Electronic Supplementary Material (ESI) for Dalton Transactions


**Electronic Supporting Information**

*belonging to*

# Smooth $C_{alkyl}$–H bond activation in rhodium complexes comprising abnormal carbene ligands

Anneke Krüger,[a] L. Jonas L. Häller,[b] Helge Müller-Bunz,[a] Olha Serada,[c] Antonia Neels,[c] Stuart A. Macgregor*[b] and Martin Albrecht*[a]

**Table S1. Crystallographic data for complexes 3b, 4 – 6**

| | 3b | 4 | 5b | 6 |
|---|---|---|---|---|
| CCDC no. | 817392 | 817393 | 817394 | 817395 |
| color, shape | orange, rod | red, rod | orange, rod | yellow, lath |
| cryst size /mm | 0.40, 0.35, 0.25 | 0.45, 0.40, 0.23 | 0.30, 0.28, 0.25 | 0.25, 0.10, 0.01 |
| formula | $C_{58}H_{70}F_6I_3N_8PRh_2$ ×0.5$CH_2Cl_2$ ×$C_6H_{14}$ | $C_{21}H_{32}I_2N_6Rh$ | $C_{19}H_{31}Br_2N_4O_2Rh$ | $C_{19}H_{30}I_2N_5Rh$ |
| Fw | 1739.34 | 725.24 | 610.21 | 685.19 |
| T /K | 173(2) | 173(2) | 173(2) | 100(2) |
| crystal system | orthorhombic | monoclinic | monoclinic | triclinic |
| space group | *Pnna* (No. 52) | $P2_1/c$ (No. 14) | *Cc* (No. 9) | *P*1 (No. 1) |
| unit cell | | | | |
| *a* /Å | 26.7628(17) | 16.7813(9) | 11.8107(11) | 7.6131(11) |
| *b* /Å | 26.7351(18) | 11.0963(4) | 12.0520(9) | 8.3587(11) |
| *c* /Å | 20.3079(11) | 14.6937(7) | 16.1426(16) | 10.6771(15) |
| $\alpha$ | 90 | 90 | 90 | 68.734(3) |
| $\beta$ | 90 | 97.152(4) | 95.827(12) | 73.159(3) |
| $\gamma$ | 90 | 90 | 90 | 66.537(3) |
| $V$ /Å$^3$ | 14530.4(16) | 2714.8(2) | 2285.9(4) | 572.37(14) |
| $Z$ | 8 | 4 | 4 | 1 |
| $D_{calc}$/g cm$^{-3}$ | 1.590 | 1.774 | 1.773 | 1.988 |
| $\mu$ /mm$^{-1}$ | 1.845 | 2.922 | 4.265 | 3.457 |
| total, unique reflections | 57955, 12927 | 51616, 7338 | 44953, 2234 | 9954, 4798 |
| $R_{int}$ | 0.1184 | 0.0322 | --- | 0.0353 |
| transmission range | 0.611–0.750 | 0.308–0.511 | --- | 0.547–0.966 |
| no. parameters, restraints | 399, 53 | 271, 0 | 190, 2 | 247, 83 |
| $R$,[a] $R_w$[b] | 0.0827, 0.1977 | 0.0296 0.0792 | 0.0274, 0.0431 | 0.0436, 0.0904 |
| GOF | 0.837 | 1.061 | 0.673 | 1.072 |
| largest hole, peak /e Å$^{-3}$ | –0.586, 2.074 | –1.631, 1.225 | –1.137, 0.604 | –2.919, 1.168 |

[*a*] $R_1 = \Sigma||F_O|-|F_C||/\Sigma|F_O|$ for all $I > 2\sigma(I)$; [*b*] $wR_2 = [\Sigma w(F_O^2-F_C^2)^2/\Sigma(w(F_O^4)]^{1/2}$.

