

Mechanistic Studies for Dirhodium-Catalyzed Ring Expansion Reactions

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Shanghai 200237, P. R. China

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The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 3 and archive entries

Table S1^a

	$E_{\text{tot}} (E_{\text{h}})$	$H_{298, \text{toluene}}$	$G_{298, \text{toluene}}$	# of imaginary frequencies
1a	-781.7926124	-781.5330448	-781.5959628	0
Rh₂(esp)₂	-2067.153012	-2066.450934	-2066.56452	0
IN1	-2848.952860	-2847.986559	-2848.142651	0
TS1	-2848.917718	-2847.9545	-2848.107292	1 (-586.10 cm ⁻¹)
N₂	-109.5462206	-109.5375433	-109.5593163	0
¹IN2	-2739.421785	-2738.467887	-2738.617711	0
³IN2	-2739.424139	-2738.470662	-2738.622242	0
TS1'	-781.7268584	-781.4690828	-781.5334438	1 (-277.80 cm ⁻¹)
³IN2'	-672.2286479	-671.9801546	-672.0390496	0

a. SMD/BPW91/BS2// BPW91/BS1

1a

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  Card Required\0,1\C,0,-0.0023485306,0.0360867041,0.03562248\C,0,-0
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  ,3.3652161185,-0.2023119963,-0.487115092\H,0,1.2135464249,-0.063749180
  4,-1.7599891341\C,0,1.1821437068,0.0250389938,3.6595367132\C,0,-0.0269
  898379,-0.4987859862,4.3720008572\C,0,-0.4418175379,-1.8291519383,4.15
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Rh₂(esp)₂

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INI

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TS1

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³IN2

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TS1'

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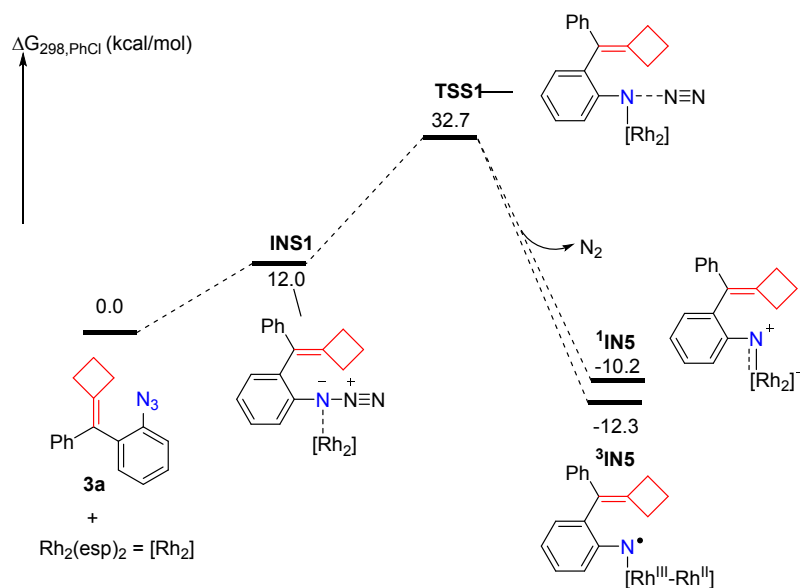
³IN2'

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91,-0.6702544873\C,0,-1.2563286195,-0.1456251094,2.2303398826\C,0,1.23
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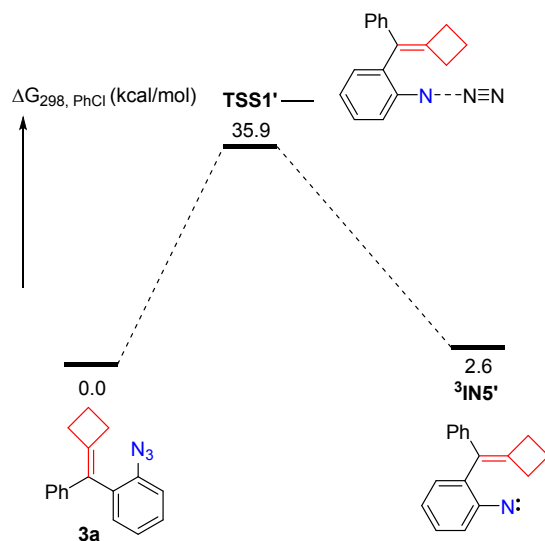
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Solvation Gibbs free energy profiles for catalyzed and uncatalyzed N₂ extrusion using substrates 3a and 3b

(a) The energetic profile for generation of nitrene intermediate catalyzed by Rh₂(esp)₂

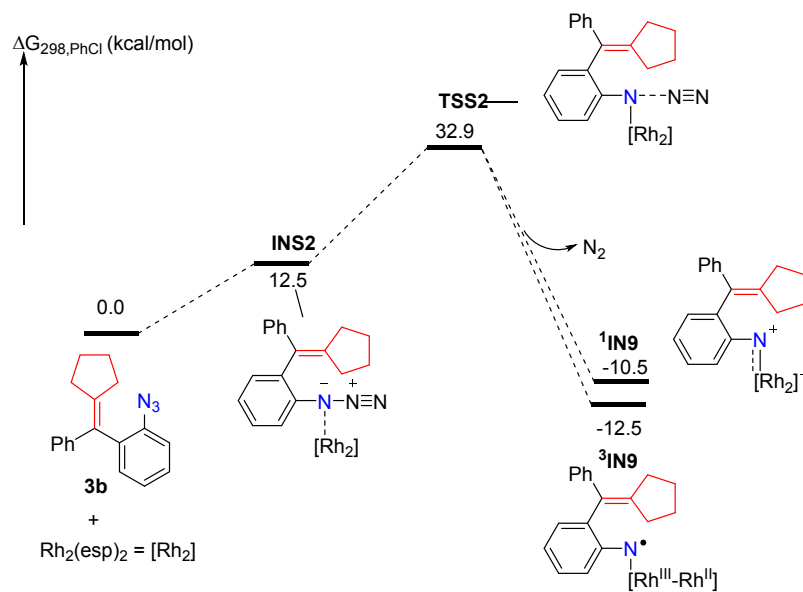


(b) The energetic profile for generation of nitrene intermediate uncatalyzed by Rh catalyst

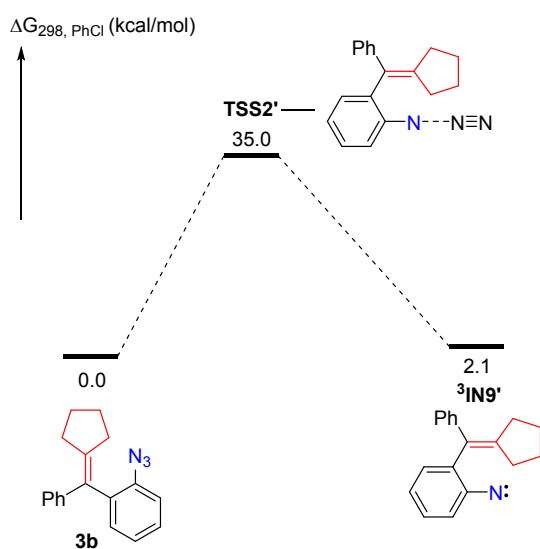


Scheme S1. Solvation Gibbs free energy profiles for catalyzed and uncatalyzed N₂ extrusion for substrate 3a.

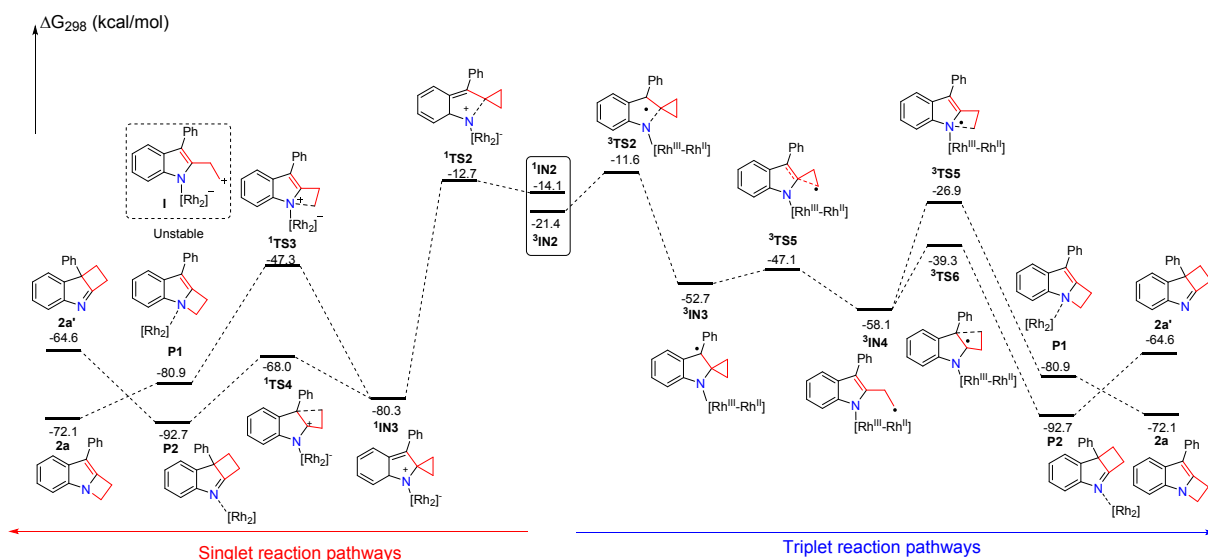
(a) The energetic profile for generation of nitrene intermediate catalyzed by $\text{Rh}_2(\text{esp})_2$



(b) The energetic profile for generation of nitrene intermediate uncatalyzed by Rh catalyst



Scheme S2. Solvation Gibbs free energy profiles for catalyzed and uncatalyzed N_2 extrusion for substrate **3b**.



Scheme S3. The Gibbs free energy profile for the reaction of **1a** having three-member ring calculated at B3PW91-D3/BS1//BPW91-D3/BS1 level.

In order to investigate whether the dispersion corrections affect the energy profile significantly, we calculated the Gibbs free energy profile for the reaction of **1a** having three-member ring calculated at B3PW91-D3/BS1//BPW91/BS1 level. Although the energy values are different, the relative stabilities of key intermediates are not reversed and the energy barriers do not vary significantly.

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 4 and archive entries

Table S2^a

	E_{tot} (E _h)	H _{298, toluene}	G _{298, toluene}	# of imaginary frequencies
¹TS2	-2739.418163	-2738.465179	-2738.611127	1 (-137.90 cm ⁻¹)
¹IN3	-2739.504832	-2738.548297	-2738.694895	0
¹TS3	-2739.456138	-2738.50174	-2738.647929	1 (-422.75 cm ⁻¹)
¹TS4	-2739.486433	-2738.531659	-2738.678459	1 (-352.67 cm ⁻¹)
³TS2	-2739.40918	-2738.457029	-2738.605513	1 (-137.94 cm ⁻¹)
³IN3	-2739.463016	-2738.508387	-2738.655884	0
³TS5	-2739.455919	-2738.502722	-2738.648314	1 (-492.28 cm ⁻¹)
³IN4	-2739.470209	-2738.516936	-2738.667435	0
³TS6	-2739.432577	-2738.478967	-2738.62936	1 (-334.91 cm ⁻¹)
³TS7	-2739.45103	-2738.497116	-2738.648105	1 (-411.89 cm ⁻¹)
P1	-2739.510165	-2738.552256	-2738.69835	0
P2	-2739.50604	-2738.570063	-2738.716178	0
2a	-672.3477786	-672.0944309	-672.1485019	0
2a'	-672.3291797	-672.0769934	-672.1304824	0

