1.00 d . . .
C10   C  0.1635(2)  0.3807(6)  1.4222(2)  0.094(1)   Uani 1.00 d . . .
C11   C  0.1980(2)  0.2577(5)  1.4469(2)  0.0710(10) Uani 1.00 d . . .
C12   C  0.2051(2)  0.1576(6)  1.3847(2)  0.087(1)   Uani 1.00 d . . .
C13   C  0.1747(2)  0.1789(5)  1.2988(2)  0.081(1)   Uani 1.00 d . . .
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C16   C  0.1618(2)  -0.0757(5) 1.5168(3)  0.083(1)   Uani 1.00 d . . .
C17   C  0.1138(2)  -0.1622(7) 1.4955(3)  0.109(2)   Uani 1.00 d . . .
C18   C  0.0694(2)  -0.1158(9) 1.5229(4)  0.121(2)   Uani 1.00 d . . .
C19   C  0.0726(2)  0.0189(9)  1.5688(4)  0.116(2)   Uani 1.00 d . . .
C20   C  0.1195(2)  0.1040(6)  1.5905(3)  0.091(1)   Uani 1.00 d . . .
C21   C  0.2511(1)  0.1556(5)  1.6791(2)  0.0676(9)  Uani 1.00 d . . .
C22   C  0.2345(2)  0.0719(5)  1.7410(2)  0.081(1)   Uani 1.00 d . . .
C23   C  0.2646(2)  0.0832(6)  1.8275(3)  0.100(2)   Uani 1.00 d . . .
C24   C  0.3104(2)  0.1736(7)  1.8503(3)  0.108(2)   Uani 1.00 d . . .
C25   C  0.3287(2)  0.2513(6)  1.7882(3)  0.103(2)   Uani 1.00 d . . .
C26   C  0.2984(2)  0.2418(6)  1.7028(2)  0.086(1)   Uani 1.00 d . . .
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C28   C  0.1633(2)  0.2082(5)  1.0961(2)  0.075(1)   Uani 1.00 d . . .
C29   C  0.1736(2)  0.1012(5)  1.0380(2)  0.078(1)   Uani 1.00 d . . .
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C31   C  0.0850(2)  -0.0124(5) 1.0223(2)  0.073(1)   Uani 1.00 d . . .
C32   C  0.0759(1)  0.0964(5)  1.0802(2)  0.0688(9)  Uani 1.00 d . . .
C33   C  0.1219(1)  -0.1463(5) 0.8679(2)  0.0697(9)  Uani 1.00 d . . .
C34   C  0.1406(1)  -0.2781(5) 0.8255(2)  0.0732(10) Uani 1.00 d . . .
C35   C  0.1668(2)  -0.4046(6) 0.8730(3)  0.097(1)   Uani 1.00 d . . .
C36   C  0.1875(2)  -0.5217(7) 0.8374(4)  0.118(2)   Uani 1.00 d . . .
C37   C  0.1844(3)  -0.5154(8) 0.7521(6)  0.132(2)   Uani 1.00 d . . .
C38   C  0.1586(3)  -0.3976(8) 0.7019(4)  0.132(2)   Uani 1.00 d . . .
C39   C  0.1357(2)  -0.2744(6) 0.7381(3)  0.100(1)   Uani 1.00 d . . .
C40   C  0.0762(2)  -0.0446(5) 0.8191(2)  0.072(1)   Uani 1.00 d . . .
C41   C  0.0271(2)  -0.1096(6) 0.7735(3)  0.091(1)   Uani 1.00 d . . .
C42   C  -0.0176(2) -0.018(1)  0.7306(4)  0.127(2)   Uani 1.00 d . . .
C43   C  -0.0103(4) 0.145(1)   0.7335(4)  0.151(3)   Uani 1.00 d . . .
C44   C  0.0392(4)  0.2091(8)  0.7764(3)  0.156(3)   Uani 1.00 d . . .
C45   C  0.0830(2)  0.1139(6)  0.8192(3)  0.109(2)   Uani 1.00 d . . .
C48   C  0.0055(8)  0.481(2)   0.429(2)   0.133(8)   Uani 0.30 d P . .
```

C49	C	0.045(1)	0.417(4)	0.485(4)	0.16(2)	Uani 0.20 d P . .
H4	H	-0.0954	0.5157	0.9759	0.0881	Uiso 1.00 calc . . .
H5	H	-0.0386	0.4448	1.1116	0.0842	Uiso 1.00 calc . . .