## Computational Details

All geometries were optimised without constraints using Gaussian 03, Revision C.02[1] employing the BP86 functional.[2] The SDD relativistic ECPs and the associated basis sets was

used for Rh and I,[3] with a set of d-orbital polarisation functions added for I.[4] 6-31G** basis sets were employed for all other atoms.[5] Stationary points were confirmed as either minima or transition states through analytical frequency calculations and the latter were characterised through IRC calculations and subsequent geometry optimisation. Energies quoted in the text are free energies computed at 298.15 K and 1 atm and include a correction for the effect of MeCN solvent via the PCM approach. Details of the computed structures are summarised in Table S2.

**Table S2. Computed Structures**

(Cartesian coordinates in Å; energies in atomic units; labeling scheme according to main text)

**5a′**

BP86 Energy = -1010.05583686
Enthalpy 0K= -1009.741878
Enthalpy 298K= -1009.718080
Free Energy 298K= -1009.796263
E(MeCN) = -1010.08168210

| | | | |
|---|---|---|---|
| C | 1.45850 | -1.91892 | 3.13012 |
| N | 1.36106 | -1.57230 | 1.78563 |
| C | 0.34675 | -0.66024 | 1.57130 |
| N | -0.18354 | -0.46097 | 2.83108 |
| C | 0.49137 | -1.21462 | 3.78511 |
| C | 2.17674 | -2.21612 | 0.75474 |
| C | 1.48757 | -3.48004 | 0.21441 |
| C | 0.12999 | -3.16440 | -0.43603 |
| N | 0.29566 | -2.24374 | -1.56222 |
| C | 0.59841 | -2.69328 | -2.84421 |
| C | 0.82965 | -1.58289 | -3.60162 |
| N | 0.67142 | -0.47911 | -2.77058 |
| C | 0.33556 | -0.86484 | -1.48710 |
| Rh | -0.18887 | 0.41284 | -0.03325 |
| O | -0.95660 | 2.07782 | -1.24563 |
| C | -1.23181 | 2.73782 | -0.17572 |
| C | -1.88417 | 4.09547 | -0.25571 |
| C | 0.91655 | 0.88749 | -3.25474 |
| C | -1.28181 | 0.44348 | 3.19589 |
| I | -2.70716 | -0.66213 | -0.14856 |
| I | 2.29981 | 1.55392 | 0.10301 |
| O | -0.97213 | 2.20051 | 0.96199 |
| H | 0.59859 | -3.74968 | -3.09863 |
| H | 1.07688 | -1.47350 | -4.65394 |
| H | -0.34233 | -4.08298 | -0.82062 |
| H | -0.57620 | -2.70441 | 0.27281 |
| H | 2.15806 | -3.96128 | -0.52122 |
| H | 1.32795 | -4.20445 | 1.03420 |
| H | 3.15017 | -2.46384 | 1.20842 |
| H | 2.36403 | -1.47166 | -0.03531 |
| H | 0.22605 | -1.17282 | 4.83782 |
| H | 2.20360 | -2.62293 | 3.49054 |
| H | -1.66839 | 0.12239 | 4.17442 |
| H | -2.07676 | 0.37218 | 2.44048 |
| H | -0.92592 | 1.48168 | 3.24437 |
| H | 1.93086 | 1.20687 | -2.96919 |
| H | 0.18793 | 1.57700 | -2.81307 |
| H | 0.81333 | 0.87943 | -4.35014 |
| H | -2.98054 | 3.96801 | -0.27042 |
| H | -1.61609 | 4.69970 | 0.62344 |
| H | -1.58476 | 4.61031 | -1.18055 |

**5a′$_{ab}$**

BP86 Energy = -1010.02146072
Enthalpy 0K= -1009.709295
Enthalpy 298K= -1009.683662
Free Energy 298K= -1009.768253
E(MeCN) = -1010.06997437

| | | | |
|---|---|---|---|
| C | -1.52737 | -0.68961 | -0.03117 |
| N | -1.67322 | -2.08225 | 0.16172 |
| C | -2.97759 | -2.44691 | 0.08363 |
| N | -3.70092 | -1.33548 | -0.15846 |
| C | -2.83514 | -0.25254 | -0.23918 |
| C | -0.57850 | -3.03164 | 0.39083 |
| C | 0.03099 | -3.54794 | -0.92458 |
| C | 0.62337 | -2.44432 | -1.81834 |
| N | 1.70409 | -1.71128 | -1.15026 |
| C | 1.53523 | -0.59528 | -0.30089 |
| C | 2.83440 | -0.30252 | 0.11292 |