a. SMD/BPW91/BS2// BPW91/BS1

'TS2

```
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IN3

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'TS4

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[X(C48H53N1O8Rh2)]\@

³TS5

1\1\GINC-A739\FTS\UBPW91\GenECP\C48H53N1O8Rh2(3)\SIOC001\07-Jun-2016\0
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-1.3329337385,2.0559783949\O,1.447072741,-0.1723731837,1.612713039\O,-
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, -1.481791061,-0.1555576714,-1.3382632896\O,1.2855299732,-2.5542078084
, -1.2452208318\C,1.7531414283,-1.465928677,-1.7334170895\O,1.421438330
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\H,3.7708616229,-2.841134332,4.5040754153\H,2.0784685307,-3.2227829342
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³IN4

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11\O,0,-0.2486041786,-2.3126333357,2.0531733492\O,0,-2.077150584,0.013
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³TS6

1\1\GINC-SHI_02\FTS\UBPW91\GenECP\C48H53N108Rh2(3)\YIN\13-Jun-2016\0\#\p opt=(calcfc,ts,noeigen) genecp bpw91\Title Card Required\0,3\Rh,-1.530511554,1.6219777572,-0.4745738525\Rh,-0.1030060486,-0.2096906348,0.1581425955\O,-0.1821737897,2.1398435278,-1.925511938\C,0.8933400633,1.4507549953,-2.0598103264\O,1.2166165951,0.4251168224,-1.3570596186\O,-2.5665495982,0.5456423058,-1.8590161421\C,-2.3035702217,-0.7044319178,-2.0802115574\O,-1.3897938862,-1.3543853319,-1.4942373564\O,-2.8437400595,1.0513866203,1.0129525129\C,-2.595321014,-0.010916159,1.6953109409\O,-1.5524217714,-0.7456563312,1.5736145864\O,-0.6574973006,2.9275976728,0.8002080896\C,0.3153978927,2.5633837344,1.5735100496\O,0.774763684,1.3851065175,1.6374120861\C,1.7922132871,-1.8845545131,2.0142826405\C,3.0936468785,-2.4993653454,1.9585558155\C,1.2586230632,-1.3867204981,3.2253038645\C,3.3206802216,-2.9082635083,0.5981656927\C,3.8767399124,-2.565826025,3.1369576696\C,2.0370537322,-1.5018857037,4.37198658\H,0.2701364892,-0.9277430296,3.2352852392\C,3.3371288874,-2.0784947903,4.3243509757\H,4.8821406497,-2.9931836549,3.1138892641\H,1.6509194437,-1.135046486,5.3268736743\H,3.9256840901,-2.1369962314,5.2446794798\N,1.2334683141,-1.8272110169,0.7512063402\C,4.4410262587,-3.689379928,0.0505574096\C,4.9992312101,-4.7695837585,0.7752912724\C,4.9795209882,-3.3937720008,-1.2247299421\C,6.0539169266,-5.5227458803,0.2446312993\H,4.5816988919,-5.0309985159,1.7513960237\C,6.0280843914,-4.1547184568,-1.7569608238\H,4.5868375672,-2.5386750867,-1.7824043343\C,6.5720339523,-5.2214495125,-1.024634355\H,6.4669239065,-6.355325928,0.8217182176\H,6.4322615415,-3.9035658135,-2.7420049048\H,7.3955454988,-5.8103645199,-1.4379070139\C,1.8768964954,1.8784482563,-3.1732505541\C,0.9319464971,3.6571370447,2.4792800896\C,1.3394010058,3.0991688001,-3.9435010207\H,2.0537198166,3.3764094206,-4.7377512261\H,0.370236312,2.8749216254,-4.4146625571\C,2.480723604,3.7064284997,2.2253196508\H,2.8961970963,4.4510663449,2.927817271\H,2.8960792568,2.7249637993,2.5077072221\C,0.7014956151,3.2297920534,3.9506554416\H,1.1445844031,2.2420389296,4.1490320629\H,1.1617822286,3.9652772674,4.6322493857\H,-0.3753935426,3.1823953097,4.1833255196\C,2.0468132972,0.6836901964,-4.1449644781\H,2.7547245874,0.9502547974,-4.9478777246\H,2.433308119,-0.2036282126,-3.6211583898\H,1.0863856572,0.4179195393,-4.6169802172\C,3.2777021004,2.1913239601,-2.5346198409\H,3.6520859491,1.2623814766,-2.0728788393\H,3.9585152415,2.436330982,-3.3695587928\C,-3.1784536482,-1.3898062671,-3.1613580455\C,-3.6327555894,-0.3984209872,2.775118293\C,-4.6976615294,-1.2180372119,-2.8038503188\H,-5.2719096198,-1.7340416754,-3.5944721157\C,-5.0768823587,-0.3959797699,2.1593988906\H,-5.7703545358,-0.6520138479,2.9805183002\H,-5.3098705785,0.6358076745,1.849400544\C,-5.2941417602,-1.3330221495,0.9858255796\C,-5.7830164297,-2.6444077386,1.150975368\C,-

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05487,0.1783053134\H,-5.730842858,-3.7063558378,-2.1045715699\C,-2.917
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-3.4255236447,-3.348779209,-4.0756628883\H,-1.7534296643,-3.0058354145
, -3.5559257323\H,-2.9901847521,-3.4214377938,-2.344849158\C,-3.5785865
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³TS7

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5,-2.1042792616,-2.0756113941\O,-0.981478834,-1.1365552527,-1.63534435
5\O,2.4305742543,0.1022306781,-1.8686625764\C,1.7288234469,1.168480922
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\\@

P1

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,0,-1.7977147608,-0.3727801303,-4.7648678055\H,0,-3.4724492335,-0.6198
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-2.9293708173,-2.4261373914,-3.2940609246\H,0,-3.5383758087,-2.8529841
237,-4.10917939\H,0,-1.870282285,-2.6112145691,-3.5299311997\H,0,-3.17
24439246,-2.9622557567,-2.3651634882\C,0,-3.6984042084,1.0221309835,3.
8416007177\H,0,-4.4766100136,0.8487625895,4.6041320699\H,0,-2.71740054
78,0.9705982024,4.3422398121\H,0,-3.8254337916,2.0362552381,3.43392457
58\C,0,-3.6006735831,-1.448498675,3.3262975599\H,0,-2.6231750665,-1.52
47660106,3.826269258\H,0,-4.3822732396,-1.6441498011,4.080142416\H,0,-
3.6538530886,-2.2351550612,2.5599333615\H,0,-4.9187047697,0.4198488051
, -2.9508672521\C,0,-0.19520378,-3.3857154085,-0.0481100884\C,0,0.73761
62108,-3.3927285798,-1.2991895116\H,0,-1.2370323672,-3.072325689,-0.17
54773199\H,0,-0.1119854299,-4.3060277743,0.549198778\H,0,0.3295245756,
-2.8088327317,-2.1362238438\H,0,1.0874098343,-4.3737968488,-1.65021800
98\C,0,1.6976471014,-2.6486731057,-0.3956271647\H,0,1.7803674747,4.015
5922775,-2.8682016122\C,0,1.0909967283,4.2664401263,2.8467301622\H,0,1
.6919971564,4.7334136876,3.6458935605\H,0,1.3266687515,4.7664456875,1.
8963406952\H,0,0.027595707,4.4446307763,3.0671978286\C,0,3.6623000759,
2.6293905473,-1.252012369\C,0,3.2950074033,2.1899485043,0.0329786956\C
,0,4.2404138478,3.9072881025,-1.3821424744\C,0,3.4307786244,3.00678832
6,1.1704354605\H,0,2.8787935778,1.1869478953,0.1501218105\C,0,4.424919

4678, 4.7203075606, -0.2540314116\H, 0, 4.5569052588, 4.2625169466, -2.36815
62201\C, 0, 4.013582348, 4.2796958406, 1.0125623611\H, 0, 4.8899370077, 5.704
7994297, -0.3631478358\H, 0, 4.1542682205, 4.9244478749, 1.8860830262\Version=ES64L-G09RevD.01\State=1-A\HF=-2739.5101651\RMSD=4.793e-09\Dipole=
0.0287065, -1.6886904, -0.0993367\Quadrupole=-9.4155792, -6.6891518, 16.10
47309, 4.3089113, -4.4718553, 5.1563581\PG=C01 [X(C48H53N1O8Rh2)]\@

P2

1\1\GINC-A743\FOpt\RBPW91\GenECP\C48H53N1O8Rh2\SIOC001\12-Apr-2016\0\
#p opt genecp bpw91\Title Card Required\0, 1\Rh, 0.080753014, 0.0104158
03, 0.0926255324\Rh, -0.1616147605, 0.0963788499, 2.4979494252\O, 2.1145085
999, 0.0547483898, 0.3428949811\C, 2.5990651508, 0.0909513556, 1.5269771856
\O, 1.9138283913, 0.1024036134, 2.6197279825\O, 0.1346597519, -2.0451028941
, 0.2221642982\C, 0.0105234811, -2.5993720112, 1.3735525536\O, -0.126663738
6, -1.9824157633, 2.4934280536\O, -1.9722405398, -0.010658506, -0.067014294
8\C, -2.674940412, 0.0007675884, 1.0083754855\O, -2.2129164586, 0.047375349
6, 2.20669028\O, 0.0484263086, 2.0588840224, 0.0512050585\C, -0.0822429964,
2.6991571591, 1.1521894755\O, -0.208865681, 2.1681225268, 2.3204131239\C, -
1.2026567796, 1.004222904, 5.4308287724\C, -1.0014058532, 0.7726823002, 6.8
190489787\C, -2.2494870281, 1.8093932495, 4.9669239972\C, 0.266334668, -0.0
351412461, 6.9482936136\C, -1.8280159581, 1.3915492306, 7.7603188388\C, -3.
0952027733, 2.3926443797, 5.9236959566\H, -2.3888950719, 1.9641848749, 3.89
76855864\C, -2.8906481773, 2.1890548854, 7.3013167761\H, -1.6564884421, 1.2
545509119, 8.831582371\H, -3.9252258478, 3.0226362666, 5.5914150375\H, -3.5
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09819, 9.2764014203\C, 2.2029271328, 1.5090722755, 7.527751796\C, 2.1952616
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, 6.4883037607\C, 3.1138431327, 1.6255355927, 9.7794074169\H, 2.1854518016,
0.3116685858, 11.2343401254\H, 3.8270471602, 2.8131818673, 8.1095365822\H,
3.8252594038, 2.0497657188, 10.4934428675\C, 4.1393632723, 0.1018808822, 1.
6696620423\C, -0.1158811964, 4.2438973192, 1.0853149766\C, 4.8141230196, 0.
136778642, 0.2852086342\H, 5.9105812143, 0.1279746178, 0.4107492133\H, 4.52
8894324, -0.7390118159, -0.3169198417\C, 0.9805055028, 4.838718905, 2.03929
97029\H, 0.9029147079, 5.9382183266, 1.9648324944\H, 0.7122836591, 4.564818
6095, 3.0732622558\C, -1.5011928802, 4.7140731275, 1.5973016797\H, -1.67846
74796, 4.3783765923, 2.6302419582\H, -1.5542923599, 5.8158268815, 1.5748790
69\H, -2.3111492285, 4.3248898131, 0.958517104\C, 4.558917229, -1.187455350
6, 2.4196480202\H, 5.6536847576, -1.2033285553, 2.5552287966\H, 4.083381307
9, -1.244867862, 3.4103956496\H, 4.2771289447, -2.0858117859, 1.8460261499\
C, 4.5809352971, 1.3358046084, 2.5346322723\H, 4.1720467032, 1.2002941614, 3
.5496896874\H, 5.681412243, 1.286999013, 2.6194219013\C, 0.0568327488, -4.1
463974857, 1.4037274129\C, -4.2129950712, -0.0167958733, 0.8361511497\C, -1
.0194876405, -4.7228207576, 0.4154703194\H, -0.9332885686, -5.8234020375, 0

.4593230246\C,-4.6277439692,-1.234780827,-0.0644063226\H,-5.72616263,-1.188801825,-0.1736372955\H,-4.1950048364,-1.0773143996,-1.0660519041\C,-4.2133534975,-2.5978779548,0.4554834021\C,-5.0705641381,-3.3977598574,1.236495458\C,-2.9235157126,-3.0825958692,0.1722432184\C,-4.6312538792,-4.634972037,1.7307783532\H,-6.0887196555,-3.0563316037,1.4491989376\C,-2.4496596854,-4.3010742732,0.6912922236\H,-2.2639353115,-2.4860822436,-0.4614969682\C,-3.3269634611,-5.0809792405,1.4703624912\H,-5.310241584,-5.2560611418,2.3230416156\H,-2.9926848866,-6.0461866831,1.8646555796\C,1.4548687117,-4.584580956,0.8967758817\H,2.2510800157,-4.2173845614,1.5653587116\H,1.5166613473,-5.6858833583,0.8713531739\H,1.6478380269,-4.19878441,-0.1155682131\C,-0.1712434878,-4.6863128189,2.8273512983\H,-0.1361329561,-5.7891836245,2.8131230043\H,0.6119002664,-4.3333821089,3.5158057697\H,-1.1454051234,-4.3744540385,3.2308375901\C,-4.6165283379,1.2851744838,0.0977185086\H,-5.7064279076,1.2968081939,-0.0732344999\H,-4.3601361299,2.1741764482,0.6975870693\H,-4.107491665,1.3650101413,-0.8747021872\C,-4.9256298026,-0.0830754856,2.1997773556\H,-4.6732492142,0.7864124013,2.8247438868\H,-6.0181359477,-0.0873929535,2.0432279133\H,-4.6505926786,-0.9886191857,2.7594568864\H,-0.737068186,-4.4158673075,-0.6049249068\C,0.3158435869,-1.6444951284,6.846108788\C,1.2461927483,-1.5678576945,5.5824265284\H,-0.6702751798,-2.0621078778,6.6037486625\H,0.7467432142,-2.1253539164,7.7362464648\H,1.0475152425,-2.2408353782,4.7414131952\H,2.310038643,-1.5717459473,5.8622039471\C,0.6401047964,-0.1965261509,5.4843881198\H,4.5350225334,1.037666988,-0.2797575741\C,0.093606657,4.7301540465,-0.3613712123\H,0.0459951107,5.8323590531,-0.3889781087\H,1.0677841253,4.4129070375,-0.7604180151\H,-0.686863,4.3345865692,-1.0288434228\C,4.1618231713,2.6912172279,1.9976856184\C,2.8765874699,3.1858705068,2.2861433854\C,5.0144345423,3.4743665528,1.1951656497\C,2.4037133942,4.3993857456,1.753913229\H,2.2183139356,2.6005969906,2.9323222101\C,4.5755589199,4.7051543523,0.685153818\H,6.028040614,3.1236046157,0.9759919929\C,3.2766692308,5.1617916553,0.9531301682\H,5.2499826574,5.3120904803,0.0734882601\H,2.9419199746,6.1211140498,0.5453877568\\Version=ES64L-G09RevD.01\State=1-A\HF=-2738.7800936\RMSD=2.406e-09\RMSF=8.994e-06\Dipole=0.1572322,-0.1492848,2.1936327\Quadrupole=1.8638266,-0.3392755,-1.5245511,-5.7374528,2.5640935,-5.4207868\PG=C01 [X(C48H53N1O8Rh2)]\@

2a

1\1\GINC-A721\SP\RBPW91\6-311++G(d,p)\C16H13N1\ROOT\22-Mar-2016\0\#\p
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e Card Required\0,1\C,0,-0.0013058269,-0.0339638292,-0.0024136642\C,0
,0.0033660694,-0.0383077592,1.4418157982\C,0,1.1750342127,-0.011014794
4,-0.7659342292\C,0,-1.3789077296,-0.0458227458,1.9277519058\C,0,1.255
0981662,-0.0763588161,2.0940278393\C,0,2.3921067947,0.0016020031,-0.07
76276468\H,0,1.139297599,-0.0051036692,-1.8585560585\C,0,2.4289350899,
-0.0436277936,1.3352038423\H,0,1.3074044324,-0.1351737707,3.1840716123

\H,0,3.3283796322,0.0336235982,-0.6416980879\H,0,3.3967127543,-0.06063
85281,1.8444772502\N,0,-1.3352909801,-0.1364709253,-0.3581828679\C,0,-
1.8712997693,0.0246626819,3.3099695054\C,0,-1.1991875158,0.7777734997,
4.3015103859\C,0,-3.0642702657,-0.6402821038,3.681208462\C,0,-1.696954
6118,0.8549461409,5.6083258318\H,0,-0.2965566666,1.3320697869,4.032579
9257\C,0,-3.5662347201,-0.5527016882,4.9846507972\H,0,-3.5853406432,-1
.2489590885,2.9362111265\C,0,-2.8828023616,0.1918719987,5.9585218264\H
,0,-1.1594824354,1.447093701,6.3552567543\H,0,-4.4894217859,-1.0794546
635,5.2449265054\H,0,-3.2699672172,0.2538138495,6.9795034761\C,0,-2.42
52738257,0.2668851012,-1.2808479704\C,0,-3.3986700066,0.1595903626,-0.
0451238226\H,0,-2.5912395781,-0.4372222207,-2.1112400188\H,0,-2.305054
6342,1.2899439865,-1.6722367544\H,0,-4.1242835828,-0.666878204,-0.1044
56094\H,0,-3.9317098722,1.0894301964,0.2052475128\C,0,-2.1356037524,-0
.10721855,0.7654133606\\Version=ES64L-G09RevD.01\State=1-A\HF=-672.347
7786\RMSD=4.918e-09\Dipole=-0.9553521,0.2714996,-1.0783375\Quadrupole=
1.1698142,-8.2226733,7.0528591,2.1992474,4.3176177,0.0687901\PG=C01 [X
(C16H13N1)]\@

2a'

1\1\GINC-A763\SP\RBPW91\6-311++G(d,p)\C16H13N1\SIOC001\24-Mar-2016\0\\
#p bpw91/6-311++G(d,p) geom=check scrf=(iefpcm,smd,solvent=toluene)\T
itle Card Required\\0,1\C,0,-0.0101358724,-0.0119013125,-0.0006286397\
C,0,0.0098486572,-0.0232712752,1.4263836879\C,0,1.1823208527,0.0293358
87,-0.7374942336\C,0,-1.4266039157,-0.1611527667,1.8673260875\C,0,1.22
45858462,-0.0460755454,2.1152736046\C,0,2.3952416923,0.0425964006,-0.0
322854203\H,0,1.1540730873,0.0501810426,-1.8296655621\C,0,2.4192747371
,0.0056094639,1.3748666319\H,0,1.25097128,-0.093414331,3.2078909817\H,
0,3.3386920107,0.0782522871,-0.5848641401\H,0,3.3790551303,0.019873773
9,1.899043794\N,0,-1.3280097471,0.0250601901,-0.5279580639\C,0,-1.6850
716887,-1.2435122866,2.8989916835\C,0,-1.6299169971,-0.9516000982,4.27
61302895\C,0,-1.9394746231,-2.5703848783,2.5003246682\C,0,-1.826730454
2,-1.9594442606,5.2311220029\H,0,-1.4285339482,0.0727558207,4.60554367
13\C,0,-2.1431777747,-3.577290646,3.4539944725\H,0,-1.9779641441,-2.80
98970652,1.4336871589\C,0,-2.0874120105,-3.2755892472,4.822769688\H,0,
-1.778314231,-1.7140311992,6.2961022328\H,0,-2.3464585084,-4.600635648
,3.1252695194\H,0,-2.2464462468,-4.0611446722,5.5668605459\C,0,-3.3754
661582,0.5233395157,0.8990477979\C,0,-2.4322441345,1.0907160332,2.0191
643552\H,0,-4.1563074591,-0.1285946052,1.3191852615\H,0,-3.7996325225,
1.2267309174,0.1702354391\H,0,-2.8719344767,1.1754855682,3.0236310495\
H,0,-1.9541222946,2.0310874058,1.7145067176\C,0,-2.1090922078,-0.18638
92463,0.4933209677\\Version=ES64L-G09RevD.01\State=1-A\HF=-672.3291797
\RMSD=4.195e-09\Dipole=-0.3368496,0.1118352,1.2576596\Quadrupole=2.285
3192,0.4771962,-2.7625154,-0.0543251,-1.98253,1.2298625\PG=C01 [X(C16H
13N1)]\@

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 5 and archive entries

Table S3^a

	$E_{\text{tot}} (E_h)$	$H_{298,\text{toluene}}$	$G_{298,\text{toluene}}$	# of imaginary frequencies
IN3-1	-672.3301891	-672.0783376	-672.1329126	0
TS3-1	-672.2781201	-672.0279747	-672.0811297	1 (-467.34 cm ⁻¹)
TS4-1	-672.3090265	-672.0587802	-672.1116532	1 (-362.69 cm ⁻¹)

a. SMD/BPW91/6-311++G(d,p)//BPW91/6-31G(d)

IN3-1

