Supporting Information

Preparation of 1,6-Diaminohex-3-yne (10):

To a round-bottom flask (2000 ml), equipped with a magnetic stirrer flea, dropping funnel (100 ml) and reflux condenser, were added under argon 3-hexyne-1,6-diol (25 g, 219 mmol), ether (500 ml), THF (250 ml) and triethylamine (67 g, 662 mmol). The solution was cooled to 0 °C, and methanesulphonyl chloride (75 g, 655 mmol) was added dropwise over ca. 45 min. After stirring for 3 h at 0 °C the reaction mixture was quenched with 400 ml ice-cooled water. The precipitate was removed by filtration, washed with ice-cooled water and ether and dried in vacuo, yielding 40.1 g (148 mmol, 67.7%) of 3-hexyne-1,6-diol bismethanesulphonate.

Dry DMF (125 ml), 3-hexyne-1,6-diol-bismethanesulphonate (15 g, 56 mmol) and sodium azide (35 g, 538 mmol) were added under argon to a round-bottom flask (500 ml), equipped with a magnetic stirrer flea and reflux condenser, and the suspension was stirred for 48 h at room temperature. 200 ml water were added to dissolve the excess of sodium azide, and the mixture was transferred to a separatory funnel and extracted with ether (3×100 ml). The combined organic extract was washed with water (5×25 ml), dried ($MgSO_4$) and concentrated in vacuo (30 ml). The residue was dissolved in methanol (200 ml) and transferred to a round-bottom flask (500 ml), equipped with a magnetic stirrer flea and reflux condenser. The solution was cooled to 0 °C, and tin(II) chloride (60 g, 266 mmol) was added gradually. After 15 min stirring at 0 °C, the reaction mixture was allowed to warm up to room temperature and stirred for 24 h. The solvent was removed in vacuo and the residue dissolved in sodium hydroxide solution (10%, 250 ml). The solution was saturated with NaCl and extracted with $CHCl_3$ (15×200 ml). The combined organic extract was dried ($MgSO_4$) and concentrated in vacuo (500 ml). HCl-saturated ether was added, and the precipitate was removed by filtration and washed with ethanol and ether, yielding 5.75 g (31 mmol, 56.0%) of **10·2HCl**.

$CHCl_3$ (100 ml) was added to a concentrated solution of 3 g **10·2HCl** in water, and the mixture was cooled to 0 °C. NaCl-saturated sodium hydroxide solution (10%) was added dropwise until pH = 11. The layers were separated, and the aqueous layer was extracted with $CHCl_3$ (5×100 ml). The combined organic extract was dried ($MgSO_4$) and the solvent evaporated in vacuo. The residual red oil was distilled in vacuo to furnish **10** as a colorless liquid (1.34 g, 74 %).

Spectroscopic and analytical properties of 10:

- Melting point: -25 °C
- Boiling point: 70 °C (1.2 Torr)
- ^1H NMR (in $CDCl_3$, 300 MHz): δ 2.73 (4H, t, CH_2N), 2.23 (4H, t, CH_2CC), 1.27 (4H, s, NH_2)
- ^{13}C NMR (in $CDCl_3$, 75 MHz): δ 79.2 (CC), 41.2 (CH_2N), 23.6 (CH_2CC)
- IR (**10·2HCl**, KBr pellet): 2937 cm^{-1}, 2715, 2617, 2555, 2474, 2005, 1599, 1515
- UV (**10·2HCl**, in EtOH): (λ_{max}/log ε) 206 nm/2.73, 292/2.16
- CIMS: (m/z) 113.2 $[M+1]^+$ (100%), 96.1 (20), 84.1 (26), 72.1 (2)
- Elementary Analysis (**10·2HCl**): $C_6H_{14}Cl_2N_2$
  calc. (%) C 38.12, H 7.62, N 15.13
  found (%) C 39.12, H 7.75, N 14.68

Total Energies, Imaginary Wavenumbers and Cartesian Coordinates for AM1-Geometries:

7-TS(monorot): 0,1\C,1.6917446626,-0.2
836463873,3.4859511605\H,1.8852690669,-1.3723393113,3.2696236329\H,3.7
191197992,0.233039127,3.0237011743\C,1.0296845073,0.4438675272,-3.7180
669165\H,1.1297182943,1.5493938557,-3.5246694125\H,1.1126285517,0.2848
235471,-4.835854002\N,-0.2816941845,0.0290211701,-3.2392456766\N,0.279
2212344,-0.0287590447,3.2394354839\C,-0.595347041,-1.1023257205,3.6779
024928\H,-1.6584674171,-0.7394985561,3.5846117351\H,-0.4163027942,-1.3
4551511,4.7694205084\C,-0.4915317856,-2.4250726349,2.9077847181\H,0.53
5604048,-2.8600129549,3.0339525261\H,-1.2101120121,-3.1344277238,3.406
5954517\C,-0.831044628,-2.3578227028,1.4607836131\C,-2.038424459,-1.80
50008698,1.0210389389\H,-2.7630191205,-1.4209912291,1.7545331724\C,-2.