| | | | |
|---|---|---|---|
| N | 3.71770 | -1.19695 | -0.47726 |
| C | 3.01357 | -2.05417 | -1.24344 |
| Rh | -0.00622 | 0.56010 | 0.14747 |
| I | -0.21878 | 1.25646 | -2.49393 |
| C | 5.17120 | -1.19441 | -0.31730 |
| C | -5.15605 | -1.27804 | -0.29079 |
| O | -1.13434 | 2.35616 | 0.68540 |
| C | -0.03271 | 3.01656 | 0.77397 |
| O | 1.08423 | 2.41350 | 0.56001 |
| I | 0.21866 | -0.12362 | 2.79074 |
| C | -0.05340 | 4.49478 | 1.08762 |
| H | 3.42973 | -2.85855 | -1.84342 |
| H | 3.17640 | 0.49158 | 0.77067 |
| H | 1.02864 | -2.88168 | -2.74589 |
| H | -0.13005 | -1.69126 | -2.10566 |
| H | 0.81425 | -4.28611 | -0.66933 |
| H | -0.73813 | -4.08507 | -1.51068 |
| H | -0.97446 | -3.87259 | 0.98402 |
| H | 0.16296 | -2.50444 | 1.01518 |
| H | -3.37663 | -3.44901 | 0.21323 |
| H | -3.19531 | 0.75721 | -0.41535 |
| H | 0.86559 | 4.78595 | 1.61785 |
| H | -0.10198 | 5.06275 | 0.14228 |
| H | -0.93937 | 4.74601 | 1.68937 |
| H | 5.59111 | -0.25831 | -0.71749 |
| H | 5.42645 | -1.28016 | 0.75028 |
| H | 5.60138 | -2.04711 | -0.86166 |
| H | -5.42332 | -0.85592 | -1.27200 |
| H | -5.57230 | -2.29204 | -0.20704 |
| H | -5.57917 | -0.64522 | 0.50488 |

**rh_i_oac_bis_normal_me_nonagostic**

BP86 Energy = -998.325751122
Enthalpy 0K= -998.012242
Enthalpy 298K= -997.989646
Free Energy 298K= -998.065252
E(MeCN) = -998.394891696

| | | | |
|---|---|---|---|
| C | 2.12136 | 3.28097 | -0.96201 |
| N | 1.89055 | 1.91061 | -0.94955 |
| C | 0.60115 | 1.62613 | -0.53841 |
| N | 0.05194 | 2.86827 | -0.28198 |
| C | 0.96523 | 3.87843 | -0.54539 |
| C | 2.97313 | 0.94509 | -1.18624 |
| C | 3.67427 | 0.54807 | 0.12361 |
| C | 2.73108 | -0.16754 | 1.10800 |
| N | 2.14932 | -1.36458 | 0.48711 |
| C | 2.81440 | -2.58316 | 0.46008 |
| C | 2.09845 | -3.40598 | -0.36454 |
| N | 1.01178 | -2.67636 | -0.82602 |
| C | 1.02351 | -1.39266 | -0.31212 |
| Rh | -0.46975 | -0.07218 | -0.58532 |
| O | -2.16001 | -1.39168 | -0.94080 |
| C | -2.90964 | -0.36987 | -1.19505 |
| C | -4.35233 | -0.53494 | -1.56948 |
| C | 0.07774 | -3.22804 | -1.82137 |
| C | -1.31849 | 3.17337 | 0.16518 |
| I | -0.97289 | -0.18791 | 1.97365 |
| O | -2.37229 | 0.80048 | -1.08601 |
| H | 3.72124 | -2.76045 | 1.03272 |
| H | 2.26217 | -4.43979 | -0.65753 |
| H | 3.27667 | -0.48656 | 2.00982 |
| H | 1.90423 | 0.48012 | 1.43548 |
| H | 4.52986 | -0.10424 | -0.12745 |
| H | 4.08711 | 1.44460 | 0.61919 |
| H | 3.68692 | 1.41603 | -1.88024 |
| H | 2.54889 | 0.06714 | -1.69609 |
| H | 0.71030 | 4.92808 | -0.42470 |
| H | 3.07397 | 3.70463 | -1.26945 |
| H | -1.29555 | 4.14550 | 0.67732 |
| H | -1.65876 | 2.40064 | 0.86500 |
| H | -2.00171 | 3.21079 | -0.69440 |
| H | 0.46437 | -3.05030 | -2.83824 |
| H | -0.91028 | -2.76784 | -1.70334 |
| H | -0.00753 | -4.31095 | -1.65210 |
| H | -4.96000 | -0.51872 | -0.64742 |
| H | -4.68168 | 0.29518 | -2.21114 |
| H | -4.51439 | -1.50172 | -2.06750 |

