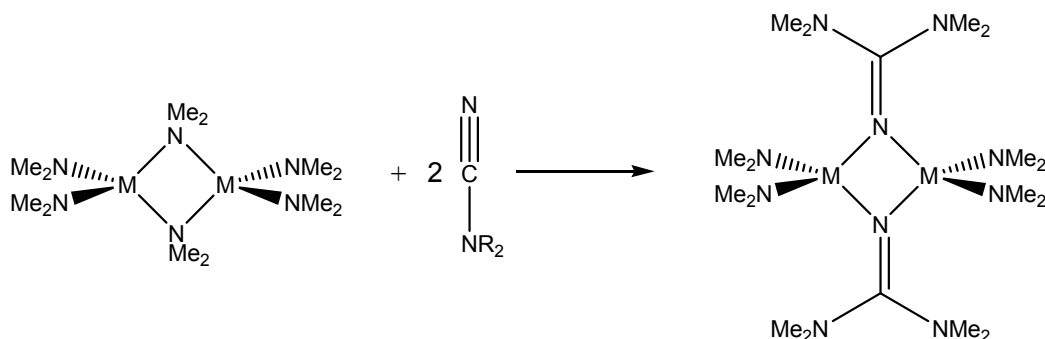


# Atom Efficient Cyclotrimerization of Dimethylcyanamide Catalyzed by Aluminium Amide: A Combined Experimental and Theoretical Investigation

## Electronic Supplementary Information

<sup>5</sup> Peter Dornan,<sup>a</sup> Christopher N. Rowley,<sup>a</sup> Jessica Priem,<sup>a</sup> Seán T. Barry,<sup>b</sup> Tara J. Burchell, Tom K. Woo<sup>\*a</sup>, Darrin S. Richeson,<sup>\*a</sup>

### Experimental



Insertion of a cyanamide in an existing M-N bond

**General Considerations:** The homoleptic amides of aluminium and gallium were synthesized by literature preparations.<sup>1</sup> Hexane was sparged with nitrogen and then dried by passage through a column of activated alumina using an apparatus purchased from Anhydrous Engineering. <sup>1</sup>H and <sup>13</sup>C NMR were collected on a Bruker AVANCE 300 MHz spectrometer, using the residual  
15 protons of the deuterated solvent for reference where applicable.

**Catalytic formation of hexamethylmelamine:** Al<sub>2</sub>(NMe<sub>2</sub>)<sub>6</sub> (0.10 g, 0.31 mmol) was added to a solution of dimethylcyanamide (0.50g, 7.1 mmol) in hexane (10 mL) and stirred overnight. The reaction mixture was quenched with aqueous NaCl. This solution was extracted with CH<sub>2</sub>Cl<sub>2</sub> (3 × 50 mL), the combined extracts were dried (MgSO<sub>4</sub>). Evaporation of the solvent provided white  
20 solid hexamethylmelamine (0.43g, 6.2mmol, 86% yield)  
m.p. 174-6°C. <sup>1</sup>H NMR (CDCl<sub>3</sub>): δ 3.25 (s, CH<sub>3</sub>N); MS (EI): m/z (%) = 210 (M<sup>+</sup>, 100)

**(Al(NMe<sub>2</sub>)<sub>2</sub>[NC(NMe<sub>2</sub>)<sub>2</sub>])<sub>2</sub> (458.4):** In a 50 mL flask, Al<sub>2</sub>(NMe<sub>2</sub>)<sub>6</sub> (1.00 g, 3.14 mmol) was taken up in 20 mL of hexanes. To this solution, NCNMe<sub>2</sub> (0.44 g, 6.28 mmol) was added drop wise. The clear, slightly yellow solution was stirred for 48 hours.  
25 Removal of the solvent and crystallization from hexane gave white, microcrystalline **1** (g, 87% yield) was collected.  
<sup>1</sup>H NMR (C<sub>6</sub>D<sub>6</sub>): δ 2.65 (s, CH<sub>3</sub>N), 2.87 (s, CH<sub>3</sub>N). <sup>13</sup>C NMR (C<sub>6</sub>D<sub>6</sub>): δ 39.47 (CH<sub>3</sub>N), 42.79 (CH<sub>3</sub>N), 165.59 (CN<sub>3</sub>).  
Anal. Calcd for C<sub>18</sub>H<sub>48</sub>Al<sub>2</sub>N<sub>10</sub>: C, 47.14; H, 10.55; N, 30.54. Found: C, 46.83; H, 10.29; N, 30.89.

### Computational Details

30 Except where noted, all calculations presented here used the PBE functional<sup>2</sup> with the 6-311G\*\* basis set, within Jaguar 6.0.<sup>3</sup> For specific large systems (indicated by italics), the smaller 6-31G\* basis set was used instead. The energies reported are Gibbs free energies, calculated using standard gas phase thermodynamic approximations.<sup>4</sup>

### References

- 35
1. K. M. Waggoner, M. M. Olmstead and P. P. Power, 1990, **9**, 257-263.
  2. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868.
  3. Jaguar, Schrodinger, LLC, New York, NY, 2005.
  4. C. J. Cramer, *Essentials of Computational Chemistry, 2nd Edition*, 2004.

## Calculated Cartesian Coordinates

### Dimethylcyanamide (1)

Gibbs free energy: -227.110735

|    |    |               |               |               |
|----|----|---------------|---------------|---------------|
| 5  | C1 | 0.0261204990  | 0.9246594764  | 0.0000000000  |
|    | N1 | -0.0978319735 | 2.0925912388  | 0.0000000000  |
|    | N2 | 0.2192138020  | -0.3989572615 | 0.0000000000  |
|    | C2 | -0.0553821275 | -1.1206469505 | 1.2467607042  |
| 10 | H1 | 0.5179247477  | -2.0598861932 | 1.2452318848  |
|    | H4 | -1.1297067805 | -1.3566662324 | 1.3657397367  |
|    | H5 | 0.2724405627  | -0.5109491624 | 2.0980561151  |
|    | C3 | -0.0553821275 | -1.1206469505 | -1.2467607042 |
|    | H2 | 0.2724405627  | -0.5109491624 | -2.0980561151 |
| 15 | H6 | -1.1297067805 | -1.3566662324 | -1.3657397367 |
|    | H7 | 0.5179247477  | -2.0598861932 | -1.2452318848 |

### Dimethylcyanamide dimer

Gibbs free energy: -454.213127

|    |     |               |               |               |
|----|-----|---------------|---------------|---------------|
| 20 | C1  | -0.0062212697 | 0.8724081650  | 0.0007557147  |
|    | N1  | 1.0870524266  | 0.0083222920  | 0.0008714886  |
|    | C2  | 0.0062212697  | -0.8724081650 | 0.0007557147  |
|    | N2  | -1.0870524266 | -0.0083222920 | 0.0008714886  |
|    | N3  | 0.0167800123  | -2.2035607153 | 0.0007072677  |
| 25 | N4  | -0.0167800123 | 2.2035607153  | 0.0007072677  |
|    | C3  | 1.2824949792  | -2.9224824888 | -0.0007185028 |
|    | H3  | 1.3634982373  | -3.5593579433 | -0.8976661674 |
|    | H6  | 1.3640114893  | -3.5620388478 | 0.8942448592  |
|    | H7  | 2.0927242791  | -2.1827848788 | 0.0001685067  |
| 30 | C4  | -1.2376324877 | -2.9420757306 | -0.0011840946 |
|    | H2  | -2.0592784660 | -2.2150716936 | 0.0003066796  |
|    | H8  | -1.3091656601 | -3.5835010523 | 0.8932859675  |
|    | H9  | -1.3088112375 | -3.5794235887 | -0.8986199027 |
|    | C5  | -1.2824949792 | 2.9224824888  | -0.0007185028 |
| 35 | H1  | -1.3634982373 | 3.5593579433  | -0.8976661674 |
|    | H10 | -1.3640114893 | 3.5620388478  | 0.8942448592  |
|    | H11 | -2.0927242791 | 2.1827848788  | 0.0001685067  |
|    | C6  | 1.2376324877  | 2.9420757306  | -0.0011840946 |
|    | H4  | 2.0592784660  | 2.2150716936  | 0.0003066796  |
| 40 | H12 | 1.3091656601  | 3.5835010523  | 0.8932859675  |
|    | H13 | 1.3088112375  | 3.5794235887  | -0.8986199027 |

### Hexamethylmelamine (2)

Gibbs free energy: -681.437100

|    |     |               |               |               |
|----|-----|---------------|---------------|---------------|
| 45 | C1  | -0.0634480978 | -1.2335653815 | 0.4294278857  |
|    | N1  | -0.4555635084 | -1.0074434390 | -0.8425598511 |
|    | C2  | -0.4073769133 | 0.2890694671  | -1.2162260930 |
|    | N2  | -0.0131644627 | 1.3195771079  | -0.4380350874 |
|    | C3  | 0.3537016989  | 0.9631021456  | 0.8114909385  |
| 50 | N3  | 0.3522673928  | -0.2936034356 | 1.3049732627  |
|    | N4  | -0.0912234485 | -2.5342598830 | 0.8721693315  |
|    | N5  | -0.7899740304 | 0.5853018280  | -2.5025164563 |
|    | N6  | 0.7618588838  | 1.9676912827  | 1.6558378386  |
|    | C4  | 0.3258916636  | -2.8974896428 | 2.2135290753  |
| 55 | H6  | 0.6289167025  | -1.9923661729 | 2.7489696365  |
|    | H10 | 1.1750975500  | -3.6043276258 | 2.1776437600  |

|    |     |               |               |               |
|----|-----|---------------|---------------|---------------|
|    | H11 | -0.5024675843 | -3.3860438156 | 2.7583498732  |
|    | C5  | -0.5173524831 | -3.6268655977 | 0.0179076075  |
|    | H7  | -1.3633290059 | -4.1685085929 | 0.4787731909  |
|    | H12 | 0.3071191250  | -4.3475161992 | -0.1351973827 |
| 5  | H13 | -0.8283040822 | -3.2212331933 | -0.9499082793 |
|    | C6  | 0.8175192110  | 3.3533540055  | 1.2292352524  |
|    | H4  | 0.1999602464  | 3.9852311295  | 1.8929755626  |
|    | H14 | 0.4413808723  | 3.4251410426  | 0.2039409023  |
|    | H15 | 1.8557090653  | 3.7322304543  | 1.2654069385  |
| 10 | C7  | 1.1977286294  | 1.6993515029  | 3.0134951645  |
|    | H5  | 2.2513338406  | 2.0045850740  | 3.1520064858  |
|    | H16 | 1.1015432833  | 0.6274713620  | 3.2125030229  |
|    | H17 | 0.5807174379  | 2.2640992094  | 3.7357827293  |
|    | C8  | -0.7883928655 | 1.9445826076  | -3.0099390086 |
| 15 | H9  | -0.4123946152 | 2.6146956409  | -2.2305840699 |
|    | H18 | -1.8097912688 | 2.2545696855  | -3.2981349176 |
|    | H19 | -0.1429957204 | 2.0216772276  | -3.9037842947 |
|    | C9  | -1.2426803544 | -0.4399031413 | -3.4240199092 |
|    | H8  | -0.6120710161 | -0.4485323699 | -4.3316087480 |
| 20 | H20 | -2.2866945108 | -0.2511435559 | -3.7351015649 |
|    | H21 | -1.1821574281 | -1.4144057693 | -2.9295347445 |