3212057347,-1.7062289726,-0.3399119461\H,-3.2634402208,-1.2369423728,-
0.6612645352\C,-1.4096874402,-2.1650542087,-1.2991177895\C,-0.23725521
05,-2.7894218474,-0.8567037072\H,0.4792312149,-3.1881593009,-1.5902202
487\C,0.0494127697,-2.8813945023,0.5040363621\H,0.9918010275,-3.348987
2323,0.8269405078\C,-1.7134567543,-2.0118860672,-2.7475864969\H,-1.860
0983907,-3.0379759922,-3.187905683\H,-2.6845258078,-1.4623487491,-2.87
20762245\C,-0.6242903138,-1.338575358,-3.5918146504\H,0.3094648769,-1.
9624995841,-3.4936207868\H,-0.9621582978,-1.4022382704,-4.6707431036\C
,2.6978860467,0.5259094211,2.6553033555\H,2.5777758335,1.6236447587,2.
863199261\C,2.6182885817,0.3153340006,1.1860150232\C,3.7613389579,0.29
3285847,0.373720309\H,4.7567738547,0.4025038078,0.8280104035\C,3.65129
52914,0.1385248289,-1.0094547721\H,4.5608001499,0.1385314542,-1.627522
1633\C,2.3967304591,-0.0213870415,-1.6155901831\C,1.2680247053,-0.0173
586367,-0.7973563443\H,0.2562821496,-0.1691172691,-1.2094769766\C,1.37
46937705,0.1757044383,0.5716534146\H,0.4373212631,0.2157599751,1.15151
93689\C,2.2486208142,-0.2367863865,-3.078884453\H,3.1518596673,0.16697
31656,-3.6132070615\H,2.2212810096,-1.3431930769,-3.2733217384\C,-0.15
49496765,1.2934113555,3.6581253168\H,0.6696802164,2.0202463794,3.40794
58629\H,-0.3089613928,1.3288239387,4.7794301585\C,-1.4427095873,1.8271
113641,3.0183943288\H,-2.3080338018,1.1701315866,3.3013401746\H,-1.630
127991,2.8338029313,3.4871363461\C,-1.4100327097,1.9995063064,1.540834
4946\C,-0.412236783,2.7535396287,0.9114782472\H,0.3661353032,3.2421396
784,1.5162842509\C,-0.3742011879,2.8644576395,-0.4772108127\H,0.437378
9494,3.436898257,-0.9511723138\C,-1.3363221647,2.2303540617,-1.2752673
275\C,-2.3770333478,1.5429585722,-0.6419602699\H,-3.1650271519,1.06790
42286,-1.2452119306\C,-2.4104738288,1.4257600716,0.7462349747\H,-3.221
8560644,0.8514015771,1.2185605771\C,-1.2586397586,2.3226500629,-2.7581
395984\H,-2.1299778619,2.9378161577,-3.1197082702\H,-0.3263064334,2.87
39486633,-3.0529818147\C,-1.3362167092,0.9895201595,-3.5133148437\H,-2
.3190917513,0.5064937822,-3.2464185707\H,-1.3727337635,1.2415009051,-4
.6168522784\H,1.9434569743,-0.1029696146,4.5748335199\\Version=IBM-RS6
000-G98RevA.7\HF=0.1307598\RMSD=0.000e+00\RMSF=1.775e-05\Dipole=-0.314
4259,-0.0181645,0.0268486\PG=C01 [X(C30H36N2)]\\@

NIMAG=1: 49.74 icm^{-1}, A

7-TS(dirot): 0,1\C,-0.5968495
012,-0.174900003,-3.5755376335\H,-1.6472412441,-0.0009481059,-3.207114
6858\H,-0.6586603731,-0.4209112883,-4.6794032116\C,0.1536917653,1.1875
265343,-3.5019792947\H,1.2538895481,1.0528705849,-3.6665108627\H,-0.23
60400697,1.7889404731,-4.3686240022\C,-0.0530825114,1.9774635271,-2.25
09038636\C,-0.3912894691,1.2314365184,-1.1248277509\H,-0.1100021691,0.
1672179492,-1.115532754\C,-0.9639383624,1.8422472479,-0.0226612747\H,-
1.6121385037,1.3030125492,0.6826287294\C,-0.7332449416,3.1922064768,0.
2318288016\C,-0.2268798442,3.9564077244,-0.8280119053\H,-0.0421168226,
5.0314742791,-0.6949421201\C,0.0179708665,3.3684257527,-2.0838091411\H
,0.2946631576,4.0120218777,-2.9304773986\C,-1.0772379687,3.5968780308,
1.6237384437\H,-0.8482743068,4.6859342463,1.7748708224\H,-2.1862607198
,3.4624652227,1.7547214069\C,-0.3624342631,2.8590044933,2.7833218113\H
,0.6686565416,3.3201197727,2.824946139\H,-0.9115062117,3.1836970517,3.
7191905163\C,1.3037758679,-1.6409201262,-3.1516249239\H,1.8392041734,-
0.697685894,-3.4482903808\H,1.3735842246,-2.3405047149,-4.0395001919\C
,2.1059171343,-2.2790325078,-2.0124792337\H,1.6279073016,-3.2476979401
,-1.7064206382\H,3.1213470311,-2.5256494398,-2.4297567596\C,2.27592095
92,-1.4062701825,-0.8210457512\C,2.6746033862,-0.0703109492,-0.9428936
323\H,2.9257410867,0.341497583,-1.9316515604\C,2.7206537058,0.76039862
,0.174041003\H,2.9975354605,1.8183404206,0.0520584245\C,2.3814956783,0
.2707151762,1.4415772907\C,2.0894190114,-1.0912343389,1.5776143114\H,1
.8733750487,-1.5117186911,2.5710038588\C,2.0307192677,-1.9188444496,0.
4589558988\H,1.7596399999,-2.9781994268,0.5816652069\C,2.3343502377,1.
1965678402,2.6040095032\H,3.212955124,0.983363162,3.2738429121\H,2.437