**rh_i_oac_bis_abnormal_me_nonagostic**

BP86 Energy = -998.311415633
Enthalpy 0K= -997.998994
Enthalpy 298K= -997.975699
Free Energy 298K= -998.054313
E(MeCN) = -998.391148493

| | | | |
|---|---|---|---|
| C | 1.54248 | -0.62409 | -0.47516 |
| N | 1.72717 | -1.98397 | -0.82039 |
| C | 3.03715 | -2.32196 | -0.72966 |
| N | 3.72340 | -1.23525 | -0.32783 |
| C | 2.82898 | -0.18691 | -0.16116 |
| C | 0.67192 | -2.93085 | -1.21180 |
| C | 0.01177 | -3.61946 | -0.00540 |
| C | -0.68200 | -2.65646 | 0.97340 |
| N | -1.73253 | -1.85693 | 0.32342 |
| C | -1.53966 | -0.63336 | -0.35800 |
| C | -2.81841 | -0.29624 | -0.80375 |
| N | -3.71365 | -1.28246 | -0.41113 |
| C | -3.03554 | -2.22252 | 0.27570 |
| Rh | -0.01300 | 0.60197 | -0.61743 |
| I | 0.03814 | 1.12598 | 1.93071 |
| C | -5.16162 | -1.27867 | -0.65752 |
| C | 5.17594 | -1.16749 | -0.12079 |
| O | 1.06750 | 2.40192 | -1.12978 |
| C | -0.05108 | 3.01654 | -1.33220 |
| O | -1.15115 | 2.36178 | -1.13538 |
| C | -0.07684 | 4.45772 | -1.75591 |
| H | -3.46875 | -3.11425 | 0.72230 |
| H | -3.14783 | 0.59971 | -1.32471 |
| H | -1.14604 | -3.22241 | 1.79696 |
| H | 0.02639 | -1.94132 | 1.42189 |
| H | -0.71845 | -4.35224 | -0.39449 |
| H | 0.76776 | -4.19346 | 0.56005 |
| H | 1.11881 | -3.68384 | -1.88075 |
| H | -0.06757 | -2.36084 | -1.79561 |
| H | 3.46857 | -3.29117 | -0.96721 |
| H | 3.16085 | 0.80001 | 0.15116 |
| H | -0.96753 | 4.66420 | -2.36723 |
| H | -0.12932 | 5.09053 | -0.85251 |

```
H    0.84087  4.71565 -2.30374
H   -5.61455 -0.39720 -0.17923
H   -5.35219 -1.24973 -1.74074
H   -5.60480 -2.19037 -0.23422
H    5.38687 -0.89645  0.92454
H    5.62096 -2.14756 -0.34037
H    5.60928 -0.41138 -0.79249
```