H9	H	0.1094	0.4906	1.3209	0.1015	Uiso 1.00 calc . . .
H10	H	0.1602	0.4548	1.4652	0.1119	Uiso 1.00 calc . . .
H12	H	0.2308	0.0711	1.4008	0.1068	Uiso 1.00 calc . . .
H13	H	0.1801	0.1092	1.2553	0.0971	Uiso 1.00 calc . . .
H16	H	0.1937	-0.1117	1.5012	0.0987	Uiso 1.00 calc . . .
H17	H	0.1116	-0.2564	1.4592	0.1310	Uiso 1.00 calc . . .
H18	H	0.0368	-0.1789	1.5086	0.1404	Uiso 1.00 calc . . .
H19	H	0.0410	0.0475	1.5850	0.1375	Uiso 1.00 calc . . .
H20	H	0.1218	0.1958	1.6253	0.1092	Uiso 1.00 calc . . .
H22	H	0.2019	0.0066	1.7249	0.0986	Uiso 1.00 calc . . .
H23	H	0.2520	0.0289	1.8705	0.1151	Uiso 1.00 calc . . .
H24	H	0.3301	0.1796	1.9104	0.1242	Uiso 1.00 calc . . .
H25	H	0.3617	0.3124	1.8066	0.1216	Uiso 1.00 calc . . .
H26	H	0.3103	0.2988	1.6599	0.1013	Uiso 1.00 calc . . .
H28	H	0.1913	0.2835	1.1232	0.0903	Uiso 1.00 calc . . .
H29	H	0.2077	0.1041	1.0222	0.0917	Uiso 1.00 calc . . .
H31	H	0.0581	-0.0893	0.9962	0.0859	Uiso 1.00 calc . . .
H32	H	0.0416	0.0936	1.0951	0.0805	Uiso 1.00 calc . . .
H35	H	0.1711	-0.4069	0.9341	0.1168	Uiso 1.00 calc . . .
H36	H	0.2032	-0.6140	0.8691	0.1393	Uiso 1.00 calc . . .
H37	H	0.2017	-0.5971	0.7258	0.1575	Uiso 1.00 calc . . .
H38	H	0.1551	-0.3934	0.6396	0.1507	Uiso 1.00 calc . . .
H39	H	0.1175	-0.1887	0.7033	0.1197	Uiso 1.00 calc . . .
H41	H	0.0223	-0.2224	0.7723	0.1100	Uiso 1.00 calc . . .
H42	H	-0.0518	-0.0636	0.7003	0.1468	Uiso 1.00 calc . . .
H43	H	-0.0403	0.2103	0.7028	0.1715	Uiso 1.00 calc . . .
H44	H	0.0426	0.3218	0.7811	0.1858	Uiso 1.00 calc . . .
H45	H	0.1185	0.1605	0.8468	0.1312	Uiso 1.00 calc . . .

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O47	0.039(9)	0.10(1)	0.35(4)	-0.011(8)	0.03(2)	0.10(2)
N1	0.070(2)	0.088(2)	0.037(1)	0.008(2)	0.004(1)	0.002(1)
N2	0.080(2)	0.110(2)	0.038(1)	-0.020(2)	-0.006(1)	0.007(2)
N3	0.082(2)	0.107(3)	0.053(2)	0.022(2)	0.005(1)	-0.008(2)
C4	0.060(2)	0.109(3)	0.053(2)	0.009(2)	0.007(2)	0.018(2)
C5	0.073(2)	0.095(3)	0.046(2)	0.013(2)	0.013(2)	0.011(2)
C6	0.064(2)	0.078(2)	0.037(2)	0.011(2)	0.001(1)	0.001(1)
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C8	0.062(2)	0.081(2)	0.037(2)	-0.002(2)	0.001(1)	0.001(2)
C9	0.114(3)	0.085(3)	0.044(2)	0.021(2)	0.001(2)	-0.001(2)
C10	0.130(4)	0.102(3)	0.038(2)	0.009(3)	0.004(2)	-0.008(2)
C11	0.072(2)	0.094(3)	0.037(2)	-0.011(2)	-0.001(1)	0.004(2)
C12	0.081(3)	0.115(3)	0.050(2)	0.018(2)	-0.008(2)	0.008(2)
C13	0.082(2)	0.112(3)	0.039(2)	0.015(2)	-0.001(2)	-0.005(2)
C14	0.064(2)	0.083(2)	0.036(2)	0.004(2)	0.003(1)	-0.001(2)
