

Supporting Information – DFT for,

Water Oxidation Catalysis with Ligand Substituted Ru-bpp-type Complexes

Stephan Roeser,[a] Fernando Bozoglian,[a] Craig J. Richmond,[a] Aaron B. League,[c]

Mehmed Z. Ertem,[c] Laia Francàs,[a] Pere Miró,[c] Jordi Benet-Buchholz,[a]

Christopher J. Cramer*[c] and Antoni Llobet*[a],[b]

DFT Key

Min-1 = bisoxo

TS-1 = peroxy formation

Min-2 = peroxy

TS-2 = one-water-assisted WNA on a Ru center

Min-3 = Ru-OO_Ru-OH₂-OH₂

TS-3 = two-water-assisted WNA on the second Ru center

A = first WNA on center with substituted terpyridine ligand

B = first WNA on center with unsubstituted terpyridine ligand

NO₂-Trpy Substituted Complex (22²⁺)[IV,IV]⁺³ pathway

| | Low Spin | (singlet) | | | low-spin | high-spin |
|--------|--------------|--------------|------------------|-------------------|--------------|--------------|
| | E | G | E _{sol} | <S ² > | single point | single point |
| Min-1 | -2748.788 55 | -2748.196 09 | -2749.883 36 | 2.01 | -2749.484 02 | -2749.484 04 |
| TS-1 | -2748.765 75 | -2748.172 29 | -2749.861 17 | 0.99 | -2749.461 46 | -2749.459 80 |
| Min-2 | -2748.774 93 | -2748.179 42 | -2749.870 66 | 0.58 | -2749.472 78 | -2749.465 86 |
| TS-2A | -2901.602 58 | -2900.960 56 | -2902.772 28 | 0.58 | -2902.371 32 | -2902.365 19 |
| TS-2B | -2901.603 11 | -2900.961 78 | -2902.774 03 | 0.56 | -2902.371 91 | -2902.365 11 |
| Min-3A | -2901.610 74 | -2900.967 18 | -2902.777 61 | 0.41 | -2902.378 27 | -2902.371 32 |
| Min-3B | -2901.611 14 | -2900.968 07 | -2902.778 68 | 0.47 | -2902.378 43 | -2902.372 44 |
| TS-3A | -2977.993 72 | -2977.330 11 | -2979.208 77 | 1.00 | -2978.798 45 | -2978.809 89 |
| TS-3B | -2977.991 62 | -2977.329 00 | -2979.205 35 | 1.01 | -2978.796 29 | -2978.807 92 |

| | High spin | (quintet/triplet) | | |
|--------|--------------|-------------------|------------------|-------------------|
| | E | G | E _{sol} | <S ² > |
| Min-1 | -2748.788 61 | -2748.197 27 | -2749.883 41 | 6.03 |
| TS-1 | -2748.764 44 | -2748.171 99 | -2749.860 69 | 2.01 |
| Min-2 | -2748.771 56 | -2748.178 20 | -2749.869 22 | 2.01 |
| TS-2A | -2901.597 46 | -2900.956 46 | -2902.767 72 | 2.02 |
| TS-2B | -2901.597 59 | -2900.957 03 | -2902.767 98 | 2.02 |
| Min-3A | -2901.607 29 | -2900.967 71 | -2902.773 73 | 2.02 |
| Min-3B | -2901.607 97 | -2900.967 13 | -2902.776 68 | 2.02 |
| TS-3A | -2978.006 06 | -2977.344 41 | -2979.220 58 | 2.02 |
| TS-3B | -2978.003 79 | -2977.342 12 | -2979.218 85 | 2.02 |

[IV,V]⁺⁴ pathway

| | Low Spin | (doublet) | | | low-spin | high-spin |
|--------|--------------|--------------|------------------|-------------------|--------------|--------------|
| | E | G | E _{sol} | <S ² > | single point | single point |
| Min-1 | N/A | N/A | N/A | N/A | | N/A |
| TS-1 | -2748.266 41 | -2747.674 36 | -2749.656 73 | 0.79 | | N/A |
| Min-2 | -2748.277 97 | -2747.685 02 | -2749.671 86 | 0.98 | -2748.973 11 | -2748.960 87 |
| TS-2A | -2901.123 02 | -2900.483 72 | -2902.584 50 | 0.81 | -2901.890 99 | -2901.868 65 |
| TS-2B | -2901.122 81 | -2900.483 81 | -2902.587 28 | 0.79 | -2901.891 12 | -2901.867 88 |
| Min-3A | -2901.130 99 | -2900.491 84 | -2902.592 98 | 1.28 | -2901.895 64 | -2901.883 53 |
| Min-3B | -2901.131 06 | -2900.491 66 | -2902.592 98 | 1.32 | -2901.894 56 | -2901.884 57 |
| TS-3A | -2977.537 41 | -2976.876 79 | -2979.039 26 | 1.67 | -2978.338 71 | -2978.337 21 |
| TS-3B | -2977.533 13 | -2976.870 98 | -2979.040 05 | 1.72 | -2978.334 28 | -2978.333 82 |

| | High Spin | (quartet) | | |
|--------|--------------|--------------|------------------|-------------------|
| | E | G | E _{sol} | <S ² > |
| Min-1 | -2748.291 22 | -2747.699 90 | -2749.675 48 | 3.78 |
| TS-1 | -2748.268 52 | -2747.677 14 | -2749.659 22 | 3.77 |
| Min-2 | -2748.271 86 | -2747.680 75 | -2749.667 82 | 3.77 |
| TS-2A | -2901.106 90 | -2900.468 87 | -2902.572 47 | 3.78 |
| TS-2B | -2901.108 88 | -2900.471 34 | -2902.577 69 | 3.78 |
| Min-3A | -2901.129 15 | -2900.490 98 | -2902.590 73 | 3.77 |
| Min-3B | -2901.130 82 | -2900.492 35 | -2902.587 81 | 3.77 |
| TS-3A | -2977.536 04 | -2976.875 85 | -2979.037 24 | 3.78 |
| TS-3B | -2977.532 85 | -2976.871 49 | -2979.040 81 | 3.78 |

CH₃O-Trpy Substituted Complex (20²⁺)

[IV,IV]⁺³ pathway

| | Low Spin | (singlet) | | | low-spin | high spin |
|--------|--------------|--------------|------------------|-------------------|-----------------|-----------------|
| | E | G | E _{sol} | <S ² > | single point | single point |
| Min-1 | -2658.839 91 | -2658.215 78 | -2659.888 72 | 2.01 | -2659.888 72 | -2659.888 74 |
| TS-1 | | | | | | |
| Min-2 | -2657.741 90 | -2657.117 97 | -2659.455 90 | | | |
| TS-2A | | | | | | |
| TS-2B | | | | | | |
| Min-3A | | | | | | |
| Min-3B | | | | | | |
| TS-3A | | | | | | |
| TS-3B | | | | | | |

| | High spin | (quintet/triplet) | | |
|--------|--------------|-------------------|------------------|-------------------|
| | E | G | E _{sol} | <S ² > |
| Min-1 | -2658.839 98 | -2658.216 99 | -2659.888 20 | |
| TS-1 | -2658.814 88 | -2658.191 22 | -2659.863 52 | |
| Min-2 | -2658.821 22 | -2658.196 25 | -2659.455 70 | |
| TS-2A | | | | |
| TS-2B | | | | |
| Min-3A | | | | |
| Min-3B | | | | |
| TS-3A | | | | |
| TS-3B | | | | |

[IV,V]⁺⁴ pathway

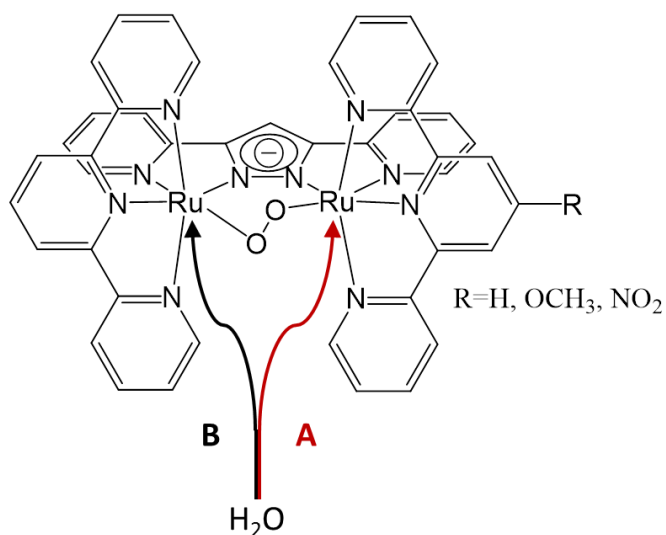
| | Low Spin | (doublet) | | | low-spin | high spin |
|--------|--------------|--------------|------------------|-------------------|-----------------|-----------------|
| | E | G | E _{sol} | <S ² > | single point | single point |
| Min-1 | -2658.350 35 | -2657.726 74 | -2659.680 10 | 1.77 | -2659.014 26 | -2659.020 07 |
| TS-1 | | | | | | |
| Min-2 | -2658.341 79 | -2657.715 94 | -2659.677 40 | 0.81 | -2659.008 31 | -2658.993 43 |
| TS-2A | -2811.184 01 | -2810.512 85 | -2812.591 20 | | | |
| TS-2B | -2811.183 30 | -2810.512 91 | -2812.592 60 | | | |
| Min-3A | -2811.189 80 | -2810.518 45 | -2812.596 60 | 1.07 | -2811.926 15 | -2811.910 20 |
| Min-3B | -2811.191 32 | -2810.518 34 | -2812.596 10 | | | |
| TS-3A | -2887.587 09 | -2886.891 89 | -2889.037 20 | | | |
| TS-3B | -2887.589 90 | -2886.896 42 | -2889.039 70 | | | |

| | High Spin | (quartet) | | |
|--------|--------------|--------------|------------------|-------------------|
| | E | G | E _{sol} | <S ² > |
| Min-1 | -2658.356 49 | -2657.733 76 | -2659.685 70 | |
| TS-1 | -2658.332 91 | -2657.709 60 | -2659.668 10 | |
| Min-2 | -2658.334 08 | -2657.710 49 | -2659.670 70 | |
| TS-2A | | | | |
| TS-2B | | | | |
| Min-3A | -2811.188 34 | -2810.518 62 | -2812.595 30 | |
| Min-3B | -2811.188 46 | -2810.518 35 | -2812.593 80 | |
| TS-3A | -2887.596 09 | -2886.904 54 | -2889.042 50 | |
| TS-3B | -2887.589 14 | -2886.896 45 | -2889.039 80 | |

DFT calculated structures and energies

Structures and electronic energies relevant to the pathway in main text figure 9 are reported here for complexes **15**³⁺, **20**³⁺, and **22**³⁺. Many of the structures for complex **15**³⁺ have been previously reported^[1] but are reproduced here for completeness. A key for structure identification can be found in the table below.

| Identifier | Structure |
|------------|---|
| Min-1 | Ru=O_Ru=O |
| TS-1 | O-O bond formation |
| Min-2 | Ru-OO-Ru |
| TS-2 | one-water-assisted O displacement on first Ru center |
| Min-3 | Ru-OO_Ru-OH ₂ -OH ₂ |
| TS-3 | one-water-assisted O displacement on second Ru center |



- | | |
|----------|---|
| A | first displacement occurs on Ru with substituted trpy |
| B | first displacement occurs on Ru with unsubstituted trpy |

In the original version of this article's supporting information, a typographical error resulted in erroneous extra atoms being appended to the cartesian coordinates for **Min-1** and **TS-1** of complex **15³⁺**. Corrected versions of these structures were supplied in July 2016, and appear below.

Structures for complex 15³⁺

Min-1 (3+ quintet)

E= -2544.318 57 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.196511 | 0.064405 | -0.233382 | C | -2.227736 | 4.191348 | -2.822793 |
| Ru | 2.196503 | -0.064412 | -0.233392 | H | -2.277619 | 5.085013 | -3.439885 |
| N | -3.139809 | 0.970983 | 1.578841 | C | -3.226451 | 3.226159 | -2.909145 |
| O | -1.211840 | -0.797540 | -1.411846 | H | -4.058941 | 3.361328 | -3.594761 |
| O | 1.211802 | 0.797614 | -1.411772 | C | -3.150680 | 2.085732 | -2.115843 |
| C | -4.388017 | 1.459366 | 1.680028 | C | -4.161343 | 1.019292 | -2.125071 |
| H | -4.945288 | 1.543271 | 0.747139 | C | -5.336446 | 0.988057 | -2.874661 |
| N | -0.633879 | 0.216028 | 1.202748 | H | -5.583919 | 1.795014 | -3.558954 |
| C | -4.953183 | 1.842133 | 2.887230 | C | -6.196409 | -0.099039 | -2.734121 |
| H | -5.964254 | 2.238246 | 2.913385 | H | -7.114846 | -0.138018 | -3.314446 |
| N | 0.633875 | -0.216231 | 1.202722 | C | -5.893248 | -1.133475 | -1.850702 |
| C | -4.196319 | 1.704225 | 4.049910 | H | -6.573466 | -1.973686 | -1.741193 |
| H | -4.608594 | 1.988658 | 5.015073 | C | -4.709229 | -1.069037 | -1.118132 |
| N | 3.139833 | -0.971132 | 1.578742 | C | -4.234796 | -2.049969 | -0.130241 |
| C | -2.903393 | 1.206171 | 3.959732 | C | -4.932395 | -3.209441 | 0.199855 |
| H | -2.285394 | 1.100190 | 4.848234 | H | -5.876112 | -3.437710 | -0.288795 |
| N | -2.104088 | 1.904260 | -1.249638 | C | -4.416399 | -4.075280 | 1.158697 |
| C | -2.390681 | 0.851612 | 2.711284 | H | -4.955598 | -4.981745 | 1.422624 |
| N | -3.887577 | -0.005722 | -1.283845 | C | -3.206777 | -3.763813 | 1.771047 |
| C | -1.039269 | 0.367019 | 2.497357 | H | -2.770624 | -4.413448 | 2.524780 |
| N | -3.045970 | -1.754539 | 0.480278 | C | -2.553899 | -2.593704 | 1.401864 |
| C | -0.000012 | -0.000238 | 3.354384 | H | -1.604301 | -2.301281 | 1.848119 |
| H | -0.000015 | -0.000304 | 4.437547 | C | 1.144927 | -2.835682 | -1.172985 |
| N | 2.104152 | -1.904174 | -1.249827 | H | 0.333761 | -2.615011 | -0.484506 |
| C | 1.039267 | -0.367343 | 2.497316 | C | 1.171745 | -3.993670 | -1.941257 |
| N | 3.887569 | 0.005877 | -1.283845 | H | 0.371485 | -4.722028 | -1.847533 |
| C | 2.390697 | -0.851908 | 2.711195 | C | 2.227898 | -4.191113 | -2.823194 |
| N | 3.045894 | 1.754495 | 0.480445 | H | 2.277820 | -5.084719 | -3.440367 |
| C | 2.903418 | -1.206578 | 3.959608 | C | 3.226573 | -3.225876 | -2.909453 |
| H | 2.285412 | -1.100712 | 4.848119 | H | 4.059071 | -3.360947 | -3.595078 |
| C | 4.196363 | -1.704591 | 4.049739 | C | 3.150754 | -2.085526 | -2.116045 |
| H | 4.608647 | -1.989107 | 5.014874 | C | 4.161377 | -1.019047 | -2.125168 |
| C | 4.953237 | -1.842347 | 2.887047 | C | 5.336482 | -0.987699 | -2.874749 |
| H | 5.964324 | -2.238423 | 2.913165 | H | 5.583988 | -1.794582 | -3.559117 |
| C | 4.388060 | -1.459477 | 1.679883 | C | 6.196404 | 0.099416 | -2.734102 |
| H | 4.945337 | -1.543266 | 0.746987 | H | 7.114843 | 0.138483 | -3.314419 |
| C | -1.144823 | 2.835719 | -1.172710 | C | 5.893201 | 1.133757 | -1.850588 |
| H | -0.333669 | 2.614949 | -0.484248 | H | 6.573387 | 1.973983 | -1.740997 |
| C | -1.171592 | 3.993780 | -1.940874 | C | 4.709181 | 1.069206 | -1.118029 |
| H | -0.371302 | 4.722096 | -1.847081 | C | 4.234708 | 2.050029 | -0.130048 |

| | | | |
|---|----------|----------|-----------|
| C | 4.932260 | 3.209500 | 0.200150 |
| H | 5.875966 | 3.437852 | -0.288481 |
| C | 4.416228 | 4.075233 | 1.159069 |
| H | 4.955388 | 4.981698 | 1.423075 |

| | | | |
|---|----------|----------|----------|
| C | 3.206619 | 3.763662 | 1.771391 |
| H | 2.770438 | 4.413214 | 2.525180 |
| C | 2.553788 | 2.593559 | 1.402104 |
| H | 1.604200 | 2.301062 | 1.848329 |

Min-1 (4+ doublet)

E= -2543.824 18 a.u.

| | | | |
|----|-----------|-----------|-----------|
| Ru | -2.184908 | 0.073756 | -0.253701 |
| Ru | 2.184351 | -0.045451 | -0.213929 |
| N | -3.125882 | 0.793756 | 1.627400 |
| O | -1.142583 | -0.563393 | -1.470729 |
| C | -4.366317 | 1.292654 | 1.769009 |
| H | -4.925035 | 1.463498 | 0.849861 |
| N | -0.610064 | 0.123097 | 1.204090 |
| C | -4.929286 | 1.573042 | 3.007918 |
| H | -5.937370 | 1.974874 | 3.065679 |
| N | 0.657340 | -0.309189 | 1.169934 |
| C | -4.183065 | 1.321148 | 4.159691 |
| H | -4.598995 | 1.523050 | 5.144049 |
| N | 3.158703 | -1.103590 | 1.492475 |
| C | -2.894813 | 0.818097 | 4.029910 |
| H | -2.281871 | 0.630426 | 4.908362 |
| N | -2.181215 | 2.025017 | -1.033420 |
| C | -2.380668 | 0.573082 | 2.754853 |
| N | -3.900040 | 0.070927 | -1.265226 |
| C | -1.028905 | 0.124427 | 2.503673 |
| N | -2.991309 | -1.821856 | 0.305171 |
| C | 0.009241 | -0.332136 | 3.330677 |
| H | -0.003690 | -0.445141 | 4.408030 |
| N | 2.156321 | -1.786042 | -1.407217 |
| C | 1.053650 | -0.609444 | 2.458804 |
| N | 3.876612 | 0.167660 | -1.292818 |
| C | 2.407107 | -1.109145 | 2.630422 |
| N | 3.032901 | 1.726145 | 0.630430 |
| C | 2.911233 | -1.594495 | 3.835865 |
| H | 2.292350 | -1.586905 | 4.730125 |
| C | 4.207825 | -2.099193 | 3.876867 |
| H | 4.617565 | -2.485055 | 4.807411 |
| C | 4.967145 | -2.107396 | 2.709684 |
| H | 5.980118 | -2.500366 | 2.697034 |
| C | 4.407022 | -1.595898 | 1.544077 |
| H | 4.971240 | -1.576879 | 0.612477 |
| C | -1.258481 | 2.978735 | -0.842888 |
| H | -0.434299 | 2.712205 | -0.186461 |
| C | -1.338747 | 4.218975 | -1.465675 |
| H | -0.569221 | 4.964156 | -1.285388 |
| C | -2.407740 | 4.478210 | -2.317213 |
| H | -2.497741 | 5.438075 | -2.820378 |
| C | -3.367761 | 3.489947 | -2.519883 |
| H | -4.209654 | 3.675854 | -3.181915 |

| | | | |
|---|-----------|-----------|-----------|
| C | -3.242325 | 2.266031 | -1.870744 |
| C | -4.210066 | 1.172055 | -1.996511 |
| C | -5.383427 | 1.175075 | -2.749286 |
| H | -5.660412 | 2.038034 | -3.348935 |
| C | -6.204919 | 0.049489 | -2.723463 |
| H | -7.121386 | 0.037771 | -3.309153 |
| C | -5.868620 | -1.059116 | -1.945262 |
| H | -6.522504 | -1.926822 | -1.923840 |
| C | -4.688461 | -1.031872 | -1.206163 |
| C | -4.180874 | -2.089532 | -0.321692 |
| C | -4.844269 | -3.292743 | -0.097488 |
| H | -5.787207 | -3.500054 | -0.597148 |
| C | -4.296523 | -4.231965 | 0.772888 |
| H | -4.811050 | -5.172589 | 0.955755 |
| C | -3.087862 | -3.948278 | 1.401956 |
| H | -2.628533 | -4.655009 | 2.087739 |
| C | -2.467106 | -2.732734 | 1.140388 |
| H | -1.519129 | -2.464723 | 1.604164 |
| C | 1.239291 | -2.764138 | -1.373754 |
| H | 0.443271 | -2.640652 | -0.643961 |
| C | 1.294620 | -3.859865 | -2.225913 |
| H | 0.534200 | -4.632918 | -2.161904 |
| C | 2.331405 | -3.942282 | -3.149685 |
| H | 2.402551 | -4.785568 | -3.832603 |
| C | 3.285252 | -2.929044 | -3.188200 |
| H | 4.104336 | -2.978431 | -3.901056 |
| C | 3.186455 | -1.855817 | -2.308108 |
| C | 4.152905 | -0.755368 | -2.245749 |
| C | 5.292114 | -0.604002 | -3.034744 |
| H | 5.535259 | -1.327822 | -3.807943 |
| C | 6.120966 | 0.495198 | -2.820246 |
| H | 7.011611 | 0.627864 | -3.430058 |
| C | 5.817892 | 1.422963 | -1.825870 |
| H | 6.471088 | 2.275303 | -1.660184 |
| C | 4.668456 | 1.241061 | -1.058546 |
| C | 4.201192 | 2.108196 | 0.028607 |
| C | 4.879737 | 3.246726 | 0.456273 |
| H | 5.808564 | 3.543137 | -0.024255 |
| C | 4.366727 | 4.004150 | 1.504786 |
| H | 4.892655 | 4.892505 | 1.846769 |
| C | 3.176283 | 3.606300 | 2.105834 |
| H | 2.742747 | 4.168406 | 2.928569 |
| C | 2.539765 | 2.462817 | 1.638497 |

| | | | | | | | |
|---|----------|----------|----------|---|----------|----------|-----------|
| H | 1.606179 | 2.112325 | 2.075536 | O | 1.178705 | 0.902279 | -1.315261 |
|---|----------|----------|----------|---|----------|----------|-----------|