```
1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C16H13N1\YIN\26-May-2016\0\#p
bpw91/6-311++g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluene)\Title
Card Required\0,1\C,0,-0.016712397,0.070484693,0.0251448067\C,0,0.
0090916909,0.0204589317,1.4976192254\C,0,1.2232937214,0.0611048392,-0.
7030876564\C,0,-1.3215931617,0.0251224823,1.9129415606\C,0,1.261154054
7,-0.0519970952,2.190925319\C,0,2.4000265726,0.0004376735,0.0068350125
\H,0,1.205260348,0.099129616,-1.7950952423\C,0,2.4218618974,-0.0598730
046,1.4496926481\H,0,1.2875250926,-0.1097630499,3.2827714258\H,0,3.355
0976105,-0.0090917077,-0.5271537709\H,0,3.3900457747,-0.1188602281,1.9
552719873\N,0,-1.2433615805,0.1248563794,-0.4841452871\C,0,-1.82929928
02,0.0433766853,3.2946286339\C,0,-1.352490394,1.0120586522,4.211363685
4\C,0,-2.7801664744,-0.8969696846,3.7577102768\C,0,-1.8161684962,1.044
1546815,5.5322678358\H,0,-0.6277054332,1.7544297927,3.8663929548\C,0,-
3.2423723193,-0.8627392537,5.079392286\H,0,-3.1217100337,-1.6903956103
,3.0883711719\C,0,-2.7660157946,0.1094470624,5.9716577446\H,0,-1.43793
46544,1.8065942479,6.2195699121\H,0,-3.9695842274,-1.6071487966,5.4166
205336\H,0,-3.1289120742,0.1355168582,7.0029361299\C,0,-3.3523979791,1
.0442243285,0.551953119\C,0,-3.538671147,-0.4144129344,0.4170355311\H,
0,-3.3616621375,1.6699121449,-0.3414491405\H,0,-3.6427569742,1.5277480
057,1.4874230327\H,0,-3.6798130071,-0.8356528013,-0.5797035984\H,0,-4.
0070641687,-0.9612972287,1.2357864348\C,0,-2.098782453,0.109276529,0.6
519831786\Version=EM64L-G09RevA.01\State=1-A\HF=-672.3301891\RMSD=4.4
98e-09\Dipole=-0.5329801,0.0736814,1.1359568\Quadrupole=5.873895,-3.45
13747,-2.4225203,2.4980824,-1.3713793,0.7865474\PG=C01 [X(C16H13N1)]\
```

TS3-1

```
1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C16H13N1\YIN\10-Oct-2016\0\#p
bpw91/6-311++g(d,p) scrf=(iefpcm,smd,solvent=toluene)\Title Card Req
uired\0,1\C,0,2.2303212321,0.3532291551,-0.1205897452\C,0,1.103408939
8,-0.5582080467,-0.1232829964\C,0,3.5655341603,-0.1272659199,-0.087835
9258\C,0,-0.0809121799,0.245588571,-0.163242337\C,0,1.3491179562,-1.95
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68113353,-0.1409703784\C,0,3.7694050774,-1.4991155307,-0.0745618459\H,
0,4.3987369324,0.5806353471,-0.0859812758\C,0,2.6652484988,-2.40304599
67,-0.106050816\H,0,0.5217048974,-2.6701855644,-0.1815896683\H,0,4.786
2027101,-1.9008880082,-0.050740375\H,0,2.8654508361,-3.4789183078,-0.1
08672694\N,0,1.8332377754,1.6541263631,-0.2281259296\C,0,-1.4887151665
, -0.1742487866,-0.1174283605\C,0,-1.9090561984,-1.2322444007,0.7246349
464\C,0,-2.4736778553,0.4746732461,-0.9014583502\C,0,-3.2525360866,-1.
6228382867,0.7783878879\H,0,-1.1723078593,-1.7326185334,1.358937559\C,
0,-3.8188989897,0.0910827707,-0.8365236958\H,0,-2.1672666397,1.2657401
145,-1.592242722\C,0,-4.2166320145,-0.9613453202,0.0021450771\H,0,-3.5
500399755,-2.4424600073,1.4395368289\H,0,-4.5580254138,0.6066617947,-1
.4572439864\H,0,-5.2660773732,-1.2657302786,0.0470293722\C,0,0.7238229
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787e-09\Dipole=-0.6428779,0.7930025,0.7892607\Quadrupole=-0.9739282,5.
9562373,-4.9823091,-1.8894617,2.4332436,0.4213865\PG=C01 [X(C16H13N1)]