C15	0.063(2)	0.094(3)	0.040(2)	0.000(2)	0.006(1)	0.003(2)
C16	0.078(2)	0.100(3)	0.064(2)	-0.005(2)	0.008(2)	-0.007(2)
C17	0.104(4)	0.121(4)	0.084(3)	-0.026(3)	-0.003(3)	-0.007(3)
C18	0.075(3)	0.158(5)	0.111(4)	-0.026(4)	-0.002(3)	0.030(4)
C19	0.069(3)	0.180(6)	0.100(4)	0.002(3)	0.026(3)	0.024(4)
C20	0.072(2)	0.131(4)	0.068(2)	0.012(2)	0.018(2)	0.006(2)
C21	0.074(2)	0.084(2)	0.035(2)	0.010(2)	-0.001(1)	-0.004(2)
C22	0.097(3)	0.093(3)	0.046(2)	0.007(2)	0.007(2)	0.007(2)
C23	0.141(4)	0.103(3)	0.041(2)	0.028(3)	0.001(2)	0.007(2)
C24	0.140(4)	0.113(4)	0.042(2)	0.031(3)	-0.023(2)	-0.008(2)
C25	0.113(3)	0.111(3)	0.058(2)	-0.005(3)	-0.020(2)	-0.013(3)
C26	0.092(3)	0.106(3)	0.045(2)	-0.007(2)	-0.007(2)	-0.004(2)
C27	0.056(2)	0.082(2)	0.036(1)	0.005(2)	-0.004(1)	0.002(1)
C28	0.067(2)	0.100(3)	0.052(2)	-0.010(2)	0.008(2)	-0.007(2)
C29	0.066(2)	0.113(3)	0.053(2)	0.003(2)	0.011(2)	-0.009(2)
C30	0.069(2)	0.092(3)	0.041(2)	0.017(2)	-0.001(2)	-0.002(2)

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 C31   0.066(2)   0.094(3)   0.045(2)   0.006(2)   -0.005(2)   -0.009(2)
 C32   0.059(2)   0.097(3)   0.045(2)   0.003(2)   0.005(1)    -0.004(2)
 C33   0.071(2)   0.088(3)   0.048(2)   0.003(2)   0.014(2)    -0.003(2)
 C34   0.066(2)   0.090(3)   0.063(2)   0.002(2)   0.016(2)    -0.010(2)
 C35   0.096(3)   0.102(3)   0.083(3)   0.028(3)   0.007(2)    -0.008(3)
 C36   0.119(4)   0.106(4)   0.117(4)   0.025(3)   0.014(3)    -0.022(3)
 C37   0.109(4)   0.112(4)   0.174(7)   0.017(3)   0.042(4)    -0.049(5)
 C38   0.171(6)   0.137(5)   0.105(4)   0.023(4)   0.067(4)    -0.030(4)
 C39   0.132(4)   0.105(3)   0.070(3)   0.013(3)   0.039(3)    -0.016(2)
 C40   0.084(2)   0.092(3)   0.038(2)   0.013(2)   0.013(2)    0.001(2)
 C41   0.082(3)   0.123(4)   0.067(2)   0.003(2)   0.018(2)    0.024(2)
 C42   0.079(3)   0.214(7)   0.086(4)   0.026(4)   0.019(3)    0.047(4)
 C43   0.170(6)   0.198(8)   0.078(4)   0.100(6)   0.024(4)    0.039(5)
 C44   0.257(9)   0.120(5)   0.061(3)   0.073(5)   -0.005(4)   0.005(3)
 C45   0.160(5)   0.092(3)   0.053(2)   0.014(3)   -0.007(3)   -0.001(2)
 C48   0.09(1)    0.07(1)    0.24(3)    -0.029(10) 0.05(2)     0.01(1)
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 C4    H4    0.959     . . no
 C5    C6    1.367(5)  . . yes
 C5    H5    0.965     . . no
 C7    C8    1.494(4)  . . yes
 C7    C27   1.497(5)  . . yes
 C8    C9    1.378(5)  . . yes
 C8    C13   1.368(6)  . . yes
 C9    C10   1.383(5)  . . yes