Min-1 (4+ quartet)

E= -2543.827 18 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.170209 | 0.048482 | -0.252538 | C | -4.140750 | 0.999489 | -2.147809 |
| Ru | 2.170195 | -0.047950 | -0.252581 | C | -5.274453 | 0.931617 | -2.956638 |
| N | -3.161757 | 0.875733 | 1.562505 | H | -5.538071 | 1.750047 | -3.621300 |
| O | -1.089617 | -0.659497 | -1.393849 | C | -6.075448 | -0.207801 | -2.898953 |
| C | -4.427309 | 1.327953 | 1.648159 | H | -6.960544 | -0.276467 | -3.527334 |
| H | -4.980653 | 1.388573 | 0.711781 | C | -5.761692 | -1.254764 | -2.031318 |
| N | -0.636383 | 0.210436 | 1.211383 | H | -6.403404 | -2.130430 | -1.981277 |
| C | -5.012968 | 1.699779 | 2.849077 | C | -4.620399 | -1.154327 | -1.238310 |
| H | -6.036786 | 2.063179 | 2.864499 | C | -4.150195 | -2.128984 | -0.244453 |
| N | 0.636351 | -0.212452 | 1.211037 | C | -4.819105 | -3.312141 | 0.056200 |
| C | -4.262631 | 1.593931 | 4.019651 | H | -5.731223 | -3.575161 | -0.473519 |
| H | -4.692672 | 1.871816 | 4.979223 | C | -4.320736 | -4.155061 | 1.046446 |
| N | 3.161783 | -0.878123 | 1.561105 | H | -4.842223 | -5.077684 | 1.291053 |
| C | -2.951703 | 1.135843 | 3.944519 | C | -3.155776 | -3.797077 | 1.719316 |
| H | -2.340281 | 1.057560 | 4.840396 | H | -2.739417 | -4.425599 | 2.501873 |
| N | -2.190903 | 1.958096 | -1.120929 | C | -2.524715 | -2.607417 | 1.377459 |
| C | -2.417829 | 0.788196 | 2.705273 | H | -1.612310 | -2.279511 | 1.873271 |
| N | -3.846533 | -0.045889 | -1.336063 | C | 1.321193 | -2.955491 | -0.913080 |
| C | -1.047989 | 0.345193 | 2.503276 | H | 0.539342 | -2.751814 | -0.185408 |
| N | -2.999744 | -1.792595 | 0.421951 | C | 1.407044 | -4.164718 | -1.591230 |
| C | -0.000089 | -0.003002 | 3.359710 | H | 0.684026 | -4.950151 | -1.390292 |
| H | -0.000108 | -0.004015 | 4.443036 | C | 2.425630 | -4.343722 | -2.522898 |
| N | 2.191076 | -1.956218 | -1.123725 | H | 2.518976 | -5.278126 | -3.071415 |
| C | 1.047870 | -0.349607 | 2.502687 | C | 3.333545 | -3.311260 | -2.742050 |
| N | 3.846379 | 0.048200 | -1.336181 | H | 4.139511 | -3.437663 | -3.460457 |
| C | 2.417726 | -0.792889 | 2.703966 | C | 3.208119 | -2.121439 | -2.031838 |
| N | 2.999826 | 1.791967 | 0.424894 | C | 4.140602 | -0.995903 | -2.149567 |
| C | 2.951528 | -1.142902 | 3.942582 | C | 5.274264 | -0.926721 | -2.958350 |
| H | 2.340010 | -1.066451 | 4.838553 | H | 5.537878 | -1.744111 | -3.624295 |
| C | 4.262515 | -1.600940 | 4.016946 | C | 6.075223 | 0.212637 | -2.898910 |
| H | 4.692497 | -1.880646 | 4.976015 | H | 6.960285 | 0.282318 | -3.527229 |
| C | 5.013004 | -1.704353 | 2.846251 | C | 5.761497 | 1.258201 | -2.029584 |
| H | 6.036889 | -2.067592 | 2.861079 | H | 6.403227 | 2.133774 | -1.978161 |
| C | 4.427406 | -1.330283 | 1.646000 | C | 4.620243 | 1.156475 | -1.236677 |
| H | 4.980865 | -1.388962 | 0.709564 | C | 4.150165 | 2.129472 | -0.241140 |
| C | -1.320827 | 2.956944 | -0.909104 | C | 4.819140 | 3.312109 | 0.061401 |
| H | -0.538740 | 2.752072 | -0.182022 | H | 5.731165 | 3.576021 | -0.468031 |
| C | -1.406740 | 4.167177 | -1.585460 | C | 4.320975 | 4.153344 | 1.053175 |
| H | -0.683554 | 4.952220 | -1.383613 | H | 4.842519 | 5.075540 | 1.299262 |
| C | -2.425607 | 4.347691 | -2.516531 | C | 3.156138 | 3.794231 | 1.725656 |
| H | -2.519017 | 5.282923 | -3.063622 | H | 2.739923 | 4.421420 | 2.509358 |
| C | -3.333687 | 3.315650 | -2.736942 | C | 2.524986 | 2.605168 | 1.381887 |
| H | -4.139847 | 3.443202 | -3.454927 | H | 1.612647 | 2.276455 | 1.877285 |
| C | -3.208159 | 2.124767 | -2.028523 | O | 1.089495 | 0.661923 | -1.392596 |

Min-1 (4+ sextet)**E= -2543.818 67 a.u.**

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.194806 | 0.076790 | -0.218517 | C | -4.170403 | 1.021942 | -2.130211 |
| Ru | 2.194986 | -0.076039 | -0.218604 | C | -5.326760 | 0.973056 | -2.907531 |
| N | -3.150853 | 0.964901 | 1.611383 | H | -5.570555 | 1.777857 | -3.595818 |
| O | -1.214538 | -0.758700 | -1.421318 | C | -6.170719 | -0.129726 | -2.794625 |
| C | -4.387961 | 1.462164 | 1.733644 | H | -7.073865 | -0.183040 | -3.398115 |
| H | -4.961956 | 1.559655 | 0.812884 | C | -5.866103 | -1.164068 | -1.911421 |
| N | -0.636198 | 0.193437 | 1.188583 | H | -6.529685 | -2.020414 | -1.826941 |
| C | -4.934241 | 1.842846 | 2.960544 | C | -4.701122 | -1.082689 | -1.150377 |
| H | -5.941694 | 2.248560 | 3.001181 | C | -4.228398 | -2.070179 | -0.172459 |
| N | 0.636267 | -0.196131 | 1.188147 | C | -4.916112 | -3.241390 | 0.136776 |
| C | -4.169317 | 1.688687 | 4.111985 | H | -5.856364 | -3.470515 | -0.358173 |
| H | -4.566504 | 1.968475 | 5.084916 | C | -4.396608 | -4.119116 | 1.083452 |
| N | 3.150687 | -0.969083 | 1.609071 | H | -4.929318 | -5.034216 | 1.331513 |
| C | -2.879234 | 1.175764 | 3.998050 | C | -3.190021 | -3.807262 | 1.703142 |
| H | -2.252938 | 1.056368 | 4.879227 | H | -2.750154 | -4.465467 | 2.447508 |
| N | -2.135930 | 1.924836 | -1.232493 | C | -2.546046 | -2.626476 | 1.355085 |
| C | -2.391017 | 0.829352 | 2.736580 | H | -1.598106 | -2.341702 | 1.809003 |
| N | -3.896129 | -0.001017 | -1.284470 | C | 1.184362 | -2.862842 | -1.147808 |
| C | -1.046513 | 0.343575 | 2.505372 | H | 0.375273 | -2.651805 | -0.454002 |
| N | -3.044554 | -1.772229 | 0.447655 | C | 1.220499 | -4.026405 | -1.906439 |
| C | -0.000106 | -0.004233 | 3.357015 | H | 0.431077 | -4.764816 | -1.799558 |
| H | -0.000182 | -0.005710 | 4.440088 | C | 2.273413 | -4.219053 | -2.794310 |
| N | 2.135620 | -1.921482 | -1.237162 | H | 2.329962 | -5.117464 | -3.404373 |
| C | 1.046408 | -0.349773 | 2.504564 | C | 3.260447 | -3.242359 | -2.894673 |
| N | 3.896022 | 0.004234 | -1.284804 | H | 4.089591 | -3.374824 | -3.584895 |
| C | 2.390847 | -0.836274 | 2.734592 | C | 3.178488 | -2.096845 | -2.109526 |
| N | 3.045330 | 1.771025 | 0.452308 | C | 4.169749 | -1.016453 | -2.133478 |
| C | 2.878983 | -1.185969 | 3.995190 | C | 5.325711 | -0.965571 | -2.911254 |
| H | 2.252686 | -1.068714 | 4.876654 | H | 5.569054 | -1.768517 | -3.601868 |
| C | 4.168988 | -1.699369 | 4.107843 | C | 6.169849 | 0.136814 | -2.795761 |
| H | 4.566118 | -1.981683 | 5.080068 | H | 7.072690 | 0.191676 | -3.399567 |
| C | 4.933912 | -1.850722 | 2.956029 | C | 5.865776 | 1.168788 | -1.909611 |
| H | 5.941302 | -2.256691 | 2.995660 | H | 6.529477 | 2.024847 | -1.823167 |
| C | 4.387719 | -1.466837 | 1.730083 | C | 4.701167 | 1.085467 | -1.148208 |
| H | 4.961703 | -1.562076 | 0.809081 | C | 4.229025 | 2.070384 | -0.167411 |
| C | -1.184578 | 2.865932 | -1.141386 | C | 4.917158 | 3.240546 | 0.144819 |
| H | -0.375053 | 2.653128 | -0.448630 | H | 5.857287 | 3.470799 | -0.349838 |
| C | -1.221125 | 4.031369 | -1.897138 | C | 4.398262 | 4.115759 | 1.094148 |
| H | -0.431599 | 4.769472 | -1.788899 | H | 4.931312 | 5.030021 | 1.344550 |
| C | -2.274550 | 4.226253 | -2.783911 | C | 3.191846 | 3.802493 | 1.713448 |
| H | -2.331429 | 5.126180 | -3.391705 | H | 2.752442 | 4.458728 | 2.459824 |
| C | -3.261632 | 3.249808 | -2.886151 | C | 2.547414 | 2.622855 | 1.362336 |
| H | -4.091123 | 3.383968 | -3.575626 | H | 1.599540 | 2.337102 | 1.815777 |
| C | -3.179231 | 2.102351 | -2.103903 | O | 1.214776 | 0.762798 | -1.419124 |

TS-1 (3+ unrestricted singlet)**E= -2544.295 13 a.u.**

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 0.045254 | 2.001124 | -0.090063 | C | 2.334447 | 2.895064 | -1.681805 |
| N | 0.390727 | 3.207255 | 1.718492 | C | 1.186567 | 3.684495 | -2.153265 |
| O | -0.531850 | 0.671779 | -1.225031 | C | 1.189721 | 4.634396 | -3.171506 |
| O | 0.531850 | -0.671779 | -1.225031 | H | 2.098687 | 4.861720 | -3.721799 |
| C | 0.580298 | 4.538678 | 1.745050 | C | 0.000000 | 5.291698 | -3.484054 |
| H | 0.604198 | 5.035985 | 0.775933 | H | -0.013815 | 6.032132 | -4.279814 |
| Ru | -0.045254 | -2.001124 | -0.090063 | C | -1.168767 | 5.008840 | -2.782634 |
| N | 0.085151 | 0.657039 | 1.479428 | H | -2.091686 | 5.526509 | -3.029502 |
| C | 0.741943 | 5.253993 | 2.921874 | C | -1.131251 | 4.055018 | -1.765048 |
| H | 0.897408 | 6.328430 | 2.886210 | C | -2.242583 | 3.656630 | -0.892882 |
| N | -0.085151 | -0.657039 | 1.479428 | C | -3.507591 | 4.240745 | -0.938320 |
| C | 0.698926 | 4.565089 | 4.133034 | H | -3.727779 | 5.006333 | -1.677895 |
| H | 0.819210 | 5.094487 | 5.075099 | C | -4.480549 | 3.853892 | -0.024236 |
| N | -0.390727 | -3.207255 | 1.718492 | H | -5.467319 | 4.309483 | -0.049513 |
| C | 0.501705 | 3.190868 | 4.122439 | C | -4.164572 | 2.890958 | 0.930290 |
| H | 0.466787 | 2.626094 | 5.051069 | H | -4.888265 | 2.576879 | 1.677695 |
| N | 2.072022 | 2.018120 | -0.662801 | C | -2.891060 | 2.336940 | 0.923369 |
| C | 0.350274 | 2.525947 | 2.905560 | H | -2.588335 | 1.587227 | 1.653709 |
| N | 0.035734 | 3.426545 | -1.487054 | C | -3.070809 | -1.278402 | -0.162497 |
| C | 0.149149 | 1.096198 | 2.766341 | H | -2.790635 | -0.609749 | 0.648382 |
| N | -1.951593 | 2.690451 | 0.033684 | C | -4.372078 | -1.357346 | -0.639545 |
| C | 0.000000 | 0.000000 | 3.625089 | H | -5.151387 | -0.743617 | -0.196003 |
| H | 0.000000 | 0.000000 | 4.708128 | C | -4.650586 | -2.240014 | -1.678644 |
| N | -2.072022 | -2.018120 | -0.662801 | H | -5.658494 | -2.331771 | -2.075774 |
| C | -0.149149 | -1.096198 | 2.766341 | C | -3.620401 | -3.015075 | -2.201372 |
| N | -0.035734 | -3.426545 | -1.487054 | H | -3.819866 | -3.714289 | -3.009233 |
| C | -0.350274 | -2.525947 | 2.905560 | C | -2.334447 | -2.895064 | -1.681805 |
| N | 1.951593 | -2.690451 | 0.033684 | C | -1.186567 | -3.684495 | -2.153265 |
| C | -0.501705 | -3.190868 | 4.122439 | C | -1.189721 | -4.634396 | -3.171506 |
| H | -0.466787 | -2.626094 | 5.051069 | H | -2.098687 | -4.861720 | -3.721799 |
| C | -0.698926 | -4.565089 | 4.133034 | C | 0.000000 | -5.291698 | -3.484054 |
| H | -0.819210 | -5.094487 | 5.075099 | H | 0.013815 | -6.032132 | -4.279814 |
| C | -0.741943 | -5.253993 | 2.921874 | C | 1.168767 | -5.008840 | -2.782634 |
| H | -0.897408 | -6.328430 | 2.886210 | H | 2.091686 | -5.526509 | -3.029502 |
| C | -0.580298 | -4.538678 | 1.745050 | C | 1.131251 | -4.055018 | -1.765048 |
| H | -0.604198 | -5.035985 | 0.775933 | C | 2.242583 | -3.656630 | -0.892882 |
| C | 3.070809 | 1.278402 | -0.162497 | C | 3.507591 | -4.240745 | -0.938320 |
| H | 2.790635 | 0.609749 | 0.648382 | H | 3.727779 | -5.006333 | -1.677895 |
| C | 4.372078 | 1.357346 | -0.639545 | C | 4.480549 | -3.853892 | -0.024236 |
| H | 5.151387 | 0.743617 | -0.196003 | H | 5.467319 | -4.309483 | -0.049513 |
| C | 4.650586 | 2.240014 | -1.678644 | C | 4.164572 | -2.890958 | 0.930290 |
| H | 5.658494 | 2.331771 | -2.075774 | H | 4.888265 | -2.576879 | 1.677695 |
| C | 3.620401 | 3.015075 | -2.201372 | C | 2.891060 | -2.336940 | 0.923369 |
| H | 3.819866 | 3.714289 | -3.009233 | H | 2.588335 | -1.587227 | 1.653709 |

TS-1 (4+ quartet)

E= -2543.804 00 a.u.

| | | | | | | | |
|----|----------|----------|-----------|---|-----------|-----------|-----------|
| Ru | 0.000000 | 0.000000 | 0.000000 | O | 0.997572 | 1.436771 | -2.293917 |
| N | 0.000000 | 0.000000 | 2.179172 | C | -1.018678 | -0.400052 | 2.962355 |
| O | 0.559145 | 0.000000 | -1.781205 | H | -1.920052 | -0.730411 | 2.448481 |

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.843368 | 1.706508 | -2.219003 | H | -4.946204 | -0.040488 | -1.095754 |
| N | 1.790268 | 0.845361 | 0.534207 | C | -4.149152 | -2.041812 | -1.023818 |
| C | -0.942485 | -0.402485 | 4.348700 | H | -5.095394 | -2.506545 | -1.291333 |
| H | -1.794695 | -0.735617 | 4.934880 | C | -3.031017 | -2.838898 | -0.783792 |
| N | 2.805489 | 1.228523 | -0.225221 | H | -3.106958 | -3.920161 | -0.861823 |
| C | 0.237962 | 0.019404 | 4.959383 | C | -1.825652 | -2.225191 | -0.445163 |
| H | 0.329595 | 0.024178 | 6.043025 | C | -0.558728 | -2.893020 | -0.124121 |
| N | 4.855292 | 2.128294 | -1.495781 | C | -0.409732 | -4.275956 | -0.048038 |
| C | 1.297785 | 0.436882 | 4.163385 | H | -1.250071 | -4.929204 | -0.269102 |
| H | 2.228605 | 0.776982 | 4.611271 | C | 0.813564 | -4.819529 | 0.332774 |
| N | -1.277464 | 1.668345 | -0.052000 | H | 0.934255 | -5.897991 | 0.404550 |
| C | 1.161678 | 0.426483 | 2.775463 | C | 1.868279 | -3.962984 | 0.636878 |
| N | -1.770938 | -0.873776 | -0.358656 | H | 2.832426 | -4.346626 | 0.960155 |
| C | 2.182805 | 0.862715 | 1.843729 | C | 1.666342 | -2.592007 | 0.537396 |
| N | 0.493640 | -2.060727 | 0.156646 | H | 2.455804 | -1.880058 | 0.774776 |
| C | 3.513954 | 1.291883 | 1.908799 | C | 3.774661 | -1.244084 | -2.462694 |
| H | 4.126707 | 1.420343 | 2.792754 | H | 3.682241 | -1.220627 | -1.379078 |
| N | 3.479097 | -0.096372 | -3.092768 | C | 4.178450 | -2.384743 | -3.143398 |
| C | 3.875519 | 1.517785 | 0.575152 | H | 4.416739 | -3.290039 | -2.591599 |
| N | 3.032554 | 2.248682 | -4.142176 | C | 4.282840 | -2.335622 | -4.530786 |
| C | 5.044828 | 1.985083 | -0.142816 | H | 4.600383 | -3.208839 | -5.096004 |
| N | 2.533791 | 3.805823 | -2.110121 | C | 3.991010 | -1.144330 | -5.190394 |
| C | 6.278625 | 2.261875 | 0.445480 | H | 4.083777 | -1.084370 | -6.271788 |
| H | 6.402665 | 2.142919 | 1.519332 | C | 3.596358 | -0.028739 | -4.458232 |
| C | 7.339062 | 2.679481 | -0.349632 | C | 3.327305 | 1.287421 | -5.051993 |
| H | 8.307188 | 2.896878 | 0.095530 | C | 3.374736 | 1.618565 | -6.404123 |
| C | 7.143612 | 2.812923 | -1.723813 | H | 3.606947 | 0.870139 | -7.157088 |
| H | 7.946908 | 3.135804 | -2.380555 | C | 3.117901 | 2.936035 | -6.784697 |
| C | 5.891423 | 2.532004 | -2.253787 | H | 3.149217 | 3.208960 | -7.837050 |
| H | 5.697165 | 2.632672 | -3.320468 | C | 2.830023 | 3.907178 | -5.826996 |
| C | -0.956141 | 2.945384 | 0.207846 | H | 2.640247 | 4.932735 | -6.132287 |
| H | 0.080728 | 3.119923 | 0.486689 | C | 2.791065 | 3.538000 | -4.482972 |
| C | -1.883010 | 3.976382 | 0.133954 | C | 2.541763 | 4.419166 | -3.335996 |
| H | -1.580811 | 4.994987 | 0.361864 | C | 2.372819 | 5.797920 | -3.440856 |
| C | -3.194910 | 3.674115 | -0.220605 | H | 2.383603 | 6.277258 | -4.416504 |
| H | -3.948225 | 4.455976 | -0.284030 | C | 2.211078 | 6.564041 | -2.290272 |
| C | -3.538997 | 2.349508 | -0.478369 | H | 2.089199 | 7.642253 | -2.363763 |
| H | -4.562748 | 2.094374 | -0.740009 | C | 2.227060 | 5.931959 | -1.049793 |
| C | -2.571272 | 1.354058 | -0.383817 | H | 2.126953 | 6.496741 | -0.126609 |
| C | -2.846012 | -0.076104 | -0.574530 | C | 2.391856 | 4.553196 | -1.003890 |
| C | -4.067014 | -0.653279 | -0.915390 | H | 2.422328 | 4.013140 | -0.058438 |

Min-2 (3+ unrestricted singlet)