**A**

```
BP86 Energy =  -998.316590772
Enthalpy 0K=  -998.004001
Enthalpy 298K=  -997.981500
Free Energy 298K=  -998.056418
E(MeCN) = -998.388906846

C    0.84556  1.60512  0.05881
N    2.12650  1.77473  0.54696
C    2.57039  3.07817  0.33752
C    1.55005  3.73756 -0.28689
N    0.50287  2.83022 -0.44435
C    2.92551  0.73171  1.21207
C    2.07236 -0.29451  2.00620
C    2.24561 -1.76249  1.57884
N    2.07016 -1.91686  0.13041
C    1.14619 -1.18750 -0.58625
N    1.38796 -1.51884 -1.89225
C    2.41481 -2.45980 -1.97850
C    2.85097 -2.70700 -0.70730
Rh  -0.12778 -0.08261  0.50463
O   -1.23291 -1.58607  1.60062
C   -1.84619 -0.66172  2.26635
C   -2.88836 -1.00188  3.29072
O   -1.54722  0.56752  1.99751
I   -2.13144 -0.13191 -1.19893
H    3.63118 -3.36503 -0.33373
H    2.74141 -2.86347 -2.93321
C    0.72763 -0.98189 -3.08999
H    3.26220 -2.11056  1.82608
H    1.52249 -2.39765  2.11772
H    2.29623 -0.23294  3.08734
H    0.97822  0.02585  2.05230
H    3.62284  1.25037  1.88766
H    3.53055  0.20762  0.45091
H    3.55238  3.41977  0.65398
H    1.46911  4.76919 -0.61862
C   -0.79855  3.20952 -1.01611
H   -2.68874 -1.98928  3.73161
H   -2.93402 -0.22577  4.06841
H   -3.87113 -1.04322  2.78888
H   -1.60792  2.82661 -0.38033
H   -0.84671  4.30669 -1.05373
H   -0.91131  2.79852 -2.02948
H    1.46935 -0.93737 -3.90126
H   -0.11611 -1.62268 -3.38724
H    0.34886  0.02396 -2.87549
```

**$A_{ab}$**

```
BP86 Energy =  -998.304440743
Enthalpy 0K=  -997.993018
Enthalpy 298K=  -997.969856
Free Energy 298K=  -998.047383
E(MeCN) = -998.388619129

C   -0.80091  1.35829  0.03355
N   -1.77066  1.73111  0.99369
C   -2.59581  2.68506  0.49262
N   -2.21121  2.93434 -0.77225
C   -1.11852  2.12751 -1.07799
C   -1.74035  1.33363  2.41077
C   -1.03214  0.00020  2.70592
C   -1.74076 -1.33303  2.41088
N   -1.77088 -1.73080  0.99387
C   -2.59609 -2.68475  0.49294
N   -2.21139 -2.93435 -0.77183
C   -1.11860 -2.12770 -1.07764
C   -0.80100 -1.35830  0.03376
Rh   0.56014 -0.00002  0.52062
O    2.26315 -1.10805  1.29999
C    2.87553  0.00000  1.55696
C    4.27648  0.00012  2.10270
I    1.65562 -0.00020 -1.85754
O    2.26312  1.10807  1.29989
H   -3.40888 -3.17906  1.01889
H   -0.63911 -2.16387 -2.05201
C   -2.84095 -3.89839 -1.68297
H   -1.21509 -2.12402  2.97374
H   -2.77910 -1.28937  2.78285
H   -0.86486  0.00025  3.80034
H    0.05860 -0.00002  2.37634
H   -2.77862  1.29042  2.78299
H   -1.21425  2.12455  2.97333
H   -3.40848  3.17958  1.01856
C   -2.84058  3.89844 -1.68345
H   -0.63908  2.16346 -2.05240
H    4.46008  0.90575  2.69890
H    4.46061 -0.90594  2.69805
H    4.98060  0.00078  1.25229
H   -2.09178 -4.63500 -2.00962
H   -3.65603 -4.41677 -1.15978
H   -3.24564 -3.37195 -2.56055
H   -2.09178  4.63609 -2.00863
H   -3.24361  3.37220 -2.56191
H   -3.65688  4.41556 -1.16092
```