Tris(dimethylamino)Aluminum (monomer) (4)

Gibbs free energy: -645.446192

|    |     |               |               |               |
|----|-----|---------------|---------------|---------------|
| 25 | Al1 | -0.0587217628 | -0.1614605462 | 0.0410402715  |
|    | N1  | -1.6660078137 | -0.1398721963 | 0.8592517981  |
|    | N2  | 0.0634050398  | 0.2126494025  | -1.7191862621 |
|    | N3  | 1.4278407917  | -0.5611004701 | 0.9817331890  |
|    | C1  | -1.8525067626 | 0.1732457591  | 2.2674689069  |
| 30 | H3  | -0.8874965803 | 0.4002966066  | 2.7465207237  |
|    | H8  | -2.3172484765 | -0.6678991650 | 2.8245312173  |
|    | H9  | -2.5113080976 | 1.0560222444  | 2.4083050083  |
|    | C2  | 1.0934881165  | -0.3285080500 | -2.5921965508 |
|    | H4  | 1.7661452862  | -0.9962646314 | -2.0320000694 |
| 35 | H10 | 1.7142671381  | 0.4703563277  | -3.0505879447 |
|    | H11 | 0.6575455116  | -0.9166633332 | -3.4270354007 |
|    | C3  | -0.8568610344 | 1.0897057522  | -2.4264176488 |
|    | H6  | -1.3872480712 | 0.5631496738  | -3.2480759894 |
|    | H12 | -0.3310387568 | 1.9537922612  | -2.8843966661 |
| 40 | H13 | -1.6175380344 | 1.4909936397  | -1.7389521365 |
|    | C4  | 1.4381830577  | -1.4238329554 | 2.1527909216  |
|    | H2  | 1.7992828922  | -0.8928634505 | 3.0591817852  |
|    | H14 | 2.1006280175  | -2.3034688181 | 2.0095386039  |
|    | H15 | 0.4264839481  | -1.8021543217 | 2.3663013908  |
| 45 | C5  | 2.7508982904  | -0.0491512765 | 0.6600472183  |
|    | H1  | 3.1778990182  | 0.5433170362  | 1.4966336980  |
|    | H16 | 2.7096465220  | 0.6067308198  | -0.2234252362 |
|    | H17 | 3.4723048383  | -0.8652848359 | 0.4424283970  |
|    | C6  | -2.9219154663 | -0.4332278655 | 0.1865468466  |
| 50 | H7  | -3.6268630628 | 0.4242772477  | 0.2266905103  |
|    | H18 | -3.4424534320 | -1.2996296813 | 0.6463916947  |
|    | H19 | -2.7482946431 | -0.6756718257 | -0.8733318219 |

Tris(dimethylamino)Aluminum (dimer) (3)

Gibbs free energy: -1290.926265

|    |     |               |               |               |
|----|-----|---------------|---------------|---------------|
| 55 | Al1 | -0.3631433550 | 0.4553142658  | 1.0531797660  |
|    | N1  | -1.6588632794 | 1.6686472509  | 1.5441244879  |
|    | N2  | -0.4867332088 | -0.1054812884 | -0.6889033812 |

|        |               |               |               |
|--------|---------------|---------------|---------------|
| C1     | -3.0014748686 | 1.3395913407  | 1.9987968278  |
| H1     | -3.2917716292 | 1.9270015811  | 2.8972651448  |
| H8     | -3.0971040696 | 0.2760100254  | 2.2572636632  |
| H9     | -3.7673989554 | 1.5552491933  | 1.2208049254  |
| 5 C2   | -1.6218034326 | 3.0509269802  | 1.0850375112  |
| H6     | -0.6532549586 | 3.3032463644  | 0.6282338445  |
| H10    | -1.7964038884 | 3.7710455981  | 1.9139323367  |
| H11    | -2.4023949233 | 3.2552034403  | 0.3188583661  |
| C3     | -1.6155702811 | 0.3457877908  | -1.4963524626 |
| 10 H5  | -2.2320911055 | -0.5052901264 | -1.8586288885 |
| H12    | -1.2827590210 | 0.9048923279  | -2.3975268380 |
| H13    | -2.2684507106 | 1.0093413176  | -0.9099832446 |
| C4     | 0.3669435498  | -0.9825875575 | -1.4693005814 |
| H4     | 0.7682545947  | -0.4737823017 | -2.3729916789 |
| 15 H14 | -0.1800787698 | -1.8805617672 | -1.8319337249 |
| H15    | 1.2297997638  | -1.3411293993 | -0.8899413476 |
| N3     | 1.4626665189  | 1.0930011005  | 1.6212266225  |
| N4     | -0.1423707242 | -1.0208471848 | 2.4058231002  |
| Al2    | 1.3883508736  | -0.0549241008 | 3.2605099878  |
| 20 C5  | -1.2725331582 | -1.3038555194 | 3.3235359327  |
| H2     | -1.5810433857 | -0.3930112220 | 3.8507662068  |
| H16    | -0.9764276161 | -2.0523698200 | 4.0805335343  |
| H20    | -2.1389300612 | -1.7124504161 | 2.7719315922  |
| C6     | 0.2325107438  | -2.2920030689 | 1.7290234594  |
| 25 H19 | 1.1867069621  | -2.1827396624 | 1.1954376128  |
| H22    | -0.5437318075 | -2.6019271109 | 1.0083090864  |
| H23    | 0.3616892065  | -3.0998662722 | 2.4693857545  |
| C7     | 1.6103633021  | 2.5425978321  | 1.9046286142  |
| H18    | 2.5844157352  | 2.7462141191  | 2.3845796884  |
| 30 H24 | 0.8166348179  | 2.8878136823  | 2.5779106977  |
| H25    | 1.5670924470  | 3.1329003000  | 0.9714801197  |
| C8     | 2.5211595642  | 0.7034226408  | 0.6514006337  |
| H17    | 3.5048470983  | 1.0789379161  | 0.9818012014  |
| H26    | 2.3132990104  | 1.1166652045  | -0.3507609832 |
| 35 H27 | 2.5985397761  | -0.3901732829 | 0.5774067413  |
| N5     | 0.8796409045  | 0.8804753939  | 4.7467859477  |
| N6     | 2.8681561631  | -1.1234228050 | 3.4325970857  |
| C9     | 1.6175838254  | 0.7550564031  | 5.9950998863  |
| H3     | 2.0285874478  | 1.7302144108  | 6.3363921614  |
| 40 H30 | 2.4621739630  | 0.0590289308  | 5.8727736299  |
| H31    | 0.9793045197  | 0.3718675089  | 6.8211242535  |
| C10    | -0.2409367427 | 1.7950601523  | 4.8791299298  |
| H28    | -0.7907981505 | 1.8872269914  | 3.9265193618  |
| H32    | 0.0868532374  | 2.8151997297  | 5.1797173911  |
| 45 H33 | -0.9638222171 | 1.4603825449  | 5.6565177488  |
| C11    | 4.2265718902  | -0.6087214972 | 3.3988932971  |
| H7     | 4.8966414050  | -1.2331987614 | 2.7685255828  |
| H34    | 4.6904948916  | -0.5682245806 | 4.4103529729  |
| H35    | 4.2559235448  | 0.4152115363  | 2.9925906294  |
| 50 C12 | 2.8242693825  | -2.4323495323 | 4.0623293632  |
| H21    | 3.2638632022  | -2.4262561122 | 5.0854006589  |
| H36    | 3.3850421372  | -3.1971311346 | 3.4817952937  |
| H37    | 1.7876753998  | -2.7929286647 | 4.1625228948  |

55 Dimethylcyanamide coordinated to Al(NMe<sub>2</sub>)<sub>3</sub>:

Gibbs free energy: -872.559836

|    |              |               |               |
|----|--------------|---------------|---------------|
| C1 | 4.4791329564 | -3.3881051872 | -0.2631951429 |
| N2 | 4.4899067323 | -2.2393915507 | -0.0886671284 |