E= -2544.303 90 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| Ru | 0.000000 | 2.006922 | -0.055967 | Ru | 0.000000 | -2.006922 | -0.055967 |
| N | 0.179038 | 3.210806 | 1.721424 | N | 0.046800 | 0.660417 | 1.505284 |
| O | -0.491565 | 0.488437 | -1.172456 | C | 0.359399 | 5.293935 | 2.897233 |
| O | 0.491565 | -0.488437 | -1.172456 | H | 0.428703 | 6.376751 | 2.846546 |
| C | 0.263534 | 4.554025 | 1.728716 | N | -0.046800 | -0.660417 | 1.505284 |
| H | 0.253847 | 5.037328 | 0.752801 | C | 0.361291 | 4.620688 | 4.118019 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 0.432546 | 5.170817 | 5.053093 | C | -1.290321 | 4.765877 | -2.970331 |
| N | -0.179038 | -3.210806 | 1.721424 | H | -2.238945 | 5.179366 | -3.302009 |
| C | 0.269910 | 3.235632 | 4.125612 | C | -1.234529 | 3.870826 | -1.901469 |
| H | 0.269404 | 2.682042 | 5.061573 | C | -2.358433 | 3.407741 | -1.083202 |
| N | 2.054802 | 2.192485 | -0.501230 | C | -3.668295 | 3.860012 | -1.235232 |
| C | 0.180131 | 2.542557 | 2.918472 | H | -3.911986 | 4.564561 | -2.026358 |
| N | -0.037085 | 3.368197 | -1.511949 | C | -4.655981 | 3.422588 | -0.361202 |
| C | 0.080287 | 1.102655 | 2.793060 | H | -5.678187 | 3.776744 | -0.468227 |
| N | -2.034292 | 2.518611 | -0.091350 | C | -4.309715 | 2.542297 | 0.660723 |
| C | 0.000000 | 0.000000 | 3.652918 | H | -5.045882 | 2.195794 | 1.381264 |
| H | 0.000000 | 0.000000 | 4.735948 | C | -2.991957 | 2.116943 | 0.759392 |
| N | -2.054802 | -2.192485 | -0.501230 | H | -2.665366 | 1.437136 | 1.545268 |
| C | -0.080287 | -1.102655 | 2.793060 | C | -3.083076 | -1.583575 | 0.107356 |
| N | 0.037085 | -3.368197 | -1.511949 | H | -2.812263 | -0.928139 | 0.932910 |
| C | -0.180131 | -2.542557 | 2.918472 | C | -4.402958 | -1.778071 | -0.276217 |
| N | 2.034292 | -2.518611 | -0.091350 | H | -5.203128 | -1.269738 | 0.254991 |
| C | -0.269910 | -3.235632 | 4.125612 | C | -4.671824 | -2.643473 | -1.332489 |
| H | -0.269404 | -2.682042 | 5.061573 | H | -5.693458 | -2.825386 | -1.656744 |
| C | -0.361291 | -4.620688 | 4.118019 | C | -3.612623 | -3.286852 | -1.964240 |
| H | -0.432546 | -5.170817 | 5.053093 | H | -3.802872 | -3.973915 | -2.784721 |
| C | -0.359399 | -5.293935 | 2.897233 | C | -2.308684 | -3.054522 | -1.535148 |
| H | -0.428703 | -6.376751 | 2.846546 | C | -1.127424 | -3.705669 | -2.119733 |
| C | -0.263534 | -4.554025 | 1.728716 | C | -1.112079 | -4.600724 | -3.185696 |
| H | -0.253847 | -5.037328 | 0.752801 | H | -2.032534 | -4.886895 | -3.687380 |
| C | 3.083076 | 1.583575 | 0.107356 | C | 0.108369 | -5.126366 | -3.610117 |
| H | 2.812263 | 0.928139 | 0.932910 | H | 0.135407 | -5.823247 | -4.443839 |
| C | 4.402958 | 1.778071 | -0.276217 | C | 1.290321 | -4.765877 | -2.970331 |
| H | 5.203128 | 1.269738 | 0.254991 | H | 2.238945 | -5.179366 | -3.302009 |
| C | 4.671824 | 2.643473 | -1.332489 | C | 1.234529 | -3.870826 | -1.901469 |
| H | 5.693458 | 2.825386 | -1.656744 | C | 2.358433 | -3.407741 | -1.083202 |
| C | 3.612623 | 3.286852 | -1.964240 | C | 3.668295 | -3.860012 | -1.235232 |
| H | 3.802872 | 3.973915 | -2.784721 | H | 3.911986 | -4.564561 | -2.026358 |
| C | 2.308684 | 3.054522 | -1.535148 | C | 4.655981 | -3.422588 | -0.361202 |
| C | 1.127424 | 3.705669 | -2.119733 | H | 5.678187 | -3.776744 | -0.468227 |
| C | 1.112079 | 4.600724 | -3.185696 | C | 4.309715 | -2.542297 | 0.660723 |
| H | 2.032534 | 4.886895 | -3.687380 | H | 5.045882 | -2.195794 | 1.381264 |
| C | -0.108369 | 5.126366 | -3.610117 | C | 2.991957 | -2.116943 | 0.759392 |
| H | -0.135407 | 5.823247 | -4.443839 | H | 2.665366 | -1.437136 | 1.545268 |

Min-2 (4+ doublet)

E= -2543.812 87 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 0.000000 | 2.026830 | -0.063230 | H | 0.076031 | 6.385394 | 2.845448 |
| N | 0.042129 | 3.216874 | 1.705282 | N | -0.006216 | -0.662999 | 1.473348 |
| O | -0.459834 | 0.501201 | -1.193381 | C | 0.075867 | 4.625096 | 4.112185 |
| O | 0.459834 | -0.501201 | -1.193381 | H | 0.090514 | 5.176241 | 5.049563 |
| C | 0.044926 | 4.562691 | 1.715181 | N | -0.042129 | -3.216874 | 1.705282 |
| H | 0.037930 | 5.051587 | 0.742720 | C | 0.063689 | 3.235477 | 4.114460 |
| Ru | 0.000000 | -2.026830 | -0.063230 | H | 0.066554 | 2.680791 | 5.049888 |
| N | 0.006216 | 0.662999 | 1.473348 | N | 2.070972 | 2.333058 | -0.317959 |
| C | 0.065912 | 5.299723 | 2.892131 | C | 0.045281 | 2.544869 | 2.902865 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| N | 0.045393 | 3.393293 | -1.540914 | C | -2.298483 | 3.420236 | -1.270915 |
| C | 0.016643 | 1.104469 | 2.769438 | C | -3.598671 | 3.861595 | -1.509754 |
| N | -2.030022 | 2.562732 | -0.235727 | H | -3.800954 | 4.543151 | -2.332172 |
| C | 0.000000 | 0.000000 | 3.627694 | C | -4.632275 | 3.445979 | -0.677507 |
| H | 0.000000 | 0.000000 | 4.710895 | H | -5.647894 | 3.794365 | -0.849987 |
| N | -2.070972 | -2.333058 | -0.317959 | C | -4.341827 | 2.596238 | 0.387303 |
| C | -0.016643 | -1.104469 | 2.769438 | H | -5.117355 | 2.266389 | 1.073540 |
| N | -0.045393 | -3.393293 | -1.540914 | C | -3.030800 | 2.177814 | 0.573245 |
| C | -0.045281 | -2.544869 | 2.902865 | H | -2.750513 | 1.518444 | 1.392739 |
| N | 2.030022 | -2.562732 | -0.235727 | C | -3.056522 | -1.810797 | 0.433509 |
| C | -0.063689 | -3.235477 | 4.114460 | H | -2.735282 | -1.186652 | 1.265520 |
| H | -0.066554 | -2.680791 | 5.049888 | C | -4.397706 | -2.056609 | 0.176506 |
| C | -0.075867 | -4.625096 | 4.112185 | H | -5.161092 | -1.625232 | 0.818500 |
| H | -0.090514 | -5.176241 | 5.049563 | C | -4.735212 | -2.880440 | -0.894847 |
| C | -0.065912 | -5.299723 | 2.892131 | H | -5.776031 | -3.103091 | -1.118433 |
| H | -0.076031 | -6.385394 | 2.845448 | C | -3.719862 | -3.436099 | -1.668586 |
| C | -0.044926 | -4.562691 | 1.715181 | H | -3.965658 | -4.094383 | -2.497990 |
| H | -0.037930 | -5.051587 | 0.742720 | C | -2.390393 | -3.160614 | -1.363351 |
| C | 3.056522 | 1.810797 | 0.433509 | C | -1.243989 | -3.743858 | -2.069930 |
| H | 2.735282 | 1.186652 | 1.265520 | C | -1.290596 | -4.606911 | -3.161302 |
| C | 4.397706 | 2.056609 | 0.176506 | H | -2.240028 | -4.903633 | -3.599117 |
| H | 5.161092 | 1.625232 | 0.818500 | C | -0.094698 | -5.094315 | -3.690575 |
| C | 4.735212 | 2.880440 | -0.894847 | H | -0.115860 | -5.766898 | -4.544762 |
| H | 5.776031 | 3.103091 | -1.118433 | C | 1.123097 | -4.733211 | -3.121827 |
| C | 3.719862 | 3.436099 | -1.668586 | H | 2.052139 | -5.124990 | -3.527373 |
| H | 3.965658 | 4.094383 | -2.497990 | C | 1.128181 | -3.869275 | -2.025843 |
| C | 2.390393 | 3.160614 | -1.363351 | C | 2.298483 | -3.420236 | -1.270915 |
| C | 1.243989 | 3.743858 | -2.069930 | C | 3.598671 | -3.861595 | -1.509754 |
| C | 1.290596 | 4.606911 | -3.161302 | H | 3.800954 | -4.543151 | -2.332172 |
| H | 2.240028 | 4.903633 | -3.599117 | C | 4.632275 | -3.445979 | -0.677507 |
| C | 0.094698 | 5.094315 | -3.690575 | H | 5.647894 | -3.794365 | -0.849987 |
| H | 0.115860 | 5.766898 | -4.544762 | C | 4.341827 | -2.596238 | 0.387303 |
| C | -1.123097 | 4.733211 | -3.121827 | H | 5.117355 | -2.266389 | 1.073540 |
| H | -2.052139 | 5.124990 | -3.527373 | C | 3.030800 | -2.177814 | 0.573245 |
| C | -1.128181 | 3.869275 | -2.025843 | H | 2.750513 | -1.518444 | 1.392739 |

Min-2 (4+ quartet)

E= -2543.806 65 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 0.000000 | 2.011735 | -0.030504 | H | 0.395629 | 5.157691 | 5.076159 |
| N | 0.147989 | 3.227386 | 1.724538 | N | -0.147989 | -3.227386 | 1.724538 |
| O | -0.395123 | 0.558748 | -1.308859 | C | 0.258018 | 3.225989 | 4.131870 |
| O | 0.395123 | -0.558748 | -1.308859 | H | 0.276169 | 2.666039 | 5.064045 |
| C | 0.206050 | 4.571794 | 1.742592 | N | 2.060732 | 2.203840 | -0.414193 |
| H | 0.181736 | 5.066284 | 0.773152 | C | 0.168728 | 2.548114 | 2.917535 |
| Ru | 0.000000 | -2.011735 | -0.030504 | N | 0.033507 | 3.374547 | -1.532010 |
| N | 0.042141 | 0.675187 | 1.482537 | C | 0.080585 | 1.108339 | 2.771595 |
| C | 0.298319 | 5.298587 | 2.922015 | N | -2.013512 | 2.626671 | -0.152264 |
| H | 0.348827 | 6.383409 | 2.882986 | C | 0.000000 | 0.000000 | 3.626972 |
| N | -0.042141 | -0.675187 | 1.482537 | H | 0.000000 | 0.000000 | 4.710866 |
| C | 0.324913 | 4.614676 | 4.136622 | N | -2.060732 | -2.203840 | -0.414193 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -0.080585 | -1.108339 | 2.771595 | C | -4.601524 | 3.584772 | -0.501708 |
| N | -0.033507 | -3.374547 | -1.532010 | H | -5.611551 | 3.964299 | -0.637733 |
| C | -0.168728 | -2.548114 | 2.917535 | C | -4.298361 | 2.730420 | 0.555823 |
| N | 2.013512 | -2.626671 | -0.152264 | H | -5.056381 | 2.429534 | 1.274218 |
| C | -0.258018 | -3.225989 | 4.131870 | C | -2.994336 | 2.275594 | 0.697160 |
| H | -0.276169 | -2.666039 | 5.064045 | H | -2.703905 | 1.617389 | 1.514266 |
| C | -0.324913 | -4.614676 | 4.136622 | C | -3.053204 | -1.627862 | 0.286330 |
| H | -0.395629 | -5.157691 | 5.076159 | H | -2.741780 | -1.011435 | 1.127449 |
| C | -0.298319 | -5.298587 | 2.922015 | C | -4.391181 | -1.813926 | -0.030843 |
| H | -0.348827 | -6.383409 | 2.882986 | H | -5.161449 | -1.339031 | 0.571020 |
| C | -0.206050 | -4.571794 | 1.742592 | C | -4.717516 | -2.629938 | -1.111226 |
| H | -0.181736 | -5.066284 | 0.773152 | H | -5.756107 | -2.804614 | -1.382531 |
| C | 3.053204 | 1.627862 | 0.286330 | C | -3.694742 | -3.238121 | -1.833061 |
| H | 2.741780 | 1.011435 | 1.127449 | H | -3.932025 | -3.891940 | -2.668377 |
| C | 4.391181 | 1.813926 | -0.030843 | C | -2.368678 | -3.021742 | -1.469263 |
| H | 5.161449 | 1.339031 | 0.571020 | C | -1.219896 | -3.658075 | -2.121756 |
| C | 4.717516 | 2.629938 | -1.111226 | C | -1.257855 | -4.502655 | -3.229175 |
| H | 5.756107 | 2.804614 | -1.382531 | H | -2.199659 | -4.744188 | -3.714665 |
| C | 3.694742 | 3.238121 | -1.833061 | C | -0.065036 | -5.038271 | -3.713199 |
| H | 3.932025 | 3.891940 | -2.668377 | H | -0.078662 | -5.697531 | -4.577821 |
| C | 2.368678 | 3.021742 | -1.469263 | C | 1.141987 | -4.736283 | -3.088778 |
| C | 1.219896 | 3.658075 | -2.121756 | H | 2.070848 | -5.160011 | -3.461433 |
| C | 1.257855 | 4.502655 | -3.229175 | C | 1.136346 | -3.886878 | -1.982197 |
| H | 2.199659 | 4.744188 | -3.714665 | C | 2.293184 | -3.487137 | -1.180145 |
| C | 0.065036 | 5.038271 | -3.713199 | C | 3.586740 | -3.966999 | -1.372614 |
| H | 0.078662 | 5.697531 | -4.577821 | H | 3.797740 | -4.652254 | -2.189745 |
| C | -1.141987 | 4.736283 | -3.088778 | C | 4.601524 | -3.584772 | -0.501708 |
| H | -2.070848 | 5.160011 | -3.461433 | H | 5.611551 | -3.964299 | -0.637733 |
| C | -1.136346 | 3.886878 | -1.982197 | C | 4.298361 | -2.730420 | 0.555823 |
| C | -2.293184 | 3.487137 | -1.180145 | H | 5.056381 | -2.429534 | 1.274218 |
| C | -3.586740 | 3.966999 | -1.372614 | C | 2.994336 | -2.275594 | 0.697160 |
| H | -3.797740 | 4.652254 | -2.189745 | H | 2.703905 | -1.617389 | 1.514266 |

TS-2 (3+ unrestricted singlet)

E= -2697.131 32 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.014006 | 0.025010 | -0.006476 | H | 2.400601 | -0.119110 | 5.097887 |
| Ru | -2.193648 | -0.012303 | -0.071890 | N | 2.406458 | -2.058049 | 0.103504 |
| N | 3.043304 | 0.207418 | 1.795910 | C | 2.339039 | 0.015358 | 2.955705 |
| O | 0.273792 | 0.989485 | -1.002930 | N | 3.644893 | -0.112697 | -1.161449 |
| O | -0.745806 | 0.146771 | -1.357231 | C | 0.926442 | -0.177015 | 2.758977 |
| C | 4.369668 | 0.445246 | 1.869597 | N | 2.508875 | 2.044401 | -0.358901 |
| H | 4.883437 | 0.600095 | 0.924378 | C | -0.174254 | -0.433186 | 3.580505 |
| N | 0.514865 | -0.086538 | 1.459792 | H | -0.188921 | -0.550610 | 4.657024 |
| C | 5.053102 | 0.488893 | 3.072212 | N | -2.534854 | 2.036911 | 0.264325 |
| H | 6.121296 | 0.685565 | 3.074441 | C | -1.253115 | -0.487979 | 2.694144 |
| N | -0.798602 | -0.279986 | 1.423697 | N | -3.668226 | 0.335647 | -1.360416 |
| C | 4.347935 | 0.275982 | 4.257280 | C | -2.685965 | -0.665820 | 2.820414 |
| H | 4.858118 | 0.298729 | 5.217048 | N | -2.506765 | -1.927076 | -0.874520 |
| N | -3.379489 | -0.527057 | 1.649013 | C | -3.342451 | -0.961213 | 4.015164 |
| C | 2.983302 | 0.041291 | 4.194031 | H | -2.767195 | -1.066380 | 4.931976 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -4.721434 | -1.120829 | 4.019275 | C | -1.929139 | 2.841372 | 1.151206 |
| H | -5.244718 | -1.350840 | 4.944111 | H | -1.162402 | 2.367305 | 1.762633 |
| C | -5.422084 | -0.986245 | 2.821763 | C | -2.260022 | 4.182005 | 1.297542 |
| H | -6.500779 | -1.107000 | 2.779851 | H | -1.749199 | 4.789337 | 2.040112 |
| C | -4.714917 | -0.691860 | 1.666108 | C | -3.264873 | 4.714376 | 0.494783 |
| H | -5.221068 | -0.576805 | 0.708676 | H | -3.556127 | 5.757828 | 0.585934 |
| C | 1.775464 | -2.985885 | 0.836813 | C | -3.904647 | 3.886986 | -0.421972 |
| H | 0.982523 | -2.616245 | 1.485423 | H | -4.698117 | 4.282175 | -1.051086 |
| C | 2.107318 | -4.334053 | 0.786091 | C | -3.532443 | 2.548816 | -0.524364 |
| H | 1.570134 | -5.048014 | 1.404754 | C | -4.169071 | 1.593976 | -1.444404 |
| C | 3.142554 | -4.734792 | -0.051962 | C | -5.203322 | 1.863220 | -2.337231 |
| H | 3.433711 | -5.780299 | -0.116909 | H | -5.622148 | 2.862534 | -2.420684 |
| C | 3.816289 | -3.773644 | -0.798294 | C | -5.701091 | 0.829148 | -3.129682 |
| H | 4.637514 | -4.066976 | -1.446724 | H | -6.507671 | 1.026330 | -3.831026 |
| C | 3.439409 | -2.436846 | -0.708563 | C | -5.174156 | -0.454626 | -3.022711 |
| C | 4.131852 | -1.351720 | -1.417768 | H | -5.568575 | -1.259834 | -3.636804 |
| C | 5.235634 | -1.492173 | -2.254774 | C | -4.140542 | -0.687347 | -2.115005 |
| H | 5.642798 | -2.474217 | -2.478608 | C | -3.479277 | -1.966429 | -1.841194 |
| C | 5.823281 | -0.352963 | -2.803798 | C | -3.801951 | -3.161851 | -2.481349 |
| H | 6.682282 | -0.452345 | -3.462452 | H | -4.575783 | -3.178418 | -3.244729 |
| C | 5.326232 | 0.908997 | -2.496709 | C | -3.133513 | -4.331395 | -2.139707 |
| H | 5.794336 | 1.799501 | -2.907397 | H | -3.379736 | -5.267663 | -2.634067 |
| C | 4.218886 | 1.008052 | -1.655398 | C | -2.150661 | -4.281817 | -1.154682 |
| C | 3.578721 | 2.236484 | -1.186584 | H | -1.606662 | -5.173272 | -0.854469 |
| C | 4.008591 | 3.521129 | -1.510525 | C | -1.871583 | -3.064231 | -0.549407 |
| H | 4.860145 | 3.659551 | -2.171767 | H | -1.117302 | -2.967233 | 0.229325 |
| C | 3.342683 | 4.620819 | -0.983600 | O | 1.414589 | -1.187134 | -2.276249 |
| H | 3.671236 | 5.628121 | -1.227345 | H | 1.598366 | -0.442992 | -2.898752 |
| C | 2.255818 | 4.412217 | -0.138058 | H | 0.444631 | -1.160698 | -2.192674 |
| H | 1.713312 | 5.245484 | 0.300120 | H | 1.051633 | 1.545287 | -2.746985 |
| C | 1.870148 | 3.109958 | 0.147095 | O | 1.750751 | 1.294147 | -3.380239 |
| H | 1.024186 | 2.880654 | 0.789931 | H | 1.469475 | 1.631967 | -4.242320 |

TS-2 (4+ doublet)