2914593,2.2562684776,2.247647602\C,1.0764271679,1.0589792425,3.4686005
97\H,1.0346757976,-0.0052896188,3.8291541351\H,1.2330294644,1.70172468
32,4.3878193615\N,-0.1782782884,1.4015144146,2.8021243527\N,-0.0907643
836,-1.3365972111,-2.8374074034\C,-0.9133827291,-2.5485486019,-2.95177
62775\H,-0.229506698,-3.4277849586,-2.7598934387\H,-1.2958809219,-2.64
80875059,-4.0131490234\C,-2.1495036554,-2.8080546733,-2.054917981\H,-3
.003600945,-2.1916489335,-2.4494202378\H,-2.411852587,-3.8888375028,-2
.2109264666\C,-2.0177278359,-2.5204163275,-0.5991201241\C,-1.666272636
8,-1.2000870564,-0.3281225241\H,-1.8010751876,-0.4693401126,-1.1381495
179\C,-1.1731407926,-0.8499683498,0.9168062003\H,-0.4478038686,-0.0315
91465,1.042576302\C,-1.5012268216,-1.5988046285,2.0439237526\C,-2.0292
624318,-2.8780514606,1.8152728517\H,-2.2942462471,-3.5248049931,2.6632
765884\C,-2.1937634021,-3.3656125857,0.5045648822\H,-2.4898762798,-4.4
134332334,0.3562552741\C,-1.2768343192,-0.9144421063,3.3527898835\H,-2
.0982433635,-1.2203818245,4.0573138663\H,-0.3147426379,-1.2833124975,3
.7931866616\C,-1.3204816624,0.6418368494,3.3206813756\H,-2.2078440004,
0.9408020614,2.6941468195\H,-1.5349365013,0.9551089887,4.3878126965\\V
ersion=SGI-G98RevA.5\HF=0.2050782\RMSD=0.000e+00\RMSF=2.043e-05\Dipole
=0.0620038,-0.0154078,0.0089025\PG=C01 [X(C30H36N2)]\\@

NIMAG=1: 78.86 icm^{-1} A

7-TS(trirot): 0,1\C,-0.6506447363,1.30123
85452,-3.4785080278\H,-1.6863292829,1.2211334796,-3.1806735247\H,-0.62
5119492,1.3797446276,-4.5664139486\C,-0.1370268591,2.7141941612,-2.932
8288748\H,0.9047915364,2.8526943252,-3.2018116573\H,-0.7062083227,3.44
56697794,-3.4982745139\C,-0.3017922485,2.9545695114,-1.4201346722\C,-0
.1838127062,1.8189941331,-0.6772151487\H,-0.0074899985,0.9408964266,-1
.2129368709\C,-0.2914532365,1.8047874131,0.6773293509\H,-0.2350708728,
0.9108344275,1.2130442567\C,-0.4709555944,2.9323247686,1.420181886\C,-
0.5792846012,4.1298079981,0.7017963375\H,-0.7272396033,5.0632901993,1.
2118865079\C,-0.5064633523,4.1393773484,-0.7017513176\H,-0.6047519166,
5.0793728475,-1.2118695639\C,-0.5681726482,2.6576009419,2.9328316365\H
,-0.2066216199,3.5111263894,3.4981023905\H,-1.6104209691,2.5228554979,
3.2021081621\C,0.2926468544,1.4250020104,3.4783927919\H,1.3140393523,1
.6149829128,3.1809508702\H,0.2473416609,1.4941087728,4.5662782333\C,1.
4522280046,-0.0871444021,-3.4785080278\H,1.9006972562,0.8498372583,-3.
1806735247\H,1.5074536443,-0.1485029533,-4.5664139486\C,2.4190745239,-
1.2384283396,-2.9328288748\H,2.0181099867,-2.2099196182,-3.2018116573\
H,3.3371417233,-1.1112405419,-3.4982745139\C,2.7096283784,-1.215925001
8,-1.4201346722\C,1.6672014816,-0.7503105935,-0.6772151487\H,0.8185852
07,-0.4639616843,-1.2129368709\C,1.7087183664,-0.6499877997,0.67732935
09\H,0.9063411893,-0.2518398662,1.2130442567\C,2.7749455389,-1.0583028
754,1.420181886\C,3.8661609397,-1.5632288183,0.7017963375\H,4.74855774
1,-1.9018371286,1.2118865079\C,3.8380376157,-1.631078545,-0.7017513176
\H,4.7012418795,-2.015955901,-1.2118695639\C,2.5856362529,-0.836748523
9,2.9328316365\H,3.1440354591,-1.5766236229,3.4981023905\H,2.990067435
8,0.1332377211,3.2021081621\C,1.0877645143,-0.9659406154,3.4783927919\
H,0.741596553,-1.9454829171,3.1809508702\H,1.1702653229,-0.9612585481,
4.5662782333\N,0.,0.,3.0660985459\N,0.,0.,-3.066507451\C,-0.8015832684
,-1.214094143,-3.4785080278\H,-0.2143679733,-2.0709707379,-3.180673524
7\H,-0.8823341523,-1.2312416743,-4.5664139486\C,-2.2820476648,-1.47576
58216,-2.9328288748\H,-2.922901523,-0.642774707,-3.2018116573\H,-2.630
9334006,-2.3344292375,-3.4982745139\C,-2.4078361298,-1.7386445096,-1.4
201346722\C,-1.4833887755,-1.0686835396,-0.6772151487\H,-0.8110952085,
-0.4769347423,-1.2129368709\C,-1.41726513,-1.1547996134,0.6773293509\H
,-0.6712703165,-0.6589945613,1.2130442567\C,-2.3039899445,-1.874021893
1,1.420181886\C,-3.2868763385,-2.5665791798,0.7017963375\H,-4.02131813
77,-3.1614530707,1.2118865079\C,-3.3315742634,-2.5082988034,-0.7017513
176\H,-4.096489963,-3.0634169465,-1.2118695639\C,-2.0174636047,-1.8208
524181,2.9328316365\H,-2.9374138392,-1.9345027665,3.4981023905\H,-1.37