|    |      |              |               |               |
|----|------|--------------|---------------|---------------|
|    | N3   | 4.5061258833 | -4.6805233696 | -0.4638365560 |
|    | C4   | 4.8885558759 | -5.5783981865 | 0.6380722396  |
|    | H5   | 5.4864717985 | -6.4038554226 | 0.2334266900  |
|    | H6   | 4.0004272213 | -5.9871059128 | 1.1428247531  |
| 5  | H7   | 5.4923162178 | -5.0261971658 | 1.3638516775  |
|    | C8   | 3.7721902880 | -5.2553870464 | -1.6022135627 |
|    | H9   | 3.6332393096 | -4.4904550944 | -2.3689589644 |
|    | H10  | 2.7895458933 | -5.6369318779 | -1.2893173537 |
|    | H11  | 4.3598299335 | -6.0763319422 | -2.0271634884 |
| 10 | H12  | 1.1279550519 | -0.9252742139 | 1.3621259499  |
|    | C13  | 1.7115636271 | -0.3783074062 | 0.5886199116  |
|    | N14  | 2.9872645719 | 0.0904224785  | 1.0899910692  |
|    | H15  | 1.0579036577 | 0.4483332400  | 0.2340696080  |
|    | H16  | 1.8483235027 | -1.0631007308 | -0.2612407093 |
| 15 | Al17 | 4.6025012152 | -0.2559328209 | 0.2988622047  |
|    | C18  | 2.8398987182 | 0.9877992919  | 2.2179271858  |
|    | N19  | 4.8455561227 | 0.3837377646  | -1.4054900698 |
|    | N20  | 6.0282768668 | -0.1304467798 | 1.4455769305  |
|    | H21  | 3.8270471009 | 1.3213997652  | 2.5683605634  |
| 20 | H22  | 2.3212443631 | 0.5060503833  | 3.0759342945  |
|    | H23  | 2.2510430832 | 1.8951385941  | 1.9641895690  |
|    | C24  | 5.8773129934 | -0.0457007587 | -2.3251977772 |
|    | C25  | 4.0272528176 | 1.4513569039  | -1.9547909705 |
|    | C26  | 6.0518272099 | -0.7283948138 | 2.7621554654  |
| 25 | C27  | 7.2734392233 | 0.5344274309  | 1.1205795165  |
|    | H28  | 6.4802060505 | -0.8594015382 | -1.8913439538 |
|    | H29  | 6.5793971111 | 0.7748570885  | -2.5927766980 |
|    | H30  | 5.4592723899 | -0.4207352834 | -3.2875315900 |
|    | H31  | 3.5182364170 | 1.1521581909  | -2.8999243334 |
| 30 | H32  | 4.6186774281 | 2.3638685056  | -2.1910756522 |
|    | H33  | 3.2525622748 | 1.7397131293  | -1.2305557909 |
|    | H34  | 6.2666598669 | 0.0145569467  | 3.5582406228  |
|    | H35  | 6.8275000459 | -1.5178585023 | 2.8624734832  |
|    | H36  | 5.0807895089 | -1.1849062021 | 2.9981918019  |
| 35 | H37  | 7.5234180740 | 1.3293106038  | 1.8541212981  |
|    | H38  | 7.2030744369 | 1.0106401476  | 0.1343147483  |
|    | H39  | 8.1415212920 | -0.1587289461 | 1.1041890949  |

TS to 1<sup>st</sup> insertion product

40 Gibbs free energy: -872.549634

|    |     |              |               |               |
|----|-----|--------------|---------------|---------------|
|    | N1  | 3.5984403242 | 0.1915494811  | 0.7339049245  |
|    | Al2 | 4.0387051375 | 1.2776585976  | -0.8027534808 |
|    | N3  | 3.0487813104 | 0.8701994369  | -2.2830472906 |
|    | N4  | 4.2918912550 | 3.0346811334  | -0.3645313283 |
| 45 | C5  | 1.6038414297 | 0.7545027223  | -2.2711733430 |
|    | H6  | 1.2199057193 | 0.7335201108  | -1.2373695458 |
|    | H7  | 1.2542387994 | -0.1760351180 | -2.7717739075 |
|    | H8  | 1.0974403633 | 1.6001159949  | -2.7903877359 |
|    | C9  | 3.5855092702 | 0.8973954162  | -3.6308564462 |
| 50 | H10 | 3.3106260140 | -0.0161958365 | -4.2030630124 |
|    | H11 | 4.6859396774 | 0.9520352171  | -3.6104841413 |
|    | H12 | 3.2186792187 | 1.7648214334  | -4.2255012160 |
|    | C13 | 3.5997512698 | 4.1010701848  | -1.0661344426 |
|    | H14 | 4.3029352629 | 4.7863409755  | -1.5896378371 |
| 55 | H15 | 2.9922963951 | 4.7323725499  | -0.3801576481 |
|    | H16 | 2.9202342061 | 3.6784114828  | -1.8231323202 |
|    | C17 | 5.2482379897 | 3.5478972416  | 0.5941612887  |
|    | H18 | 5.9956211700 | 4.2224488450  | 0.1205207041  |

|    |     |              |               |               |
|----|-----|--------------|---------------|---------------|
|    | H19 | 5.8117450619 | 2.7283998068  | 1.0704026349  |
|    | H20 | 4.7650157911 | 4.1367821724  | 1.4068716560  |
|    | H21 | 8.1552362184 | -1.9761186725 | 0.4432838985  |
|    | C22 | 7.1148101616 | -2.2584178680 | 0.2032900347  |
| 5  | N23 | 6.1524534313 | -1.3247234348 | 0.8059649739  |
|    | H24 | 6.9163371083 | -3.2696109530 | 0.5895744381  |
|    | H25 | 6.9853925168 | -2.2566643695 | -0.8855390018 |
|    | C26 | 5.7670411150 | -0.2882525766 | 0.0666454629  |
|    | C27 | 6.0786191062 | -1.2820199603 | 2.2639994397  |
| 10 | N28 | 5.8327100144 | 0.4226948861  | -0.9077724114 |
|    | H29 | 5.2753487863 | -0.5973756141 | 2.5541577769  |
|    | H30 | 7.0317698441 | -0.9367817023 | 2.7039301895  |
|    | H31 | 5.8541983695 | -2.2890133423 | 2.6468176546  |
|    | C32 | 3.1679701945 | 0.8235940159  | 1.9793873690  |
| 15 | H33 | 3.3379122034 | 0.1684360890  | 2.8591932643  |
|    | H34 | 3.7019751205 | 1.7714836322  | 2.1368038851  |
|    | H35 | 2.0811982222 | 1.0518226599  | 1.9688984857  |
|    | C36 | 2.9107499266 | -1.0808374015 | 0.5305059952  |
|    | H37 | 3.1565631922 | -1.4924104161 | -0.4600483918 |
| 20 | H38 | 3.1948623977 | -1.8275751286 | 1.3006861285  |
|    | H39 | 1.8079690950 | -0.9686178276 | 0.5828795885  |

1<sup>st</sup> insertion product (5)

Gibbs free energy: -872.573812

|    |     |               |               |               |
|----|-----|---------------|---------------|---------------|
| 25 | C1  | -0.3832268282 | -1.1728251436 | 1.1452744135  |
|    | N1  | 0.1621448805  | -0.5522635068 | 0.1722379735  |
|    | N2  | -1.5665041952 | -0.7557352205 | 1.8037284660  |
|    | C2  | -1.5813126680 | -0.6892324625 | 3.2657749502  |
|    | H2  | -0.8632176617 | -1.4052213340 | 3.6810201887  |
| 30 | H6  | -2.5859452176 | -0.9224606951 | 3.6571916780  |
|    | H7  | -1.3016501506 | 0.3231171518  | 3.6221837752  |
|    | C3  | -2.3140522148 | 0.3183081178  | 1.1727948119  |
|    | H5  | -1.8430899141 | 1.3143191098  | 1.3133987605  |
|    | H8  | -3.3237556403 | 0.3519671556  | 1.6116644925  |
| 35 | H9  | -2.4035794154 | 0.1294305175  | 0.0948940289  |
|    | N3  | 0.1415264078  | -2.3654248495 | 1.6728562217  |
|    | C4  | 1.4457464058  | -2.7812263004 | 1.1822951299  |
|    | H3  | 2.0886845351  | -1.9019744420 | 1.0589989277  |
|    | H11 | 1.3823005518  | -3.2957614963 | 0.2027881523  |
| 40 | H12 | 1.8988389844  | -3.4712526189 | 1.9120308301  |
|    | C5  | -0.7395360426 | -3.4772234921 | 2.0226867494  |
|    | H10 | -1.7628738286 | -3.1126555991 | 2.1651276268  |
|    | H13 | -0.4017138292 | -3.9742628375 | 2.9484925049  |
|    | H14 | -0.7535438749 | -4.2356470288 | 1.2145929811  |
| 45 | Al1 | 0.4967100729  | 0.7616216922  | -0.9574277207 |
|    | N4  | 0.0143870265  | 0.5505620656  | -2.6857199311 |
|    | N5  | 1.3975465691  | 2.2360470744  | -0.4269143315 |
|    | C6  | -0.1829115714 | 1.6134260831  | -3.6552237375 |
|    | H15 | 0.0166896419  | 2.5987583132  | -3.2071309890 |
| 50 | H18 | -1.2263753361 | 1.6293728235  | -4.0368622758 |
|    | H19 | 0.4792860683  | 1.5038731682  | -4.5407475604 |
|    | C7  | -0.3188550878 | -0.7586163071 | -3.2276175631 |
|    | H16 | -1.3727900655 | -0.8066777188 | -3.5763390425 |
|    | H20 | -0.1829257054 | -1.5352193812 | -2.4596266379 |
| 55 | H21 | 0.3206568864  | -1.0208053855 | -4.0970881771 |
|    | C8  | 2.1725933244  | 3.1191554982  | -1.2816248372 |
|    | H1  | 3.2387173531  | 3.1541077866  | -0.9709838059 |
|    | H22 | 1.7972281140  | 4.1649019457  | -1.2570883991 |

|       |              |              |               |
|-------|--------------|--------------|---------------|
| H23   | 2.1475209256 | 2.7778397224 | -2.3275055675 |
| C9    | 1.4819925736 | 2.6164725727 | 0.9745639242  |
| H17   | 2.5323077693 | 2.6296835195 | 1.3367056072  |
| H24   | 0.9243543637 | 1.9024970663 | 1.6013429703  |
| 5 H25 | 1.0643790227 | 3.6298462959 | 1.1580168532  |

1<sup>st</sup> intermediate bridged with amide (**10**)