E= -2696.656 83 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 1.940588 | 0.022263 | 0.033722 | H | 2.269631 | -0.146779 | 5.185090 |
| Ru | -2.187572 | 0.003354 | -0.053853 | N | 2.356795 | -2.060203 | 0.095689 |
| N | 2.962965 | 0.134651 | 1.884988 | C | 2.242686 | -0.027111 | 3.039990 |
| O | 0.396328 | 0.756029 | -0.972585 | N | 3.618087 | -0.077875 | -1.060228 |
| O | -0.593828 | -0.144445 | -1.219619 | C | 0.824394 | -0.160414 | 2.829739 |
| C | 4.294089 | 0.342617 | 1.975660 | N | 2.444293 | 2.056472 | -0.207013 |
| H | 4.831179 | 0.476853 | 1.041035 | C | -0.302475 | -0.321853 | 3.648357 |
| N | 0.438492 | -0.085637 | 1.527010 | H | -0.332042 | -0.401553 | 4.728179 |
| C | 4.962241 | 0.370066 | 3.189177 | N | -2.531843 | 2.082150 | 0.082479 |
| H | 6.036752 | 0.531267 | 3.202965 | C | -1.372412 | -0.340156 | 2.755337 |
| N | -0.884606 | -0.203223 | 1.482591 | N | -3.516988 | 0.314589 | -1.541962 |
| C | 4.239340 | 0.182828 | 4.367521 | C | -2.818270 | -0.414870 | 2.840644 |
| H | 4.738959 | 0.196673 | 5.333310 | N | -2.677657 | -1.956670 | -0.639462 |
| N | -3.460103 | -0.285274 | 1.635153 | C | -3.536504 | -0.604883 | 4.020069 |
| C | 2.868170 | -0.012499 | 4.287245 | H | -3.005812 | -0.705536 | 4.963918 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -4.924128 | -0.668268 | 3.975442 | C | -2.056193 | 2.911244 | 1.028476 |
| H | -5.496513 | -0.816361 | 4.888096 | H | -1.439947 | 2.447561 | 1.797639 |
| C | -5.569021 | -0.542610 | 2.745863 | C | -2.340012 | 4.269645 | 1.040101 |
| H | -6.651921 | -0.586445 | 2.667762 | H | -1.946852 | 4.898829 | 1.834387 |
| C | -4.804026 | -0.355337 | 1.603272 | C | -3.155612 | 4.792431 | 0.039102 |
| H | -5.266441 | -0.249688 | 0.623450 | H | -3.408921 | 5.849979 | 0.024068 |
| C | 1.681095 | -3.008405 | 0.761400 | C | -3.665257 | 3.937659 | -0.933739 |
| H | 0.851157 | -2.658044 | 1.371910 | H | -4.319876 | 4.325273 | -1.710224 |
| C | 2.021346 | -4.353560 | 0.691008 | C | -3.352176 | 2.581530 | -0.895217 |
| H | 1.451734 | -5.087507 | 1.254733 | C | -3.893647 | 1.585177 | -1.826952 |
| C | 3.110047 | -4.727420 | -0.090237 | C | -4.749116 | 1.829243 | -2.898667 |
| H | 3.411342 | -5.769828 | -0.162612 | H | -5.066961 | 2.839962 | -3.140695 |
| C | 3.823976 | -3.743897 | -0.770066 | C | -5.204070 | 0.752947 | -3.660572 |
| H | 4.683154 | -4.018721 | -1.376253 | H | -5.871680 | 0.928221 | -4.500692 |
| C | 3.434672 | -2.413019 | -0.666724 | C | -4.820063 | -0.545343 | -3.338207 |
| C | 4.148494 | -1.301505 | -1.308439 | H | -5.191035 | -1.384594 | -3.920600 |
| C | 5.310351 | -1.398789 | -2.068217 | C | -3.965186 | -0.748131 | -2.253649 |
| H | 5.760798 | -2.366039 | -2.274235 | C | -3.505125 | -2.035342 | -1.730080 |
| C | 5.908203 | -0.233759 | -2.551475 | C | -3.910812 | -3.272552 | -2.226832 |
| H | 6.819490 | -0.299336 | -3.141443 | H | -4.568798 | -3.323904 | -3.090680 |
| C | 5.359924 | 1.010499 | -2.258762 | C | -3.490516 | -4.440343 | -1.599760 |
| H | 5.840105 | 1.918629 | -2.613286 | H | -3.810229 | -5.409378 | -1.975549 |
| C | 4.197591 | 1.069979 | -1.490427 | C | -2.674318 | -4.346426 | -0.474987 |
| C | 3.526607 | 2.278446 | -1.014184 | H | -2.342979 | -5.234162 | 0.056945 |
| C | 3.960240 | 3.576190 | -1.280330 | C | -2.292164 | -3.089156 | -0.027215 |
| H | 4.819832 | 3.743598 | -1.924458 | H | -1.664246 | -2.959571 | 0.851769 |
| C | 3.296130 | 4.654667 | -0.706165 | O | 1.589141 | -1.291720 | -2.461604 |
| H | 3.630638 | 5.670659 | -0.902042 | H | 1.892880 | -0.706261 | -3.198555 |
| C | 2.208738 | 4.411951 | 0.129614 | H | 0.624462 | -1.318424 | -2.545143 |
| H | 1.673637 | 5.227419 | 0.608723 | H | 2.297962 | 0.983040 | -4.892409 |
| C | 1.812238 | 3.099505 | 0.350054 | O | 2.763340 | 0.295921 | -4.393714 |
| H | 0.965894 | 2.848794 | 0.985553 | H | 3.189232 | -0.236799 | -5.082424 |

Min-3 (3+ triplet)

E= -2697.135 78 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.217294 | 0.003869 | -0.031227 | H | 2.270347 | 0.427555 | 5.030520 |
| Ru | -2.309093 | -0.051687 | -0.115340 | N | 2.710885 | -2.017540 | 0.297022 |
| N | 3.116294 | 0.493179 | 1.757485 | C | 2.352442 | 0.355032 | 2.882606 |
| O | -0.275203 | 1.456193 | -1.152676 | N | 3.873982 | -0.167698 | -1.128796 |
| O | -1.049400 | 0.440463 | -1.575059 | C | 0.971638 | 0.034390 | 2.625646 |
| C | 4.410721 | 0.848379 | 1.889786 | N | 2.562964 | 1.990978 | -0.624165 |
| H | 4.973941 | 0.952521 | 0.965120 | C | -0.108695 | -0.266240 | 3.449897 |
| N | 0.576957 | 0.014925 | 1.307949 | H | -0.125338 | -0.328850 | 4.530913 |
| C | 5.001753 | 1.064673 | 3.122863 | N | -2.872485 | 1.918108 | 0.386816 |
| H | 6.048286 | 1.351059 | 3.173979 | C | -1.167307 | -0.456913 | 2.562764 |
| N | -0.732081 | -0.273369 | 1.274568 | N | -3.898387 | 0.200424 | -1.271838 |
| C | 4.234311 | 0.903842 | 4.277622 | C | -2.564568 | -0.777690 | 2.751299 |
| H | 4.672928 | 1.059403 | 5.260060 | N | -2.455873 | -1.934568 | -1.011516 |
| N | -3.321052 | -0.736551 | 1.614524 | C | -3.126551 | -1.131151 | 3.979968 |
| C | 2.900308 | 0.548973 | 4.152652 | H | -2.501883 | -1.156763 | 4.869675 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -4.472795 | -1.457973 | 4.048642 | C | -2.280426 | 2.741237 | 1.265536 |
| H | -4.923350 | -1.736020 | 4.998175 | H | -1.404937 | 2.335941 | 1.770923 |
| C | -5.235665 | -1.431168 | 2.880974 | C | -2.746873 | 4.024143 | 1.519735 |
| H | -6.292101 | -1.684004 | 2.889518 | H | -2.240747 | 4.650752 | 2.248964 |
| C | -4.623927 | -1.067058 | 1.692005 | C | -3.870237 | 4.476685 | 0.833504 |
| H | -5.181944 | -1.023953 | 0.758168 | H | -4.265979 | 5.473603 | 1.010875 |
| C | 2.103012 | -2.894935 | 1.112022 | C | -4.485242 | 3.633192 | -0.084863 |
| H | 1.272055 | -2.500644 | 1.695276 | H | -5.361594 | 3.969368 | -0.633064 |
| C | 2.502428 | -4.221042 | 1.216457 | C | -3.975263 | 2.354462 | -0.296643 |
| H | 1.983363 | -4.890299 | 1.897142 | C | -4.552135 | 1.389101 | -1.240817 |
| C | 3.575895 | -4.659385 | 0.447279 | C | -5.660259 | 1.587855 | -2.061173 |
| H | 3.918770 | -5.689464 | 0.505673 | H | -6.198974 | 2.531593 | -2.048045 |
| C | 4.216578 | -3.755125 | -0.392629 | C | -6.072766 | 0.559450 | -2.906525 |
| H | 5.064569 | -4.075281 | -0.992390 | H | -6.934492 | 0.702515 | -3.553091 |
| C | 3.776778 | -2.435138 | -0.453826 | C | -5.386858 | -0.651377 | -2.921731 |
| C | 4.423433 | -1.398705 | -1.268581 | H | -5.711752 | -1.455243 | -3.576981 |
| C | 5.524939 | -1.570226 | -2.104428 | C | -4.284770 | -0.816925 | -2.082787 |
| H | 5.981127 | -2.548347 | -2.230175 | C | -3.467518 | -2.023425 | -1.934898 |
| C | 6.039792 | -0.467023 | -2.782631 | C | -3.688597 | -3.206350 | -2.638140 |
| H | 6.896092 | -0.587966 | -3.441057 | H | -4.493615 | -3.263042 | -3.366456 |
| C | 5.465734 | 0.789129 | -2.613827 | C | -2.881558 | -4.312494 | -2.402256 |
| H | 5.868805 | 1.651688 | -3.137692 | H | -3.049359 | -5.238726 | -2.945932 |
| C | 4.364894 | 0.921409 | -1.767581 | C | -1.863921 | -4.215237 | -1.456385 |
| C | 3.648084 | 2.154669 | -1.440908 | H | -1.214890 | -5.058442 | -1.237016 |
| C | 4.027439 | 3.417472 | -1.887165 | C | -1.687050 | -3.013912 | -0.785324 |
| H | 4.891660 | 3.528552 | -2.537029 | H | -0.909215 | -2.880973 | -0.034966 |
| C | 3.298573 | 4.532311 | -1.492665 | O | 1.326112 | -0.790642 | -1.849876 |
| H | 3.585076 | 5.523972 | -1.833747 | H | 1.505166 | -0.124110 | -2.577192 |
| C | 2.204950 | 4.357301 | -0.648874 | H | 0.349650 | -0.723700 | -1.770863 |
| H | 1.613250 | 5.203158 | -0.310251 | H | 0.771817 | 1.733890 | -2.757433 |
| C | 1.872197 | 3.074860 | -0.235089 | O | 1.476753 | 1.390886 | -3.348897 |
| H | 1.016698 | 2.876417 | 0.406402 | H | 1.133675 | 1.473031 | -4.250408 |

Min-3 (4+ doublet)

E= -2696.666 42 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.191991 | -0.063222 | -0.035939 | H | -2.128501 | -1.894247 | 4.701945 |
| Ru | 2.355760 | 0.071774 | -0.159777 | N | -2.812263 | 1.720689 | 0.926313 |
| N | -3.040428 | -1.081235 | 1.550119 | C | -2.257971 | -1.228336 | 2.660070 |
| O | 0.253004 | -1.095317 | -1.484724 | N | -3.911946 | 0.376604 | -1.007797 |
| O | 1.110341 | -0.114863 | -1.621516 | C | -0.895639 | -0.785606 | 2.485556 |
| C | -4.320556 | -1.503882 | 1.588919 | N | -2.549785 | -1.795099 | -1.168041 |
| H | -4.900724 | -1.368415 | 0.679095 | C | 0.179829 | -0.641076 | 3.352879 |
| N | -0.529773 | -0.400969 | 1.214460 | H | 0.213280 | -0.855169 | 4.414145 |
| C | -4.876699 | -2.078878 | 2.720246 | N | 2.944592 | -1.964948 | -0.012134 |
| H | -5.911642 | -2.409076 | 2.701347 | C | 1.210609 | -0.161713 | 2.540733 |
| N | 0.766789 | -0.032448 | 1.253928 | N | 3.984295 | 0.050798 | -1.315770 |
| C | -4.090222 | -2.217998 | 3.864518 | C | 2.592811 | 0.183519 | 2.806287 |
| H | -4.502284 | -2.659283 | 4.768898 | N | 2.543737 | 2.104625 | -0.648242 |
| N | 3.334831 | 0.464233 | 1.694181 | C | 3.146605 | 0.268781 | 4.083619 |
| C | -2.770245 | -1.789777 | 3.830394 | H | 2.537914 | 0.039071 | 4.954919 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.471711 | 0.661270 | 4.229412 | C | 2.358860 | -2.942764 | 0.697348 |
| H | 4.917715 | 0.733594 | 5.218559 | H | 1.487652 | -2.646742 | 1.279643 |
| C | 5.216356 | 0.969118 | 3.091205 | C | 2.831175 | -4.249204 | 0.700768 |
| H | 6.252934 | 1.286890 | 3.162717 | H | 2.332472 | -5.005775 | 1.300375 |
| C | 4.612923 | 0.858191 | 1.846857 | C | 3.953955 | -4.556452 | -0.061806 |
| H | 5.160139 | 1.078321 | 0.931972 | H | 4.356368 | -5.566653 | -0.077337 |
| C | -2.206041 | 2.325224 | 1.963056 | C | 4.564204 | -3.549187 | -0.805158 |
| H | -1.328047 | 1.822743 | 2.364137 | H | 5.441418 | -3.773584 | -1.406506 |
| C | -2.667070 | 3.520010 | 2.501189 | C | 4.049542 | -2.256974 | -0.768278 |
| H | -2.148881 | 3.967066 | 3.345240 | C | 4.632830 | -1.125073 | -1.504991 |
| C | -3.797944 | 4.114172 | 1.948734 | C | 5.752106 | -1.163173 | -2.332464 |
| H | -4.190307 | 5.045305 | 2.350936 | H | 6.291737 | -2.091472 | -2.499819 |
| C | -4.429705 | 3.493001 | 0.876057 | C | 6.178984 | 0.012473 | -2.951306 |
| H | -5.319151 | 3.937862 | 0.437301 | H | 7.049396 | -0.005754 | -3.602723 |
| C | -3.927696 | 2.293499 | 0.377847 | C | 5.503126 | 1.209001 | -2.731115 |
| C | -4.549123 | 1.534760 | -0.711568 | H | 5.845823 | 2.124559 | -3.205811 |
| C | -5.713852 | 1.879808 | -1.395822 | C | 4.389135 | 1.210808 | -1.890431 |
| H | -6.244678 | 2.798877 | -1.162061 | C | 3.584200 | 2.371503 | -1.503129 |
| C | -6.207665 | 1.018408 | -2.373028 | C | 3.853976 | 3.676109 | -1.911744 |
| H | -7.119147 | 1.271462 | -2.909255 | H | 4.682355 | 3.876529 | -2.586598 |
| C | -5.549872 | -0.177204 | -2.644656 | C | 3.068735 | 4.722810 | -1.441248 |
| H | -5.948945 | -0.865981 | -3.384824 | H | 3.277578 | 5.744723 | -1.748574 |
| C | -4.387472 | -0.485790 | -1.937898 | C | 2.022670 | 4.441435 | -0.566166 |
| C | -3.612372 | -1.722249 | -2.029210 | H | 1.392420 | 5.232630 | -0.169770 |
| C | -3.936463 | -2.797176 | -2.852932 | C | 1.793073 | 3.122862 | -0.195482 |
| H | -4.780135 | -2.727502 | -3.535045 | H | 0.986948 | 2.846546 | 0.482174 |
| C | -3.188262 | -3.967893 | -2.782485 | O | -1.303087 | 1.257697 | -1.501831 |
| H | -3.437485 | -4.815847 | -3.416032 | H | -1.851172 | 1.457789 | -2.316659 |
| C | -2.133354 | -4.041258 | -1.876964 | H | -0.439014 | 0.947731 | -1.834109 |
| H | -1.537011 | -4.943923 | -1.778485 | H | -2.586385 | 1.362089 | -4.523113 |
| C | -1.845727 | -2.936944 | -1.086276 | O | -2.790935 | 1.795259 | -3.680450 |
| H | -1.021968 | -2.933430 | -0.376856 | H | -2.922225 | 2.725895 | -3.918462 |

Min-3 (4+ quartet)

E= -2696.663 55 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.254317 | -0.028912 | -0.001079 | H | -2.264311 | -0.441430 | 5.050909 |
| Ru | 2.321047 | 0.043011 | -0.132451 | N | -2.917600 | 1.949256 | 0.305291 |
| N | -3.158342 | -0.501372 | 1.791224 | C | -2.377377 | -0.363172 | 2.903246 |
| O | 0.625667 | -1.518043 | -1.167481 | N | -3.911475 | 0.054104 | -1.157101 |
| O | 1.247724 | -0.526557 | -1.757020 | C | -0.999728 | -0.033093 | 2.622719 |
| C | -4.453479 | -0.847064 | 1.936869 | N | -2.518508 | -2.028228 | -0.568630 |
| H | -5.031740 | -0.945097 | 1.021001 | C | 0.084226 | 0.284353 | 3.427083 |
| N | -0.622653 | -0.007342 | 1.296238 | H | 0.114895 | 0.352496 | 4.507653 |
| C | -5.026012 | -1.063660 | 3.180258 | N | 3.053937 | -1.863870 | 0.391429 |
| H | -6.073429 | -1.344541 | 3.247517 | C | 1.133593 | 0.481556 | 2.525176 |
| N | 0.698054 | 0.292062 | 1.244791 | N | 3.953158 | -0.108893 | -1.283850 |
| C | -4.239998 | -0.911047 | 4.322981 | C | 2.531056 | 0.804338 | 2.721738 |
| H | -4.664466 | -1.068838 | 5.311563 | N | 2.411300 | 1.980241 | -0.976878 |
| N | 3.303955 | 0.732662 | 1.597925 | C | 3.078192 | 1.178141 | 3.949709 |
| C | -2.904720 | -0.558830 | 4.180051 | H | 2.443060 | 1.227466 | 4.830959 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.428031 | 1.495936 | 4.031782 | C | 2.553717 | -2.684093 | 1.329382 |
| H | 4.867131 | 1.791633 | 4.981584 | H | 1.669954 | -2.320899 | 1.852543 |
| C | 5.206600 | 1.434407 | 2.877118 | C | 3.120818 | -3.918170 | 1.619368 |
| H | 6.265236 | 1.678481 | 2.894857 | H | 2.686109 | -4.546346 | 2.392157 |
| C | 4.610206 | 1.046947 | 1.685682 | C | 4.248515 | -4.322240 | 0.909212 |
| H | 5.184753 | 0.976762 | 0.764344 | H | 4.719419 | -5.281107 | 1.112530 |
| C | -2.393544 | 2.843647 | 1.162308 | C | 4.773196 | -3.476963 | -0.063072 |
| H | -1.564975 | 2.490398 | 1.774306 | H | 5.657699 | -3.771485 | -0.622249 |
| C | -2.876124 | 4.141194 | 1.270233 | C | 4.167731 | -2.246306 | -0.306610 |
| H | -2.426096 | 4.827351 | 1.982645 | C | 4.664422 | -1.261233 | -1.271665 |
| C | -3.943928 | 4.530116 | 0.465730 | C | 5.767091 | -1.400215 | -2.115368 |
| H | -4.350641 | 5.536714 | 0.529830 | H | 6.351876 | -2.316304 | -2.121510 |
| C | -4.498646 | 3.605509 | -0.413823 | C | 6.112280 | -0.343960 | -2.953976 |
| H | -5.343347 | 3.886171 | -1.037826 | H | 6.967655 | -0.436926 | -3.618750 |
| C | -3.979532 | 2.315236 | -0.478104 | C | 5.371989 | 0.837388 | -2.936993 |
| C | -4.535354 | 1.246344 | -1.312770 | H | 5.653892 | 1.664411 | -3.583161 |
| C | -5.629573 | 1.347002 | -2.171093 | C | 4.277150 | 0.938942 | -2.080266 |
| H | -6.147680 | 2.292965 | -2.304608 | C | 3.418172 | 2.117321 | -1.898030 |
| C | -6.063182 | 0.210853 | -2.851750 | C | 3.611832 | 3.325908 | -2.562323 |
| H | -6.916731 | 0.274190 | -3.522469 | H | 4.413931 | 3.428355 | -3.288706 |
| C | -5.417561 | -1.008024 | -2.660987 | C | 2.784064 | 4.409241 | -2.283558 |
| H | -5.767457 | -1.899271 | -3.175367 | H | 2.934865 | 5.357614 | -2.793858 |
| C | -4.326419 | -1.066460 | -1.794364 | C | 1.776034 | 4.263374 | -1.334512 |
| C | -3.552179 | -2.255650 | -1.438055 | H | 1.120936 | 5.090751 | -1.076569 |
| C | -3.837312 | -3.542906 | -1.883546 | C | 1.625373 | 3.035571 | -0.703802 |
| H | -4.662552 | -3.712413 | -2.570624 | H | 0.862818 | 2.866664 | 0.054998 |
| C | -3.073382 | -4.613035 | -1.429324 | O | -1.294027 | 0.656263 | -1.802380 |
| H | -3.294741 | -5.624167 | -1.763004 | H | -1.492056 | 0.072104 | -2.596386 |
| C | -2.036356 | -4.371468 | -0.531217 | H | -0.320989 | 0.640063 | -1.749315 |
| H | -1.426563 | -5.182471 | -0.143148 | H | -1.055691 | -1.716832 | -3.899616 |
| C | -1.792581 | -3.068404 | -0.120829 | O | -1.761999 | -1.062614 | -3.784408 |
| H | -0.994676 | -2.820913 | 0.575517 | H | -1.957707 | -0.752608 | -4.682808 |

TS-3 (3+ triplet)