TS4-1

1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C16H13N1\YIN\26-May-2016\0\#\#p
bpw91/6-311++g(d,p) geom=check scrf=(iefpcm,smd,solvent=toluene)\Tit
le Card Required\0,1\C,0,0.0072520743,-0.0908186616,0.0034163208\C,0,
0.0215378696,0.0757566679,1.4393940515\C,0,1.2314784651,-0.1896661545,
-0.7044221851\C,0,-1.3555535435,0.1897018197,1.8241169032\C,0,1.246154
2804,0.1868423396,2.1414771749\C,0,2.4201453735,-0.1054207761,0.012605
3583\H,0,1.2227804555,-0.326594278,-1.7887120448\C,0,2.4329736426,0.08
89232717,1.423083408\H,0,1.260243841,0.3564253542,3.2219281959\H,0,3.3
743071507,-0.1825271577,-0.5178562307\H,0,3.3916517349,0.1660822027,1.
9435229648\N,0,-1.2603027874,-0.1468055274,-0.5251776131\C,0,-1.868651
6909,0.7123843384,3.1075909563\C,0,-2.7847428121,1.7882589656,3.133392
1435\C,0,-1.4460460317,0.1596202391,4.3386402705\C,0,-3.259498854,2.29
53932482,4.3501790107\H,0,-3.0996983325,2.2435527682,2.1904033532\C,0,
-1.920377679,0.6701887848,5.5533392155\H,0,-0.7528097109,-0.6862429957
,4.3348198961\C,0,-2.829733617,1.7392651866,5.5642071541\H,0,-3.961953
6303,3.1338687821,4.3489728012\H,0,-1.5827908877,0.2278429413,6.495090
7601\H,0,-3.2000506733,2.1367523224,6.5132417506\C,0,-2.0785701318,0.0
726215925,0.5295749516\C,0,-2.7212799573,-1.4075335898,1.3989708766\C,
0,-3.4919227903,-0.4280822779,0.5716787953\H,0,-2.2416106452,-2.249981
1673,0.8976579915\H,0,-2.9312215625,-1.5118336945,2.4656792135\H,0,-4.
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-1.4679571,-3.675267,-1.4337378,-0.3637758,0.721137\PG=C01 [X(C16H13N1]

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 6 and archive entries

Table S4^a

	$E_{\text{tot}} (E_h)$	$H_{298, \text{PhCl}}$	$G_{298, \text{PhCl}}$	# of imaginary frequencies
3a	-821.1269336	-820.8348716	-820.9001976	0
¹IN5	-2778.759321	-2777.7753860	-2777.9280410	0
¹TS8	-2778.754429	-2777.7714006	-2777.9193536	1 (-102.23 cm ⁻¹)
¹IN6	-2778.819204	-2777.8329374	-2777.9806464	0
¹TS9	-2778.760408	-2777.7781219	-2777.9271939	1 (-434.70 cm ⁻¹)
¹TS10	-2778.802188	-2777.8172716	-2777.9632846	1 (-488.86 cm ⁻¹)
³IN5	-2778.761319	-2777.7777903	-2777.9313513	0
³TS8	-2778.743625	-2777.7615381	-2777.9116171	1 (-267.80 cm ⁻¹)
³IN6	-2778.782514	-2777.7980175	-2777.9464875	0
³TS11	-2778.755729	-2777.7734593	-2777.9221543	1 (-542.86 cm ⁻¹)
³IN7	-2778.790159	-2777.8072794	-2777.9593574	0
³TS12	-2778.74318	-2777.7606770	-2777.9105550	1 (-589.22 cm ⁻¹)
³TS13	-2778.769389	-2777.7859744	-2777.9384784	1 (-467.36 cm ⁻¹)
P3	-2778.74318	-2777.7606770	-2777.9105550	0
P4	-2778.862125	-2777.8749938	-2778.0229598	0
4a	-711.6841274	-711.4016582	-711.4576382	0
4a'	-711.714235	-711.4304371	-711.4864601	0

a. SMD/BPW91/BS2// BPW91/BS1

3a

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1\1\GINC-A736\SP\RBPW91\6-311++G(d,p)\C17H15N3\SIOC001\14-Jun-2016\0\#\#p bpw91/6-311++G(d,p) scrf=(iefpcm,smd,solvent=chlorobenzene) geom=check\Title Card Required\0,1\C,0,1.8936963197,0.0455720195,-0.1503874782\C,0,1.9047862685,0.555573652,1.1536822385\C,0,1.2734812502,-0.1361307436,2.2142659749\C,0,0.6089876594,-1.3469179366,1.9064275596\C,0,0.6006420609,-1.857501222,0.6031841618\C,0,1.2457778936,-1.1661091653,-0.4332694081\H,0,2.3841184585,0.6056224835,-0.9523273833\H,0,2.3821083727,1.5180397468,1.3486291862\H,0,0.102385496,-1.8954910046,2.7044438979\H,0,0.0864348833,-2.800865985,0.3965108881\H,0,1.2357484903,-1.5624690318,-1.4525689567\C,0,1.2926121848,0.3771785168,3.6100423879\C,0,0.1096331697,0.0600767073,4.4782650484\C,0,-1.1344674528,0.6689472803,4.2193380222\C,0,0.1815522074,-0.8549098839,5.5592784918\C,0,-2.2620332546,0.4111699273,5.0085998557\H,0,-1.2033548171,1.3637903592,3.3778410886\C,0,-0.9498336832,-1.1190765939,6.3587052022\C,0,-2.1649382641,-0.485300831,6.0838374747\H,0,-3.2106523927,0.9070500381,4.7868543104\H,0,-0.8744240084,-1.8263805401,7.1897625454\H,0,-3.0362635197,-0.6976700581,6.7094813296\N,0,1.4390500026,-1.4870613821,5.7733093719\N,0,1.5556839414,-2.317656312,6.6882461354\N,0,1.8305602234,-3.1066624918,7.4897070145\C,0,2.3081957441,1.1197898776,4.1177084866\C,0,3.7005345122,1.5075039171,3.6289298019\C,0,2.5853405785,1.6829934955,5.5055545835\H,0,4.2521927924,0.7506546293,3.0465824121\H,0,3.7158111549,2.4535588552,3.0575702655\H,0,2.29457563,1.0711298418,6.3731256082\H,0,2.1592358149,2.6943553978,5.6396981363\C,0,4.0992949347,1.7275014481,5.1222252672\H,0,4.650950398,0.8679833347,5.5312052057\H,0,4.6475015371,2.6516803711,5.3600654335\Version=ES64L-G09RevD.01\State=1-A\HF=-821.1269336\RMSD=5.566e-09\Dipole=-0.3954818,0.8259818,-0.1578986\Quadrupole=3.2357617,-2.1923743,-1.0433873,5.2943544,-4.8840195,2.7098027\PG=C01 [X(C17H15N3)]\@
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1IN5

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277,-3.3882347\PG=C01 [X(C49H55N1O8Rh2)]\@

!TS8

1\1\GINC-SHI_02\SP\RBPW91\GenECP\C49H55N1O8Rh2\YIN\05-Jul-2016\0\#\#p g
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IN6

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'TS9

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'TS10

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7,-1.6318722\PG=C01 [X(C49H55N1O8Rh2)]\@

3IN5

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676,0.17849145,2.5473123518\O,0,0.1248523721,-2.0634044365,0.232285470
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,2.5427982893\H,0,4.0840651947,-1.0726860113,3.4012628079\H,0,4.291340
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³TS8

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³IN6

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H,0,4.6609311122,-0.7207833665,-3.9852423796\H,0,2.8950731297,-0.47726
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³TS13

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P3

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N1O8Rh2)]\@

P4

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668,4.9424053503\C,0,0.4296682899,0.2589408216,6.9562139463\C,0,-1.269
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0629761\H,0,-1.8029849016,-2.1911028434,3.8736149107\C,0,-2.1664457088
, -2.615073103,7.2701705144\H,0,-1.1368083468,-1.4732954142,8.811850691
\H,0,-3.0605118453,-3.5719822825,5.5446152615\H,0,-2.7222397794,-3.225
5776993,7.9874496467\N,0,0.0909967157,-0.2191673819,4.6427187663\C,0,-
0.2233464642,1.4628040144,7.6641106418\C,0,-0.119369939,1.6316349864,9
.0584891026\C,0,-0.9995229662,2.3859519978,6.933999162\C,0,-0.76359748
55,2.6984074488,9.7034337316\H,0,0.4638852614,0.926079239,9.656691685\
C,0,-1.6407356211,3.4537297567,7.5771323957\H,0,-1.1075481618,2.265361
9797,5.8519670103\C,0,-1.5237317727,3.6165725346,8.965347825\H,0,-0.66
82697516,2.8095135171,10.7875495526\H,0,-2.2344126579,4.1595310944,6.9
889141207\H,0,-2.0223082967,4.4501125435,9.4678644661\C,0,4.2483244657
, -0.1656166384,0.951822664\C,0,0.1233866178,4.1622192804,1.4564225522\
C,0,4.6834371739,-0.1127089884,-0.5251326193\H,0,5.7830604675,-0.18337
53058,-0.5868259192\H,0,4.2520862454,-0.9497932343,-1.0946079527\C,0,1