Gibbs free energy: -1518.053769

|        |               |               |               |
|--------|---------------|---------------|---------------|
| 10 N1  | 0.2229243535  | 0.7712337144  | 0.6414818744  |
| C1     | 0.0975004322  | 1.5814727931  | 1.6215846968  |
| N2     | -0.9731834332 | 2.4721621922  | 1.8264980490  |
| N3     | 1.0667435356  | 1.6889307732  | 2.6591234176  |
| C2     | -0.7917349137 | 3.7859419533  | 2.4312802594  |
| 15 H4  | 0.2478068285  | 3.8989959182  | 2.7601437066  |
| H7     | -1.4621093271 | 3.9398197423  | 3.2981165288  |
| H8     | -1.0157884092 | 4.5791788450  | 1.6919217435  |
| C3     | -2.1963642147 | 2.3309783875  | 1.0622002327  |
| H5     | -3.0666614438 | 2.5297486699  | 1.7120261016  |
| 20 H9  | -2.2768804541 | 1.3118050725  | 0.6637379338  |
| H10    | -2.2407434413 | 3.0430317503  | 0.2138291902  |
| C4     | 0.6085810766  | 1.5285298082  | 4.0409472791  |
| H2     | 0.5666555405  | 0.4569318030  | 4.3278098416  |
| H11    | -0.3939998677 | 1.9517834959  | 4.1685364787  |
| 25 H12 | 1.2977803559  | 2.0397483668  | 4.7335740877  |
| C5     | 2.3302299062  | 1.0073003143  | 2.4188423916  |
| H3     | 2.7078061889  | 1.2585216377  | 1.4206498416  |
| H13    | 2.2389905173  | -0.0955586516 | 2.4848538961  |
| H14    | 3.0593925842  | 1.3477566653  | 3.1712946739  |
| 30 A11 | -0.3473681022 | -0.1977791215 | -0.7553637468 |
| N4     | 1.2035580612  | -1.2136777926 | -1.5479144838 |
| N5     | -0.3855270843 | 0.8491867733  | -2.4767592853 |
| A12    | 1.4125565473  | 0.1291671002  | -3.0029344358 |
| N6     | 2.7575328422  | 1.3349317896  | -2.7033461839 |
| 35 N7  | 1.3851760745  | -0.6389683014 | -4.6705021645 |
| N8     | -1.8169756727 | -1.2461845010 | -0.3989530651 |
| C6     | 3.7667920861  | 1.5904196381  | -3.7200925769 |
| H16    | 4.7916190360  | 1.3477535603  | -3.3622775573 |
| H24    | 3.7832778678  | 2.6575814727  | -4.0332797228 |
| 40 H25 | 3.5705841982  | 0.9808777739  | -4.6158794390 |
| C7     | 2.2219990131  | -1.7681578631 | -5.0387319277 |
| H17    | 3.0876838112  | -1.4661741439 | -5.6711982129 |
| H26    | 1.6617727745  | -2.5353195055 | -5.6167930498 |
| H27    | 2.6346816292  | -2.2668881002 | -4.1474850230 |
| 45 C8  | 0.9287627058  | 0.0726766888  | -5.8524154453 |
| H21    | 0.2693883087  | -0.5548773356 | -6.4913587161 |
| H28    | 1.7716773338  | 0.4060756713  | -6.4997124096 |
| H29    | 0.3581388314  | 0.9754078586  | -5.5805823530 |
| C9     | 0.7710973468  | -2.5641075899 | -1.9919712164 |
| 50 H15 | 1.6285696592  | -3.1388694093 | -2.3835090377 |
| H30    | 0.0269262861  | -2.4893001321 | -2.7975595154 |
| H31    | 0.3288528663  | -3.1319595012 | -1.1547692211 |
| C10    | -2.5744909485 | -2.1022999777 | -1.2925338701 |
| H18    | -2.4520245636 | -3.1815948143 | -1.0471235445 |
| 55 H32 | -2.2714219194 | -1.9724440740 | -2.3414884238 |
| H33    | -3.6651781046 | -1.8914599557 | -1.2393987209 |
| C11    | -2.2433286819 | -1.4554651952 | 0.9788173382  |
| H23    | -1.6580880674 | -0.8289766704 | 1.6688560608  |

|        |               |               |               |
|--------|---------------|---------------|---------------|
| H34    | -2.1173926654 | -2.5138327217 | 1.2984254215  |
| H35    | -3.3184826990 | -1.2078993262 | 1.1224978933  |
| C12    | -1.4809587993 | 0.4519462156  | -3.3988137687 |
| H22    | -1.3399900093 | -0.5821560846 | -3.7438777578 |
| 5 H36  | -1.4873901059 | 1.0974964366  | -4.2944597053 |
| C13    | 2.9923543961  | 2.1301172230  | -1.5138039773 |
| H19    | 2.9605307198  | 3.2225721348  | -1.7250927949 |
| H38    | 3.9920628005  | 1.9282331245  | -1.0664393126 |
| H39    | 2.2374523114  | 1.9220950996  | -0.7378644879 |
| 10 C14 | 2.3598525388  | -1.3661186674 | -0.6322194589 |
| H20    | 3.2051552420  | -1.8545157421 | -1.1504140661 |
| H40    | 2.0875759672  | -1.9830598322 | 0.2428656882  |
| H41    | 2.6877561092  | -0.3866030710 | -0.2670319370 |
| H44    | -2.4663384316 | 0.5406036726  | -2.9080400555 |
| 15 C15 | -0.4572497182 | 2.3186113611  | -2.2815874329 |
| H1     | 0.2559345949  | 2.6421442529  | -1.5135651444 |
| H37    | -1.4700660738 | 2.6164145799  | -1.9563528922 |
| H42    | -0.2293396353 | 2.8507294997  | -3.2225680665 |

20 1<sup>st</sup> intermediate bridged with guanidinate (**11**)

Gibbs free energy: -1518.066253

|        |               |               |               |
|--------|---------------|---------------|---------------|
| N1     | 0.3726019579  | 0.6085420767  | 0.6584889173  |
| Al2    | -0.2765700253 | -0.3973415889 | -0.7469783963 |
| N3     | 1.2503807106  | -1.2673786966 | -1.5691818672 |
| 25 N4  | -0.3746734764 | 0.7037976879  | -2.4107965805 |
| Al5    | 1.4459187602  | 0.0489455752  | -2.9777845153 |
| N6     | 2.6863633541  | 1.3979909982  | -2.8551178151 |
| N7     | 1.4320020178  | -0.7636855243 | -4.6292531076 |
| N8     | -1.8585644409 | -1.2392195062 | -0.3146760498 |
| 30 C9  | 3.7513876736  | 1.5908829645  | -3.8207864958 |
| H10    | 4.7588168459  | 1.4149381906  | -3.3741202086 |
| H11    | 3.7710017980  | 2.6261058811  | -4.2268783206 |
| H12    | 3.6399324145  | 0.8982867198  | -4.6686683317 |
| C13    | 1.2795047621  | -2.1827535514 | -4.8722091890 |
| 35 H14 | 2.0556968705  | -2.5742797606 | -5.5670703144 |
| H15    | 0.2956728214  | -2.4376390575 | -5.3334576283 |
| H16    | 1.3597656895  | -2.7543653251 | -3.9340816201 |
| C17    | 1.3066240729  | -0.0036782077 | -5.8600159184 |
| H18    | 0.3191914013  | -0.1547427331 | -6.3547958585 |
| 40 H19 | 2.0782349004  | -0.2871214857 | -6.6100011303 |
| H20    | 1.4182348675  | 1.0765665422  | -5.6708515875 |
| C21    | -2.7886226595 | -1.9346631726 | -1.1816212009 |
| H22    | -2.8953720935 | -3.0101744452 | -0.9054736870 |
| H23    | -2.4703823233 | -1.9015319471 | -2.2337947611 |
| 45 H24 | -3.8124771263 | -1.5033668537 | -1.1332851472 |
| C25    | -2.2747762763 | -1.3556912731 | 1.0747619839  |
| H26    | -1.5580461839 | -0.8461491220 | 1.7355753781  |
| H27    | -2.3435226638 | -2.4190614132 | 1.4038212840  |
| H28    | -3.2783156971 | -0.9104295089 | 1.2500706404  |
| 50 C29 | -1.3776005093 | 0.2748189405  | -3.4168088742 |
| H30    | -1.2306662485 | -0.7805693544 | -3.6883658651 |
| H31    | -1.2775220865 | 0.8678898640  | -4.3439179086 |
| C32    | 2.8681961216  | 2.2502067383  | -1.6950646026 |
| H33    | 2.7919800615  | 3.3319353298  | -1.9427221702 |
| 55 H34 | 3.8733431731  | 2.1102641019  | -1.2318072771 |
| H35    | 2.1205391855  | 2.0269123530  | -0.9166188244 |
| H36    | -2.4047971280 | 0.4085097480  | -3.0325439031 |
| C37    | -0.5513820029 | 2.1570996228  | -2.1875821462 |

|        |               |               |               |
|--------|---------------|---------------|---------------|
| H38    | 0.1074384563  | 2.5043946592  | -1.3831462495 |
| H39    | -1.5957278613 | 2.3827708548  | -1.9017707856 |
| H40    | -0.3176831165 | 2.7288719866  | -3.1036873854 |
| C41    | -0.4209761010 | 1.6367740539  | 1.3090669833  |
| 5 H42  | -0.6907929160 | 1.3703748166  | 2.3565292104  |
| H43    | 0.1168684883  | 2.6096054327  | 1.3625373574  |
| H44    | -1.3656417560 | 1.8108001286  | 0.7684545477  |
| C45    | 1.5898800782  | 0.3411243669  | 1.3982793090  |
| H46    | 2.2334257542  | 1.2446615998  | 1.4914532530  |
| 10 H47 | 1.3891977960  | -0.0079251929 | 2.4370444053  |
| H48    | 2.1885913554  | -0.4364342522 | 0.8987839136  |
| C49    | 1.9695722295  | -2.3220024721 | -1.2376440495 |
| N50    | 1.4176455657  | -3.4678015832 | -0.6886190110 |
| N51    | 3.3398361599  | -2.3989809168 | -1.4148806659 |
| 15 C52 | 0.0356550902  | -3.8446514900 | -0.9525042043 |
| H53    | -0.0186732948 | -4.9427830234 | -1.0453219142 |
| H54    | -0.6520219727 | -3.5112141724 | -0.1576886113 |
| H55    | -0.2924026193 | -3.3916759014 | -1.8954845089 |
| C56    | 2.0657298567  | -4.2066351799 | 0.3893782295  |
| 20 H57 | 1.4007530014  | -4.2313215840 | 1.2706488090  |
| H58    | 2.2906646771  | -5.2501734876 | 0.1029327360  |
| H59    | 2.9994216117  | -3.7088375902 | 0.6768086399  |
| C60    | 4.0026121444  | -3.6298223011 | -1.8353889509 |
| H61    | 4.5453838562  | -3.4476735495 | -2.7793478328 |
| 25 H62 | 4.7321049795  | -3.9858280394 | -1.0855826432 |
| H63    | 3.2595632362  | -4.4164918472 | -2.0104497540 |
| C64    | 4.1776991070  | -1.2086569642 | -1.4764427577 |
| H65    | 5.1095187125  | -1.4027142715 | -0.9178173927 |
| H66    | 4.4416683596  | -0.9406688863 | -2.5143556958 |
| 30 H67 | 3.6565755987  | -0.3576815083 | -1.0268836428 |