96464666,-2.656093219,3.2021081621\C,-1.3804113686,-0.459061395,3.4783
927919\H,-2.0556359053,0.3305000043,3.1809508702\H,-1.4176069837,-0.53
28502247,4.5662782333\\Version=HP-PARisc-HPUX-G98RevA.7\State=1-A\HF=-
1258.7070324\RMSD=5.956e-09\RMSF=2.300e-05\Dipole=0.,0.,0.0005316\PG=C
03 [C3(N1N1),X(C30H36)]\\@

NIMAG=3: (52.08 icm^{-1}, E; 24.06 icm^{-1}, A)

7: 0,1\C,3.1080415932,-0.0
147877943,-0.696166524\H,3.6310249693,0.7830584087,-1.2438262946\C,2.4
232554724,-1.0084397235,-1.4069945695\C,1.7922199023,-2.0339924963,-0.
6965724261\H,1.2592841426,-2.8306413972,-1.2377859642\C,2.3534548243,-
0.9617792653,-2.8911252644\H,3.369755754,-0.7094131535,-3.3022402454\H
,2.0777460415,-1.9689408479,-3.3002724128\C,1.3934984976,0.1115163041,
-3.4146636647\H,1.7727229461,1.1016181018,-3.0291990681\H,1.4845573668
,0.1196780907,-4.5429561105\C,3.1080415932,-0.0147877943,0.696166524\H
,3.6310249693,0.7830584087,1.2438262946\C,2.4232554724,-1.0084397235,1
.4069945695\C,1.7922199023,-2.0339924963,0.6965724261\H,1.2592841426,-
2.8306413972,1.2377859642\C,2.3534548243,-0.9617792653,2.8911252644\H,
3.369755754,-0.7094131535,3.3022402454\H,2.0777460415,-1.9689408479,3.
3002724128\C,1.3934984976,0.1115163041,3.4146636647\H,1.7727229461,1.1
016181018,3.0291990681\H,1.4845573668,0.1196780907,4.5429561105\C,-1.5
668274022,-2.6842490786,-0.696166524\H,-1.13736401,-3.5360890696,-1.24
38262946\C,-2.0849621549,-1.5943809372,-1.4069945695\C,-2.6575991241,-
0.5351117164,-0.6965724261\H,-3.0810494303,0.3247486406,-1.2377859642\
C,-2.0096526887,-1.5572620318,-2.8911252644\H,-2.2992476897,-2.5635875
108,-3.3022402454\H,-2.7440258136,-0.8149104306,-3.3002724128\C,-0.600
1732965,-1.2625632511,-3.4146636647\H,0.0676677884,-2.0860321561,-3.02
91990681\H,-0.6386344166,-1.3455034384,-4.5429561105\C,-1.5668274022,-
2.6842490786,0.696166524\H,-1.13736401,-3.5360890696,1.2438262946\C,-2
.0849621549,-1.5943809372,1.4069945695\C,-2.6575991241,-0.5351117164,0
.6965724261\H,-3.0810494303,0.3247486406,1.2377859642\C,-2.0096526887,
-1.5572620318,2.8911252644\H,-2.2992476897,-2.5635875108,3.3022402454\
H,-2.7440258136,-0.8149104306,3.3002724128\C,-0.6001732965,-1.26256325
11,3.4146636647\H,0.0676677884,-2.0860321561,3.0291990681\H,-0.6386344
166,-1.3455034384,4.5429561105\N,0.,0.,-3.0020451762\C,-1.541214191,2.
6990368729,-0.696166524\H,-2.4936609593,2.7530306608,-1.2438262946\C,-
0.3382933174,2.6028206607,-1.4069945695\C,0.8653792218,2.5691042127,-0
.6965724261\H,1.8217652877,2.5058927566,-1.2377859642\C,-0.3438021355,
2.5190412971,-2.8911252644\H,-1.0705080643,3.2730006643,-3.3022402454\
H,0.6662797721,2.7838512785,-3.3002724128\C,-0.7933252011,1.151046947,
-3.4146636647\H,-1.8403907345,0.9844140543,-3.0291990681\H,-0.84592295
02,1.2258253477,-4.5429561105\N,0.,0.,3.0020451762\C,-1.541214191,2.69
90368729,0.696166524\H,-2.4936609593,2.7530306608,1.2438262946\C,-0.33
82933174,2.6028206607,1.4069945695\C,0.8653792218,2.5691042127,0.69657
24261\H,1.8217652877,2.5058927566,1.2377859642\C,-0.3438021355,2.51904
12971,2.8911252644\H,-1.0705080643,3.2730006643,3.3022402454\H,0.66627
97721,2.7838512785,3.3002724128\C,-0.7933252011,1.151046947,3.41466366
47\H,-1.8403907345,0.9844140543,3.0291990681\H,-0.8459229502,1.2258253
477,4.5429561105\\Version=IBM-RS6000-G98RevA.7\State=1-A\HF=0.1141167
\\@