**TS(A-B)**

```
BP86 Energy =  -998.291851982
Enthalpy 0K=  -997.983970
Enthalpy 298K=  -997.961394
Free Energy 298K=  -998.037840
E(MeCN) = -998.362914427
Nimag=1 (-1023.0498cm-1)

C   -0.27542 -1.09517  1.24472
N    0.24208 -2.35943  1.28393
C   -0.04393 -2.96117  2.50630
C   -0.76649 -2.04693  3.22487
N   -0.91139 -0.90447  2.43405
C    0.97233 -2.93053  0.14618
C    0.61772 -2.23327 -1.19775
```

| | | | |
|---|---|---|---|
| Rh | -0.16087 | -0.06832 | -0.38746 |
| I | -0.65702 | 2.47232 | -0.02884 |
| C | 1.83736 | -1.72870 | -1.98433 |
| N | 2.54120 | -0.69887 | -1.21289 |
| C | 1.84654 | 0.12755 | -0.36252 |
| N | 2.81418 | 0.88106 | 0.24948 |
| C | 4.07493 | 0.54431 | -0.23805 |
| C | 3.90552 | -0.45436 | -1.16093 |
| O | -2.26762 | -0.23507 | -0.54365 |
| C | -2.63914 | -0.97351 | -1.54817 |
| O | -1.81328 | -1.63057 | -2.25469 |
| C | -4.11479 | -0.99118 | -1.87624 |
| H | 4.62685 | -0.99483 | -1.76838 |
| H | 4.97670 | 1.03857 | 0.11418 |
| C | 2.61689 | 1.90342 | 1.28546 |
| H | 2.55037 | -2.54891 | -2.18230 |
| H | 1.51572 | -1.32182 | -2.95898 |
| H | 0.14770 | -2.99492 | -1.85141 |
| H | 0.73110 | -4.00489 | 0.10791 |
| H | 2.05549 | -2.83729 | 0.34562 |
| H | 0.27565 | -3.97025 | 2.75216 |
| H | -1.19808 | -2.10783 | 4.22038 |
| C | -1.68161 | 0.28442 | 2.83123 |
| H | -4.38652 | -1.93902 | -2.36165 |
| H | -4.72168 | -0.82235 | -0.97568 |
| H | -4.32296 | -0.17081 | -2.58501 |
| H | -0.51257 | -1.63448 | -1.44503 |
| H | -2.27794 | 0.62939 | 1.97591 |
| H | -2.34737 | 0.00013 | 3.65772 |
| H | -1.00667 | 1.08873 | 3.16109 |
| H | 3.49010 | 1.89328 | 1.95436 |
| H | 2.50112 | 2.89757 | 0.82897 |
| H | 1.70967 | 1.66865 | 1.85476 |

**TS(A-B)$_{ab}$**

BP86 Energy = -998.280130854
Enthalpy 0K= -997.973450
Enthalpy 298K= -997.950464
Free Energy 298K= -998.028765
E(MeCN) = -998.361943393
Nimag=1 (-869.9444cm-1)

| | | | |
|---|---|---|---|
| C | -3.39186 | -0.56019 | -1.70632 |
| N | -2.10771 | -0.13895 | -1.67673 |
| C | -1.42599 | -0.69122 | -0.57285 |
| C | -2.39107 | -1.44948 | 0.07730 |
| N | -3.58248 | -1.36159 | -0.63763 |
| C | -1.40426 | 0.62702 | -2.71856 |
| C | -0.04210 | 1.18168 | -2.24955 |
| Rh | 0.48852 | -0.20840 | -0.38366 |
| O | 2.59754 | 0.21476 | -0.36270 |
| C | 3.03559 | -0.07797 | -1.53707 |
| C | 4.52644 | -0.16058 | -1.75681 |
| C | -0.01606 | 2.57002 | -1.57551 |
| N | -0.29159 | 2.51587 | -0.13056 |
| C | -0.04228 | 1.35260 | 0.61649 |
| C | -0.25951 | 1.71500 | 1.93714 |
| N | -0.60251 | 3.06596 | 1.95682 |
| C | -0.61478 | 3.53913 | 0.69445 |
| I | 0.84538 | -1.79314 | 1.67611 |
| O | 2.23517 | -0.32727 | -2.51752 |
| H | -0.83147 | 4.56354 | 0.40346 |
| C | -0.90252 | 3.84856 | 3.16297 |
| H | -0.17905 | 1.12808 | 2.84700 |
| H | 0.99137 | 3.00075 | -1.70719 |
| H | -0.74327 | 3.25701 | -2.04493 |
| H | 0.48979 | 1.37146 | -3.20589 |
| H | -2.06721 | 1.43938 | -3.06799 |
| H | -1.22765 | -0.05067 | -3.57186 |
| H | -2.30929 | -2.05170 | 0.97831 |
| C | -4.84147 | -2.03261 | -0.28855 |
| H | -4.13969 | -0.31994 | -2.45788 |
| H | 4.78349 | 0.14746 | -2.78065 |
| H | 5.06353 | 0.44619 | -1.01467 |
| H | 4.83902 | -1.21202 | -1.63227 |
| H | 0.98952 | 0.32027 | -2.13426 |
| H | -0.03488 | 3.82755 | 3.83926 |
| H | -1.11498 | 4.88763 | 2.87670 |
| H | -1.77938 | 3.42341 | 3.67411 |
| H | -5.59425 | -1.81684 | -1.05895 |
| H | -4.67556 | -3.11906 | -0.23736 |
| H | -5.20116 | -1.66898 | 0.68589 |