Dimethylcyanamide coordinated to 1<sup>st</sup> insertion product  
Gibbs free energy: -1099.686339

|        |               |               |               |
|--------|---------------|---------------|---------------|
| C1     | 1.7196562897  | 0.9207402377  | 0.4843506719  |
| 35 N2  | 2.9117524619  | 0.9998981945  | 0.0455986117  |
| N3     | 0.5977569149  | 1.6588191910  | 0.0121588938  |
| C4     | 0.8865327458  | 2.7276736960  | -0.9309782643 |
| H5     | 1.7176670261  | 3.3436927928  | -0.5595972417 |
| H6     | -0.0072848198 | 3.3648594779  | -1.0274327368 |
| 40 H7  | 1.1631015058  | 2.3497539390  | -1.9364577722 |
| C8     | -0.6283133804 | 0.9310732282  | -0.3154147438 |
| H9     | -0.6217460512 | 0.5833931004  | -1.3699521752 |
| H10    | -1.5116353054 | 1.5780772209  | -0.1773127647 |
| H11    | -0.7248393427 | 0.0519286195  | 0.3318713625  |
| 45 N12 | 1.3581373086  | 0.0507861746  | 1.5495351285  |
| C13    | 2.3956927872  | -0.8655659864 | 1.9905436388  |
| H14    | 2.9131971978  | -1.2762243939 | 1.1149087148  |
| H15    | 1.9299931778  | -1.6818641014 | 2.5674928950  |
| H16    | 3.1570492932  | -0.3694818544 | 2.6281252663  |
| 50 C17 | 0.5532358642  | 0.5736825939  | 2.6512023784  |
| H18    | -0.1067224894 | 1.3690168380  | 2.2868107960  |
| H19    | 1.1943803624  | 0.9992246858  | 3.4523279878  |
| H20    | -0.0603566941 | -0.2271865471 | 3.0988558853  |
| Al21   | 4.0367100745  | 1.6454306064  | -1.2196229664 |
| 55 N22 | 3.7476446255  | 1.6512661579  | -3.0407905641 |
| N23    | 4.9477686791  | 3.1384862878  | -0.6621719950 |
| C24    | 3.5079629686  | 2.8656558285  | -3.7939840264 |
| H25    | 3.7290780346  | 3.7504759697  | -3.1766220959 |

|    |     |              |               |               |
|----|-----|--------------|---------------|---------------|
|    | H26 | 2.4507402951 | 2.9542706379  | -4.1389976719 |
|    | H27 | 4.1385041469 | 2.9247237967  | -4.7097292780 |
|    | C28 | 3.4364703734 | 0.4687402348  | -3.8155963955 |
|    | H29 | 2.3709624100 | 0.4357159607  | -4.1425212452 |
| 5  | H30 | 3.6268814944 | -0.4458180354 | -3.2302685226 |
|    | H31 | 4.0480178249 | 0.4017659711  | -4.7442706456 |
|    | C32 | 6.0312446641 | 3.7428627506  | -1.4059215096 |
|    | H33 | 7.0221862643 | 3.6059811813  | -0.9088937157 |
|    | H34 | 5.9001459459 | 4.8417576552  | -1.5303562714 |
| 10 | H35 | 6.1020035490 | 3.3036488410  | -2.4143778268 |
|    | C36 | 4.8287499975 | 3.6922725966  | 0.6713169262  |
|    | H37 | 5.7664001629 | 3.5814975238  | 1.2657811755  |
|    | H38 | 4.0243500720 | 3.1829683207  | 1.2241804109  |
|    | H39 | 4.5982570762 | 4.7815629717  | 0.6555648648  |
| 15 | H40 | 9.3504793343 | -0.3674038047 | -1.3603859498 |
|    | C41 | 8.5871729431 | -0.9983253834 | -1.8465730820 |
|    | N42 | 7.4506231835 | -1.2395486208 | -0.9464342912 |
|    | H43 | 9.0353264824 | -1.9642375372 | -2.1237637578 |
|    | H44 | 8.2309718792 | -0.4975002762 | -2.7547066518 |
| 20 | C45 | 6.3669263190 | -0.5052488728 | -1.0603988562 |
|    | C46 | 7.6962785247 | -1.9853609700 | 0.2952379525  |
|    | N47 | 5.3849299994 | 0.1243346878  | -1.1899393782 |
|    | H48 | 6.7455140419 | -2.1416439303 | 0.8190265719  |
|    | H49 | 8.3884000455 | -1.4372034750 | 0.9568656112  |
| 25 | H50 | 8.1315994061 | -2.9643770364 | 0.0441919329  |

TS to 2<sup>nd</sup> insertion product

Gibbs free energy: -1099.669994

|    |      |               |               |               |
|----|------|---------------|---------------|---------------|
|    | C1   | 2.7664433374  | -0.4020055485 | 1.4241954138  |
| 30 | N2   | 3.7655790395  | 0.1035741069  | 0.7759062892  |
|    | N3   | 1.6826493399  | 0.3439932665  | 1.9319534294  |
|    | C4   | 1.8699808344  | 1.7787250216  | 2.1106130415  |
|    | H5   | 2.8350518300  | 1.9643102928  | 2.5982556841  |
|    | H6   | 1.0641273308  | 2.1545016648  | 2.7612341466  |
| 35 | H7   | 1.8617920618  | 2.3487751238  | 1.1618676290  |
|    | C8   | 0.3234698400  | -0.0306406879 | 1.5400967808  |
|    | H9   | 0.0026099518  | 0.5205672263  | 0.6339419766  |
|    | H10  | -0.3885712816 | 0.1955732844  | 2.3519270009  |
|    | H11  | 0.2753109750  | -1.1038835778 | 1.3193585289  |
| 40 | N12  | 2.6606482705  | -1.7657016770 | 1.7206313676  |
|    | C13  | 3.2926971512  | -2.7562098995 | 0.8712123886  |
|    | H14  | 3.6561395060  | -2.2658420695 | -0.0389631216 |
|    | H15  | 2.5623936418  | -3.5409132928 | 0.5998762236  |
|    | H16  | 4.1484212063  | -3.2520330972 | 1.3683475950  |
| 45 | C17  | 2.0222230572  | -2.2760746389 | 2.9220357895  |
|    | H18  | 1.7132106303  | -1.4347842400 | 3.5541492750  |
|    | H19  | 2.7293470420  | -2.9104498532 | 3.4896576453  |
|    | H20  | 1.1316437492  | -2.8936342114 | 2.6939720404  |
|    | Al21 | 3.9678025510  | 1.2942485934  | -0.6847075471 |
| 50 | N22  | 2.9214252281  | 1.0063306127  | -2.1644150281 |
|    | N23  | 4.1219142935  | 3.0643805972  | -0.2425435608 |
|    | C24  | 1.5910875780  | 1.5695448847  | -2.2729550146 |
|    | H25  | 1.4468945691  | 2.3751588347  | -1.5333160850 |
|    | H26  | 0.7817763131  | 0.8168792903  | -2.1109137904 |
| 55 | H27  | 1.4057041492  | 2.0115824796  | -3.2773532792 |
|    | C28  | 3.1536965417  | -0.0248250647 | -3.1537885130 |
|    | H29  | 2.4516032546  | -0.8875495631 | -3.0592636610 |
|    | H30  | 4.1795570755  | -0.4177600697 | -3.0715090993 |

|        |              |               |               |
|--------|--------------|---------------|---------------|
| H31    | 3.0314335338 | 0.3626855955  | -4.1895529407 |
| C32    | 3.9911109390 | 4.1398055274  | -1.2084846758 |
| H33    | 4.9654608998 | 4.6293329150  | -1.4334733116 |
| H34    | 3.3098832752 | 4.9423018514  | -0.8478486973 |
| 5 H35  | 3.5860697156 | 3.7533731458  | -2.1562366534 |
| C36    | 4.7150863962 | 3.5199284233  | 0.9976280819  |
| H37    | 5.7060387608 | 4.0031254115  | 0.8413981565  |
| H38    | 4.8659348358 | 2.6734851454  | 1.6876419736  |
| H39    | 4.0798232250 | 4.2696702860  | 1.5221291090  |
| 10 H40 | 8.4653306217 | -1.5186550637 | 0.2595290706  |
| C41    | 7.5175329811 | -2.0194746777 | -0.0078129128 |
| N42    | 6.3597817201 | -1.3443598871 | 0.5976595314  |
| H43    | 7.5458188362 | -3.0598386199 | 0.3492777442  |
| H44    | 7.4080891282 | -2.0173007108 | -1.0992414903 |
| 15 C45 | 5.8270665150 | -0.3422093370 | -0.0978555412 |
| C46    | 6.2671036016 | -1.3575858858 | 2.0576006991  |
| N47    | 5.7634741060 | 0.4564525234  | -0.9953744066 |
| H48    | 5.3239790670 | -0.8748039430 | 2.3388642438  |
| H49    | 7.1149870021 | -0.8187452529 | 2.5183906779  |
| 20 H50 | 6.2745565586 | -2.4012789909 | 2.4079108673  |

2<sup>nd</sup> insertion product (7)