NIMAG=0

6-TS(monorot): 0,1\C,-3.5824463625,-1.1901345813,-
0.4694310843\H,-3.6725299809,-0.74487666,-1.5030454244\H,-4.6245116976
,-1.4764025913,-0.1304347307\C,-2.8080001679,-2.5128902841,-0.62844729
9\H,-2.8872912841,-3.0998823597,0.327029912\H,-3.342999782,-3.09504169
28,-1.4259019183\C,-1.3674690181,-2.3779928793,-0.9704809747\C,-0.6270
418765,-1.511298266,-0.1722279242\H,-1.075601498,-1.0151457882,0.69042

45217\C,0.6919008586,-1.2179200987,-0.4392102051\H,1.1356495762,-0.380
5166501,0.122605915\C,1.40419984,-1.9229024356,-1.4071066553\C,0.69398
86705,-2.8514036922,-2.1810630801\H,1.2157451911,-3.4271906732,-2.9588
967603\C,-0.6819222311,-3.0514249849,-1.9896809521\H,-1.2192428094,-3.
7524380313,-2.6440878665\C,2.8548673524,-1.6194566599,-1.5386250062\H,
3.4039629312,-2.5250668638,-1.9105668705\H,2.9856012315,-0.8064169546,
-2.3025061744\C,3.5281854046,-1.2026045705,-0.2113727762\H,3.343007722
7,-2.0263232665,0.5339488388\H,4.6414538396,-1.1676741478,-0.40881871\
C,-2.983289658,-0.4294922617,1.808516311\H,-2.7398591592,-1.5214781242
,1.9375827756\H,-3.9899776335,-0.2485948882,2.2938322176\C,-1.96310571
24,0.402096542,2.6232113764\H,-2.0175065327,1.4848630438,2.3141391404\
H,-2.3009861668,0.3417399771,3.6977648179\C,-0.5845010274,0.0005901344
,2.5678850197\C,0.5846716981,-0.2770986263,2.5244659757\C,1.9344948946
,-0.7680758245,2.4951584615\H,2.2771430335,-0.9036525432,3.5618383657\
H,1.9165374648,-1.789015858,2.0168654239\C,3.0001956246,0.1129249541,1
.8142571136\H,2.7946837834,1.1809911242,2.1070785278\H,3.9922026495,-0
.184092816,2.272310531\N,3.0793279167,0.0533133858,0.3678587956\N,-3.0
453780199,-0.1425186386,0.3854500257\C,-3.5627432209,1.1756722615,0.06
32968882\H,-3.4811059649,1.8398613359,0.9700476587\H,-4.661195788,1.12
06968626,-0.2045737533\C,-2.8528367312,1.8830645152,-1.0990220006\H,-3
.0006193608,1.2909041953,-2.0413576747\H,-3.3689763666,2.8722549937,-1
.240168837\C,-1.4015485017,2.1211689482,-0.878579234\C,-0.9423717629,2
.8385459976,0.2324519639\H,-1.6652039397,3.2810349393,0.9337795532\C,0
.4229177344,2.9802389646,0.4698179902\H,0.7641499003,3.5234663036,1.36
35594138\C,1.362891251,2.4176518183,-0.403772894\C,0.9033080247,1.7698
402139,-1.5553058664\H,1.6258535063,1.3407045483,-2.2657534514\C,-0.46
22237881,1.6220021474,-1.7892801738\H,-0.8022825677,1.0793752228,-2.68
42240229\C,2.8149940882,2.5257764179,-0.1037355772\H,3.27238791,3.2806
468876,-0.8021255732\H,2.9562105086,2.9194086428,0.9386439861\C,3.6211
14218,1.2320210378,-0.2728010097\H,3.69267106,1.0120549303,-1.37720749
31\H,4.6699623347,1.4462380147,0.096000005\\Version=SGI-G98RevA.5\HF=0
.1834184\RMSD=0.000e+00\RMSF=3.849e-05\Dipole=-0.0059259,0.1749626,0.4
00675\PG=C01 [X(C26H32N2)]\\@

