

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 (MgSO₄) 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 CHCl₃ (15 × 200 ml). The combined organic extract was dried (MgSO₄) 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**.

CHCl₃ (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 CHCl₃ (5 × 100 ml). The combined organic extract was dried (MgSO₄) 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 CDCl₃, 300 MHz): δ 2.73 (4H, t, CH₂N), 2.23 (4H, t, CH₂CC), 1.27 (4H, s, NH₂)
- ¹³C NMR (in CDCl₃, 75 MHz): δ 79.2 (CC), 41.2 (CH₂N), 23.6 (CH₂CC)
- 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**):
C₆H₁₄Cl₂N₂
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(diro): 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,0,0,0,3.0660985459\N,0,0,0,-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(diro): 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\RMSE=0.000e+00\RMSE=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**