Gibbs free energy: -1099.694878

|        |               |               |               |
|--------|---------------|---------------|---------------|
| C1     | 0.6397332284  | 0.3993592830  | -1.2449133367 |
| 25 N1  | 2.0001310136  | 0.5752462712  | -1.3752043049 |
| N2     | -0.1597788579 | 1.1880448512  | -2.0490500080 |
| C2     | -1.5603671084 | 0.8027946780  | -2.2268553270 |
| H3     | -1.6245943088 | -0.2772314412 | -2.4068861179 |
| H7     | -1.9583935728 | 1.3409402025  | -3.1003103454 |
| 30 H8  | -2.1758758448 | 1.0322832306  | -1.3377135738 |
| C3     | 2.9128645675  | 0.4173371603  | -0.2479383760 |
| H6     | 3.5605558207  | 1.3095698018  | -0.1842535105 |
| H9     | 3.5431873227  | -0.4802469259 | -0.3581036875 |
| H10    | 2.3479709705  | 0.3326421288  | 0.6871889643  |
| 35 C4  | 0.0909822181  | 2.6271068418  | -2.1569938173 |
| H5     | -0.6202852156 | 3.1869013225  | -1.5226317151 |
| H11    | -0.0256310291 | 2.9667603844  | -3.1991841151 |
| H12    | 1.1055879101  | 2.8621339822  | -1.8165920329 |
| C5     | 2.6248582770  | 0.8873889599  | -2.6545152923 |
| 40 H2  | 3.4180918379  | 0.1488797507  | -2.8664584158 |
| H13    | 3.0882753992  | 1.8912107867  | -2.6582721193 |
| H14    | 1.8753517721  | 0.8412070511  | -3.4537406288 |
| N3     | 0.0431105518  | -0.4479403479 | -0.4198220240 |
| C6     | 0.6450704098  | -1.4818173316 | 0.4064734525  |
| 45 N4  | 1.5714049375  | -2.3540940651 | -0.1744479319 |
| N5     | 0.2372179171  | -1.4982090012 | 1.6267298005  |
| C7     | 1.4364160298  | -2.7534340065 | -1.5697749445 |
| H15    | 0.7206293366  | -3.5922327234 | -1.6931248610 |
| H17    | 2.4145024761  | -3.0852197833 | -1.9556537902 |
| 50 H18 | 1.0897788735  | -1.9158351157 | -2.1851947114 |
| C8     | 2.0588486234  | -3.4159753082 | 0.7004826864  |
| H16    | 1.3603173733  | -4.2749477728 | 0.7374028588  |
| H19    | 2.1552150646  | -3.0202603854 | 1.7179334112  |
| H20    | 3.0351350361  | -3.7693288807 | 0.3315129600  |
| 55 A11 | -1.0088118671 | -0.0941823599 | 1.3526003943  |
| N6     | -0.6083063227 | 1.5163070174  | 2.1212331111  |
| N7     | -2.7930723197 | -0.3486752760 | 1.0360298883  |
| C9     | -1.3248564801 | 2.7498574601  | 1.8731772278  |

|    |     |               |               |               |
|----|-----|---------------|---------------|---------------|
|    | H4  | -1.7007832336 | 3.2205806216  | 2.8090600678  |
|    | H24 | -2.1964983512 | 2.5684248886  | 1.2236647929  |
|    | H25 | -0.6873586792 | 3.5182831421  | 1.3749637034  |
|    | C10 | 0.5487553952  | 1.7143846178  | 2.9736383016  |
| 5  | H1  | 1.2853640921  | 2.4276007176  | 2.5344177555  |
|    | H26 | 1.0655006214  | 0.7567307981  | 3.1455612546  |
|    | H27 | 0.2713121706  | 2.1270914920  | 3.9683922664  |
|    | C11 | -3.8452000375 | 0.1677694326  | 1.8935304781  |
|    | H22 | -4.3299460710 | -0.6296863665 | 2.4998144378  |
| 10 | H28 | -4.6557892793 | 0.6561768072  | 1.3083743534  |
|    | H29 | -3.4420863457 | 0.9150515399  | 2.5943113422  |
|    | C12 | -3.2852232019 | -1.3784572510 | 0.1406088668  |
|    | H23 | -3.7386304104 | -2.2371187758 | 0.6837090299  |
|    | H30 | -2.4667530264 | -1.7775631962 | -0.4800400515 |
| 15 | H31 | -4.0701852564 | -0.9916710951 | -0.5481631583 |

Dimethylcyanamide coordinated to 7

Gibbs free energy: -1326.806572

|    |      |               |               |               |
|----|------|---------------|---------------|---------------|
| 20 | C1   | 1.6543988740  | 0.7931794711  | 1.3029802606  |
|    | N2   | 2.8600639655  | 0.9327618511  | 0.8932463037  |
|    | N3   | 0.6067377173  | 1.6903151607  | 1.0329126463  |
|    | C4   | 0.8238220720  | 2.7759352667  | 0.0960555447  |
|    | H5   | 1.8488361527  | 3.1598636188  | 0.1879466170  |
| 25 | H6   | 0.1189099128  | 3.5928063813  | 0.3210201983  |
|    | H7   | 0.6674370234  | 2.4646323322  | -0.9571824081 |
|    | C8   | -0.7905920347 | 1.3613651287  | 1.2714101832  |
|    | H9   | -1.3106294128 | 1.0853617680  | 0.3311687624  |
|    | H10  | -1.3199416798 | 2.2278738048  | 1.7072622517  |
| 30 | H11  | -0.8473541402 | 0.5130788726  | 1.9605438694  |
|    | N12  | 1.2037417426  | -0.3226253597 | 2.0503913679  |
|    | Al13 | 4.0179846841  | 1.5422386281  | -0.3403046225 |
|    | N14  | 3.8086588916  | 1.2864969135  | -2.1555921819 |
|    | N15  | 4.7848124487  | 3.1821674064  | 0.0012721372  |
| 35 | C16  | 3.3379504848  | 2.3503624310  | -3.0197921813 |
|    | H17  | 3.4394175251  | 3.3247090412  | -2.5153649841 |
|    | H18  | 2.2664557072  | 2.2329640843  | -3.3095699768 |
|    | H19  | 3.9127233228  | 2.4012631347  | -3.9721064662 |
|    | C20  | 3.6641362643  | -0.0118738267 | -2.7780493907 |
| 40 | H21  | 2.6061737916  | -0.2577322143 | -3.0311181260 |
|    | H22  | 4.0330578049  | -0.8089057908 | -2.1112840623 |
|    | H23  | 4.2371330050  | -0.0832892987 | -3.7308724371 |
|    | C24  | 5.8343435069  | 3.7465394665  | -0.8201509596 |
|    | H25  | 6.8259531636  | 3.7607366427  | -0.3052628342 |
| 45 | H26  | 5.6232393226  | 4.8012348661  | -1.1083641415 |
|    | H27  | 5.9476094233  | 3.1656081398  | -1.7498551940 |
|    | C28  | 4.5936507104  | 3.9293747487  | 1.2251870828  |
|    | H29  | 5.5075459283  | 3.9576785582  | 1.8658531540  |
|    | H30  | 3.7822091256  | 3.4821810379  | 1.8215934284  |
| 50 | H31  | 4.3202250351  | 4.9913558634  | 1.0302941293  |
|    | H32  | 9.7257370891  | -0.7447484226 | 0.3068793769  |
|    | C33  | 8.8504500503  | -0.7007680049 | -0.3586134936 |
|    | N34  | 7.6440114229  | -1.0101309369 | 0.4211063121  |
|    | H35  | 8.9860460131  | -1.4173632016 | -1.1870707757 |
| 55 | H36  | 8.7662828686  | 0.3131294804  | -0.7681019904 |
|    | C37  | 6.5236921015  | -0.3717733727 | 0.1605013451  |
|    | C38  | 7.6038429402  | -2.2757279728 | 1.1649135317  |
|    | N39  | 5.5352180390  | 0.2241075545  | -0.0511822039 |

|    |     |               |               |              |
|----|-----|---------------|---------------|--------------|
|    | H40 | 6.6894331245  | -2.3118008623 | 1.7696519576 |
|    | H41 | 8.4757977118  | -2.3240927799 | 1.8346245047 |
|    | H42 | 7.6220926890  | -3.1423631736 | 0.4815330752 |
|    | C43 | 1.9376300267  | -0.8662237198 | 2.9737138749 |
| 5  | N44 | 1.8031309223  | -2.2326910868 | 3.2329897205 |
|    | N45 | 2.8562181487  | -0.2244489576 | 3.8057072626 |
|    | C46 | 1.7050033891  | -2.7194038573 | 4.6051316732 |
|    | H47 | 2.2647902355  | -3.6624793641 | 4.7296033482 |
|    | H48 | 2.1116964572  | -1.9699671722 | 5.2941475682 |
| 10 | H49 | 0.6486907741  | -2.9115857712 | 4.8814184291 |
|    | C50 | 1.0759385201  | -3.0373920865 | 2.2625265400 |
|    | H51 | -0.0172694440 | -3.0162493811 | 2.4399242392 |
|    | H52 | 1.2611729975  | -2.6477461344 | 1.2553742045 |
|    | H53 | 1.4205659099  | -4.0827468162 | 2.3310019453 |
| 15 | C54 | 4.1838762622  | -0.7889206470 | 4.0103681656 |
|    | H55 | 4.4912481139  | -0.7095279986 | 5.0691284391 |
|    | H56 | 4.1819772330  | -1.8466007428 | 3.7186929781 |
|    | H57 | 4.9268731977  | -0.2503681751 | 3.3896972549 |
|    | C58 | 2.7820136039  | 1.2146392206  | 3.9995220415 |
| 20 | H59 | 3.4102412874  | 1.7592491070  | 3.2723702139 |
|    | H60 | 1.7441779816  | 1.5503469857  | 3.8755897458 |
|    | H61 | 3.1123739772  | 1.4538949400  | 5.0253022931 |

3<sup>rd</sup> insertion product (8)