E= -2773.531 82 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.375496 | -0.087337 | -0.090673 | H | -2.422801 | -1.170873 | 4.865140 |
| Ru | 2.303511 | -0.058216 | -0.081609 | N | -2.681963 | 1.959398 | 0.167725 |
| N | -3.319290 | -0.467307 | 1.684862 | C | -2.526476 | -0.709993 | 2.768081 |
| O | 0.391590 | -2.357350 | -1.491183 | N | -3.988131 | 0.176521 | -1.182484 |
| O | 0.833849 | -1.203788 | -1.683530 | C | -1.107226 | -0.662513 | 2.508883 |
| C | -4.659550 | -0.492296 | 1.846021 | N | -2.778689 | -2.058765 | -0.678548 |
| H | -5.249166 | -0.290585 | 0.955123 | C | -0.015028 | -0.820810 | 3.354592 |
| N | -0.689293 | -0.413618 | 1.225071 | H | -0.018832 | -1.016727 | 4.419601 |
| C | -5.262574 | -0.754675 | 3.064396 | N | 3.090182 | -1.967013 | -0.568745 |
| H | -6.346435 | -0.762100 | 3.135678 | C | 1.081260 | -0.656970 | 2.516082 |
| N | 0.661315 | -0.423914 | 1.231769 | N | 3.882916 | 0.408185 | -1.185518 |
| C | -4.458139 | -1.003783 | 4.175852 | C | 2.496633 | -0.633213 | 2.764491 |
| H | -4.900359 | -1.213580 | 5.146400 | N | 2.382979 | 2.007736 | 0.229288 |
| N | 3.272007 | -0.336951 | 1.677790 | C | 3.086718 | -0.872555 | 4.009363 |
| C | -3.080689 | -0.979547 | 4.020876 | H | 2.450229 | -1.108553 | 4.858548 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.462934 | -0.810606 | 4.147729 | C | 3.299471 | -4.349672 | -0.452131 |
| H | 4.927814 | -0.996740 | 5.112624 | H | 2.942383 | -5.286468 | -0.033547 |
| C | 5.242449 | -0.507263 | 3.029356 | C | 4.365876 | -4.316614 | -1.343868 |
| H | 6.325165 | -0.446967 | 3.090558 | H | 4.863765 | -5.233289 | -1.649732 |
| C | 4.615047 | -0.280660 | 1.818457 | C | 4.800200 | -3.087747 | -1.830360 |
| H | 5.180995 | -0.043669 | 0.921706 | H | 5.643845 | -3.036770 | -2.514211 |
| C | -2.061246 | 2.799381 | 1.013404 | C | 4.158740 | -1.920957 | -1.422595 |
| H | -1.268873 | 2.349098 | 1.608177 | C | 4.589316 | -0.572046 | -1.802587 |
| C | -2.402068 | 4.138459 | 1.139748 | C | 5.638323 | -0.234814 | -2.658199 |
| H | -1.874688 | 4.767851 | 1.851824 | H | 6.208310 | -1.006525 | -3.168919 |
| C | -3.435185 | 4.645138 | 0.355805 | C | 5.951324 | 1.108545 | -2.846777 |
| H | -3.732743 | 5.688136 | 0.429642 | H | 6.766206 | 1.387095 | -3.509904 |
| C | -4.106250 | 3.782906 | -0.503521 | C | 5.234951 | 2.097244 | -2.173824 |
| H | -4.941356 | 4.145446 | -1.098075 | H | 5.496839 | 3.143866 | -2.305715 |
| C | -3.732216 | 2.442020 | -0.575759 | C | 4.190364 | 1.723699 | -1.330501 |
| C | -4.446700 | 1.440808 | -1.373046 | C | 3.377246 | 2.616668 | -0.495121 |
| C | -5.522848 | 1.665521 | -2.230282 | C | 3.612250 | 3.983974 | -0.368221 |
| H | -5.904356 | 2.670562 | -2.391064 | H | 4.408546 | 4.454608 | -0.939795 |
| C | -6.106352 | 0.583884 | -2.885483 | C | 2.850383 | 4.739041 | 0.518421 |
| H | -6.945942 | 0.744388 | -3.556464 | H | 3.042139 | 5.802949 | 0.635555 |
| C | -5.611638 | -0.702928 | -2.686796 | C | 1.865266 | 4.104532 | 1.269263 |
| H | -6.057844 | -1.546263 | -3.207490 | H | 1.266917 | 4.651299 | 1.993293 |
| C | -4.534254 | -0.891076 | -1.822182 | C | 1.666749 | 2.741344 | 1.094876 |
| C | -3.886498 | -2.163188 | -1.484734 | H | 0.918687 | 2.187976 | 1.659488 |
| C | -4.358696 | -3.405767 | -1.901517 | O | -1.400265 | 0.385650 | -2.013581 |
| H | -5.236113 | -3.467324 | -2.540595 | H | -1.448741 | -0.393573 | -2.590870 |
| C | -3.719923 | -4.565250 | -1.477290 | H | -0.431022 | 0.585504 | -1.967856 |
| H | -4.086445 | -5.539549 | -1.790316 | H | 1.467299 | 1.087597 | -3.104866 |
| C | -2.618602 | -4.453788 | -0.633688 | O | 1.187792 | 1.251814 | -2.191557 |
| H | -2.101845 | -5.334443 | -0.262464 | H | 0.937582 | 2.209016 | -2.136228 |
| C | -2.182499 | -3.189525 | -0.261438 | H | 0.292682 | 4.541286 | -2.00435 |
| H | -1.321538 | -3.047145 | 0.388346 | O | -0.02623 | 3.642262 | -1.83889 |
| C | 2.685931 | -3.154038 | -0.094947 | H | -0.86002 | 3.589295 | -2.3289 |
| H | 1.838289 | -3.124321 | 0.586532 | | | | |

TS-3 (4+ doublet)

E= -2773.066 26 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.363395 | -0.080421 | -0.081760 | N | 3.249105 | -0.461833 | 1.641311 |
| Ru | 2.294564 | -0.086868 | -0.103238 | C | -3.125086 | -0.896791 | 4.034036 |
| N | -3.342634 | -0.410440 | 1.690495 | H | -2.479600 | -1.089705 | 4.887349 |
| O | 0.157056 | -2.140282 | -1.319991 | N | -2.689036 | 1.977128 | 0.156041 |
| O | 0.837900 | -1.142610 | -1.652359 | C | -2.559582 | -0.654115 | 2.780645 |
| C | -4.684022 | -0.405470 | 1.836143 | N | -3.982678 | 0.221308 | -1.239027 |
| H | -5.264734 | -0.203745 | 0.939494 | C | -1.142664 | -0.635950 | 2.516817 |
| N | -0.728127 | -0.395658 | 1.217205 | N | -2.908451 | -2.043652 | -0.613309 |
| C | -5.297919 | -0.640039 | 3.056054 | C | -0.047259 | -0.816490 | 3.342722 |
| H | -6.382318 | -0.624923 | 3.122138 | H | -0.039776 | -1.017253 | 4.406790 |
| N | 0.624937 | -0.429822 | 1.206549 | N | 3.053136 | -2.009713 | -0.652221 |
| C | -4.505036 | -0.891126 | 4.176533 | C | 1.044676 | -0.675857 | 2.486683 |
| H | -4.959619 | -1.079375 | 5.146130 | N | 3.896932 | 0.369708 | -1.193569 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 2.462997 | -0.719718 | 2.731386 | C | 2.629377 | -3.201945 | -0.210162 |
| N | 2.469410 | 1.969856 | 0.307247 | H | 1.789104 | -3.178783 | 0.481068 |
| C | 3.035111 | -1.004816 | 3.973585 | C | 3.211273 | -4.398301 | -0.615123 |
| H | 2.388945 | -1.207605 | 4.824140 | H | 2.840872 | -5.340810 | -0.221383 |
| C | 4.414844 | -1.034099 | 4.109051 | C | 4.266025 | -4.359186 | -1.521744 |
| H | 4.870552 | -1.256133 | 5.070875 | H | 4.739805 | -5.276076 | -1.863980 |
| C | 5.205694 | -0.777808 | 2.988148 | C | 4.719615 | -3.124449 | -1.975192 |
| H | 6.290730 | -0.789849 | 3.045741 | H | 5.554580 | -3.071079 | -2.669460 |
| C | 4.592606 | -0.500242 | 1.777384 | C | 4.109501 | -1.957584 | -1.519791 |
| H | 5.173863 | -0.294698 | 0.883021 | C | 4.570349 | -0.607230 | -1.852118 |
| C | -2.057961 | 2.795264 | 1.015154 | C | 5.630145 | -0.269526 | -2.695939 |
| H | -1.315206 | 2.321119 | 1.653491 | H | 6.173874 | -1.037696 | -3.239624 |
| C | -2.341363 | 4.151200 | 1.098723 | C | 5.991513 | 1.068028 | -2.826549 |
| H | -1.818084 | 4.770799 | 1.822248 | H | 6.815121 | 1.346445 | -3.479423 |
| C | -3.320679 | 4.684810 | 0.265139 | C | 5.315661 | 2.050307 | -2.102481 |
| H | -3.577561 | 5.740505 | 0.312551 | H | 5.621048 | 3.090238 | -2.183937 |
| C | -3.993601 | 3.840323 | -0.612009 | C | 4.259422 | 1.677123 | -1.273860 |
| H | -4.782836 | 4.232401 | -1.248560 | C | 3.495195 | 2.562728 | -0.385519 |
| C | -3.676021 | 2.485037 | -0.647281 | C | 3.810208 | 3.904746 | -0.177853 |
| C | -4.390940 | 1.493859 | -1.456846 | H | 4.633443 | 4.362365 | -0.721045 |
| C | -5.433629 | 1.743573 | -2.348075 | C | 3.095950 | 4.648797 | 0.757229 |
| H | -5.782133 | 2.757055 | -2.528602 | H | 3.355391 | 5.688874 | 0.942137 |
| C | -6.032947 | 0.671599 | -3.006348 | C | 2.070730 | 4.030592 | 1.469729 |
| H | -6.847335 | 0.850095 | -3.704216 | H | 1.510123 | 4.566765 | 2.231279 |
| C | -5.595352 | -0.628449 | -2.767361 | C | 1.793394 | 2.693721 | 1.214980 |
| H | -6.065222 | -1.465665 | -3.276919 | H | 1.016441 | 2.154596 | 1.754240 |
| C | -4.549451 | -0.836192 | -1.867236 | O | -1.407758 | 0.376434 | -1.992331 |
| C | -3.972631 | -2.124966 | -1.474895 | H | -1.407076 | -0.391874 | -2.586998 |
| C | -4.469434 | -3.360152 | -1.882323 | H | -0.458196 | 0.677201 | -1.974703 |
| H | -5.312487 | -3.410884 | -2.566828 | H | 1.473600 | 1.201392 | -3.003902 |
| C | -3.897176 | -4.529129 | -1.390413 | O | 1.138444 | 1.335338 | -2.102831 |
| H | -4.284331 | -5.498599 | -1.694928 | H | 0.982903 | 2.312888 | -2.007086 |
| C | -2.836933 | -4.435249 | -0.492950 | H | 0.730397 | 4.637715 | -1.41938 |
| H | -2.373049 | -5.323671 | -0.073507 | O | 0.257949 | 3.88187 | -1.7967 |
| C | -2.373259 | -3.178542 | -0.128126 | H | -0.13849 | 4.236009 | -2.60767 |
| H | -1.539089 | -3.051259 | 0.558331 | | | | |

Structures for complex 20³⁺

Min-1 (3+ unrestricted singlet)

E= -2658.839 91 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.435707 | -0.356728 | 0.054946 | C | -5.300055 | -3.428571 | 0.256973 |
| Ru | 1.930179 | 0.106023 | 0.083894 | H | -5.470987 | -4.384855 | -0.229854 |
| N | -3.544089 | 0.872452 | -1.447852 | C | -6.186808 | -2.968887 | 1.228337 |
| O | -1.351971 | -1.020762 | 1.272340 | C | -5.982536 | -1.738197 | 1.849738 |
| O | 1.067717 | -1.401075 | -0.204725 | H | -6.684072 | -1.383376 | 2.599766 |
| C | -4.792509 | 0.661168 | -1.899060 | C | -4.869326 | -0.979146 | 1.492727 |
| H | -5.256771 | -0.277854 | -1.597744 | C | -4.503665 | 0.344180 | 2.020715 |
| N | -1.020860 | 1.052754 | -0.676225 | C | -5.243808 | 1.017768 | 2.989563 |
| C | -5.468470 | 1.567448 | -2.702005 | H | -6.138711 | 0.564089 | 3.407606 |
| H | -6.474427 | 1.345070 | -3.046165 | C | -4.832522 | 2.274558 | 3.421402 |
| N | 0.237288 | 1.336221 | -0.316455 | H | -5.405125 | 2.806752 | 4.177013 |
| C | -4.827666 | 2.756173 | -3.048458 | C | -3.684191 | 2.836390 | 2.872939 |
| H | -5.328553 | 3.492993 | -3.671861 | H | -3.330528 | 3.816044 | 3.182058 |
| N | 2.688016 | 2.211387 | 0.165338 | C | -2.985061 | 2.118810 | 1.909543 |
| C | -3.536134 | 2.985595 | -2.593596 | H | -2.080599 | 2.510793 | 1.446083 |
| H | -3.007454 | 3.898221 | -2.858423 | C | 0.918611 | 0.265139 | 3.019239 |
| N | -2.213630 | -1.980581 | -1.261070 | H | 0.047260 | 0.717403 | 2.553702 |
| C | -2.908231 | 2.025928 | -1.798298 | C | 0.997233 | 0.042182 | 4.388198 |
| N | -4.018533 | -1.456973 | 0.554127 | H | 0.175311 | 0.341302 | 5.032183 |
| C | -1.547531 | 2.142796 | -1.307418 | C | 2.134139 | -0.568877 | 4.905133 |
| N | -3.375277 | 0.907745 | 1.489364 | H | 2.227176 | -0.759275 | 5.971466 |
| C | -0.598015 | 3.165702 | -1.333563 | C | 3.156960 | -0.938428 | 4.037669 |
| H | -0.701305 | 4.157956 | -1.755517 | H | 4.052070 | -1.420877 | 4.421488 |
| N | 1.901879 | -0.084964 | 2.179301 | C | 3.026047 | -0.691268 | 2.675119 |
| C | 0.515310 | 2.618507 | -0.692603 | C | 4.055138 | -1.035558 | 1.681728 |
| N | 3.713661 | -0.710330 | 0.406978 | C | 5.283011 | -1.611802 | 1.939604 |
| C | 1.834246 | 3.130157 | -0.367245 | H | 5.598017 | -1.887452 | 2.941913 |
| N | 2.750673 | 0.094080 | -1.885481 | C | 6.167522 | -1.861276 | 0.868962 |
| C | 2.219140 | 4.459857 | -0.543966 | C | 5.791571 | -1.498033 | -0.438715 |
| H | 1.519073 | 5.173592 | -0.971830 | H | 6.463412 | -1.669491 | -1.273541 |
| C | 3.491612 | 4.858866 | -0.157425 | C | 4.544398 | -0.920238 | -0.639499 |
| H | 3.804662 | 5.892381 | -0.284871 | C | 3.999047 | -0.465501 | -1.930577 |
| C | 4.356440 | 3.919829 | 0.402673 | C | 4.685274 | -0.566954 | -3.138031 |
| H | 5.355740 | 4.193939 | 0.728465 | H | 5.676485 | -1.011790 | -3.167775 |
| C | 3.915065 | 2.612123 | 0.539170 | C | 4.098920 | -0.096694 | -4.308352 |
| H | 4.558263 | 1.842522 | 0.965735 | H | 4.629744 | -0.171673 | -5.254228 |
| C | -1.243812 | -2.174304 | -2.163864 | C | 2.829546 | 0.469212 | -4.248767 |
| H | -0.502233 | -1.382768 | -2.228300 | H | 2.337048 | 0.849446 | -5.139393 |
| C | -1.176762 | -3.321836 | -2.945241 | C | 2.191234 | 0.544573 | -3.016792 |
| H | -0.371647 | -3.438491 | -3.664890 | H | 1.197789 | 0.978804 | -2.911706 |
| C | -2.146797 | -4.303939 | -2.781894 | O | 7.316856 | -2.425024 | 1.198720 |
| H | -2.122823 | -5.214015 | -3.376122 | C | 8.277288 | -2.721037 | 0.172683 |
| C | -3.154180 | -4.110620 | -1.841385 | H | 8.606791 | -1.799812 | -0.320260 |
| H | -3.918452 | -4.869565 | -1.695547 | H | 9.115840 | -3.182969 | 0.691309 |
| C | -3.173513 | -2.942826 | -1.085365 | H | 7.855841 | -3.424173 | -0.553941 |
| C | -4.197700 | -2.642431 | -0.075379 | H | -7.049090 | -3.572725 | 1.499699 |

Min-1 (3+ quintet)

E= -2658.839 98 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.440478 | -0.359993 | 0.021401 | C | -5.316698 | -3.427105 | -0.036127 |
| Ru | 1.933526 | 0.091478 | 0.094599 | H | -5.488212 | -4.340779 | -0.598581 |
| N | -3.533094 | 0.994394 | -1.380308 | C | -6.206667 | -3.044345 | 0.964853 |
| O | -1.367200 | -1.125398 | 1.188497 | C | -6.001992 | -1.867974 | 1.683562 |
| O | 1.081650 | -1.379783 | -0.365829 | H | -6.705842 | -1.571775 | 2.456521 |
| C | -4.776745 | 0.823678 | -1.860900 | C | -4.884988 | -1.086344 | 1.393592 |
| H | -5.241608 | -0.139730 | -1.652054 | C | -4.517675 | 0.188699 | 2.027469 |
| N | -1.017027 | 1.102464 | -0.577632 | C | -5.261278 | 0.786519 | 3.042330 |
| C | -5.447341 | 1.798801 | -2.583516 | H | -6.161141 | 0.305455 | 3.416983 |
| H | -6.449515 | 1.607408 | -2.956125 | C | -4.847104 | 2.002923 | 3.575519 |
| N | 0.236920 | 1.352172 | -0.179419 | H | -5.422512 | 2.476413 | 4.367231 |
| C | -4.806088 | 3.015198 | -2.813356 | C | -3.691689 | 2.599972 | 3.081869 |
| H | -5.302855 | 3.805423 | -3.371189 | H | -3.334919 | 3.549330 | 3.471421 |
| N | 2.680670 | 2.177820 | 0.405613 | C | -2.989176 | 1.957812 | 2.068970 |
| C | -3.518931 | 3.203506 | -2.328006 | H | -2.078121 | 2.379264 | 1.646213 |
| H | -2.989668 | 4.137078 | -2.503799 | C | 0.920336 | -0.078065 | 3.030750 |
| N | -2.220458 | -1.873309 | -1.424280 | H | 0.044727 | 0.415121 | 2.617671 |
| C | -2.896053 | 2.175697 | -1.618478 | C | 1.000961 | -0.448459 | 4.367320 |
| N | -4.030734 | -1.489938 | 0.423531 | H | 0.177479 | -0.225783 | 5.039618 |
| C | -1.539717 | 2.247205 | -1.107465 | C | 2.140982 | -1.106503 | 4.814776 |
| N | -3.383332 | 0.787277 | 1.549647 | H | 2.235366 | -1.411805 | 5.853928 |
| C | -0.592328 | 3.269327 | -1.026166 | C | 3.165269 | -1.373844 | 3.912235 |
| H | -0.693746 | 4.297201 | -1.352473 | H | 4.063274 | -1.890431 | 4.240918 |
| N | 1.905012 | -0.329364 | 2.157435 | C | 3.032506 | -0.980068 | 2.584824 |
| C | 0.515620 | 2.664980 | -0.428628 | C | 4.063735 | -1.208016 | 1.560772 |
| N | 3.721277 | -0.746528 | 0.329096 | C | 5.294610 | -1.802502 | 1.755453 |
| C | 1.830568 | 3.143933 | -0.042534 | H | 5.610088 | -2.185073 | 2.721874 |
| N | 2.757386 | 0.303148 | -1.861517 | C | 6.181458 | -1.927336 | 0.665179 |
| C | 2.215029 | 4.484831 | -0.084032 | C | 5.804217 | -1.424722 | -0.595174 |
| H | 1.518197 | 5.236628 | -0.447156 | H | 6.477884 | -1.499325 | -1.442744 |
| C | 3.482657 | 4.844722 | 0.353632 | C | 4.553923 | -0.835405 | -0.732915 |
| H | 3.795357 | 5.885952 | 0.331671 | C | 4.007114 | -0.244660 | -1.966935 |
| C | 4.342916 | 3.855870 | 0.828594 | C | 4.693285 | -0.212575 | -3.178246 |
| H | 5.337916 | 4.097613 | 1.191122 | H | 5.685591 | -0.649061 | -3.256364 |
| C | 3.902632 | 2.540697 | 0.830926 | C | 4.105387 | 0.380471 | -4.290568 |
| H | 4.542493 | 1.733390 | 1.186995 | H | 4.636144 | 0.409738 | -5.239020 |
| C | -1.251017 | -1.999517 | -2.339652 | C | 2.834668 | 0.933175 | -4.169959 |
| H | -0.503916 | -1.210548 | -2.340058 | H | 2.340761 | 1.406166 | -5.014138 |
| C | -1.189140 | -3.081609 | -3.210161 | C | 2.196069 | 0.872170 | -2.937193 |
| H | -0.383765 | -3.143914 | -3.936234 | H | 1.200832 | 1.288242 | -2.785810 |
| C | -2.163289 | -4.069516 | -3.125812 | O | 7.334305 | -2.516389 | 0.932642 |
| H | -2.142540 | -4.929631 | -3.790381 | C | 8.297130 | -2.692320 | -0.118442 |
| C | -3.170329 | -3.946507 | -2.173553 | H | 8.619756 | -1.720708 | -0.508490 |
| H | -3.938239 | -4.711042 | -2.089121 | H | 9.139123 | -3.201292 | 0.347959 |
| C | -3.184933 | -2.842370 | -1.327460 | H | 7.881233 | -3.315934 | -0.917263 |
| C | -4.210952 | -2.620089 | -0.299694 | H | -7.071793 | -3.665343 | 1.183283 |

Min-1 (4+ doublet)