.4253144281,4.6535355864,2.1836612539\H,0,1.384915796,5.7574994306,2.1
956429489\H,0,1.3710485385,4.3195299203,3.233439003\C,0,-1.0981499527,
4.6203422348,2.2922338136\H,0,-1.0756545647,4.1860313332,3.3030716786\
H,0,-1.1002129215,5.7199308548,2.3818970936\H,0,-2.0417631945,4.320108
0317,1.8075467825\C,0,4.7251556462,-1.4943965122,1.5899812168\H,0,5.82
64043832,-1.5524409148,1.5573778082\H,0,4.3998786698,-1.5740344561,2.6
383097217\H,0,4.3254817258,-2.3608009081,1.0379421725\C,0,4.8919392448
,1.0196480461,1.7569772091\H,0,4.68160081,0.8540165464,2.827201211\H,0
,5.9857873479,0.9329132057,1.6288131423\C,0,0.048703538,-4.2179711002,
0.9597947448\C,0,-4.1284123908,0.1096464182,1.4450702976\C,0,-1.236504
4561,-4.6845195093,0.184205952\H,0,-1.2001076555,-5.7879000496,0.14408
4871\C,0,-4.7280126863,-1.0660404972,0.591161091\H,0,-5.8267846705,-0.
9937938648,0.680164647\H,0,-4.4744846625,-0.8757643803,-0.4647846339\C
,0,-4.2644410564,-2.4594445235,0.9710585521\C,0,-4.9757858257,-3.26896
49416,1.8787084106\C,0,-3.0783404077,-2.9701934515,0.4110908601\C,0,-4
.4953367321,-4.5420636947,2.2213389798\H,0,-5.9166180065,-2.9077582376
,2.3060880008\C,0,-2.5582715823,-4.2274641737,0.7711202455\H,0,-2.5375
971093,-2.3658773484,-0.320886125\C,0,-3.2903741598,-5.0161682166,1.68
06200499\H,0,-5.0674709055,-5.1718413211,2.909634257\H,0,-2.9242260354
, -6.0110245268,1.9538334908\C,0,1.2880756184,-4.6299818815,0.125455164
5\H,0,2.2213029769,-4.3544771482,0.6440560359\H,0,1.2943539564,-5.7234
87219,-0.0209010109\H,0,1.2833125694,-4.1431009461,-0.8613027564\C,0,0
.1194218379,-4.8751130389,2.3503867235\H,0,0.1496203668,-5.9725693297,
2.2378716498\H,0,1.024164752,-4.5596342218,2.8917616973\H,0,-0.7490096
876,-4.6137095103,2.9714543041\C,0,-4.5778109431,1.4454108245,0.800269
6356\H,0,-5.679573494,1.4995014857,0.7805288362\H,0,-4.2083457348,2.30
61858665,1.3818339731\H,0,-4.202354884,1.536356609,-0.230034803\C,0,-4
.6296016766,0.0428016955,2.8993215579\H,0,-4.2286810162,0.8772251084,3
.4946196869\H,0,-5.7311524479,0.1093218758,2.911670248\H,0,-4.33168691
62,-0.8924748365,3.3938482067\H,0,-1.1529942493,-4.3186640482,-0.85236
20204\H,0,4.3647731249,0.8215955412,-1.0090831307\C,0,0.0371772276,4.7
637738104,0.0405530104\H,0,0.0243147878,5.865140469,0.1106231421\H,0,0
.8927788298,4.4630551862,-0.5808430593\H,0,-0.8806499407,4.4401666376,
-0.4729267464\C,0,4.4307195,2.4110570231,1.3666976391\C,0,3.2505631573
,2.9286614703,1.9293505202\C,0,5.137253034,3.2127439465,0.449221978\C,
0,2.7351031609,4.1881958128,1.5760437786\H,0,2.7078619374,2.3262489492
,2.6594384143\C,0,4.6573600163,4.4852974213,0.1041595702\H,0,6.0714247
45,2.8449215507,0.012986117\C,0,3.4619399394,4.9694962788,0.6567108089
\H,0,5.2212060228,5.1059523777,-0.5987211049\H,0,3.0976295532,5.964334
4741,0.3811137177\C,0,0.7514888053,0.5254520064,5.4891596342\C,0,2.029
8173445,1.2918856411,5.3228870184\C,0,1.8900656979,-0.0153135036,7.431
2348755\C,0,2.717372857,1.0910525424,6.7144751145\H,0,1.8506703269,2.3
564127182,5.09990355\H,0,2.6039659408,0.8726590568,4.4844465678\H,0,2.
0099218927,0.0006926032,8.5249650613\H,0,2.1926980329,-1.0162063397,7.
0787884782\H,0,2.6739213569,2.0242836065,7.2981692222\H,0,3.7780253469

,0.8128157323,6.6168131748\\Version=ES64L-G09RevD.01\State=1-A\HF=-277
8.8621247\RMSD=2.749e-09\Dipole=0.5092698,0.3046792,2.4216844\Quadrupo
le=0.1469129,1.9761988,-2.1231116,-6.7964798,0.3245347,1.4136773\PG=C0
1 [X(C49H55N1O8Rh2)]\@

4a

1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C17H15N1\YIN\21-Sep-2016\0\#\p
bpw91/6-311++G(d,p) scrf=(iefpcm,smd,solvent=chlorobenzene)\Title Ca
rd Required\\0,1\C\C,1,1.4364019\C,2,1.41158657,1,118.18056459\C,3,1.3
9778598,2,119.31413689,1,-1.76280584,0\C,4,1.41468014,3,121.32760942,2
,0.58468311,0\C,5,1.39834096,4,121.01260958,3,0.68193254,0\C,2,2.26666
55,1,71.59446489,6,179.49373343,0\C,7,1.39170628,2,38.24900099,1,179.4
7612013,0\H,3,1.09315819,2,120.34572289,1,177.84225405,0\H,4,1.0937639
5,3,119.40923885,2,-179.66054808,0\H,5,1.09357528,4,119.59092528,3,-17
9.70397533,0\H,6,1.09351892,5,121.17884549,4,179.18866748,0\C,8,1.4734
1499,7,127.13588256,2,-179.03972315,0\C,13,1.41492672,8,120.87179036,7
,138.03034769,0\C,13,1.41425473,8,121.36701716,7,-41.54836489,0\C,14,1
.40059911,13,121.05847391,8,-179.62282387,0\H,14,1.0931595,13,119.1111
6666,8,-1.25785379,0\C,15,1.40026065,13,121.15694284,8,179.06905283,0\
H,15,1.09371256,13,119.13286756,8,-2.68017546,0\C,16,1.40298022,14,120
.40593304,13,0.42996557,0\H,16,1.09429674,14,119.54322934,13,179.77776
965,0\H,18,1.09435444,15,119.60333634,13,179.80018351,0\H,20,1.0937271
7,16,120.36988764,14,179.8666485,0\N,1,1.38166328,6,130.80774948,5,177
.88301082,0\C,24,1.45853465,1,135.25988543,6,10.22547922,0\C,7,1.50622
734,2,174.98681364,1,98.38467393,0\H,26,1.10629884,7,110.44256922,2,5.
84656068,0\H,26,1.10018648,7,113.91238339,2,125.90216479,0\H,25,1.1064
5427,24,110.58286813,1,68.40843746,0\H,25,1.10202379,24,111.32353124,1
, -51.7730293,0\C,25,1.55166345,24,101.71178203,1,-172.30665804,0\H,31,
1.10185186,25,109.2340842,24,91.16132857,0\H,31,1.10004778,25,112.0940
057,24,-149.42362921,0\\Version=EM64L-G09RevA.01\State=1-A\HF=-711.714
235\RMSD=5.843e-09\Dipole=-1.232575,-0.0426347,-1.3621363\Quadrupole=-
0.5005682,-7.9347552,8.4353235,-3.0752705,3.908041,-0.9305575\PG=C01 [X
(C17H15N1)]\@

4a'

1\1\GINC-A719\SP\RBPW91\6-311++G(d,p)\C17H15N1\SIOC001\21-Sep-2016\0\#\p
bpw91/6-311++G(d,p) scrf=(iefpcm,smd,solvent=chlorobenzene)\Title
Card Required\\0,1\C\C,1,1.42143838\C,2,1.39382204,1,120.33373499\C,3,
1.40925283,2,118.59213651,1,-1.6402718,0\C,4,1.40516172,3,120.83217473
,2,1.0696479,0\C,1,1.39881142,2,121.22957124,3,1.37239241,0\C,1,2.1720
6951,6,161.25163271,5,178.90749335,0\C,2,1.52023308,1,106.56691798,6,1
77.77556729,0\H,3,1.09405758,2,121.11217407,1,178.41448136,0\H,4,1.093
70884,3,119.52816504,2,-178.94401013,0\H,5,1.09385311,4,119.53981245,3
,179.65767418,0\H,6,1.09280103,1,120.33026956,2,179.58415352,0\N,7,1.2
9785648,1,39.28408637,6,4.89904156,0\C,8,1.53662925,2,111.61594247,1,-

118.11681609,0\C,14,1.40990275,8,120.28102076,2,81.50264743,0\C,14,1.4
0831057,8,121.45217767,2,-95.29165463,0\C,15,1.40109755,14,120.9916169
6,8,-177.54446906,0\H,15,1.09415311,14,119.35112457,8,2.10318893,0\C,1
6,1.40293177,14,120.91394891,8,177.39608627,0\H,16,1.09360838,14,120.1
3330913,8,-2.24363009,0\C,19,1.40160463,16,120.30151363,14,-0.04752768
,0\H,17,1.09395036,15,119.59256508,14,-179.76021419,0\H,19,1.09405309,
16,119.54489456,14,179.99680288,0\H,21,1.0936349,19,120.30635868,16,17
9.78820521,0\C,7,1.50576138,1,162.50902894,6,61.28674838,0\C,25,1.5660
8182,7,101.94624571,1,96.1549141,0\C,26,1.55877037,25,105.62611108,7,-
9.21683405,0\H,25,1.10081007,7,110.37959919,1,-24.73525362,0\H,25,1.10
371641,7,112.25480201,1,-144.3710529,0\H,26,1.10108202,25,112.2762456,
7,-131.25109714,0\H,26,1.10158116,25,110.17395991,7,109.2255306,0\H,27
,1.10327253,26,110.47055176,25,-81.69454977,0\H,27,1.10065617,26,112.7
0803224,25,158.20962979,0\\Version=ES64L-G09RevD.01\State=1-A\HF=-711.
6841274\RMSD=2.747e-09\Dipole=-0.4914603,-0.1036477,1.2960995\Quadrupo
le=2.356139,0.1228257,-2.4789647,0.187547,-0.6520463,-1.6810788\PG=C01
[X(C17H15N1)]\@

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 7 and archive entries

Table S5^a

	$E_{\text{tot}} (E_h)$	$H_{298, \text{PhCl}}$	$G_{298, \text{PhCl}}$	# of imaginary frequencies
IN6-1	-711.6417315	-711.3602042	-711.4166402	0
TS8-1	-711.5831475	-711.3054956	-711.3649336	1 (-407.98-cm ⁻¹)
TS9-1	-711.6240879	-711.3443268	-711.3994988	1 (-493.00 cm ⁻¹)

IN6-1

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1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C17H15N1\YIN\31-May-2016\0\#\#p
bpw91/6-311++g(d,p) geom=check scrf=(iefpcm,smd,solvent=ChloroBenzene)
)\TitleCard Required\0,1\C,0,-0.027367827,0.0362724751,0.0327316552
\C,0,0.0109962128,0.0390684129,1.510982545\C,0,1.2133908847,0.00464190
25,-0.7054155649\C,0,-1.3080667829,0.057110907,1.9374156562\C,0,1.2742
420086,-0.0121303971,2.1948910548\C,0,2.3920324028,-0.0285147358,-0.00
33193112\H,0,1.1858897029,0.0045965991,-1.797755002\C,0,2.4258489428,-
0.0439803789,1.4452117178\H,0,1.3114953143,-0.0414817743,3.28731888\H,
0,3.3442326904,-0.0543181017,-0.5420716658\H,0,3.398862736,-0.09208021
28,1.9424912381\N,0,-1.2456105685,0.0676376966,-0.4702994037\C,0,-1.76
68167565,0.1715009088,3.3310315009\C,0,-1.169421694,1.1315808768,4.187
1287556\C,0,-2.7846197681,-0.6505199021,3.8738286754\C,0,-1.5713696596
,1.2626150444,5.5216234688\H,0,-0.4029976088,1.7966349437,3.780743921\
C,0,-3.1812045084,-0.5208830054,5.2103158557\H,0,-3.2447407903,-1.4211
138684,3.2523847711\C,0,-2.5792394643,0.4363126302,6.0409359296\H,0,-1
.0999674141,2.0188736462,6.156123275\H,0,-3.9616842425,-1.1771017717,5
.6064338086\H,0,-2.8942418961,0.5380606234,7.0831807051\C,0,-3.2219637
875,1.2633102774,0.6309590222\C,0,-3.3813547906,-0.890534131,0.5230463
933\H,0,-3.2597087188,1.6660867575,-0.3905653088\H,0,-3.0637201676,2.0
811414211,1.3488794613\H,0,-3.466048899,-1.1588365099,-0.5396740613\H,
0,-3.3575371057,-1.8129865583,1.1219193255\C,0,-2.147827559,0.08895244
99,0.666906918\C,0,-4.3552203978,0.2466701962,0.9185917605\H,0,-5.2760
70406,0.3440589538,0.3232788785\H,0,-4.6259807142,0.2198185822,1.98460
99433\Version=EM64L-G09RevA.01\State=1-A\HF=-711.6417315\RMSD=4.140e-
09\Dipole=-0.1349024,0.0696731,1.3716397\Quadrupole=7.0728851,-4.16235
66,-2.9105284,2.7773479,-2.0945827,1.0662865\PG=C01 [X(C17H15N1)]\@
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TS8-1

```
1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C17H15N1\YIN\31-May-2016\0\#\#p
bpw91/6-311++g(d,p) geom=check scrf=(iefpcm,smd,solvent=ChloroBenzene
```