**B**

BP86 Energy = -998.345932233
Enthalpy 0K= -998.034172
Enthalpy 298K= -998.010754
Free Energy 298K= -998.090532
E(MeCN) =

| | | | |
|---|---|---|---|
| C | 0.50534 | -1.72487 | 0.07494 |
| N | 0.74572 | -2.30719 | -1.13988 |
| C | 1.29335 | -3.57572 | -0.98566 |
| C | 1.36563 | -3.79505 | 0.36545 |
| N | 0.87723 | -2.65002 | 1.00399 |
| C | 0.55885 | -1.44888 | -2.31599 |
| C | -0.53336 | -0.43328 | -1.92810 |
| C | -1.96076 | -1.03304 | -2.10245 |
| N | -2.72577 | -0.79421 | -0.88155 |
| C | -4.07794 | -0.96728 | -0.60696 |
| C | -4.24816 | -0.60479 | 0.70407 |
| N | -2.99690 | -0.22340 | 1.19559 |
| C | -2.05320 | -0.34003 | 0.21554 |
| Rh | -0.13750 | 0.12957 | 0.03688 |
| O | -0.92307 | 2.18281 | -0.11323 |
| C | -0.47183 | 3.34762 | -0.26265 |
| C | -1.39501 | 4.53137 | -0.38052 |
| I | 2.49521 | 0.81465 | 0.23597 |
| O | 0.80880 | 3.66005 | -0.31846 |
| C | 0.81221 | -2.45760 | 2.45482 |
| C | -2.74737 | 0.28226 | 2.54738 |
| H | 1.58075 | -4.20370 | -1.82453 |
| H | 1.71797 | -4.65679 | 0.92620 |
| H | 0.27031 | -2.06915 | -3.18493 |
| H | 1.50916 | -0.93672 | -2.54366 |
| H | -0.42311 | 0.50595 | -2.49280 |
| H | -2.48324 | -0.56975 | -2.95751 |
| H | -1.91293 | -2.12229 | -2.28307 |
| H | -4.79195 | -1.32695 | -1.34305 |
| H | -5.14083 | -0.58713 | 1.32420 |

| | | | |
|---|---|---|---|
| H | -1.08599 | 5.16751 | -1.22468 |
| H | -2.43248 | 4.19778 | -0.50792 |
| H | -1.31381 | 5.14570 | 0.53256 |
| H | 1.37712 | 2.83449 | -0.17986 |
| H | 0.99780 | -1.39715 | 2.68034 |
| H | 1.59693 | -3.06123 | 2.93231 |
| H | -0.17161 | -2.76141 | 2.84729 |
| H | -3.11730 | -0.43678 | 3.29457 |
| H | -3.24619 | 1.25317 | 2.69241 |
| H | -1.66345 | 0.41409 | 2.67344 |