E= -2658.350 35 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|----------|-----------|
| Ru | -2.413244 | 0.218291 | -0.305911 | N | -3.542512 | 0.282386 | 1.606546 |
| Ru | 1.919538 | -0.119717 | -0.023144 | O | -1.237688 | 0.015616 | -1.544895 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| O | 0.957218 | 1.053118 | -0.852415 | C | -6.100706 | 1.301095 | -3.051543 |
| C | -4.794747 | 0.747333 | 1.781358 | C | -5.877609 | -0.028313 | -2.690179 |
| H | -5.253135 | 1.230577 | 0.919469 | H | -6.540750 | -0.808961 | -3.053243 |
| N | -1.016771 | -0.337879 | 1.198118 | C | -4.799082 | -0.330125 | -1.861836 |
| C | -5.480728 | 0.625666 | 2.979956 | C | -4.427953 | -1.654371 | -1.346421 |
| H | -6.488995 | 1.020113 | 3.070932 | C | -5.136612 | -2.819709 | -1.623762 |
| N | 0.237013 | -0.804100 | 1.110760 | H | -6.006329 | -2.789660 | -2.275217 |
| C | -4.850646 | -0.010610 | 4.049597 | C | -4.731794 | -4.025800 | -1.056990 |
| H | -5.362351 | -0.128190 | 5.002073 | H | -5.284395 | -4.939298 | -1.264753 |
| N | 2.697365 | -1.714728 | 1.342254 | C | -3.619317 | -4.042809 | -0.220346 |
| C | -3.554517 | -0.485760 | 3.886291 | H | -3.275449 | -4.963048 | 0.244067 |
| H | -3.034648 | -0.971656 | 4.708576 | C | -2.944875 | -2.852301 | 0.021257 |
| N | -2.318048 | 2.312187 | -0.295795 | H | -2.069452 | -2.810108 | 0.667109 |
| C | -2.914482 | -0.322856 | 2.658785 | C | 1.061973 | -2.352960 | -2.012580 |
| N | -3.994565 | 0.674793 | -1.435597 | H | 0.183717 | -2.403429 | -1.373520 |
| C | -1.546996 | -0.731625 | 2.391109 | C | 1.206731 | -3.155071 | -3.137170 |
| N | -3.329768 | -1.687259 | -0.525111 | H | 0.432111 | -3.871710 | -3.394665 |
| C | -0.595476 | -1.474173 | 3.093659 | C | 2.351722 | -3.020227 | -3.916539 |
| H | -0.696627 | -1.927605 | 4.072301 | H | 2.495149 | -3.632094 | -4.804002 |
| N | 1.990511 | -1.455724 | -1.650055 | C | 3.318808 | -2.091473 | -3.544099 |
| C | 0.518288 | -1.496541 | 2.250122 | H | 4.221144 | -1.975451 | -4.138908 |
| N | 3.708506 | 0.292481 | -0.760725 | C | 3.125777 | -1.315671 | -2.405626 |
| C | 1.849026 | -2.072837 | 2.349091 | C | 4.098538 | -0.333119 | -1.910407 |
| N | 2.675077 | 1.229254 | 1.445251 | C | 5.318448 | -0.032760 | -2.474802 |
| C | 2.245571 | -2.951544 | 3.355273 | H | 5.668214 | -0.501749 | -3.390325 |
| H | 1.550494 | -3.220450 | 4.147185 | C | 6.155594 | 0.925275 | -1.853698 |
| C | 3.527788 | -3.488644 | 3.325749 | C | 5.734221 | 1.534911 | -0.648512 |
| H | 3.851954 | -4.178878 | 4.101144 | H | 6.370948 | 2.257687 | -0.147697 |
| C | 4.385465 | -3.137255 | 2.284865 | C | 4.498404 | 1.196811 | -0.123665 |
| H | 5.390909 | -3.543710 | 2.219184 | C | 3.916654 | 1.712806 | 1.126780 |
| C | 3.932818 | -2.247795 | 1.320819 | C | 4.562094 | 2.610687 | 1.971840 |
| H | 4.573574 | -1.941225 | 0.494973 | H | 5.547703 | 2.991433 | 1.716946 |
| C | -1.433273 | 3.078742 | 0.358562 | C | 3.945044 | 3.015887 | 3.152371 |
| H | -0.712172 | 2.544662 | 0.972255 | H | 4.446451 | 3.713074 | 3.819664 |
| C | -1.429631 | 4.463175 | 0.242502 | C | 2.686595 | 2.511640 | 3.466381 |
| H | -0.696937 | 5.049415 | 0.789703 | H | 2.175695 | 2.797536 | 4.381737 |
| C | -2.370454 | 5.073038 | -0.582051 | C | 2.086118 | 1.620283 | 2.585727 |
| H | -2.392782 | 6.154481 | -0.694410 | H | 1.105326 | 1.191284 | 2.785443 |
| C | -3.291219 | 4.280990 | -1.262894 | O | 7.291129 | 1.162539 | -2.462960 |
| H | -4.035147 | 4.741463 | -1.908071 | C | 8.228262 | 2.123684 | -1.925746 |
| C | -3.256031 | 2.898737 | -1.109465 | H | 8.573561 | 1.798808 | -0.939285 |
| C | -4.203202 | 1.978933 | -1.745886 | H | 9.058961 | 2.128211 | -2.629163 |
| C | -5.272793 | 2.315852 | -2.574151 | H | 7.765523 | 3.114581 | -1.883933 |
| H | -5.466369 | 3.350386 | -2.845053 | H | -6.936537 | 1.549009 | -3.701812 |

Min-1 (4+ quartet)

E= -2658.356 49 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|----------|
| Ru | -2.435905 | 0.151461 | -0.331181 | H | -5.298771 | 1.324359 | 0.696564 |
| Ru | 1.924354 | -0.083043 | -0.027548 | N | -1.005169 | -0.048899 | 1.238289 |
| N | -3.551631 | 0.599727 | 1.542493 | C | -5.482014 | 1.182839 | 2.844348 |
| O | -1.271263 | -0.319574 | -1.519954 | H | -6.500689 | 1.559972 | 2.865883 |
| O | 0.961852 | 0.876630 | -1.076376 | N | 0.252941 | -0.517019 | 1.243851 |
| C | -4.815020 | 1.055566 | 1.634898 | C | -4.818781 | 0.816531 | 4.014613 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -5.313731 | 0.898028 | 4.979596 | C | -4.417317 | -1.935090 | -0.939600 |
| N | 2.710592 | -1.365543 | 1.633224 | C | -5.111068 | -3.142022 | -0.955834 |
| C | -3.510860 | 0.351117 | 3.934006 | H | -5.986054 | -3.262222 | -1.589625 |
| H | -2.966516 | 0.071084 | 4.832765 | C | -4.684433 | -4.194771 | -0.150485 |
| N | -2.364904 | 2.202399 | -0.786432 | H | -5.225012 | -5.138516 | -0.153842 |
| C | -2.893713 | 0.255653 | 2.688196 | C | -3.565377 | -4.019337 | 0.658628 |
| N | -4.023871 | 0.328726 | -1.528036 | H | -3.204613 | -4.815447 | 1.304183 |
| C | -1.519344 | -0.178430 | 2.493720 | C | -2.907707 | -2.795614 | 0.634153 |
| N | -3.313573 | -1.777970 | -0.141311 | H | -2.028020 | -2.605142 | 1.247132 |
| C | -0.556656 | -0.746012 | 3.331853 | C | 1.023168 | -2.661959 | -1.508135 |
| H | -0.648149 | -0.982474 | 4.385058 | H | 0.137325 | -2.550480 | -0.888094 |
| N | 1.974776 | -1.734522 | -1.330459 | C | 1.156510 | -3.686907 | -2.436595 |
| C | 0.549629 | -0.944018 | 2.503441 | H | 0.362865 | -4.419698 | -2.550756 |
| N | 3.723916 | 0.125580 | -0.806604 | C | 2.312281 | -3.750452 | -3.208647 |
| C | 1.879053 | -1.489982 | 2.707769 | H | 2.445817 | -4.539139 | -3.945326 |
| N | 2.686447 | 1.536171 | 1.130123 | C | 3.303349 | -2.790036 | -3.025969 |
| C | 2.290100 | -2.132194 | 3.874471 | H | 4.214078 | -2.825833 | -3.618327 |
| H | 1.607799 | -2.215910 | 4.717034 | C | 3.121079 | -1.786426 | -2.080406 |
| C | 3.568015 | -2.674824 | 3.940444 | C | 4.113310 | -0.744132 | -1.788853 |
| H | 3.903228 | -3.183179 | 4.841551 | C | 5.346866 | -0.597130 | -2.381334 |
| C | 4.407344 | -2.567793 | 2.832169 | H | 5.696617 | -1.257928 | -3.169760 |
| H | 5.408354 | -2.990057 | 2.838327 | C | 6.199166 | 0.455088 | -1.964295 |
| C | 3.942326 | -1.904962 | 1.706305 | C | 5.778062 | 1.319116 | -0.924136 |
| H | 4.569894 | -1.793950 | 0.823128 | H | 6.426718 | 2.118932 | -0.580135 |
| C | -1.493017 | 3.110563 | -0.324656 | C | 4.528984 | 1.129210 | -0.361105 |
| H | -0.761191 | 2.737778 | 0.387930 | C | 3.942575 | 1.915851 | 0.736858 |
| C | -1.514922 | 4.435957 | -0.740125 | C | 4.594300 | 2.966772 | 1.374364 |
| H | -0.792158 | 5.141050 | -0.339613 | H | 5.590875 | 3.266037 | 1.060271 |
| C | -2.470839 | 4.833775 | -1.670030 | C | 3.967257 | 3.633958 | 2.423794 |
| H | -2.514587 | 5.863763 | -2.016147 | H | 4.472361 | 4.453525 | 2.929765 |
| C | -3.379345 | 3.895619 | -2.152097 | C | 2.693732 | 3.233867 | 2.816239 |
| H | -4.135114 | 4.190628 | -2.875521 | H | 2.174397 | 3.725163 | 3.634563 |
| C | -3.317204 | 2.581308 | -1.699742 | C | 2.087030 | 2.179797 | 2.143340 |
| C | -4.252516 | 1.529729 | -2.113693 | H | 1.093799 | 1.823717 | 2.411930 |
| C | -5.328997 | 1.663564 | -2.989491 | O | 7.346075 | 0.532278 | -2.589550 |
| H | -5.538701 | 2.611234 | -3.478285 | C | 8.302908 | 1.566835 | -2.259278 |
| C | -6.142766 | 0.557885 | -3.230483 | H | 8.631748 | 1.453198 | -1.221731 |
| C | -5.897363 | -0.657778 | -2.591683 | H | 9.138473 | 1.400938 | -2.936835 |
| H | -6.548149 | -1.508776 | -2.773865 | H | 7.862783 | 2.552626 | -2.437976 |
| C | -4.811718 | -0.756655 | -1.723676 | H | -6.983825 | 0.646623 | -3.914257 |

TS-1 (3+ triplet)

E= -2658.814 88 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.740221 | 0.274922 | -0.234232 | N | 1.105473 | 1.471083 | -0.275772 |
| N | -2.652315 | 2.062813 | -1.154647 | C | -3.614723 | 4.460457 | -2.202005 |
| O | -0.661252 | -0.837935 | 0.743659 | H | -3.989775 | 5.395517 | -2.610963 |
| O | 0.784953 | -1.324353 | -0.096332 | N | 3.647334 | 1.463092 | 0.184184 |
| C | -3.949965 | 2.206607 | -1.477425 | C | -2.273045 | 4.329435 | -1.871077 |
| H | -4.581584 | 1.335775 | -1.304631 | H | -1.580412 | 5.155087 | -2.016415 |
| Ru | 2.201752 | -0.201632 | 0.232196 | N | -1.655010 | -0.817188 | -2.029219 |
| N | -0.187542 | 1.599091 | -0.536984 | C | -1.807060 | 3.122522 | -1.348853 |
| C | -4.471309 | 3.378345 | -2.004415 | N | -3.359515 | -0.874859 | -0.055841 |
| H | -5.526680 | 3.438432 | -2.254289 | C | -0.428055 | 2.863144 | -0.981808 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| N | -2.583380 | 0.999410 | 1.573070 | H | -4.510726 | 2.048309 | 4.762403 |
| C | 0.776289 | 3.577995 | -0.981305 | C | -2.839452 | 2.459329 | 3.456542 |
| H | 0.936533 | 4.609015 | -1.271688 | H | -2.476760 | 3.320476 | 4.011356 |
| N | 2.010672 | -0.167565 | 2.327565 | C | -2.179956 | 2.047685 | 2.305909 |
| C | 1.726803 | 2.658341 | -0.521415 | H | -1.298721 | 2.568751 | 1.933577 |
| N | 3.401993 | -1.711266 | 0.747148 | C | 1.291009 | 0.684263 | 3.069801 |
| C | 3.149398 | 2.666165 | -0.239893 | H | 0.773035 | 1.461165 | 2.511687 |
| N | 3.031193 | -0.734835 | -1.641212 | C | 1.212978 | 0.588895 | 4.452634 |
| C | 3.976086 | 3.783041 | -0.366975 | H | 0.624066 | 1.308523 | 5.014801 |
| H | 3.555321 | 4.727292 | -0.704487 | C | 1.910083 | -0.431637 | 5.091917 |
| C | 5.324944 | 3.676070 | -0.057232 | H | 1.876688 | -0.535027 | 6.173682 |
| H | 5.979144 | 4.539493 | -0.151249 | C | 2.661821 | -1.319146 | 4.328506 |
| C | 5.827177 | 2.449588 | 0.375825 | H | 3.216685 | -2.119355 | 4.811337 |
| H | 6.875598 | 2.324845 | 0.630972 | C | 2.704138 | -1.174778 | 2.944709 |
| C | 4.957201 | 1.374871 | 0.477002 | C | 3.482382 | -2.050772 | 2.055524 |
| H | 5.305865 | 0.397118 | 0.808106 | C | 4.261031 | -3.141672 | 2.433272 |
| C | -0.750808 | -0.703290 | -3.011463 | H | 4.344321 | -3.435280 | 3.476159 |
| H | 0.002531 | 0.066459 | -2.859425 | C | 4.932622 | -3.864338 | 1.447300 |
| C | -0.770876 | -1.505765 | -4.143327 | H | 5.540207 | -4.721331 | 1.726527 |
| H | -0.020384 | -1.371738 | -4.917662 | C | 4.831741 | -3.494922 | 0.109178 |
| C | -1.770768 | -2.466213 | -4.263020 | H | 5.358241 | -4.061455 | -0.654084 |
| H | -1.821365 | -3.110745 | -5.137128 | C | 4.046137 | -2.392231 | -0.229247 |
| C | -2.715565 | -2.588671 | -3.249589 | C | 3.855992 | -1.826639 | -1.569886 |
| H | -3.506912 | -3.329596 | -3.327095 | C | 4.504654 | -2.303869 | -2.708036 |
| C | -2.646393 | -1.755673 | -2.136818 | H | 5.155869 | -3.171536 | -2.639625 |
| C | -3.607165 | -1.798503 | -1.021319 | C | 4.331506 | -1.655998 | -3.925184 |
| C | -4.682468 | -2.654341 | -0.899968 | H | 4.838838 | -2.018799 | -4.815658 |
| H | -4.918004 | -3.405868 | -1.648096 | C | 3.517240 | -0.527724 | -3.978844 |
| C | -5.510214 | -2.565375 | 0.241091 | H | 3.374837 | 0.023705 | -4.904451 |
| C | -5.229064 | -1.601037 | 1.226297 | C | 2.888600 | -0.102752 | -2.816001 |
| H | -5.852281 | -1.517389 | 2.110893 | H | 2.249442 | 0.779484 | -2.800342 |
| C | -4.133946 | -0.763024 | 1.047056 | O | -6.513773 | -3.425567 | 0.283031 |
| C | -3.708339 | 0.315644 | 1.952837 | C | -7.408519 | -3.409084 | 1.406063 |
| C | -4.405304 | 0.679989 | 3.103118 | H | -7.919072 | -2.442166 | 1.474257 |
| H | -5.297018 | 0.131760 | 3.395792 | H | -8.133336 | -4.196494 | 1.205612 |
| C | -3.968222 | 1.755928 | 3.866785 | H | -6.865004 | -3.629903 | 2.331270 |

TS-1 (4+ quartet)

E= -2658.332 91 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 1.744585 | -0.258705 | 0.222924 | C | 2.272552 | -2.590469 | 3.899045 |
| N | 2.647236 | -1.460632 | 1.803628 | H | 1.584452 | -2.885528 | 4.687757 |
| O | 0.571763 | 0.847212 | -0.719913 | N | 1.807406 | -1.875232 | -1.112893 |
| O | -0.701464 | 0.076788 | -1.273963 | C | 1.803580 | -1.849641 | 2.814516 |
| C | 3.943472 | -1.817479 | 1.870248 | N | 3.378982 | 0.177538 | -0.830199 |
| H | 4.574869 | -1.488803 | 1.046267 | C | 0.424946 | -1.441246 | 2.630526 |
| Ru | -2.204001 | 0.243106 | -0.180972 | N | 2.508911 | 1.422929 | 1.274724 |
| N | 0.184850 | -0.791537 | 1.452840 | C | -0.771287 | -1.520994 | 3.352967 |
| C | 4.463368 | -2.559948 | 2.921037 | H | -0.930593 | -1.973085 | 4.324320 |
| H | 5.517700 | -2.822637 | 2.926251 | N | -2.149449 | 2.320646 | 0.135718 |
| N | -1.095511 | -0.454719 | 1.399977 | C | -1.716429 | -0.886569 | 2.536747 |
| C | 3.613297 | -2.949890 | 3.955513 | N | -3.422767 | 0.890576 | -1.636233 |
| H | 3.991774 | -3.529145 | 4.794453 | C | -3.138265 | -0.605554 | 2.581061 |
| N | -3.634871 | -0.029113 | 1.437537 | N | -2.969529 | -1.585109 | -0.946644 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -3.965256 | -0.867919 | 3.672771 | H | 1.172510 | 1.446261 | 2.847942 |
| H | -3.548551 | -1.326381 | 4.566534 | C | -1.532968 | 2.976450 | 1.131227 |
| C | -5.312142 | -0.532516 | 3.609020 | H | -1.018727 | 2.349596 | 1.856466 |
| H | -5.967715 | -0.729602 | 4.453987 | C | -1.554502 | 4.360512 | 1.237559 |
| C | -5.808509 | 0.061593 | 2.449144 | H | -1.049962 | 4.849000 | 2.066738 |
| H | -6.854895 | 0.340443 | 2.359721 | C | -2.242862 | 5.095493 | 0.276364 |
| C | -4.941132 | 0.291873 | 1.390419 | H | -2.285009 | 6.180837 | 0.330925 |
| H | -5.291183 | 0.746483 | 0.464905 | C | -2.895304 | 4.421754 | -0.752884 |
| C | 0.986606 | -2.937630 | -1.135577 | H | -3.450493 | 4.980077 | -1.502269 |
| H | 0.220209 | -2.952644 | -0.363833 | C | -2.846559 | 3.032138 | -0.808128 |
| C | 1.106476 | -3.949485 | -2.077154 | C | -3.550245 | 2.227988 | -1.816467 |
| H | 0.425334 | -4.795839 | -2.053884 | C | -4.322345 | 2.703962 | -2.873669 |
| C | 2.116823 | -3.860723 | -3.031462 | H | -4.443715 | 3.770350 | -3.044135 |
| H | 2.242982 | -4.638117 | -3.781420 | C | -4.944685 | 1.786108 | -3.720151 |
| C | 2.977901 | -2.767540 | -3.006841 | H | -5.548439 | 2.142807 | -4.551398 |
| H | 3.780280 | -2.689294 | -3.735897 | C | -4.806494 | 0.416109 | -3.504269 |
| C | 2.815539 | -1.782952 | -2.037368 | H | -5.302410 | -0.291145 | -4.163647 |
| C | 3.699252 | -0.617406 | -1.891807 | C | -4.026554 | -0.022486 | -2.434663 |
| C | 4.775919 | -0.303553 | -2.690645 | C | -3.795829 | -1.413740 | -2.027007 |
| H | 5.064123 | -0.907431 | -3.546718 | C | -4.402334 | -2.509239 | -2.637697 |
| C | 5.544528 | 0.850445 | -2.398556 | H | -5.058198 | -2.364705 | -3.492523 |
| C | 5.199652 | 1.645984 | -1.281983 | C | -4.183676 | -3.788776 | -2.136370 |
| H | 5.784252 | 2.526588 | -1.033841 | H | -4.662255 | -4.647576 | -2.601267 |
| C | 4.104816 | 1.281334 | -0.514571 | C | -3.362424 | -3.947279 | -1.023138 |
| C | 3.622872 | 1.968994 | 0.693420 | H | -3.186002 | -4.926630 | -0.586059 |
| C | 4.251128 | 3.071209 | 1.266810 | C | -2.776696 | -2.820876 | -0.458979 |
| H | 5.135971 | 3.498851 | 0.802523 | H | -2.135503 | -2.889918 | 0.419158 |
| C | 3.754435 | 3.614664 | 2.447806 | O | 6.546243 | 1.080646 | -3.211774 |
| H | 4.246047 | 4.469846 | 2.905734 | C | 7.406306 | 2.226028 | -3.014220 |
| C | 2.634518 | 3.036976 | 3.039412 | H | 7.915352 | 2.149299 | -2.048375 |
| H | 2.229156 | 3.417353 | 3.973291 | H | 8.131969 | 2.174674 | -3.823930 |
| C | 2.043291 | 1.942398 | 2.421587 | H | 6.823141 | 3.149142 | -3.089240 |

Min-2 (3+ triplet)