)\\Title Card Required\\0,1\C,0,2.1760464129,-0.455587325,-0.497570120
6\C,0,0.8918723775,-1.1019348963,-0.2407870025\C,0,3.3614961203,-1.227
1231603,-0.4922702239\C,0,-0.0651611386,-0.0617719882,-0.2809349757\C,
0,0.8237844571,-2.5103541526,-0.0484258991\C,0,3.2621340207,-2.5970457
392,-0.2647867076\H,0,4.3259760465,-0.7464709327,-0.6759263772\C,0,2.0
036758045,-3.239693722,-0.0508014845\H,0,-0.1413922167,-3.0083003263,0
.0836862414\H,0,4.1706415685,-3.2074566553,-0.2622225936\H,0,1.9776173
756,-4.3225630015,0.0990957879\N,0,2.0531773958,0.8916575046,-0.710348
0455\C,0,-1.5120538737,-0.1548940177,-0.0993896468\C,0,-2.0586490407,-
0.9547534118,0.9387727328\C,0,-2.41865908,0.5417615007,-0.9409786278\C
,0,-3.4406631807,-1.0366120789,1.134466462\H,0,-1.3788500308,-1.480616
5909,1.6139808013\C,0,-3.8017262185,0.4576205809,-0.7398064854\H,0,-2.
0267365049,1.1060221253,-1.7911592972\C,0,-4.3210070714,-0.3285816994,
0.2993720012\H,0,-3.8347068207,-1.6500358357,1.9502465469\H,0,-4.47808
91232,0.9960767961,-1.410327078\H,0,-5.4015207557,-0.396104547,0.45352
79849\C,0,0.6640640232,3.3169851798,1.0945895913\C,0,0.2413387105,2.48
39315804,-0.6019544778\H,0,0.1341705434,4.256363236,0.8945543772\H,0,0
.123849358,2.6364662472,1.7598770848\H,0,0.7743833623,3.1827430112,-1.
2525418567\H,0,-0.8438482885,2.632212338,-0.5779631882\C,0,0.722715696
4,1.1408725522,-0.5947802295\C,0,2.0519287681,3.3737879589,1.202492888
8\H,0,2.623828942,4.1793650162,0.7340144491\H,0,2.6270323608,2.5526024
534,1.6327693682\\Version=EM64L-G09RevA.01\State=1-A\HF=-711.5831475\R
MSD=5.349e-09\Dipole=-1.2350662,1.528339,0.8780036\Quadrupole=-1.67961
74,9.1653768,-7.4857593,-0.0794152,2.8703105,-1.8123814\PG=C01 [X(C17H
15N1)]\\@

TS9-1

1\1\GINC-LOCALHOST\SP\RBPW91\6-311++G(d,p)\C17H15N1\YIN\16-Jan-2017\0\
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ene)\\Title Card Required\\0,1\C\C,1,1.4510074\C,1,1.42146203,2,119.56
823975\C,2,1.42423414,1,105.57015881,3,-178.78700519,0\C,2,1.41998727,
1,120.56889886,3,-2.12490193,0\C,3,1.38782801,1,118.51074858,2,1.55806
72,0\H,3,1.09296693,1,119.70551366,2,-179.21974614,0\C,5,1.38799431,2,
118.4750837,1,1.22163924,0\H,5,1.09376853,2,120.87503481,1,-177.594702
49,0\H,6,1.09448808,3,119.45434462,1,179.28162467,0\H,8,1.09359315,5,1
19.84088792,2,-179.56792845,0\N,1,1.36264958,3,127.12121077,6,-179.106
99961,0\C,4,1.47422675,2,126.59035423,1,169.21492813,0\C,13,1.41540799
,4,120.78384063,2,50.65940247,0\C,13,1.41442845,4,120.971719,2,-127.47
604504,0\C,14,1.40031458,13,120.86766683,4,-178.28161689,0\H,14,1.0935
6473,13,119.21785751,4,2.56304246,0\C,15,1.40049015,13,120.81056793,4,
178.15307103,0\H,15,1.09271175,13,119.34592449,4,0.09696949,0\C,18,1.4
0315693,15,120.27726875,13,0.1854534,0\H,16,1.09382749,14,119.70023061
,13,-179.72951886,0\H,18,1.09378675,15,119.64185135,13,-179.42079054,0
\H,20,1.09356356,18,120.1876765,15,179.90266177,0\C,4,2.21301258,2,112
.39518106,1,-64.30632354,0\C,24,2.27535316,4,73.80044662,2,124.9890028
,0\H,24,1.0957752,4,118.9209218,2,27.92810596,0\H,24,1.09610392,4,85.1

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75,0\H,25,1.10136221,24,140.60710962,4,57.71063971,0\C,12,1.36652132,1
,105.07293136,3,-178.38764996,0\C,24,1.53020799,4,102.00863446,2,157.2
5674518,0\H,31,1.1026369,24,114.04215928,4,-170.54800825,0\H,31,1.0999
9859,24,111.03781891,4,67.0210167,0\\Version=EM64L-G09RevA.01\State=1-
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\Quadrupole=5.3680727,-1.5706457,-3.7974269,1.660918,0.0723124,-1.3508
184\PG=C01 [X(C17H15N1)]\@

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 8 and archive entries

Table S6^a

	$E_{\text{tot}} (E_h)$	$H_{298, \text{PhCl}}$	$G_{298, \text{PhCl}}$	# of imaginary frequencies
3b	-860.4702738	-860.1480818	-860.2161568	0
¹IN8	-2818.10336	-2817.0892263	-2817.2443343	0
¹TS14	-2818.09616	-2817.0829407	-2817.2331677	1 (-185.83 cm ⁻¹)
¹IN9	-2818.156256	-2817.1394976	-2817.2895336	0
¹TS15	-2818.095662	-2817.0817222	-2817.2313272	1 (-483.17 cm ⁻¹)
¹TS16	-2818.131083	-2817.1166784	-2817.2664484	1 (-456.86 cm ⁻¹)
³IN8	-2818.105215	-2817.0914428	-2817.2475168	0
³TS14	-2818.085176	-2817.0727153	-2817.2248943	1 (-245.46 cm ⁻¹)
³IN9	-2818.118506	-2817.1033855	-2817.2537195	0
³TS17	-2818.089377	-2817.0776443	-2817.2296983	1 (-373.52 cm ⁻¹)
³IN10	-2818.103077	-2817.0904301	-2817.2447311	0
³TS18	-2818.080875	-2817.0690973	-2817.2211233	1 (-334.91 cm ⁻¹)
³TS19	-2818.098449	-2817.0849928	-2817.2391958	1 (-432.18 cm ⁻¹)
P5	-2818.181063	-2817.1631598	-2817.3149548	0
P6	-2818.189514	-2817.1723194	-2817.3212114	0
5a	-751.0133886	-750.7010041	-750.7585011	0
5a'	-751.0364487	-750.7229104	-750.7808714	0