NIMAG=1: 106.44 icm^{-1}, A

6-TS(dirot): 0,1\C,3.65093218
72,0.9701662456,-1.2664622051\H,4.5343273234,1.5346262766,-1.596085887
4\C,2.4213357663,1.61958989,-1.0920575331\C,1.3565993751,0.8200264035,
-0.6894597852\H,0.3506801959,1.238081181,-0.8044218046\C,2.0332769513,
3.0488883029,-1.276460519\H,2.9484810417,3.6953937763,-1.3302493739\H,
1.490246791,3.1365984576,-2.2562287219\C,1.1392403599,3.6733299557,-0.
1646597594\H,1.8029320321,3.7728713962,0.7427495131\H,0.9072992959,4.7
188416882,-0.5311075876\C,0.1601521885,0.5795531811,2.4964226705\C,0.6
414424061,1.9317170973,2.4319752745\H,0.7719163649,2.318065576,3.48227
73102\H,1.6590317834,1.9143870828,1.9462752953\C,-0.2728453437,2.93997
8475,1.6972264809\H,-1.3388324161,2.6582784028,1.921098677\H,-0.082101
9999,3.9476643198,2.1758519451\N,-0.0970973068,3.0251239494,0.25974200
88\C,-1.5552691023,0.4507796866,-0.1953830637\H,-0.8018293462,0.885128
4364,0.472989782\C,-2.7083999231,1.16289288,-0.5100809052\C,-3.7655474
244,0.4193284577,-1.0580920553\H,-4.7109866122,0.9179960032,-1.3145029
083\C,-2.6423520714,2.6322519627,-0.254117619\H,-3.379744198,3.1518371
161,-0.9252806317\H,-2.9607000598,2.8339615152,0.8028210655\C,-1.27843
30742,3.3212949283,-0.5374002364\H,-0.9964129336,3.0717170961,-1.60133
28109\H,-1.4969054717,4.4324920802,-0.4917523909\C,-3.6509321872,-0.97
01662456,-1.2664622051\H,-4.5343273234,-1.5346262766,-1.5960858874\C,-
2.4213357663,-1.61958989,-1.0920575331\C,-1.3565993751,-0.8200264035,-
0.6894597852\H,-0.3506801959,-1.238081181,-0.8044218046\C,-2.033276951
3,-3.0488883029,-1.276460519\H,-2.9484810417,-3.6953937763,-1.33024937
39\H,-1.490246791,-3.1365984576,-2.2562287219\C,-1.1392403599,-3.67332
99557,-0.1646597594\H,-1.8029320321,-3.7728713962,0.7427495131\H,-0.90

72992959,-4.7188416882,-0.5311075876\C,-0.1601521885,-0.5795531811,2.4
964226705\C,-0.6414424061,-1.9317170973,2.4319752745\H,-0.7719163649,-
2.318065576,3.4822773102\H,-1.6590317834,-1.9143870828,1.9462752953\C,
0.2728453437,-2.939978475,1.6972264809\H,1.3388324161,-2.6582784028,1.
921098677\H,0.0821019999,-3.9476643198,2.1758519451\N,0.0970973068,-3.
0251239494,0.2597420088\C,1.5552691023,-0.4507796866,-0.1953830637\H,0
.8018293462,-0.8851284364,0.472989782\C,2.7083999231,-1.16289288,-0.51
00809052\C,3.7655474244,-0.4193284577,-1.0580920553\H,4.7109866122,-0.
9179960032,-1.3145029083\C,2.6423520714,-2.6322519627,-0.254117619\H,3
.379744198,-3.1518371161,-0.9252806317\H,2.9607000598,-2.8339615152,0.
8028210655\C,1.2784330742,-3.3212949283,-0.5374002364\H,0.9964129336,-
3.0717170961,-1.6013328109\H,1.4969054717,-4.4324920802,-0.4917523909\
\Version=IBM-RS6000-G98RevA.7\State=1-A\HF=0.2490303\RMSD=0.000e+00\RM
SF=7.596e-05\Dipole=0.,0.,0.2904436\PG=C02 [X(C26H32N2)]\\@