E= -2658.821 22 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.183046 | 0.110179 | 0.247457 | N | -3.259400 | 1.382909 | 1.349543 |
| N | -3.675097 | -1.268496 | -0.487617 | C | -1.783669 | -2.280069 | -1.489384 |
| O | -0.603660 | 1.233797 | 0.440333 | N | -2.888613 | 1.451476 | -1.214280 |
| O | 0.553597 | 0.609732 | 0.944889 | C | -0.838404 | -3.059055 | -2.168595 |
| C | -4.996484 | -1.180518 | -0.246836 | H | -1.017193 | -3.925485 | -2.793277 |
| H | -5.308804 | -0.354327 | 0.390423 | N | 1.695809 | 1.226459 | -1.805472 |
| Ru | 1.727490 | -0.276932 | -0.332368 | C | 0.390527 | -2.463233 | -1.857369 |
| N | -1.134558 | -1.278298 | -0.829000 | N | 3.300283 | 0.825943 | 0.215005 |
| C | -5.916908 | -2.078023 | -0.764679 | C | 1.783210 | -2.653702 | -2.206238 |
| H | -6.972277 | -1.963719 | -0.534455 | N | 2.508338 | -1.396547 | 1.274838 |
| N | 0.167620 | -1.401720 | -1.031112 | C | 2.265757 | -3.657445 | -3.046833 |
| C | -5.457663 | -3.114483 | -1.577208 | H | 1.569703 | -4.367077 | -3.487777 |
| H | -6.153266 | -3.834864 | -2.000688 | C | 3.625738 | -3.736779 | -3.311073 |
| N | 2.633894 | -1.740962 | -1.635642 | H | 4.012970 | -4.513871 | -3.965509 |
| C | -4.099040 | -3.214755 | -1.841093 | C | 4.485950 | -2.808372 | -2.725458 |
| H | -3.710853 | -4.010949 | -2.471869 | H | 5.556646 | -2.835629 | -2.906427 |
| N | -2.082189 | -0.811231 | 2.136668 | C | 3.950952 | -1.835102 | -1.896191 |
| C | -3.218014 | -2.283499 | -1.289775 | H | 4.583781 | -1.090317 | -1.415623 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -1.499981 | -1.977749 | 2.449466 | H | 0.247932 | 2.403776 | -4.607587 |
| H | -1.044894 | -2.508356 | 1.614815 | C | 1.906126 | 3.351210 | -3.586651 |
| C | -1.488424 | -2.486113 | 3.741267 | H | 1.995342 | 4.180455 | -4.284119 |
| H | -1.014563 | -3.442731 | 3.944670 | C | 2.776057 | 3.250879 | -2.505793 |
| C | -2.109438 | -1.757023 | 4.750847 | H | 3.548392 | 4.000606 | -2.355033 |
| H | -2.127695 | -2.126623 | 5.773155 | C | 2.661994 | 2.180463 | -1.623538 |
| C | -2.722679 | -0.549076 | 4.433884 | C | 3.552904 | 1.973358 | -0.468365 |
| H | -3.221694 | 0.028070 | 5.207994 | C | 4.570312 | 2.811986 | -0.062001 |
| C | -2.704197 | -0.088175 | 3.120475 | H | 4.806606 | 3.736758 | -0.580619 |
| C | -3.346641 | 1.161104 | 2.683175 | C | 5.334946 | 2.470826 | 1.075849 |
| C | -4.006623 | 2.083148 | 3.490953 | C | 5.046660 | 1.283056 | 1.770314 |
| H | -4.091652 | 1.927168 | 4.562982 | H | 5.616195 | 1.005062 | 2.651356 |
| C | -4.555228 | 3.224271 | 2.905180 | C | 4.010754 | 0.476523 | 1.310278 |
| C | -4.446440 | 3.432866 | 1.534164 | C | 3.580893 | -0.803236 | 1.889903 |
| H | -4.872572 | 4.324095 | 1.081375 | C | 4.225674 | -1.427238 | 2.955673 |
| C | -3.781537 | 2.482114 | 0.757951 | H | 5.074940 | -0.945961 | 3.433771 |
| C | -3.599884 | 2.503080 | -0.696033 | C | 3.794373 | -2.673464 | 3.393379 |
| C | -4.153196 | 3.472099 | -1.531498 | H | 4.297247 | -3.168919 | 4.220102 |
| H | -4.713379 | 4.300793 | -1.105937 | C | 2.723958 | -3.280720 | 2.743145 |
| C | -4.006217 | 3.362789 | -2.908722 | H | 2.369777 | -4.265552 | 3.035880 |
| H | -4.441557 | 4.109924 | -3.567577 | C | 2.113039 | -2.609522 | 1.692697 |
| C | -3.314051 | 2.271371 | -3.427005 | H | 1.279430 | -3.044791 | 1.144071 |
| H | -3.200140 | 2.131747 | -4.498788 | O | 6.287309 | 3.330560 | 1.398924 |
| C | -2.773568 | 1.343374 | -2.547604 | C | 7.115844 | 3.062937 | 2.540356 |
| H | -2.232197 | 0.467401 | -2.901458 | H | 7.809069 | 3.900892 | 2.593797 |
| C | 0.866206 | 1.327286 | -2.853971 | H | 6.509580 | 3.022388 | 3.452053 |
| H | 0.137390 | 0.523980 | -2.947099 | H | 7.671103 | 2.129037 | 2.399487 |
| C | 0.934770 | 2.370968 | -3.766057 | H | -5.069631 | 3.954596 | 3.524405 |

Min-2 (4+ doublet)

E= -2658.341 79 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.242656 | -0.055278 | -0.241708 | H | 0.983605 | -0.606605 | 4.735061 |
| N | 3.703917 | -0.351410 | 1.280888 | N | -1.885832 | 2.123275 | 0.376713 |
| O | 0.554391 | 0.539638 | -1.098422 | C | -0.401471 | -0.348917 | 2.996083 |
| O | -0.460690 | -0.363880 | -0.984716 | N | -3.393576 | 0.325781 | -0.760354 |
| C | 5.033301 | -0.393614 | 1.075368 | C | -1.800504 | -0.314201 | 3.356810 |
| H | 5.362888 | -0.281649 | 0.043942 | N | -2.443671 | -1.964621 | -0.008443 |
| Ru | -1.783911 | 0.013642 | 0.340637 | C | -2.296901 | -0.439144 | 4.654329 |
| N | 1.142410 | -0.240804 | 1.457855 | H | -1.604569 | -0.558358 | 5.484358 |
| C | 5.942155 | -0.574084 | 2.109133 | C | -3.668708 | -0.414909 | 4.870129 |
| H | 7.006064 | -0.605981 | 1.890443 | H | -4.069165 | -0.510310 | 5.876645 |
| N | -0.169745 | -0.218135 | 1.662645 | C | -4.521841 | -0.270313 | 3.776857 |
| C | 5.463755 | -0.711213 | 3.411342 | H | -5.601021 | -0.242348 | 3.900786 |
| H | 6.151582 | -0.852602 | 4.241680 | C | -3.975384 | -0.152879 | 2.506673 |
| N | -2.646009 | -0.160730 | 2.287258 | H | -4.608335 | -0.032566 | 1.629918 |
| C | 4.093026 | -0.663221 | 3.636193 | C | 2.048708 | -3.139743 | -0.087386 |
| H | 3.690564 | -0.765593 | 4.641296 | H | 1.609514 | -2.919173 | 0.883817 |
| N | 2.443614 | -2.072948 | -0.805654 | C | 2.201223 | -4.440591 | -0.544468 |
| C | 3.224847 | -0.481798 | 2.560539 | H | 1.880213 | -5.273635 | 0.075236 |
| N | 3.322413 | 0.074824 | -1.946545 | C | 2.792674 | -4.649953 | -1.788450 |
| C | 1.780918 | -0.409360 | 2.661355 | H | 2.938034 | -5.657148 | -2.172110 |
| N | 2.847793 | 1.960869 | -0.251889 | C | 3.219045 | -3.551685 | -2.529166 |
| C | 0.823044 | -0.479262 | 3.671431 | H | 3.700853 | -3.697436 | -3.492650 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.045826 | -2.267202 | -2.021503 | H | -3.947738 | 4.381605 | -1.071348 |
| C | 3.520614 | -1.046833 | -2.680676 | C | -2.911024 | 2.622821 | -0.382670 |
| C | 4.154526 | -0.962254 | -3.918072 | C | -3.751394 | 1.614031 | -1.047961 |
| H | 4.326331 | -1.851436 | -4.518922 | C | -4.827288 | 1.863610 | -1.867592 |
| C | 4.573481 | 0.285241 | -4.379936 | H | -5.148220 | 2.870514 | -2.119925 |
| C | 4.373884 | 1.422280 | -3.602623 | C | -5.556286 | 0.775583 | -2.413860 |
| H | 4.714971 | 2.391918 | -3.955601 | C | -5.171551 | -0.544983 | -2.093658 |
| C | 3.738641 | 1.293647 | -2.366702 | H | -5.715382 | -1.391032 | -2.502423 |
| C | 3.496388 | 2.357344 | -1.392051 | C | -4.083790 | -0.739591 | -1.258146 |
| C | 3.946116 | 3.668591 | -1.534371 | C | -3.555793 | -2.033482 | -0.806412 |
| H | 4.460651 | 3.972348 | -2.442538 | C | -4.139151 | -3.261465 | -1.109689 |
| C | 3.760338 | 4.578088 | -0.499220 | H | -5.022266 | -3.306809 | -1.741853 |
| H | 4.120115 | 5.599657 | -0.596882 | C | -3.597934 | -4.431821 | -0.587518 |
| C | 3.132183 | 4.152895 | 0.669416 | H | -4.051651 | -5.393903 | -0.813165 |
| H | 2.994938 | 4.824343 | 1.513015 | C | -2.479015 | -4.347473 | 0.235804 |
| C | 2.691948 | 2.839221 | 0.753667 | H | -2.036580 | -5.236039 | 0.678116 |
| H | 2.204759 | 2.454330 | 1.647866 | C | -1.933478 | -3.096514 | 0.498470 |
| C | -1.105569 | 2.973392 | 1.063271 | H | -1.063259 | -2.974256 | 1.140970 |
| H | -0.325636 | 2.510156 | 1.665008 | O | -6.559031 | 1.106648 | -3.189171 |
| C | -1.283852 | 4.349354 | 1.022336 | C | -7.387774 | 0.088997 | -3.797257 |
| H | -0.637623 | 4.998685 | 1.606953 | H | -8.127642 | 0.639030 | -4.375906 |
| C | -2.312072 | 4.868901 | 0.240674 | H | -6.782636 | -0.538870 | -4.458649 |
| H | -2.485739 | 5.941257 | 0.190435 | H | -7.881407 | -0.503606 | -3.020829 |
| C | -3.131664 | 3.993841 | -0.467049 | H | 5.067294 | 0.367577 | -5.345116 |

Min-2 (4+ quartet)

E= -2658.334 08 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.200668 | 0.240540 | -0.155030 | C | 1.790193 | -1.999517 | 2.749171 |
| N | -3.650654 | -0.190805 | 1.389170 | N | 2.454232 | 1.388257 | 1.343197 |
| O | -0.613286 | 0.202091 | -1.252835 | C | 2.258075 | -2.795547 | 3.794888 |
| O | 0.518226 | 0.880161 | -0.678700 | H | 1.564850 | -3.148439 | 4.554877 |
| C | -4.961600 | 0.103717 | 1.334297 | C | 3.604529 | -3.133848 | 3.849574 |
| H | -5.303791 | 0.607341 | 0.431651 | H | 3.982938 | -3.754799 | 4.658082 |
| Ru | 1.740570 | -0.283305 | 0.250906 | C | 4.459842 | -2.666428 | 2.852816 |
| N | -1.104621 | -0.556189 | 1.376117 | H | 5.519341 | -2.907745 | 2.858181 |
| C | -5.845478 | -0.214766 | 2.357969 | C | 3.940736 | -1.870585 | 1.839752 |
| H | -6.896247 | 0.045096 | 2.261986 | H | 4.577710 | -1.479658 | 1.048080 |
| N | 0.178407 | -0.875850 | 1.429858 | C | -1.636807 | 2.874069 | 1.403216 |
| C | -5.361246 | -0.873274 | 3.487155 | H | -1.138383 | 2.199123 | 2.095862 |
| H | -6.029823 | -1.140485 | 4.302094 | C | -1.695460 | 4.243316 | 1.625120 |
| N | 2.639912 | -1.534225 | 1.775666 | H | -1.237541 | 4.669453 | 2.513637 |
| C | -4.008574 | -1.184119 | 3.557750 | C | -2.362602 | 5.043039 | 0.701389 |
| H | -3.600004 | -1.693056 | 4.427702 | H | -2.434571 | 6.118490 | 0.845947 |
| N | -2.195979 | 2.291609 | 0.330906 | C | -2.955141 | 4.445584 | -0.407944 |
| C | -3.165242 | -0.831188 | 2.503994 | H | -3.493141 | 5.053835 | -1.130549 |
| N | -3.362869 | 0.992193 | -1.607335 | C | -2.869692 | 3.067012 | -0.578052 |
| C | -1.738725 | -1.078915 | 2.471141 | C | -3.508401 | 2.338053 | -1.682529 |
| N | -2.886158 | -1.516314 | -1.113038 | C | -4.234691 | 2.890320 | -2.734719 |
| C | -0.796971 | -1.751489 | 3.260980 | H | -4.368103 | 3.965438 | -2.820034 |
| H | -0.965791 | -2.270599 | 4.196551 | C | -4.794383 | 2.039712 | -3.688695 |
| N | 1.836227 | -1.840890 | -1.158285 | C | -4.636401 | 0.659613 | -3.584092 |
| C | 0.409143 | -1.603735 | 2.569139 | H | -5.080845 | 0.002539 | -4.326858 |
| N | 3.355685 | 0.235418 | -0.797188 | C | -3.903085 | 0.144125 | -2.515439 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -3.660688 | -1.271151 | -2.217750 | H | 5.045409 | -0.688834 | -3.570735 |
| C | -4.210161 | -2.322113 | -2.949178 | C | 5.481532 | 1.039404 | -2.361605 |
| H | -4.824777 | -2.116838 | -3.822011 | C | 5.118270 | 1.784648 | -1.217291 |
| C | -3.989643 | -3.634938 | -2.545556 | H | 5.672798 | 2.677273 | -0.944582 |
| H | -4.424801 | -4.460024 | -3.104590 | C | 4.043852 | 1.355725 | -0.454560 |
| C | -3.224142 | -3.871118 | -1.406421 | C | 3.546674 | 1.989200 | 0.775488 |
| H | -3.049926 | -4.880275 | -1.042207 | C | 4.142011 | 3.093590 | 1.378850 |
| C | -2.693372 | -2.786332 | -0.720534 | H | 5.010545 | 3.563098 | 0.924398 |
| H | -2.097856 | -2.918273 | 0.182100 | C | 3.634794 | 3.585344 | 2.577506 |
| C | 1.047170 | -2.925614 | -1.215723 | H | 4.101119 | 4.441372 | 3.059534 |
| H | 0.283160 | -2.990824 | -0.444025 | C | 2.537094 | 2.953715 | 3.155162 |
| C | 1.195635 | -3.903756 | -2.188628 | H | 2.124785 | 3.291241 | 4.102415 |
| H | 0.539607 | -4.770065 | -2.191848 | C | 1.978497 | 1.859225 | 2.507251 |
| C | 2.203041 | -3.756818 | -3.138538 | H | 1.127143 | 1.322640 | 2.923395 |
| H | 2.351917 | -4.506504 | -3.912137 | O | 6.468407 | 1.330407 | -3.173595 |
| C | 3.033020 | -2.641102 | -3.077513 | C | 7.292576 | 2.495755 | -2.942653 |
| H | 3.834661 | -2.517619 | -3.801170 | H | 8.017370 | 2.491958 | -3.754759 |
| C | 2.841846 | -1.692766 | -2.077352 | H | 6.680339 | 3.401798 | -2.988555 |
| C | 3.691839 | -0.508121 | -1.891800 | H | 7.806174 | 2.405805 | -1.980359 |
| C | 4.748197 | -0.128226 | -2.688753 | H | -5.362351 | 2.457271 | -4.516735 |

TS-2 A (4+ doublet)

E= -2811.184 01 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 1.677704 | 0.088295 | 0.295167 | C | -5.558114 | -0.240054 | 3.579724 |
| Ru | -2.436930 | -0.018368 | -0.212309 | H | -6.218177 | -0.283281 | 4.442786 |
| N | 2.482084 | 0.543194 | 2.204324 | C | -6.075422 | -0.307391 | 2.286778 |
| O | 0.219768 | 0.655829 | -0.938396 | H | -7.143142 | -0.401415 | 2.108754 |
| O | -0.741237 | -0.281348 | -1.189892 | C | -5.200988 | -0.249265 | 1.211376 |
| C | 3.791720 | 0.811077 | 2.400654 | H | -5.561911 | -0.294664 | 0.185402 |
| H | 4.424962 | 0.818950 | 1.518825 | C | 1.268433 | -2.776364 | 1.501209 |
| N | 0.016515 | 0.194450 | 1.626147 | H | 0.369777 | -2.332928 | 1.924986 |
| C | 4.323207 | 1.049732 | 3.657148 | C | 1.595769 | -4.109578 | 1.713071 |
| H | 5.386280 | 1.250984 | 3.756751 | H | 0.947047 | -4.738181 | 2.317197 |
| N | -1.290274 | 0.014201 | 1.464000 | C | 2.770559 | -4.605626 | 1.157330 |
| C | 3.481444 | 1.018702 | 4.769113 | H | 3.063588 | -5.641928 | 1.308342 |
| H | 3.873016 | 1.197999 | 5.767576 | C | 3.579454 | -3.750671 | 0.414057 |
| N | -3.869294 | -0.124886 | 1.366091 | H | 4.506939 | -4.118671 | -0.016653 |
| C | 2.131868 | 0.763738 | 4.577392 | C | 3.199422 | -2.425606 | 0.232028 |
| H | 1.441280 | 0.746496 | 5.417087 | C | 4.009392 | -1.437180 | -0.496729 |
| N | 2.037916 | -1.953417 | 0.774326 | C | 5.239684 | -1.667828 | -1.070291 |
| C | 1.645618 | 0.535774 | 3.289553 | H | 5.709024 | -2.647666 | -1.062459 |
| N | 3.471795 | -0.183944 | -0.523368 | C | 5.940416 | -0.599588 | -1.681117 |
| C | 0.261734 | 0.322671 | 2.957915 | C | 5.383743 | 0.694574 | -1.649449 |
| N | 2.232010 | 2.050962 | -0.249032 | H | 5.914125 | 1.536724 | -2.083128 |
| C | -0.940568 | 0.236374 | 3.671503 | C | 4.141821 | 0.869624 | -1.059548 |
| H | -1.084444 | 0.314000 | 4.742223 | C | 3.431962 | 2.141928 | -0.898473 |
| N | -2.792962 | 2.058826 | -0.368182 | C | 3.921211 | 3.378067 | -1.314677 |
| C | -1.907521 | 0.044918 | 2.684935 | H | 4.875419 | 3.442687 | -1.831306 |
| N | -3.623207 | 0.080346 | -1.838252 | C | 3.187838 | 4.531361 | -1.057638 |
| C | -3.352698 | -0.066989 | 2.635047 | H | 3.563822 | 5.501401 | -1.373931 |
| N | -2.841437 | -2.047254 | -0.594514 | C | 1.973703 | 4.423943 | -0.384556 |
| C | -4.184508 | -0.120487 | 3.752419 | H | 1.376354 | 5.302450 | -0.156388 |
| H | -3.751830 | -0.072679 | 4.748966 | C | 1.529769 | 3.165485 | -0.000618 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 0.585551 | 3.015959 | 0.517657 | C | -3.910104 | -3.571226 | -2.114151 |
| C | -2.402383 | 3.010492 | 0.497518 | H | -4.488300 | -3.739801 | -3.019165 |
| H | -1.845085 | 2.660434 | 1.365590 | C | -3.528162 | -4.646658 | -1.319921 |
| C | -2.698815 | 4.353869 | 0.313154 | H | -3.798336 | -5.660833 | -1.604152 |
| H | -2.377304 | 5.086126 | 1.049138 | C | -2.813976 | -4.401067 | -0.149760 |
| C | -3.435253 | 4.729448 | -0.807809 | H | -2.514890 | -5.212018 | 0.508789 |
| H | -3.696340 | 5.771348 | -0.978167 | C | -2.492243 | -3.090560 | 0.176414 |
| C | -3.855174 | 3.748554 | -1.701308 | H | -1.943408 | -2.843098 | 1.082575 |
| H | -4.446573 | 4.022349 | -2.571302 | O | 1.556742 | -1.568900 | -1.905107 |
| C | -3.533964 | 2.414531 | -1.464871 | H | 2.075110 | -1.266335 | -2.691093 |
| C | -3.985361 | 1.299562 | -2.307643 | H | 0.624593 | -1.494844 | -2.160794 |
| C | -4.746809 | 1.393492 | -3.469871 | H | 3.088921 | -0.317937 | -4.672062 |
| H | -5.051838 | 2.360193 | -3.861647 | O | 3.313676 | -0.898670 | -3.930416 |
| C | -5.123126 | 0.223100 | -4.129424 | H | 3.622002 | -1.710099 | -4.361493 |
| H | -5.716754 | 0.281511 | -5.038467 | O | 7.095476 | -0.917553 | -2.219820 |
| C | -4.755263 | -1.018346 | -3.619524 | C | 7.915687 | 0.100755 | -2.83207 |
| H | -5.065065 | -1.929385 | -4.124611 | H | 8.79565 | -0.42635 | -3.19666 |
| C | -3.996119 | -1.070378 | -2.449315 | H | 7.380871 | 0.563124 | -3.66796 |
| C | -3.568018 | -2.274554 | -1.735043 | H | 8.208396 | 0.846235 | -2.08591 |

TS-2 B (4+ doublet)