a. SMD/BPW91/BS2// BPW91/BS1

3b

```
1\1\GINC-A737\SP\RBPW91\6-311++G(d,p)\C18H17N3\SIOC001\20-Jun-2016\0\
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1596555,-1.9102966818,0.6085280078\C,0,1.1416869786,-0.9787907524,-0.4
189058954\H,0,1.5868287423,1.0922387118,-0.8854909171\H,0,1.7201933726
,1.794598056,1.4983859615\H,0,0.8361154105,-2.2438386225,2.7453322094\
H,0,0.6961566766,-2.9516046739,0.3647662031\H,0,1.0757584149,-1.288100
0257,-1.4659694249\C,0,1.3754470776,0.2389796028,3.7323304726\C,0,0.11
13315494,0.0225891949,4.5125123215\C,0,-1.0443567099,0.7667880884,4.20
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,4.539311776,0.6223315101,6.3166653836\H,0,4.275124747,2.3311541414,6.
7332053829\C,0,4.6175888629,1.9265450134,4.5744619441\H,0,5.7102442555
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```

¹IN8

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,-2.0058142868,2.5628241422\O,-2.0065944605,-0.0502895898,-0.046930425
6\C,-2.7398171956,-0.0138407206,1.0027581361\O,-2.311698401,0.01987803
36,2.2168981464\O,0.0238341047,1.9929900173,0.0923883231\C,-0.15023029
8,2.6494982978,1.1786772616\O,-0.3196645685,2.1341788884,2.3470798926\
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¹TS14

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IN9

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'TS16

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³IN8

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³TS14

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606646,2.4741360421\C,4.2221839331,1.7717440465,1.0311798318\H,3.36453
14422,1.2947210207,-0.9348831522\H,2.6504033879,0.408218516,0.40542160
67\H,1.6301254539,3.195699067,2.8196504035\H,1.8300133892,1.363558013,
2.6645363805\H,4.9484576925,2.4072869878,0.4998794032\H,4.760432776,0.
8466945044,1.298699999\C,3.7205745787,2.5202186346,2.3078327254\H,3.96
50728091,3.5917612863,2.2265290599\H,4.2730533853,2.1458333319,3.19394
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4391906,0.0719812\Quadrupole=1.6249914,-5.5482316,3.9232402,-5.2936237
, -2.8346127,-1.1318149\PG=C01 [X(C50H57N1O8Rh2)]\@

³IN10

1\1\GINC-SHI_02\FOpt\UBPW91\GenECP\C50H57N1O8Rh2(3)\YIN\24-Jun-2016\0\
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779764,-0.0365697068\Rh,0.0777094847,-0.1653736384,2.3638384257\O,1.94
05522871,0.0796125974,-0.1598469191\C,2.6371596628,-0.0550090296,0.907
0032972\O,2.158973316,-0.1882364597,2.0970372616\O,-0.0723766112,-1.95
28341422,-0.2205004194\C,0.0012667078,-2.6657538157,0.8451054611\O,0.0
698269413,-2.2078586272,2.04468202\O,-2.1298336158,0.1223608923,0.1175
831448\C,-2.6483996951,0.0199232473,1.2884846917\O,-1.9900765703,-0.10
40160837,2.3841027908\O,-0.0820246815,2.1163708992,0.2087991845\C,-0.0
060178767,2.6039452861,1.3921229409\O,0.0791838852,1.9186263185,2.4800

822503\C,-0.9534386858,-1.1936272225,5.1234829288\C,-0.9830913755,-0.8
918460849,6.5187568818\C,-1.8017478809,-2.1620983294,4.5828215921\C,0.
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595852775\C,-2.7031342204,-2.8207956179,5.447434492\H,-1.7674226656,-2
.4074313155,3.5234996857\C,-2.7688878824,-2.5015217626,6.8134735518\H,
-1.9777976552,-1.2670326413,8.4194343154\H,-3.3663387874,-3.5852053919
,5.0340984394\H,-3.4886826666,-3.0126160505,7.4589906115\N,0.027949666
, -0.3987787981,4.4853597804\C,0.3532827322,0.7433709944,8.0193217761\C
,0.4405768631,-0.0420550226,9.19783507\C,0.5592536964,2.1408935142,8.1
392784264\C,0.7281715678,0.5436860129,10.4359408448\H,0.3147454071,-1.
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051,-0.8415941517\H,4.1344760826,-0.7850864909,-1.3322220633\C,1.28401
88955,4.6396367524,2.2201957166\H,1.2174797383,5.7408916477,2.27326226
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9,2.4442026647\H,-1.1515974852,4.0308869261,3.4260573\H,-1.2528448828,
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.2380900163\H,4.4270570355,-1.5416804142,2.3682103097\H,4.3127252263,-
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6328805926,0.9014746268,2.6358156233\H,5.9007453385,1.046846532,1.4052
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C,-5.0151049767,-3.347180933,1.6254660362\C,-3.1192426979,-2.949763676
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66,-6.0700313909,1.5515643306\C,1.2632244447,-4.5535951286,-0.20183630
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475,-0.4023977069\H,1.2504620035,-4.018516083,-1.1632178563\C,0.100793
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8317,2.6401795074\C,-4.6587987146,1.4266334688,0.8075798585\H,-5.76099
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93\H,-4.3037243053,1.5744528393,-0.2235341297\C,-4.671378586,-0.088313
1864,2.8297324385\H,-4.267889171,0.7134323018,3.4664017174\H,-5.772942
9567,-0.0296434784,2.8577021714\H,-4.3610093812,-1.0471727587,3.267736

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285356,1.2281840984\C,3.1320024749,2.9681087772,1.8413858588\C,4.96321
82236,3.3389104581,0.3137605284\C,2.5779837151,4.2256936548,1.54529208
56\H,2.6282587677,2.3365332216,2.574159096\C,4.4431688007,4.609168146,
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5.0499801506,0.6261246477\H,4.9703156986,5.2632798431,-0.6789500582\H,
2.862196814,6.0445273793,0.3929586821\C,0.6320632746,0.3493626858,5.45
57888564\C,1.8424876963,1.1933535554,5.162731016\C,2.9042775994,-1.741
5388014,6.1053898055\C,3.1178550546,0.8219805004,5.9601934163\H,1.6179
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824\H,2.8028154073,-1.9343517759,7.176657129\H,2.3220839918,-2.3608325
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84,1.5859386275,5.732393257\C,3.7081745665,-0.5785334778,5.6253292561\
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6854,-3.0732519,3.2017694\PG=C01 [X(C50H57N1O8Rh2)]\@

³TS18

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24.74115718,1,-0.29633319,0\O,1,2.06112102,3,88.72658711,4,-87.8867330
1,0\C,6,1.28260107,1,119.25067154,3,91.16823062,0\O,7,1.28704986,6,125
.49202395,1,-1.09511941,0\O,1,2.04247779,3,179.40844266,4,137.00841563
,0\C,9,1.28775178,1,118.14826894,3,-136.08583766,0\O,10,1.27947103,9,1
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0\C,12,1.28155415,1,118.85905542,3,-90.58659504,0\O,13,1.28761144,12,1
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.84898881,0\C,16,1.40905164,15,119.73867606,11,95.14555416,0\C,17,1.40
717179,15,118.15676637,11,-123.52010054,0\H,17,1.08993323,15,120.55511
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,19,1.09352055,16,120.56635606,15,-177.20008794,0\H,20,1.09327359,17,1
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C,28,1.39986576,27,121.040587,18,-179.91363636,0\H,28,1.0932196,27,119

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,0\H,32,1.09414384,29,119.60749552,27,-179.5156625,0\H,34,1.09363398,3
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92885423,0\C,13,1.54664916,12,117.33001009,1,-178.73486348,0\C,38,1.54
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4,-178.57059688,0\H,40,1.10061499,38,111.19121977,4,-59.21181044,0\C,3
9,1.57126831,13,109.45014142,12,-119.69729673,0\H,43,1.10459287,39,106
.59075638,13,179.31520799,0\H,43,1.10265343,39,107.80165731,13,-66.129
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067,39,111.3177388,13,57.13645816,0\H,46,1.1031145,39,109.79156387,13,
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\H,50,1.1023952,38,110.97075644,4,62.27316462,0\C,38,1.57081336,4,109.
68601457,3,120.53173546,0\H,54,1.1030228,38,107.9925537,4,66.77452293,
0\H,54,1.10459193,38,106.55894938,4,-178.78195759,0\C,7,1.54636788,6,1
16.5004109,1,179.78271256,0\C,10,1.54497023,9,116.57445769,1,178.89157
024,0\C,57,1.57252485,7,109.11039726,6,-56.14570212,0\H,59,1.10472488,
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.75850851,0\H,61,1.10461644,58,106.53008638,10,178.99226615,0\H,61,1.1
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,64,1.4073778,61,119.4474525,58,-86.39044219,0\C,65,1.40297552,64,120.
37602507,61,-178.45308315,0\H,65,1.09446467,64,119.73791022,61,2.27881
773,0\C,66,1.40725806,64,122.25793514,61,176.3774315,0\H,66,1.09233663
,64,118.83114975,61,-3.08199695,0\C,67,1.40316775,65,120.44194163,64,1
.12622711,0\H,67,1.09426493,65,119.78527425,64,-178.64278886,0\H,71,1.
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,58,1.53877292,10,111.14179209,9,179.4660089,0\H,86,1.10038153,58,111.
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61.40323179,0\H,99,1.10051141,39,111.11832932,13,59.0765804,0\C,54,1.5
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0\C,104,1.40607479,103,122.50310823,54,-177.52408865,0\H,104,1.0917701
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87101,26,-84.94084212,0\C,91,1.49197292,26,106.90396035,15,-150.059100
13,0\H,116,1.10083246,91,109.26566139,26,-81.29874786,0\H,116,1.114495
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³TS19

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2.4507232763,-1.813471731\O,-0.9965582452,-1.2950472776,-1.6372545721\
O,2.6623678589,-0.9654360135,-1.3716954555\C,2.3223589087,0.1991643554
,-1.8032267478\O,1.3190584951,0.8779202978,-1.3923300628\O,2.782839622
7,-0.9921130264,1.5625921438\C,2.513073836,0.1703273111,2.0718339331\
O,1.511128423,0.8733962422,1.7584006373\O,0.4367449133,-2.6529390731,1.
6358777882\C,-0.6215605765,-2.0447298166,2.0364832044\O,-1.0526769403,
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,-1.7061806367,4.0925721394,-0.1829097602\C,0.6754439795,3.5543389677,
0.1948765554\C,-2.9271069747,3.3480936177,-0.2902784373\C,-1.423459218
5,5.4800434587,-0.1781434292\C,0.9288435122,4.923357249,0.1841329051\H
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P5

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P6

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3.5337864987,-4.31034298\H,0,2.3441982349,-4.1623402605,-3.031059412\C
,0,3.511115956,-0.8960322993,-3.4469222864\H,0,4.2818034961,-1.1466631
088,-4.1960003778\H,0,2.6293042077,-0.5059824599,-3.9773989337\H,0,3.8
997498797,-0.0908635756,-2.8073396852\C,0,2.3059267516,-0.6692163296,4
.4782297888\H,0,3.0321174097,-0.4520357334,5.2799168952\H,0,1.40054418
4,-0.0706756041,4.6723849962\H,0,2.0346480494,-1.7344560867,4.52839084
29\C,0,3.2428142119,1.1934352744,3.0537416871\H,0,2.3355552567,1.79723
63063,3.2071059186\H,0,3.9602157902,1.4409245117,3.8549929649\H,0,3.68
01251063,1.4898573777,2.0899848641\H,0,4.1525865099,-3.6931006656,-1.4
588709242\H,0,-3.2780406185,-4.4173007632,-1.7289927392\C,0,-3.1642949
533,-1.9922944103,3.8037885852\H,0,-3.9438532657,-1.7936889009,4.55940
35156\H,0,-3.4935312667,-2.8311689078,3.1741154019\H,0,-2.2484194832,-
2.3052579899,4.3275963838\C,0,-4.6572471544,-1.9816343495,-1.161383985
2\C,0,-4.2636752372,-1.1166257761,-0.1258593962\C,0,-5.6246323643,-2.9
638724094,-0.8726509982\C,0,-4.7642412052,-1.2224381313,1.1830608107\H
,0,-3.5328269275,-0.3366844685,-0.3431997968\C,0,-6.1597930287,-3.0715
503955,0.4202538388\H,0,-5.9690878286,-3.6377523688,-1.6635121812\C,0,
-5.7306336066,-2.2132488878,1.4443736151\H,0,-6.9208660952,-3.82892983
45,0.6308210204\H,0,-6.1578536699,-2.3059171716,2.4480198482\C,0,-0.95
09315289,2.7281495714,-0.911760975\C,0,-2.3799358853,2.3476249181,-1.0
975033449\C,0,-1.0461249413,4.6621439439,-2.4507180301\C,0,-2.87432007
37,2.8942729139,-2.4678512341\H,0,-2.9856758833,2.8004037454,-0.290846
0385\H,0,-2.4894552379,1.2582517764,-1.045708814\H,0,-0.8014907385,5.7
261701991,-2.6080969349\H,0,-0.4676172503,4.1019432165,-3.2068995139\H
,0,-3.9606597847,2.7213712158,-2.5521753\H,0,-2.3914818235,2.311586059
8,-3.272895376\C,0,-2.5489619718,4.387370553,-2.6485509863\H,0,-3.1386
312048,4.9858784682,-1.931693435\H,0,-2.8489815653,4.7157392927,-3.659
1957279\\Version=ES64L-G09RevD.01\State=1-A\HF=-2818.1895144\RMSD=8.23
6e-09\Dipole=-0.758495,2.3440239,-0.727732\Quadrupole=-5.3788624,-1.38
80598,6.7669222,-2.6155087,-0.1364475,2.5956094\PG=C01 [X(C50H57N108Rh
2)]\@

5a

1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C18H17N1\YIN\21-Sep-2016\0\#p
bpw91/6-311++G(d,p) scrf=(iefpcm,smd,solvent=chlorobenzene)\Title Ca
rd Required\0,1\C\C,1,1.41624052\C,2,1.39418094,1,120.61361756\C,3,1.
40888557,2,118.41148151,1,-0.75300513,0\C,4,1.40588353,3,120.82513327,

2,0.40056208,0\C,1,1.39961049,2,121.19307137,3,0.70565008,0\C,1,2.1834
1741,6,161.28899169,5,179.2605042,0\C,2,1.52287894,1,106.91172779,6,-1
79.90296662,0\H,3,1.0942911,2,121.21714959,1,178.77022163,0\H,4,1.0937
3401,3,119.54709749,2,-179.82496067,0\H,5,1.09388191,4,119.50963353,3,
179.85126388,0\H,6,1.09287183,1,120.36766536,2,179.71930556,0\N,7,1.30
286084,1,38.72787411,6,1.78478129,0\C,8,1.53855203,2,111.45095235,1,-1
19.13904163,0\C,14,1.40740072,8,122.94623535,2,-108.1477619,0\C,14,1.4
1184938,8,118.98977528,2,69.11080899,0\C,15,1.40436188,14,120.93735373
,8,177.58228435,0\H,15,1.0925969,14,120.37620581,8,-2.3475547,0\C,16,1
.3997542,14,121.15660336,8,-177.78164992,0\H,16,1.09426088,14,119.2503
5617,8,1.79999012,0\C,17,1.40041552,15,120.40499597,14,0.00616008,0\H,
17,1.09407127,15,119.43880938,14,179.93896797,0\H,19,1.0939457,16,119.
58626501,14,-179.90438781,0\H,21,1.0936227,17,120.36497206,15,179.8137
1818,0\C,7,1.49596006,1,162.76494874,6,21.68878844,0\C,25,2.5621461,7,
85.91796685,1,126.4145561,0\C,26,1.5426328,25,90.23164138,7,-2.2424702
3,0\H,25,1.10082489,7,109.97436452,1,-21.31054831,0\H,25,1.1061123,7,1
09.64423433,1,-140.18840015,0\H,26,1.1042799,25,143.88800365,7,-126.40
659418,0\H,26,1.10461114,25,94.20922241,7,107.61183957,0\H,27,1.104497
3,26,109.34793728,25,-87.96133844,0\H,27,1.10334867,26,111.42066543,25
,155.23683019,0\C,26,1.53990485,25,34.31057305,7,-133.10537504,0\H,34,
1.10520241,26,109.41950908,25,120.31071686,0\H,34,1.10345847,26,110.47
081998,25,-122.24672856,0\Version=EM64L-G09RevA.01\State=1-A\HF=-751.
0133886\RMSD=5.077e-09\Dipole=-0.5808071,-0.2412194,1.3207511\Quadrupo
le=2.3951515,0.4705216,-2.8656731,0.783537,-1.1600626,-1.5987802\PG=C0
1 [X(C18H17N1)]\@

5a'

1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C18H17N1\YIN\21-Sep-2016\0\#\#p
bpw91/6-311++G(d,p) scrf=(iefpcm,smd,solvent=chlorobenzene)\Title Ca
rd Required\0,1\C\C,1,1.4291763\C,2,1.41131229,1,118.58716456\C,3,1.3
9760292,2,119.19671373,1,-1.72942465,0\C,4,1.41413489,3,121.18186281,2
,0.36169231,0\C,5,1.39903794,4,121.02275214,3,0.71428077,0\C,1,2.26775
121,6,165.37733543,5,-179.83340554,0\C,7,1.39594043,1,74.14115639,6,17
8.81107526,0\H,3,1.09315553,2,120.36816175,1,177.82701357,0\H,4,1.0937
6911,3,119.49847059,2,-179.82211596,0\H,5,1.09359727,4,119.62254743,3,
-179.66202633,0\H,6,1.09337655,5,120.82101981,4,179.4071635,0\C,8,1.47
41545,7,126.71325862,1,-178.98229361,0\C,13,1.41577882,8,120.51578126,
7,135.73330099,0\C,13,1.41445673,8,121.80012149,7,-44.17015035,0\C,14,
1.40009056,13,121.1237057,8,-179.87159649,0\H,14,1.09329154,13,119.062
41738,8,-1.37460376,0\C,15,1.40116868,13,121.16393803,8,179.40046108,0
\H,15,1.0933831,13,119.2461501,8,-2.43224338,0\C,18,1.40259181,15,120.
35125632,13,0.59932368,0\H,16,1.09430857,14,119.55959003,13,179.746736
46,0\H,18,1.09434844,15,119.56836942,13,179.75856814,0\H,20,1.0937397,
18,120.35426388,15,179.63695225,0\N,1,1.38871787,6,129.83144056,5,178.
55087494,0\C,24,1.46274975,1,124.46294558,6,10.21094755,0\C,7,1.504586

42,1,155.17747532,24,3.01487942,0\H,26,1.10249162,7,109.25696988,1,146
.14816013,0\H,26,1.10831417,7,110.00676312,1,-97.90874821,0\H,25,1.107
51095,24,108.99536599,1,66.39090492,0\H,25,1.10331971,24,108.55894307,
1,-50.1106671,0\C,26,1.54105996,7,111.77606424,1,22.28423695,0\H,31,1.
10261216,26,109.84868633,7,-172.02165499,0\H,31,1.10543858,26,110.0432
0246,7,70.41334625,0\C,25,1.53429197,24,111.36796215,1,-172.24552322,0
\H,34,1.10514333,25,109.74828043,24,74.54364464,0\H,34,1.10269865,25,1
08.47983907,24,-168.81586721,0\\Version=EM64L-G09RevA.01\State=1-A\HF=
-751.0364487\RMSD=6.906e-09\Dipole=-1.2279465,-0.0619131,-1.3829535\Qu
adrupole=-1.006802,-7.6417244,8.6485264,-3.2470462,2.7564202,-0.773176
9\PG=C01 [X(C18H17N1)]\@

The total energies, enthalpies and free energies of the lowest conformers of all species shown in Scheme 9 and archive entries

Table S7^a

	$E_{\text{tot}} (E_h)$	$H_{298, \text{PhCl}}$	$G_{298, \text{PhCl}}$	# of imaginary frequencies
IN10-1	-750.9788892	-750.6691195	-750.7281315	0
TS14-1	-750.9197341	-750.6104334	-750.6692894	1 (-589.32 cm^{-1})
TS15-1	-750.9556516	-750.6458573	-750.7031483	1 (-460.91 cm^{-1})

IN10-1