NIMAG=1: 110.98 icm^{-1}, A

6: 0,1\C,3.4622125959,1.1101920118,-0.547309
0693\H,3.4007092831,0.720199303,-1.6046700693\H,4.5566978843,1.2874033
237,-0.3146180693\C,2.7732311685,2.4757126066,-0.5108810693\H,3.010428
5809,2.9951948772,0.4556869307\H,3.2340175068,3.0907854246,-1.33303606
93\C,1.3027433577,2.4221690196,-0.7149900693\C,0.7603868222,1.78854997
14,-1.8380790693\H,1.4288176691,1.345699673,-2.5912860693\C,-0.6191502
209,1.674354254,-1.9871240693\H,-1.0289452324,1.1367349227,-2.85525606
93\C,-1.4844705363,2.1993532721,-1.0209070693\C,-0.9429647205,2.896834
9904,0.0650469307\H,-1.6119667559,3.3428503431,0.8155969307\C,0.436899
6083,3.0019290914,0.2198679307\H,0.8480005288,3.5242509986,1.096361930
7\C,-2.9510121341,1.9869211702,-1.1359840693\H,-3.4717653981,2.9821001
949,-1.1783190693\H,-3.1865240645,1.4448297661,-2.0901020693\C,-3.5432
051398,1.217505416,0.0510429307\H,-3.4481810104,1.872006011,0.96260693
07\H,-4.6510027939,1.0945596433,-0.1464270693\C,2.8636448247,0.4274891
109,1.7142529307\H,2.4674942175,1.4800864037,1.7891049307\H,3.90093221
21,0.4158571465,2.1668529307\C,1.9757871561,-0.4645338714,2.5953519307
\H,2.0825708672,-1.5511138086,2.3193829307\H,2.3454652265,-0.352118583
7,3.6548729307\C,0.5873219784,-0.1230284241,2.5565599307\C,-0.58453925
61,0.1235000769,2.5562799307\C,-1.9729518278,0.4653354282,2.5952419307
\H,-2.3422403709,0.3537514265,3.6549719307\H,-2.0794148002,1.551772776
,2.3187239307\C,-2.8612743826,-0.4271697012,1.7150849307\H,-2.46408018
41,-1.47944591,1.7890799307\H,-3.8978835967,-0.416532984,2.1693149307\
N,-2.9074772099,-0.0692812477,0.3074729307\N,2.9073385791,0.0695632651
,0.3064049307\C,3.5429831988,-1.2173922459,0.0496279307\H,3.4483142249
,-1.8718084929,0.9612689307\H,4.6506226272,-1.0945691828,-0.1485500693
\C,2.9498242185,-1.986793226,-1.1369150693\H,3.1845231926,-1.444677328
9,-2.0912170693\H,3.4704895066,-2.9819590891,-1.1798770693\C,1.4833683
966,-2.1993474857,-1.0206320693\C,0.9424874896,-2.894701348,0.06699493
07\H,1.6119608023,-3.3389325632,0.8182149307\C,-0.4373303462,-3.000071
5348,0.2223829307\H,-0.8481445345,-3.5209059661,1.0999359307\C,-1.3036
30653,-2.4227926288,-0.7136300693\C,-0.7618636801,-1.7916575021,-1.838
3890693\H,-1.430607833,-1.3511516322,-2.5926250693\C,0.6175552704,-1.6
76967567,-1.9878990693\H,1.0268329111,-1.1411832887,-2.8573740693\C,-2
.7740405199,-2.475822358,-0.5086940693\H,-3.2354838085,-3.0914119704,-
1.3300590693\H,-3.0109492285,-2.9943771573,0.4584399307\C,-3.462384432
3,-1.1100219335,-0.5458430693\H,-3.4003970864,-0.7205561145,-1.6034110
693\H,-4.5570895433,-1.2865918407,-0.3134830693\\Version=IBM-RS6000-G9
8RevA.7\HF=0.1537018\RMSD=0.000e+00\RMSF=2.446e-05\Dipole=0.0011693,-0
.0005446,0.2347706\PG=C01 [X(C26H32N2)]\\@

NIMAG=0

5-TS: 0,1\C,-1

.1148480137,-1.1502550779,-3.1025137812\H,-0.3022615183,-1.9282442215,
-3.0226681988\H,-1.6266027127,-1.2891718803,-4.104382601\C,-2.18796930
42,-1.4739025843,-2.041750227\H,-2.9638410495,-0.6593137738,-2.0077825
916\H,-2.7091328922,-2.4055218154,-2.4100640633\C,-1.7272689285,-1.722
6324665,-0.7071708541\C,-1.3950472224,-1.9247766824,0.4293048989\C,-0.
8902879172,-2.2574750286,1.7293619577\H,-1.2648395501,-3.287359294,1.9
962949032\H,0.2344614769,-2.3137625844,1.6616680598\C,-1.2899743318,-1
.3286104066,2.8951153274\H,-2.3697016553,-1.041759933,2.7670755623\H,-
1.2215769734,-1.9657260507,3.8298172842\C,-1.2807823696,1.3272283187,-
2.8938964141\H,-2.3612631582,1.0449765975,-2.7613899392\H,-1.211472604
,1.9538481002,-3.8352790067\C,-0.8755404453,2.2629248744,-1.7358406436
\H,0.2494373363,2.3177933924,-1.6720463268\H,-1.2501773546,3.291829090
5,-2.0053686368\C,-1.3774337248,1.9310812463,-0.4347420411\C,-1.711180
6371,1.7233912752,0.7000470439\C,-2.1767204689,1.4698698499,2.03178769
08\H,-2.7044862059,2.3983319329,2.3988117135\H,-2.9487035221,0.6519193
636,1.9926685287\C,-1.1049884114,1.1515964875,3.0948768275\H,-0.283922
3327,1.9188673157,2.9992093834\H,-1.6127080316,1.3154499468,4.09528150
78\N,-0.4987935334,-0.1488948412,3.0930308618\N,-0.4907458423,0.141943
2566,-3.0685458382\C,0.8524938351,0.2893487662,-3.5686753283\H,1.10313
23674,1.3892902012,-3.5581905039\H,0.8783349149,-0.0580233806,-4.64639
24723\C,2.0163333974,-0.4448730477,-2.8666329967\H,1.8973989913,-1.551
9362443,-3.0218892379\H,2.9541648345,-0.1306458634,-3.3982686119\C,2.1
472772252,-0.1960933458,-1.4073504716\C,0.9666181908,-0.1269402124,-0.
6755319826\H,-0.0194848347,-0.2419384117,-1.1426834491\C,0.9631639682,
0.1009860852,0.6813562512\H,-0.0267382071,0.1957954824,1.1447199376\C,
2.1422663183,0.201252126,1.4119293931\C,3.3453816195,0.1091414615,0.69
76141692\H,4.3044356749,0.185090384,1.2298284798\C,3.3478967049,-0.073
3997435,-0.6935981913\H,4.3086324036,-0.1242677865,-1.2257484658\C,2.0
079802533,0.4463949361,2.871285584\H,2.9485776106,0.1393875418,3.40250
18849\H,1.8797743728,1.5518184803,3.029905345\C,0.8516371812,-0.302744
1844,3.5690776593\H,1.1035763811,-1.4019124665,3.535718154\H,0.8877203
547,0.0247710878,4.6529349681\\Version=IBM-RS6000-G94RevE.2\HF=0.23038
58\RMSD=0.000e+00\RMSF=3.515e-05\Dipole=0.0024605,-0.0455936,-0.360620
2\PG=C01 [X(C22H28N2)]\\@