 C9    H9    0.967     . . no
 C10   C11   1.357(6)  . . yes
 C10   H10   0.963     . . no
 C11   C12   1.372(6)  . . yes
 C12   C13   1.397(5)  . . yes
 C12   H12   0.974     . . no
 C13   H13   0.961     . . no
 C14   C15   1.493(5)  . . yes
 C14   C21   1.502(4)  . . yes
 C15   C16   1.378(6)  . . yes
 C15   C20   1.386(6)  . . yes
 C16   C17   1.383(7)  . . yes
 C16   H16   0.963     . . no
 C17   C18   1.379(9)  . . yes
 C17   H17   0.990     . . no
 C18   C19   1.36(1)   . . yes
 C18   H18   0.961     . . no
 C19   C20   1.356(7)  . . yes
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C20     H20     0.961     . . no
C21     C22     1.388(6)  . . yes
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C22     H22     0.971     . . no
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C23     H23     0.962     . . no
C24     C25     1.388(8)  . . yes
C24     H24     0.961     . . no
C25     C26     1.382(5)  . . yes
C25     H25     0.961     . . no
C26     H26     0.963     . . no
C27     C28     1.382(5)  . . yes
C27     C32     1.372(5)  . . yes
C28     C29     1.389(6)  . . yes
C28     H28     0.970     . . no
C29     C30     1.376(5)  . . yes
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C31     H31     0.956     . . no
C32     H32     0.965     . . no
C33     C34     1.467(6)  . . yes
C33     C40     1.488(5)  . . yes
C34     C35     1.386(6)  . . yes
C34     C39     1.383(6)  . . yes
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C40     C41     1.373(6)  . . yes
C40     C45     1.371(7)  . . yes
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C41     H41     0.974     . . no
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C42     H42     0.953     . . no
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C45     H45     0.972     . . no
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N1	C7	C27	124.7(3)	1_555	1_555	1_555 yes
C8	C7	C27	116.9(3)	1_555	1_555	1_555 yes
C7	C8	C9	120.8(3)	1_555	1_555	1_555 yes
C7	C8	C13	122.2(3)	1_555	1_555	1_555 yes
C9	C8	C13	117.0(3)	1_555	1_555	1_555 yes
C8	C9	C10	121.1(4)	1_555	1_555	1_555 yes
C8	C9	H9	118.8(3)	1_555	1_555	1_555 no
C10	C9	H9	120.1(4)	1_555	1_555	1_555 no
C9	C10	C11	121.6(4)	1_555	1_555	1_555 yes
C9	C10	H10	119.8(5)	1_555	1_555	1_555 no
C11	C10	H10	118.6(3)	1_555	1_555	1_555 no
N2	C11	C10	120.1(3)	1_555	1_555	1_555 yes
N2	C11	C12	121.1(4)	1_555	1_555	1_555 yes
C10	C11	C12	118.4(3)	1_555	1_555	1_555 yes
C11	C12	C13	119.8(4)	1_555	1_555	1_555 yes