```
1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C18H17N1\YIN\04-Jan-2017\0\#p
bpw91/6-311++G(d,p) geom=check scrf=(iefpcm,smd,solvent=chlorobenzene)
\\TitleCard Required\\0,1\C,0,-0.0251115143,0.0230163562,0.038430673
2\C,0,0.009932532,0.0213210747,1.5156266063\C,0,1.2186688303,0.0006502
249,-0.6975363297\C,0,-1.3072052461,0.0302565467,1.9416862321\C,0,1.27
16984093,-0.0285187263,2.2034506377\C,0,2.3949377802,-0.0314135363,0.0
075508896\H,0,1.1939371468,0.0057569465,-1.7899469273\C,0,2.4249129425
,-0.0524316324,1.4568457729\H,0,1.3050699134,-0.0595671399,3.295965444
4\H,0,3.3488902702,-0.0514196265,-0.5283867372\H,0,3.3970952085,-0.096
7263883,1.9561344722\N,0,-1.239759848,0.047172252,-0.466801337\C,0,-1.
7455448306,0.0897676285,3.3471129497\C,0,-1.2006811866,1.0750039948,4.
2085980195\C,0,-2.6733624481,-0.8276401041,3.8973318402\C,0,-1.5731689
693,1.1441852216,5.5566127059\H,0,-0.497972768,1.8052103711,3.79840545
08\C,0,-3.0384831242,-0.7606337664,5.2474417459\H,0,-3.0862014633,-1.6
187636795,3.2681724539\C,0,-2.4936194027,0.2261488099,6.0833691633\H,0
,-1.1453081121,1.9216490517,6.1963926107\H,0,-3.7489285899,-1.48853708
16,5.6500914958\H,0,-2.7839740571,0.2781821287,7.1364020331\C,0,-2.162
8997776,0.0750893696,0.6704537186\C,0,-3.261517766,-1.0353125981,0.508
7972194\C,0,-3.0322446064,1.3830472803,0.5969523139\C,0,-4.6056373885,
-0.4444822959,1.0275354396\H,0,-2.9680168692,-1.9748809291,1.001205847
2\H,0,-3.3193781301,-1.2454857007,-0.5697350955\H,0,-2.4983326283,2.26
2776304,0.9888813778\H,0,-3.2357617326,1.558592439,-0.4719878195\H,0,-
4.982139946,-0.9817800872,1.912674731\H,0,-5.380188524,-0.5413192001,0
.2490248601\C,0,-4.3273376977,1.0469345821,1.3534824701\H,0,-4.1821158
613,1.180797934,2.437304922\H,0,-5.1560668448,1.7100679169,1.054659468
6\\Version=EM64L-G09RevA.01\State=1-A\HF=-750.9788892\RMSD=4.430e-09\D
ipole=-0.1448389,0.0675138,1.3638383\Quadrupole=6.5617664,-3.5286561,-
3.0331103,2.6889548,-1.4851567,0.6426493\PG=C01 [X(C18H17N1)]\@
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TS14-1

```
1\1\GINC-LOCALHOST\SP\RBPW91\6-311++G(d,p)\C18H17N1\YIN\06-Jan-2017\0\
\#p bpw91/6-311++g(d,p) geom=check scrf=(iefpcm,smd,solvent=ChloroBenz
ene)\Title Card Required\0,1\C,0,2.2000746494,-0.1358819219,-0.31693
96364\C,0,1.0401013799,-0.9867252924,-0.1464583895\C,0,3.516070752,-0.
6681844339,-0.255001121\C,0,-0.1035848874,-0.1495434038,-0.2614986116\
C,0,1.2260941722,-2.3831775268,0.0520494911\C,0,3.662571381,-2.0327881
396,-0.0592227133\H,0,4.3783213969,-0.0073573843,-0.3805820984\C,0,2.5
212438549,-2.8810500727,0.0908322272\H,0,0.36622936,-3.0489710097,0.16
82032169\H,0,4.6618692252,-2.4758624555,-0.0237022886\H,0,2.679812026,
-3.9537190685,0.2391914361\N,0,1.8551494185,1.1628864597,-0.5368332435
\C,0,-1.5152194812,-0.5684097089,-0.1181088109\C,0,-1.9427056067,-1.24
31890923,1.0501152201\C,0,-2.4715802375,-0.3436573215,-1.1355754182\C,
0,-3.2718710331,-1.659966437,1.2016989263\H,0,-1.2182177603,-1.4302977
337,1.8482537273\C,0,-3.8025895995,-0.7535325449,-0.9815029439\H,0,-2.
1552638863,0.1252206145,-2.0714884671\C,0,-4.2101640033,-1.4113148675,
0.1888775143\H,0,-3.5765078243,-2.1771484286,2.1166535082\H,0,-4.52110
50707,-0.5718354417,-1.7865052895\H,0,-5.2484421225,-1.7343427547,0.30
69522711\C,0,1.148073339,2.0155635669,1.2290792418\C,0,-0.3370529417,2
.3854750388,-0.9828567849\H,0,2.1846422705,1.8793490899,1.5438461957\H
,0,0.4596578635,1.4345020139,1.8552608483\H,0,0.2762941841,2.836264353
3,-1.7806215148\H,0,-1.2951234934,2.0829174309,-1.4278281746\C,0,0.411
4557251,1.1716600205,-0.4564043188\C,0,-0.5639620992,3.4164438361,0.14
88408367\H,0,-0.8336915501,4.4091249079,-0.2473660253\H,0,-1.397641652
1,3.080972023,0.7909311175\C,0,0.7357460317,3.4386293292,0.9571656171\
H,0,1.5364876831,3.9544125484,0.4019720837\H,0,0.6102215364,3.96444180
69,1.924073371\Version=EM64L-G09RevA.01\State=1-A\HF=-750.9197341\RMS
D=2.278e-09\Dipole=-0.7500694,1.0241963,0.9390495\Quadrupole=-1.101749
7,3.5955639,-2.4938143,0.1279132,3.7359197,-0.0790573\PG=C01 [X(C18H17
N1)]\@
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TS15-1

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1\1\GINC-SHI_02\SP\RBPW91\6-311++G(d,p)\C18H17N1\YIN\05-Jan-2017\0\#p
bpw91/6-311++G(d,p) geom=check scrf=(iefpcm,smd,solvent=chlorobenzene
)\Title Card Required\0,1\C,0,2.3290924254,0.1957363345,-0.338902187
3\C,0,1.2811352136,-0.7297515855,0.0331107176\C,0,3.6828583743,-0.2336
153849,-0.3241917241\C,0,0.058447092,0.0034464823,-0.1022422572\C,0,1.
5874066346,-2.0714364838,0.3723075716\C,0,3.9560057678,-1.5518267454,0
.0184483631\H,0,4.4772616757,0.4671973446,-0.5935092407\C,0,2.91897033
51,-2.4695166017,0.3579081576\H,0,0.7948357143,-2.783312794,0.62056056
52\H,0,4.9924566877,-1.9033978012,0.0220475995\H,0,3.1802581803,-3.502
0171522,0.6063748508\N,0,1.8590157856,1.4353469936,-0.669305944\C,0,-1
.2983552914,-0.5881342128,-0.0988068202\C,0,-1.7210028045,-1.404742337
3,0.9765728149\C,0,-2.1859739536,-0.4007342837,-1.1818106283\C,0,-2.98
72047546,-2.0032386756,0.9727772932\H,0,-1.0493606895,-1.5609991796,1.
8256500024\C,0,-3.4518915209,-1.0009818019,-1.1850776729\H,0,-1.867750
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3386,0.1946552651,-2.0404743189\C,0,-3.8592162121,-1.8016752809,-0.107
5430021\H,0,-3.2937715643,-2.627913763,1.8167599043\H,0,-4.1197591017,
-0.8474213453,-2.037589954\H,0,-4.8480203154,-2.2686842307,-0.11169916
06\C,0,-0.3488869657,2.505123792,-1.0353646027\C,0,0.1162987224,1.4744
643453,1.4370441534\C,0,0.5017001906,1.3616750007,-0.516331369\C,0,-1.
2435121148,3.0452839327,0.1003622428\H,0,-0.9398190172,2.2064201037,-1.
.9171772042\H,0,0.3616429621,3.2790243491,-1.366007494\H,0,-0.62668158
31,0.8293079261,1.9234128708\H,0,1.1220543677,1.3086867616,1.836506042
4\H,0,-2.1512880879,2.4261203342,0.2072540078\H,0,-1.570076276,4.08152
47953,-0.0861827481\C,0,-0.3712445007,2.9176153376,1.3590049627\H,0,-0.
.9292078268,3.1764850449,2.2774516418\H,0,0.4929867896,3.5982545162,1.
2768315662\\Version=EM64L-G09RevA.01\State=1-A\HF=-750.9556516\RMSD=3.
821e-09\Dipole=-1.9627415,-0.0963707,0.9132661\Quadrupole=-0.1624415,1.
.1129968,-0.9505554,-3.1080937,3.3132961,-0.8763584\PG=C01 [X(C18H17N1
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