NIMAG=1: 29.30 icm^{-1}, A

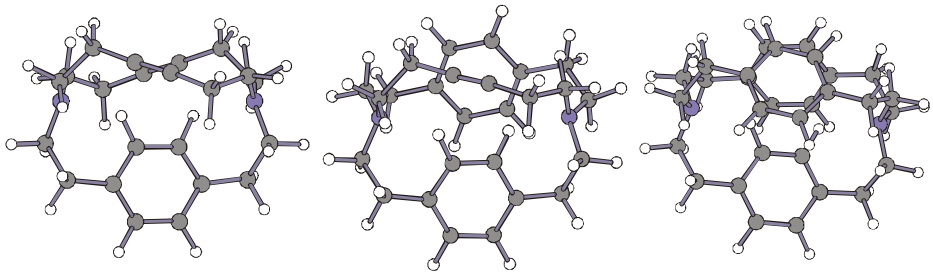
5: 0,1\C,-3.205694208
3,-0.241762542,-1.0783295787\H,-2.9981933454,0.5580051444,-1.845934401
7\H,-4.3271913189,-0.3953110506,-1.0388200106\C,-2.5978907854,-1.55157
08622,-1.5940696382\H,-2.7970858875,-2.3930433866,-0.8738030951\H,-3.1
420486944,-1.8031075805,-2.5500703931\C,-1.1957863233,-1.4885842253,-1
.8635303737\C,-0.0221082322,-1.4789506937,-2.1009957648\C,1.3729835579
,-1.4463647717,-2.4140532676\H,1.5561286197,-2.0605757344,-3.340895927
9\H,1.6697696231,-0.3847110996,-2.6466457367\C,2.2640381964,-2.0217630
374,-1.3017818211\H,1.7845281244,-2.9697787663,-0.9313053044\H,3.24934
7251,-2.3099428519,-1.7779886597\C,-2.9564310137,-0.6323243858,1.32299
14446\H,-3.0053818541,-1.6989241049,0.9684741631\H,-3.9538830618,-0.39
48753202,1.8024587022\C,-1.8911287584,-0.550987595,2.427731406\H,-1.62
6637077,0.5232142816,2.6416014901\H,-2.3465655622,-0.9809626544,3.3646
044387\C,-0.693819706,-1.2702088999,2.1192960535\C,0.3224268982,-1.859
7134038,1.8879092471\C,1.5132043793,-2.6057642267,1.6266680891\H,1.867
5483784,-3.0768400448,2.5888518084\H,1.2724134965,-3.4479923123,0.9197
732362\C,2.6832054733,-1.7708803086,1.0925988574\H,2.9026017803,-0.963
820559,1.8489637365\H,3.5829505454,-2.4574993668,1.0533565816\N,2.4695
528124,-1.115392203,-0.1845305193\N,-2.6995428098,0.2433111554,0.19201
94313\C,-3.0784167536,1.6247702231,0.4554007766\H,-2.9430480828,1.8251
483721,1.5570755663\H,-4.1695622452,1.8020535783,0.2146917711\C,-2.262
1203131,2.6744771428,-0.3083065244\H,-2.5429996045,2.6550518403,-1.394
5774553\H,-2.55597721,3.681274324,0.0952334339\C,-0.796742626,2.480183
1779,-0.1570053008\C,-0.2134869502,2.4054852149,1.1128183018\H,-0.8247

598389,2.5955233604,2.0072123726\C,1.1242837198,2.0468825628,1.2538953
323\H,1.5577589157,1.9434585361,2.2594470747\C,1.9057187228,1.77331292
41,0.1259197542\C,1.3537777508,1.967330069,-1.1458144502\H,1.974276527
2,1.8125941551,-2.0406633895\C,0.0119372958,2.3097521568,-1.2867225402
\H,-0.4220855982,2.4112129807,-2.2922635032\C,3.2785260054,1.225837528
6,0.2798840091\H,4.0263125311,1.9546418035,-0.1356713258\H,3.517320079
4,1.0859007148,1.3674173521\C,3.4739728243,-0.0988840406,-0.4668082965
\H,3.4476245769,0.1265293279,-1.5715526662\H,4.5140739888,-0.474288296
,-0.2275665343\\Version=IBM-RS6000-G94RevD.2\HF=0.1904636\RMSD=0.000e+
00\RMSF=9.264e-05\Dipole=0.0340199,0.2703869,0.1122302\PG=C01 [X(C22H2
8N2)]\\@

NIMAG=0

Supporting Information:

AM1-geometries of the transition states for rotation of one benzene ring of **5**-**7**



5-TS(monorot) **6**-TS(monorot) **7**-TS(monorot)