C11	C12	H12	119.8(3)	1_555	1_555	1_555 no
C13	C12	H12	120.4(4)	1_555	1_555	1_555 no
C8	C13	C12	122.0(4)	1_555	1_555	1_555 yes
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C12	C13	H13	119.5(4)	1_555	1_555	1_555 no
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C15	C14	C21	118.5(3)	1_555	1_555	1_555 yes
C14	C15	C16	120.9(4)	1_555	1_555	1_555 yes
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C14	C21	C22	119.7(3)	1_555	1_555	1_555 yes
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C28	C27	C32	118.1(3)	1_555	1_555	1_555 yes
C27	C28	C29	121.3(3)	1_555	1_555	1_555 yes
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C28	C29	H29	120.9(4)	1_555	1_555	1_555 no
C30	C29	H29	119.2(4)	1_555	1_555	1_555 no
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C29	C30	C31	119.7(4)	1_555	1_555	1_555	yes
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C36	C37	C38	121.5(7)	1_555	1_555	1_555	yes
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C38	C37	H37	118.3(8)	1_555	1_555	1_555	no
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C37	C38	H38	122.3(8)	1_555	1_555	1_555	no
C39	C38	H38	117.7(6)	1_555	1_555	1_555	no
C34	C39	C38	118.5(4)	1_555	1_555	1_555	yes
C34	C39	H39	120.3(5)	1_555	1_555	1_555	no
C38	C39	H39	121.2(5)	1_555	1_555	1_555	no
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C40	C41	C42	121.7(5)	1_555	1_555	1_555	yes
C40	C41	H41	120.2(4)	1_555	1_555	1_555	no
C42	C41	H41	118.0(5)	1_555	1_555	1_555	no
C41	C42	C43	117.5(6)	1_555	1_555	1_555	yes
C41	C42	H42	121.3(8)	1_555	1_555	1_555	no
C43	C42	H42	121.1(7)	1_555	1_555	1_555	no
C42	C43	C44	120.7(7)	1_555	1_555	1_555	yes
C42	C43	H43	119.0(8)	1_555	1_555	1_555	no
C44	C43	H43	120.3(10)	1_555	1_555	1_555	no
C43	C44	C45	120.3(7)	1_555	1_555	1_555	yes
C43	C44	H44	119.4(8)	1_555	1_555	1_555	no
C45	C44	H44	120.0(7)	1_555	1_555	1_555	no
C40	C45	C44	119.7(5)	1_555	1_555	1_555	yes
C40	C45	H45	120.6(5)	1_555	1_555	1_555	no
C44	C45	H45	119.6(5)	1_555	1_555	1_555	no
O46	C48	O47	129(2)	1_555	1_555	3_566	yes
O46	C48	C49	106(3)	1_555	1_555	1_555	yes
O47	C48	C49	124(3)	3_566	1_555	1_555	yes
O47	C49	C48	108(3)	1_555	1_555	1_555	yes

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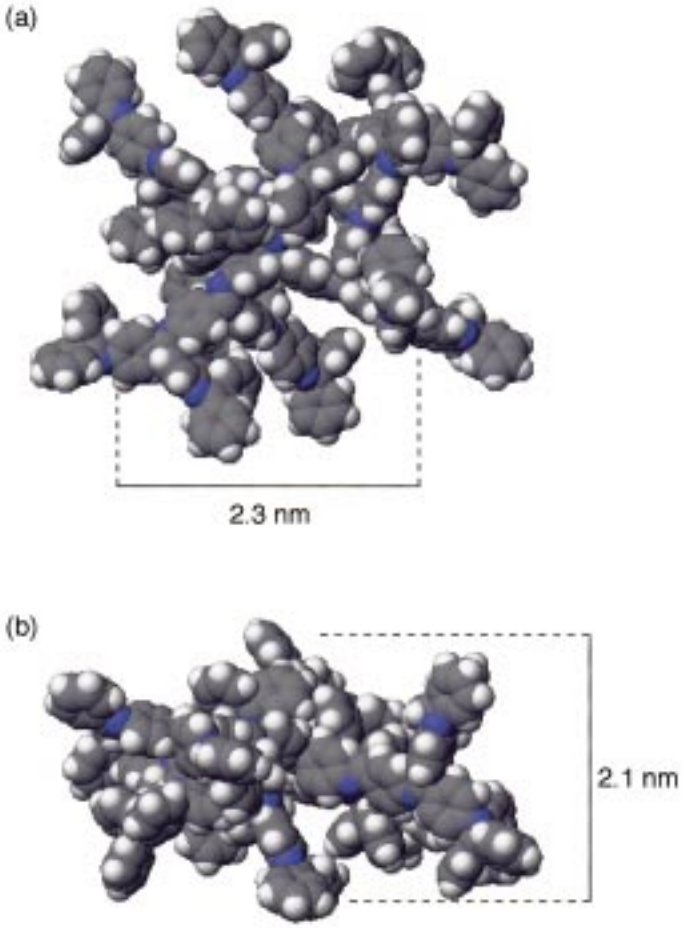
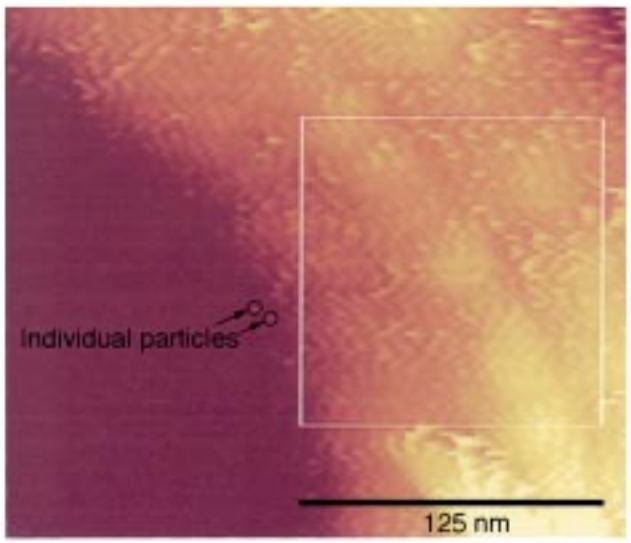


SI Figure 1. Molecular Dynamics calculation on DPA G4. (a) Top view and (b) side view. Potential energy: 351.62 kcal/mol.



SI Figure 2. The AFM picture including individual particles of DPA G4