25 Gibbs free energy: -1326.815782

|    |     |               |               |               |
|----|-----|---------------|---------------|---------------|
|    | C1  | -1.0499174347 | 1.7975278973  | -1.7043270837 |
|    | N1  | -1.3487701487 | 0.5962530383  | -1.2887822043 |
|    | N2  | -0.6031089120 | 1.9459750201  | -3.0168611307 |
|    | N3  | -1.1207010651 | 2.9692680883  | -0.9726175821 |
| 30 | C2  | -2.0988398049 | 0.2681665754  | -0.1804111162 |
|    | N4  | -1.6492002896 | -0.5084934005 | 0.7854516475  |
|    | C3  | -0.2950829003 | -0.6464091597 | 0.9667523630  |
|    | N5  | 0.6662037321  | 0.1957379214  | 1.0101972270  |
|    | A11 | 2.0046914610  | -1.1176101312 | 1.2997155118  |
| 35 | N6  | 2.7310229735  | -1.2401599815 | 2.9717187549  |
|    | N7  | 3.0448584026  | -1.5734086923 | -0.1297319848 |
|    | N8  | 0.1257214645  | -2.0962201817 | 1.2583701558  |
|    | N9  | -3.4330462078 | 0.6387008137  | -0.1363153743 |
|    | C4  | 0.6088295965  | 2.7274136136  | -3.2765245874 |
| 40 | H7  | 0.7792562616  | 3.4463723161  | -2.4679756215 |
|    | H14 | 0.5191791777  | 3.2733404337  | -4.2299874827 |
|    | H15 | 1.4920033096  | 2.0627941084  | -3.3346506157 |
|    | C5  | -0.7575414235 | 0.8066770923  | -3.9145387095 |
|    | H4  | -0.7124174506 | 1.1678689094  | -4.9538842705 |
| 45 | H16 | -1.7236483835 | 0.3197889910  | -3.7384680674 |
|    | H17 | 0.0359740069  | 0.0503153571  | -3.7644295781 |
|    | C6  | -1.5292206999 | 4.2300238723  | -1.5810261182 |
|    | H5  | -2.4505125762 | 4.5990564311  | -1.0936111598 |
|    | H18 | -1.7312542579 | 4.0835309021  | -2.6489820295 |
| 50 | H19 | -0.7542725114 | 5.0102301936  | -1.4679359878 |
|    | C7  | -1.0518199301 | 2.9600030032  | 0.4859091584  |
|    | H6  | -2.0563323206 | 2.9445050008  | 0.9486996134  |
|    | H20 | -0.5333890122 | 3.8770727112  | 0.8111596618  |
|    | H21 | -0.4579322261 | 2.0923192752  | 0.8225727811  |
| 55 | C8  | -4.2616617632 | 0.1541383859  | 0.9611954336  |
|    | H3  | -3.6496599802 | 0.0649365530  | 1.8647737118  |
|    | H22 | -4.6965668529 | -0.8394897104 | 0.7388708933  |
|    | H23 | -5.0831670974 | 0.8676176167  | 1.1303370558  |

|        |               |               |               |
|--------|---------------|---------------|---------------|
| C9     | -4.1725620056 | 1.0468896589  | -1.3210136887 |
| H13    | -3.4913923533 | 1.3910248753  | -2.1050049921 |
| H24    | -4.8603300890 | 1.8699348047  | -1.0668591971 |
| H25    | -4.7754910754 | 0.2101195580  | -1.7257288740 |
| 5 C10  | -0.2633568817 | -3.0226876374 | 0.1752398370  |
| H8     | 0.1003736211  | -2.6371390869 | -0.7864770664 |
| H26    | -1.3610257889 | -3.1290205020 | 0.1277859635  |
| H27    | 0.1978301261  | -4.0050370013 | 0.3575336715  |
| C11    | -0.3978183787 | -2.5673454043 | 2.5603079358  |
| 10 H12 | 0.0010767733  | -3.5725209801 | 2.7656860784  |
| H28    | -1.5003667520 | -2.6000988962 | 2.5475602377  |
| H29    | -0.0513121738 | -1.8888457506 | 3.3514410438  |
| C12    | 2.6114310456  | -0.1680748748 | 3.9429181895  |
| H2     | 2.0381099375  | 0.6731857858  | 3.5209690847  |
| 15 H30 | 3.6020499964  | 0.2264673209  | 4.2611229761  |
| H31    | 2.0904315176  | -0.4966412988 | 4.8715219006  |
| C13    | 3.4437634195  | -2.3827367519 | 3.5050771884  |
| H1     | 4.4865965755  | -2.1350929561 | 3.8071150720  |
| H32    | 3.5049713809  | -3.1951492296 | 2.7622565930  |
| 20 H33 | 2.9475747305  | -2.8012878354 | 4.4105410327  |
| C14    | 4.4086914069  | -2.0599657092 | -0.0446799554 |
| H10    | 4.5248038183  | -3.0880342688 | -0.4564227080 |
| H34    | 4.7515790739  | -2.0759283143 | 1.0009382078  |
| H35    | 5.1124891071  | -1.4117575788 | -0.6127253577 |
| 25 C15 | 2.6041440153  | -1.4299835750 | -1.5042553541 |
| H11    | 1.6098208668  | -0.9552188807 | -1.5485279689 |
| H36    | 2.5451247206  | -2.4025078211 | -2.0453866183 |
| H37    | 3.2986927377  | -0.7879689181 | -2.0919400824 |

30 TS for cyclization (mono Al)

Gibbs free energy: -1326.800926

|        |               |               |               |
|--------|---------------|---------------|---------------|
| C1     | -0.5202661608 | -0.6740688601 | 1.1951007450  |
| N2     | -0.6366706284 | -0.2585995663 | -0.1269772749 |
| N3     | -0.7579553050 | -2.0442021365 | 1.3358622067  |
| 35 C4  | -0.8478572627 | -2.6353195152 | 2.6556465169  |
| H5     | 0.1128819693  | -3.0665138841 | 2.9988074671  |
| H6     | -1.5969698517 | -3.4448204412 | 2.6407522710  |
| H7     | -1.1543068552 | -1.8669204723 | 3.3774214800  |
| C8     | -0.8103717491 | -2.9702761076 | 0.2179444403  |
| 40 H9  | -0.6851628121 | -2.4071183264 | -0.7120382296 |
| H10    | -1.7792140192 | -3.5030900364 | 0.1908859016  |
| H11    | -0.0084167634 | -3.7288909821 | 0.2958982802  |
| C12    | -0.1353027919 | 0.8919934904  | -0.5454585690 |
| N13    | -0.2706325296 | 1.1983852365  | -1.8869513894 |
| 45 C14 | 0.3743406947  | 2.3538320238  | -2.4800838684 |
| H15    | 0.7928240767  | 2.9826796644  | -1.6860981324 |
| H16    | -0.3524455586 | 2.9420681864  | -3.0682538031 |
| H17    | 1.1952107143  | 2.0495053030  | -3.1572126720 |
| C18    | -0.8568067379 | 0.2474727068  | -2.8146972206 |
| 50 H19 | -0.0806177721 | -0.2901992112 | -3.3927250478 |
| H20    | -1.5072185381 | 0.7829495555  | -3.5262148178 |
| H21    | -1.4472452450 | -0.4799144431 | -2.2476371588 |
| N22    | 0.6254555367  | 1.7594665891  | 0.1907247655  |
| C23    | 0.3189205096  | 2.2946137237  | 1.3384985368  |
| 55 N24 | -0.2911367480 | 0.0848317433  | 2.2235280224  |
| N25    | -0.8948471462 | 2.9844997378  | 1.6583098610  |
| N26    | 1.3711048187  | 2.4997962336  | 2.2801803341  |
| C27    | -0.8645794461 | 4.3719385375  | 1.1568065823  |

|        |               |               |              |
|--------|---------------|---------------|--------------|
| H28    | 0.0709100793  | 4.8773458189  | 1.4271390541 |
| H29    | -1.6990631657 | 4.9305943949  | 1.6077895674 |
| H30    | -0.9713444613 | 4.4117147579  | 0.0531858453 |
| C31    | -2.1380370242 | 2.3351799018  | 1.2295049474 |
| 5 H32  | -2.1681030102 | 1.3208083348  | 1.6415049940 |
| H33    | -2.2450015468 | 2.2966916866  | 0.1273290585 |
| H34    | -2.9765235992 | 2.9233509337  | 1.6340240251 |
| C35    | 2.7315233025  | 2.2376197251  | 1.7759450911 |
| H36    | 3.0562165386  | 3.0441358993  | 1.0936805551 |
| 10 H37 | 2.7489998970  | 1.2879638732  | 1.2338055339 |
| H38    | 3.4138591052  | 2.1831926379  | 2.6333865441 |
| C39    | 1.3370921292  | 3.6406962995  | 3.2129839301 |
| H40    | 1.9460536715  | 3.3863359811  | 4.0910391953 |
| H41    | 0.3099560640  | 3.8191201842  | 3.5443270205 |
| 15 H42 | 1.7519098727  | 4.5544300766  | 2.7471686534 |
| Al43   | 0.7438491474  | 0.5136950994  | 3.6093751795 |
| N44    | 2.3964840502  | -0.2500610963 | 3.7851657080 |
| N45    | 0.0325373154  | 1.2473464129  | 5.1184155909 |
| C46    | 2.8536703798  | -1.2872718530 | 2.8769241915 |
| 20 H47 | 3.1912590530  | -2.1965050510 | 3.4200466555 |
| H48    | 3.7160268907  | -0.9527908617 | 2.2557383639 |
| H49    | 2.0469983333  | -1.5880767142 | 2.1908430693 |
| C50    | 3.4543167918  | 0.1764725902  | 4.6792840351 |
| H51    | 4.3501380397  | 0.5416564716  | 4.1245530161 |
| 25 H52 | 3.8124948998  | -0.6480491954 | 5.3339434109 |
| H53    | 3.1173225078  | 0.9944666739  | 5.3350848940 |
| C54    | -1.1685007356 | 2.0638145394  | 5.1228463932 |
| H55    | -1.0060781429 | 3.0426880698  | 5.6293757470 |
| H56    | -2.0053767186 | 1.5678703426  | 5.6613071582 |
| 30 H57 | -1.5025989967 | 2.2719456704  | 4.0953284000 |
| C58    | 0.4700036234  | 0.9400012013  | 6.4685926405 |
| H59    | 1.3131183086  | 0.2335834779  | 6.4607664408 |
| H60    | -0.3441878596 | 0.4726238597  | 7.0642885300 |
| H61    | 0.7892294129  | 1.8470519560  | 7.0294719141 |