BP86 Energy = -11.5555831350
E(MeCN) = -11.6496156540

**$B_{ab}$**

BP86 Energy = -998.323547139
Enthalpy 0K= -998.012508
Enthalpy 298K= -997.988893
Free Energy 298K= -998.070123
E(MeCN =

| | | | |
|---|---|---|---|
| C | 0.13173 | 1.34784 | 0.58382 |
| N | -0.02407 | 2.63172 | 0.03259 |
| C | 0.02330 | 3.56844 | 1.00313 |
| N | 0.18871 | 2.92699 | 2.18102 |
| C | 0.25268 | 1.55242 | 1.95112 |
| C | -0.09410 | 2.74911 | -1.43553 |
| C | -0.46395 | 1.35884 | -2.00630 |
| Rh | 0.17152 | -0.13273 | -0.64631 |
| I | 0.80658 | -2.27319 | 0.95527 |
| C | -1.97084 | 1.17468 | -2.31979 |
| N | -2.58401 | 0.32534 | -1.27950 |
| C | -1.75208 | -0.41267 | -0.40983 |
| C | -2.63609 | -1.16730 | 0.35183 |
| N | -3.93205 | -0.89228 | -0.07683 |
| C | -3.88113 | 0.01802 | -1.07494 |
| O | 2.21148 | 0.30330 | -1.35880 |
| C | 3.37543 | -0.08488 | -1.08374 |
| O | 3.67715 | -0.95954 | -0.14359 |
| C | 4.56839 | 0.42248 | -1.85137 |
| C | -5.15629 | -1.49611 | 0.46332 |
| C | 0.29238 | 3.57471 | 3.49431 |
| H | -0.04864 | 4.64534 | 0.87595 |
| H | 0.39290 | 0.84183 | 2.76047 |
| H | 0.90177 | 3.05238 | -1.79829 |
| H | -0.81462 | 3.54653 | -1.69561 |
| H | 0.11396 | 1.20329 | -2.93158 |
| H | -2.52616 | 2.12968 | -2.36651 |
| H | -2.09961 | 0.66365 | -3.28931 |
| H | -2.43975 | -1.88803 | 1.14095 |
| H | -4.73963 | 0.41017 | -1.61408 |
| H | 2.83153 | -1.33969 | 0.26961 |
| H | 4.92914 | -0.37820 | -2.51985 |
| H | 4.29477 | 1.29854 | -2.45289 |
| H | 5.39129 | 0.66370 | -1.16110 |
| H | -5.25520 | -1.24890 | 1.53120 |
| H | -5.11373 | -2.58896 | 0.34155 |
| H | -6.02569 | -1.10453 | -0.08235 |
| H | -0.50719 | 3.20727 | 4.15515 |
| H | 0.19008 | 4.66161 | 3.37095 |
| H | 1.27217 | 3.35042 | 3.94258 |

**Iodide**

## References


1 Gaussian 03, Revision C.02; M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian Inc., Wallingford, CT, USA, 2004.

2 (*a*) H. L. Schmider and A. D. Becke, *J. Chem. Phys.*, 1998, **108**, 9624. (*b*) J. P. Perdew, *Phys. Rev. B*, 1986, **33**, 8822.

3 (*a*) A. Bergner, M. Dolg, H. Kuechle, H. Stoll and H. Preuss, *Mol. Phys.,* 1993, **80**, 1431. (*b*) M. Kaupp, P. v. R. Schleyer, H. Stoll and H. Preuss, *J. Chem. Phys.,* 1991, **94**, 1360. (*c*) M. Dolg, H. Stoll, H. Preuss and R. M. Pitzer, *J. Phys. Chem.,* 1993, **97**, 5852.

4 A. Höllwarth, M. Böhme, S. Dapprich, A. W. Ehlers, A. Gobbi, V. Jonas, K. F. Köhler, R. Stegmann, A. Veldkamp and G. Frenking. *Chem. Phys. Lett*., 1993, **208**, 237.

5 (*a*) W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.*, 1972, **56**, 2257. (*b*) P. Hariharan and J. A. Pople, *Theor. Chim. Acta*, 1973, **28**, 213