35  
Cyclized intermediate (mono Al) (9)  
Gibbs free energy: -1326.844390

|       |               |               |               |
|-------|---------------|---------------|---------------|
| C1    | -0.4184957988 | -0.2872726879 | 0.9974241996  |
| N1    | -0.4832593306 | -0.1218762303 | -0.3224627277 |
| 40 N2 | -0.6918681556 | -1.5320057305 | 1.5137291344  |
| C2    | -0.8410656874 | -1.7824224595 | 2.9376176775  |
| H3    | 0.0548344074  | -2.2642525414 | 3.3715155814  |
| H6    | -1.7029429679 | -2.4523519223 | 3.0993522623  |
| H7    | -1.0264075528 | -0.8448055344 | 3.4798486221  |
| 45 C3 | -0.8307945295 | -2.6893730775 | 0.6442906087  |
| H4    | -0.6170937074 | -2.3816271435 | -0.3843709732 |
| H8    | -1.8563591978 | -3.0968849670 | 0.6934799973  |
| H9    | -0.1272461671 | -3.4835164052 | 0.9509704838  |
| C4    | -0.0611825753 | 1.1053153390  | -0.7782417055 |
| 50 N3 | 0.0458711989  | 1.2157265633  | -2.1519798131 |
| C5    | 0.5402112103  | 2.4402550475  | -2.7513890993 |
| H10   | 0.4023551405  | 3.2633426237  | -2.0411999422 |
| H12   | -0.0158424157 | 2.6468381991  | -3.6813311094 |
| H13   | 1.6169139192  | 2.3717353014  | -3.0034267114 |
| 55 C6 | -0.0682908684 | 0.0668973295  | -3.0310043511 |
| H11   | 0.9226469780  | -0.2800782197 | -3.3854206454 |
| H14   | -0.6706893838 | 0.3348580216  | -3.9161812646 |
| H15   | -0.5582699018 | -0.7484450828 | -2.4896332217 |

|        |               |               |               |
|--------|---------------|---------------|---------------|
| N4     | 0.2295358889  | 2.1718548566  | -0.0475657677 |
| C7     | -0.0384425816 | 2.0594184168  | 1.3275726425  |
| N5     | -0.0825579628 | 0.6981960381  | 1.8760876962  |
| N6     | -1.2255156156 | 2.8346557126  | 1.7783176743  |
| 5 N7   | 1.2055363532  | 2.5918522634  | 2.2063851305  |
| C8     | -1.4498277707 | 4.0586148870  | 0.9953931706  |
| H5     | -0.5153702652 | 4.6123376138  | 0.8513450337  |
| H19    | -2.1583384782 | 4.7001644238  | 1.5443926792  |
| H20    | -1.8645057154 | 3.8476020537  | -0.0097069528 |
| 10 C9  | -2.4718755100 | 2.0609210573  | 1.8167355821  |
| H2     | -2.3745274362 | 1.2003965233  | 2.4883639479  |
| H21    | -2.7920664873 | 1.7037221826  | 0.8149165615  |
| H22    | -3.2648730098 | 2.7145319802  | 2.2119613891  |
| C10    | 2.4765936972  | 2.4157537101  | 1.4583065188  |
| 15 H1  | 2.5254301579  | 3.1220861609  | 0.6157719375  |
| H23    | 2.5436479436  | 1.3947635288  | 1.0649747935  |
| H24    | 3.3155081986  | 2.5827895436  | 2.1498332615  |
| C11    | 1.1531376431  | 3.9644945748  | 2.7533154812  |
| H16    | 1.9118614882  | 4.0519043380  | 3.5460478241  |
| 20 H25 | 0.1644047786  | 4.1507656606  | 3.1843266049  |
| H26    | 1.3736015493  | 4.7158577421  | 1.9761072585  |
| Al1    | 0.9678474617  | 0.9690651852  | 3.4466303501  |
| N8     | 2.4667660465  | -0.0705823403 | 3.5678211018  |
| N9     | 0.1593794074  | 1.3112222003  | 5.0448206272  |
| 25 C12 | 2.8797744739  | -1.0430295767 | 2.5730397741  |
| H27    | 3.1039182142  | -2.0315349273 | 3.0307363090  |
| H30    | 3.8027134870  | -0.7337461533 | 2.0310695872  |
| H31    | 2.0917564393  | -1.2012104497 | 1.8203023996  |
| C13    | 3.5033664029  | 0.1405475830  | 4.5640671489  |
| 30 H28 | 4.4550189666  | 0.4983304487  | 4.1101034227  |
| H32    | 3.7504959478  | -0.7920762598 | 5.1171831577  |
| H33    | 3.1903505253  | 0.8903797101  | 5.3079228751  |
| C14    | -0.8758737693 | 2.3068280614  | 5.2725477641  |
| H18    | -0.5574433586 | 3.0901676926  | 5.9952962102  |
| 35 H34 | -1.7968326867 | 1.8471679760  | 5.6931672806  |
| H35    | -1.1553848059 | 2.8013393063  | 4.3291877922  |
| C15    | 0.4587451426  | 0.5690860235  | 6.2595006310  |
| H17    | 1.1860947719  | -0.2317318039 | 6.0590145176  |
| H36    | -0.4540924466 | 0.0942031176  | 6.6808834591  |
| 40 H37 | 0.8764543092  | 1.2167009792  | 7.0614387148  |

3<sup>rd</sup> insertion product with bridging Al (**12**)

Gibbs free energy:

45 TS for cyclization (bis Al) **TS1**

Gibbs free energy:

Cyclized intermediate (bis Al) (**13**)

Gibbs free energy:

50

Hexamethylmelamine coordinated to catalyst (**14**)

Gibbs free energy: -1326.870171

|       |              |              |               |
|-------|--------------|--------------|---------------|
| C1    | 1.6657491820 | 2.1753951055 | -0.6701057291 |
| N1    | 2.0146073373 | 3.0876008896 | -1.6233279004 |
| 55 C2 | 1.3036118406 | 4.3477415514 | -1.7701153307 |
| H2    | 2.0279714641 | 5.1772576329 | -1.8334364799 |
| H6    | 0.6510944222 | 4.4925578921 | -0.9035436655 |
| H7    | 0.6916120188 | 4.3503355322 | -2.6896662953 |

|    |     |               |               |               |
|----|-----|---------------|---------------|---------------|
|    | C3  | 3.0483404375  | 2.8088250983  | -2.6065555927 |
|    | H4  | 3.7549815273  | 3.6546531250  | -2.6533298935 |
|    | H8  | 2.6097102378  | 2.6683374125  | -3.6106285555 |
|    | H9  | 3.5819584056  | 1.8983002949  | -2.3170658447 |
| 5  | N2  | 2.3731534152  | 1.0263537744  | -0.6057847480 |
|    | N3  | 0.6953340727  | 2.5240732557  | 0.2065368683  |
|    | C4  | 1.8641208714  | 0.0921208862  | 0.2121296031  |
|    | C5  | 0.2399505941  | 1.5233390049  | 0.9651464036  |
|    | N4  | 0.6254885496  | 0.1949906500  | 0.8292352143  |
| 10 | N5  | -0.6774289832 | 1.8222207548  | 1.9228523021  |
|    | N6  | 2.6051406301  | -1.0205276487 | 0.4450170041  |
|    | C6  | -0.9567617100 | 0.9516934807  | 3.0588502889  |
|    | H10 | -0.8150659838 | 1.5280546272  | 3.9902436370  |
|    | H13 | -0.2704502955 | 0.1004713973  | 3.0467817336  |
| 15 | H14 | -1.9849033433 | 0.5601784313  | 3.0196915516  |
|    | C7  | -1.2538435242 | 3.1589638916  | 1.9968943402  |
|    | H3  | -0.6850388978 | 3.8050331899  | 2.6896252700  |
|    | H15 | -2.2895393834 | 3.0760062611  | 2.3605465287  |
|    | H16 | -1.2482698427 | 3.6185593389  | 1.0034821738  |
| 20 | C8  | 2.2287249875  | -2.0257153184 | 1.4280801297  |
|    | H1  | 3.1418314900  | -2.3898784954 | 1.9251369420  |
|    | H17 | 1.6987401639  | -2.8661807133 | 0.9515265581  |
|    | H18 | 1.5678904028  | -1.5742306660 | 2.1766740147  |
|    | C9  | 3.8413418654  | -1.2715528241 | -0.2847927383 |
| 25 | H5  | 3.9147516129  | -0.5738518189 | -1.1240209195 |
|    | H19 | 3.8419435589  | -2.3070527415 | -0.6601324325 |
|    | H20 | 4.7165225104  | -1.1324499005 | 0.3738013773  |
|    | A11 | -0.9599922890 | -1.0303921766 | 0.0290905852  |
|    | N7  | -0.0687782666 | -2.3759005712 | -0.8687650658 |
| 30 | N8  | -1.9041523870 | 0.1174692095  | -1.0630677555 |
|    | N9  | -1.9768987300 | -1.6255343952 | 1.4482342225  |
|    | C10 | -2.7587165926 | 1.2016458540  | -0.6269223339 |
|    | H22 | -2.3548964256 | 2.2069814018  | -0.8922270453 |
|    | H26 | -2.8997660188 | 1.1773195757  | 0.4648650667  |
| 35 | H27 | -3.7684229425 | 1.1397804144  | -1.0918075920 |
|    | C11 | -1.8135044259 | 0.0746315267  | -2.5108615430 |
|    | H24 | -2.8192715686 | -0.0003061019 | -2.9810586147 |
|    | H28 | -1.2338105889 | -0.8005047496 | -2.8384896003 |
|    | H29 | -1.3338328816 | 0.9840493065  | -2.9430256577 |
| 40 | C12 | -3.4263327093 | -1.6760886404 | 1.3684626679  |
|    | H11 | -3.8119727729 | -2.7207934645 | 1.3548944715  |
|    | H30 | -3.7776348976 | -1.1815469185 | 0.4507915530  |
|    | H31 | -3.9157872801 | -1.1754771240 | 2.2363602661  |
|    | C13 | -1.4964778566 | -2.3433806398 | 2.6070061684  |
| 45 | H21 | -0.3960522220 | -2.3366974745 | 2.6577867138  |
|    | H32 | -1.8125171900 | -3.4120127425 | 2.6102861898  |
|    | H33 | -1.8726823468 | -1.9110735374 | 3.5645044357  |
|    | C14 | -0.4853685270 | -3.7559583281 | -0.6862768262 |
|    | H25 | 0.3661460569  | -4.4256998738 | -0.4189042765 |
| 50 | H34 | -0.9395070340 | -4.1859745888 | -1.6070169626 |
|    | H35 | -1.2344613269 | -3.8241225469 | 0.1174986630  |
|    | C15 | 0.8621955417  | -2.2534933918 | -1.9692028146 |
|    | H12 | 1.1667834494  | -1.2067344447 | -2.1289320154 |
|    | H36 | 0.4356314291  | -2.6219752972 | -2.9306898568 |
| 55 | H37 | 1.7915272626  | -2.8485320020 | -1.8049622207 |