E= -2811.183 30 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.174757 | 0.109470 | 0.068791 | H | 4.456671 | -4.455464 | -3.720585 |
| Ru | 1.942879 | -0.265122 | -0.230826 | C | 4.840543 | -2.897736 | -2.272721 |
| N | -3.450474 | -0.812191 | -1.343814 | H | 5.920702 | -3.014956 | -2.271398 |
| O | -0.476634 | 1.141682 | 0.270212 | C | 4.252721 | -1.936733 | -1.464007 |
| O | 0.522861 | 0.460341 | 0.893813 | H | 4.852144 | -1.291202 | -0.824977 |
| C | -4.774315 | -0.556792 | -1.419784 | C | -2.098902 | -2.759073 | 1.320425 |
| H | -5.167790 | 0.180026 | -0.724887 | H | -1.363800 | -2.942573 | 0.538935 |
| N | -0.903473 | -1.040097 | -1.161432 | C | -2.459478 | -3.745414 | 2.230140 |
| C | -5.605459 | -1.201846 | -2.320382 | H | -2.004539 | -4.730542 | 2.170713 |
| H | -6.665734 | -0.964767 | -2.333677 | C | -3.422825 | -3.449810 | 3.189178 |
| N | 0.403250 | -1.275587 | -1.145359 | H | -3.736722 | -4.198972 | 3.912234 |
| C | -5.060164 | -2.148535 | -3.188421 | C | -3.996385 | -2.181217 | 3.202354 |
| H | -5.689773 | -2.672316 | -3.903812 | H | -4.758451 | -1.938583 | 3.938170 |
| N | 2.921043 | -1.735205 | -1.429550 | C | -3.594046 | -1.231910 | 2.269366 |
| C | -3.698116 | -2.405443 | -3.130771 | C | -4.175246 | 0.113520 | 2.173649 |
| H | -3.236996 | -3.126485 | -3.801436 | C | -5.202965 | 0.622942 | 2.961525 |
| N | -2.638295 | -1.530950 | 1.339389 | H | -5.630055 | 0.033902 | 3.768595 |
| C | -2.903414 | -1.724520 | -2.207927 | C | -5.699855 | 1.899196 | 2.692151 |
| N | -3.668629 | 0.872910 | 1.170476 | C | -5.185942 | 2.644334 | 1.636407 |
| C | -1.474334 | -1.863514 | -2.086028 | H | -5.590883 | 3.626922 | 1.409554 |
| N | -2.597617 | 1.918515 | -0.928023 | C | -4.154866 | 2.101845 | 0.869832 |
| C | -0.483139 | -2.639717 | -2.696313 | C | -3.539631 | 2.698365 | -0.314258 |
| H | -0.604924 | -3.379369 | -3.478087 | C | -3.899147 | 3.933289 | -0.851534 |
| N | 2.202497 | 1.188701 | -1.747759 | H | -4.647493 | 4.546876 | -0.356232 |
| C | 0.698622 | -2.231428 | -2.074424 | C | -3.306224 | 4.369473 | -2.031313 |
| N | 3.524368 | 0.734828 | 0.457135 | H | -3.584999 | 5.328229 | -2.462029 |
| C | 2.111933 | -2.519424 | -2.210237 | C | -2.363577 | 3.555791 | -2.655093 |
| N | 2.484888 | -1.408144 | 1.457711 | H | -1.889048 | 3.854888 | -3.585778 |
| C | 2.649465 | -3.501115 | -3.041498 | C | -2.034935 | 2.340606 | -2.069269 |
| H | 1.986924 | -4.110776 | -3.651265 | H | -1.300611 | 1.667015 | -2.504648 |
| C | 4.024824 | -3.693014 | -3.076664 | C | 1.537635 | 1.286919 | -2.911473 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|-----------|----------|
| H | 0.769415 | 0.533211 | -3.079718 | C | 3.456255 | -2.753225 | 3.694683 |
| C | 1.816545 | 2.269514 | -3.851581 | H | 3.837852 | -3.277089 | 4.567773 |
| H | 1.264299 | 2.297896 | -4.787421 | C | 2.387765 | -3.267709 | 2.965809 |
| C | 2.829224 | 3.186292 | -3.581139 | H | 1.912673 | -4.203698 | 3.246556 |
| H | 3.081859 | 3.964057 | -4.298048 | C | 1.934495 | -2.565528 | 1.856399 |
| C | 3.534999 | 3.080333 | -2.386463 | H | 1.107674 | -2.925901 | 1.247744 |
| H | 4.342839 | 3.774281 | -2.169001 | O | -1.473806 | 0.513905 | 2.827755 |
| C | 3.217794 | 2.069988 | -1.483372 | H | -1.617897 | 1.473305 | 3.013095 |
| C | 3.954753 | 1.831051 | -0.231141 | H | -0.511804 | 0.405011 | 2.821594 |
| C | 5.017272 | 2.570634 | 0.238567 | H | -1.633777 | 3.895602 | 3.148735 |
| H | 5.395447 | 3.445861 | -0.282400 | O | -2.232693 | 3.142356 | 3.254399 |
| C | 5.659060 | 2.183503 | 1.440982 | H | -2.603106 | 3.267655 | 4.141369 |
| C | 5.205800 | 1.036149 | 2.124621 | H | -6.508161 | 2.302473 | 3.297742 |
| H | 5.688372 | 0.714848 | 3.042541 | O | 6.657859 | 2.948281 | 1.817387 |
| C | 4.133633 | 0.327197 | 1.601802 | C | 7.401765 | 2.636906 | 3.01532 |
| C | 3.550215 | -0.900939 | 2.156705 | H | 8.158685 | 3.415907 | 3.087392 |
| C | 4.041200 | -1.560950 | 3.280990 | H | 6.741387 | 2.672943 | 3.88769 |
| H | 4.887386 | -1.152260 | 3.827425 | H | 7.879946 | 1.657225 | 2.916579 |

Min-3 A (4+ doublet)

E= -2811.189 80 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.983311 | -0.144100 | 0.270352 | C | 5.630441 | 0.815852 | 2.812673 |
| Ru | 2.542606 | 0.140087 | -0.290888 | H | 6.649977 | 1.190630 | 2.839171 |
| N | -2.668498 | -1.352650 | 1.796349 | C | 4.920967 | 0.830424 | 1.620972 |
| O | 0.439398 | -0.964244 | -1.662064 | H | 5.369388 | 1.205853 | 0.702986 |
| O | 1.240624 | 0.067778 | -1.638489 | C | -1.798207 | 2.006753 | 2.514714 |
| C | -3.940679 | -1.780995 | 1.920307 | H | -0.919219 | 1.434881 | 2.806978 |
| H | -4.616907 | -1.517773 | 1.110340 | C | -2.181425 | 3.150029 | 3.201541 |
| N | -0.199591 | -0.613309 | 1.280298 | H | -1.600654 | 3.487898 | 4.055490 |
| C | -4.372576 | -2.508484 | 3.018048 | C | -3.319738 | 3.834181 | 2.782874 |
| H | -5.407671 | -2.833959 | 3.073203 | H | -3.652994 | 4.729508 | 3.302576 |
| N | 1.085481 | -0.200143 | 1.247203 | C | -4.038377 | 3.347837 | 1.695882 |
| C | -3.463926 | -2.802770 | 4.034904 | H | -4.937758 | 3.859654 | 1.363482 |
| H | -3.776780 | -3.366232 | 4.910676 | C | -3.612630 | 2.193099 | 1.045292 |
| N | 3.658128 | 0.372855 | 1.522863 | C | -4.336663 | 1.561162 | -0.064419 |
| C | -2.150870 | -2.368466 | 3.911434 | C | -5.510740 | 2.015461 | -0.628989 |
| H | -1.416721 | -2.589687 | 4.682457 | H | -5.994414 | 2.932302 | -0.303608 |
| N | -2.484172 | 1.536611 | 1.456698 | C | -6.125967 | 1.266692 | -1.658872 |
| C | -1.768262 | -1.648119 | 2.779798 | C | -5.530721 | 0.057139 | -2.069063 |
| N | -3.771641 | 0.400512 | -0.491859 | H | -5.988659 | -0.549728 | -2.844105 |
| C | -0.430436 | -1.168872 | 2.520565 | C | -4.348568 | -0.346819 | -1.462386 |
| N | -2.455663 | -1.730702 | -1.018805 | C | -3.611104 | -1.582356 | -1.737546 |
| C | 0.720307 | -1.094423 | 3.293617 | C | -4.030605 | -2.572043 | -2.620782 |
| H | 0.860510 | -1.430811 | 4.313638 | H | -4.951555 | -2.444804 | -3.183751 |
| N | 3.198570 | -1.874792 | -0.411492 | C | -3.273620 | -3.728147 | -2.771082 |
| C | 1.654775 | -0.477460 | 2.457143 | H | -3.595532 | -4.509467 | -3.455546 |
| N | 4.117380 | 0.327705 | -1.496785 | C | -2.108363 | -3.874794 | -2.022036 |
| C | 3.039557 | -0.097953 | 2.645899 | H | -1.495722 | -4.768470 | -2.101136 |
| N | 2.605827 | 2.231079 | -0.560684 | C | -1.736707 | -2.859553 | -1.152312 |
| C | 3.704047 | -0.146352 | 3.871322 | H | -0.833307 | -2.916028 | -0.549868 |
| H | 3.191436 | -0.527570 | 4.751234 | C | 2.668637 | -2.956752 | 0.179427 |
| C | 5.013668 | 0.309636 | 3.956695 | H | 1.794949 | -2.773312 | 0.802284 |
| H | 5.545584 | 0.279964 | 4.904733 | C | 3.197732 | -4.231888 | 0.017818 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 2.741848 | -5.077294 | 0.525811 | C | 2.974821 | 4.941125 | -1.104616 |
| C | 4.318488 | -4.393946 | -0.789867 | H | 3.119121 | 5.997169 | -1.319617 |
| H | 4.763641 | -5.375647 | -0.933937 | C | 1.986496 | 4.522553 | -0.217935 |
| C | 4.869879 | -3.277055 | -1.414258 | H | 1.338994 | 5.237481 | 0.282054 |
| H | 5.743428 | -3.387700 | -2.051624 | C | 1.836710 | 3.162968 | 0.026498 |
| C | 4.299748 | -2.024055 | -1.214036 | H | 1.084889 | 2.783687 | 0.718115 |
| C | 4.813262 | -0.788718 | -1.828636 | H | -0.844954 | -0.570843 | -3.341369 |
| C | 5.907190 | -0.679393 | -2.682965 | O | -1.618676 | 0.009696 | -3.454845 |
| H | 6.485154 | -1.554773 | -2.966716 | H | -1.570723 | 0.354724 | -4.359621 |
| C | 6.256408 | 0.577367 | -3.179978 | O | -7.236726 | 1.774485 | -2.145533 |
| H | 7.106704 | 0.674233 | -3.850989 | C | -7.953832 | 1.074850 | -3.183374 |
| C | 5.529394 | 1.708051 | -2.817164 | H | -8.816261 | 1.701617 | -3.403398 |
| H | 5.811939 | 2.684450 | -3.201652 | H | -7.326005 | 0.975386 | -4.074888 |
| C | 4.443699 | 1.563799 | -1.952734 | H | -8.28543 | 0.097029 | -2.81924 |
| C | 3.596657 | 2.635329 | -1.420463 | O | -1.28901 | 1.300434 | -1.18741 |
| C | 3.788094 | 3.986106 | -1.705245 | H | -1.48706 | 0.959546 | -2.11626 |
| H | 4.576218 | 4.294459 | -2.387608 | H | -0.32184 | 1.398834 | -1.18846 |

Min-3 A (4+ quartet)

E= -2811.188 34 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.977204 | -0.117308 | 0.307900 | H | 6.779068 | 1.029010 | 2.689326 |
| Ru | 2.580368 | 0.132662 | -0.258758 | C | 5.013100 | 0.702025 | 1.520239 |
| N | -2.694696 | -1.087217 | 1.979507 | H | 5.475835 | 0.961113 | 0.570804 |
| O | 0.542404 | -1.376913 | -1.856665 | C | -1.793722 | 2.307699 | 2.242805 |
| O | 1.284365 | -0.349267 | -1.673722 | H | -0.922948 | 1.770960 | 2.616180 |
| C | -3.979404 | -1.451272 | 2.167968 | C | -2.175298 | 3.532828 | 2.771707 |
| H | -4.659355 | -1.257174 | 1.341754 | H | -1.601598 | 3.973775 | 3.582411 |
| N | -0.206103 | -0.478972 | 1.362084 | C | -3.303857 | 4.164814 | 2.255333 |
| C | -4.418118 | -2.033365 | 3.346155 | H | -3.634873 | 5.122022 | 2.651507 |
| H | -5.463062 | -2.311386 | 3.451663 | C | -4.016622 | 3.545821 | 1.233917 |
| N | 1.097015 | -0.123047 | 1.269929 | H | -4.909424 | 4.015867 | 0.829695 |
| C | -3.502441 | -2.246007 | 4.377464 | C | -3.593989 | 2.313205 | 0.743993 |
| H | -3.819678 | -2.696619 | 5.314825 | C | -4.316902 | 1.542786 | -0.275317 |
| N | 3.711394 | 0.352833 | 1.475201 | C | -5.494608 | 1.915170 | -0.890652 |
| C | -2.177653 | -1.877091 | 4.188947 | H | -5.981558 | 2.864691 | -0.686329 |
| H | -1.439020 | -2.037543 | 4.970568 | C | -6.114122 | 1.032428 | -1.804816 |
| N | -2.472624 | 1.709796 | 1.246518 | C | -5.516821 | -0.219293 | -2.053149 |
| C | -1.788374 | -1.302109 | 2.978600 | H | -5.979634 | -0.928716 | -2.732322 |
| N | -3.748989 | 0.337336 | -0.548127 | C | -4.329675 | -0.535181 | -1.404838 |
| C | -0.440142 | -0.898612 | 2.654933 | C | -3.594502 | -1.798786 | -1.510103 |
| N | -2.446912 | -1.858387 | -0.764284 | C | -4.013712 | -2.896907 | -2.254973 |
| C | 0.724004 | -0.795015 | 3.402127 | H | -4.926707 | -2.839989 | -2.842111 |
| H | 0.867679 | -1.037216 | 4.447998 | C | -3.270454 | -4.072146 | -2.230924 |
| N | 3.234958 | -1.867361 | -0.328533 | H | -3.595498 | -4.937931 | -2.803143 |
| C | 1.667888 | -0.302832 | 2.496910 | C | -2.117335 | -4.127144 | -1.451690 |
| N | 4.096595 | 0.290359 | -1.530849 | H | -1.517188 | -5.030880 | -1.394989 |
| C | 3.072774 | 0.017914 | 2.636913 | C | -1.741891 | -3.003541 | -0.729648 |
| N | 2.584685 | 2.211863 | -0.619313 | H | -0.848291 | -2.988664 | -0.110414 |
| C | 3.753914 | 0.019960 | 3.854051 | C | 2.750938 | -2.924571 | 0.341542 |
| H | 3.227246 | -0.252037 | 4.765532 | H | 1.914097 | -2.718045 | 1.007468 |
| C | 5.095465 | 0.378286 | 3.892006 | C | 3.282631 | -4.201501 | 0.209851 |
| H | 5.636862 | 0.384226 | 4.835027 | H | 2.865199 | -5.025024 | 0.782701 |
| C | 5.733578 | 0.733607 | 2.704340 | C | 4.355748 | -4.394215 | -0.654805 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 4.799588 | -5.379047 | -0.779725 | H | 3.041191 | 5.951236 | -1.524827 |
| C | 4.860815 | -3.304805 | -1.358333 | C | 1.937104 | 4.506484 | -0.356953 |
| H | 5.699775 | -3.437519 | -2.036687 | H | 1.289074 | 5.232801 | 0.125471 |
| C | 4.292803 | -2.045468 | -1.184409 | C | 1.809377 | 3.156447 | -0.058768 |
| C | 4.770585 | -0.835783 | -1.868401 | H | 1.070334 | 2.791174 | 0.652766 |
| C | 5.818482 | -0.753981 | -2.785777 | H | -1.362840 | -0.671453 | -3.994815 |
| H | 6.377765 | -1.639363 | -3.076114 | O | -1.984412 | -0.021346 | -3.633423 |
| C | 6.143818 | 0.485993 | -3.331549 | H | -2.227270 | 0.536116 | -4.389037 |
| H | 6.958148 | 0.563726 | -4.047823 | O | -7.232243 | 1.466138 | -2.344779 |
| C | 5.435297 | 1.628878 | -2.962425 | C | -7.963089 | 0.625886 | -3.261169 |
| H | 5.697034 | 2.593228 | -3.389910 | H | -8.832754 | 1.212956 | -3.551357 |
| C | 4.394555 | 1.509555 | -2.042725 | H | -7.351088 | 0.403918 | -4.141607 |
| C | 3.555994 | 2.594254 | -1.513221 | H | -8.28307 | -0.29233 | -2.75801 |
| C | 3.724935 | 3.934398 | -1.850645 | O | -1.16328 | 1.023488 | -1.3235 |
| H | 4.497183 | 4.226778 | -2.557684 | H | -1.49243 | 0.706958 | -2.21899 |
| C | 2.909909 | 4.902080 | -1.270833 | H | -0.19479 | 0.932235 | -1.38234 |

Min-3 B (4+ doublet)

E= -2811.19132 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.499720 | 0.003095 | -0.159618 | C | 4.100800 | 1.283880 | 2.166242 |
| Ru | 2.069577 | 0.056328 | 0.123359 | H | 4.743847 | 1.319415 | 1.288935 |
| N | -3.540035 | -0.622504 | 1.510308 | C | -2.609181 | 2.781372 | 1.233091 |
| O | 0.176505 | -1.425763 | -1.215220 | H | -1.835923 | 2.348462 | 1.865367 |
| O | 0.979497 | -0.393713 | -1.329534 | C | -3.046222 | 4.087429 | 1.410633 |
| C | -4.839530 | -0.981985 | 1.513193 | H | -2.616670 | 4.697935 | 2.200247 |
| H | -5.335315 | -1.002605 | 0.545485 | C | -4.042356 | 4.581911 | 0.573356 |
| N | -0.971643 | -0.096690 | 1.279979 | H | -4.413455 | 5.597515 | 0.689687 |
| C | -5.515644 | -1.304037 | 2.679167 | C | -4.570315 | 3.752405 | -0.411187 |
| H | -6.562478 | -1.590879 | 2.631272 | H | -5.357086 | 4.117566 | -1.066226 |
| N | 0.325503 | 0.272596 | 1.373702 | C | -4.098886 | 2.449142 | -0.543241 |
| C | -4.832448 | -1.247775 | 3.894398 | C | -4.632400 | 1.477330 | -1.502531 |
| H | -5.339224 | -1.489155 | 4.825679 | C | -5.653350 | 1.700231 | -2.424972 |
| N | 2.843546 | 0.846095 | 1.965517 | H | -6.120220 | 2.677529 | -2.513499 |
| C | -3.493004 | -0.882500 | 3.897990 | C | -6.079383 | 0.647522 | -3.232891 |
| H | -2.930986 | -0.838191 | 4.827763 | H | -6.873960 | 0.807953 | -3.957565 |
| N | -3.111808 | 1.976952 | 0.279549 | C | -5.501612 | -0.611946 | -3.101880 |
| C | -2.859456 | -0.578078 | 2.692745 | H | -5.845227 | -1.439085 | -3.717411 |
| N | -4.070449 | 0.248671 | -1.407393 | C | -4.482521 | -0.794206 | -2.166909 |
| C | -1.467750 | -0.215423 | 2.561671 | C | -3.788645 | -2.043112 | -1.857935 |
| N | -2.809923 | -1.932973 | -0.908172 | C | -4.093274 | -3.274876 | -2.429333 |
| C | -0.477437 | 0.095176 | 3.482490 | H | -4.875578 | -3.349688 | -3.180347 |
| H | -0.551344 | 0.104474 | 4.563068 | C | -3.398434 | -4.409520 | -2.025809 |
| N | 2.526582 | -1.909506 | 0.774511 | H | -3.630846 | -5.378217 | -2.461908 |
| C | 0.637943 | 0.396020 | 2.696097 | C | -2.414095 | -4.287430 | -1.047654 |
| N | 3.848373 | -0.196711 | -0.693601 | H | -1.857068 | -5.152060 | -0.697773 |
| C | 1.990326 | 0.791950 | 3.028771 | C | -2.153472 | -3.035834 | -0.507557 |
| N | 2.371117 | 1.938174 | -0.785146 | H | -1.389697 | -2.879884 | 0.250268 |
| C | 2.407770 | 1.143906 | 4.312298 | C | 1.785150 | -2.723883 | 1.540971 |
| H | 1.708419 | 1.090266 | 5.143175 | H | 0.825580 | -2.322864 | 1.862259 |
| C | 3.713078 | 1.575713 | 4.511827 | C | 2.208098 | -3.994798 | 1.909505 |
| H | 4.054766 | 1.854252 | 5.505863 | H | 1.578923 | -4.614283 | 2.542734 |
| C | 4.572357 | 1.655748 | 3.416886 | C | 3.446548 | -4.444553 | 1.462434 |
| H | 5.598415 | 1.995599 | 3.527603 | H | 3.811825 | -5.431968 | 1.734666 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 4.219020 | -3.609135 | 0.660065 | C | 1.894532 | 4.217765 | -1.357897 |
| H | 5.188008 | -3.944770 | 0.299657 | H | 1.216903 | 5.063979 | -1.286662 |
| C | 3.746280 | -2.343512 | 0.328221 | C | 1.574828 | 3.018145 | -0.733605 |
| C | 4.493446 | -1.385783 | -0.504982 | H | 0.656223 | 2.897198 | -0.159855 |
| C | 5.732534 | -1.591207 | -1.068433 | O | -1.450410 | 0.883614 | -1.833647 |
| H | 6.282737 | -2.519743 | -0.944032 | H | -1.527850 | 0.264374 | -2.626279 |
| C | 6.324141 | -0.565845 | -1.847646 | H | -0.488351 | 0.911637 | -1.682104 |
| C | 5.638359 | 0.656766 | -2.017180 | H | -0.772692 | -1.581273 | -3.110694 |
| H | 6.076767 | 1.455624 | -2.607261 | O | -1.482194 | -1.091472 | -3.565916 |
| C | 4.396826 | 0.814905 | -1.421164 | H | -1.246617 | -1.078745 | -4.506372 |
| C | 3.559145 | 2.022367 | -1.465996 | O | 7.499564 | -0.852179 | -2.354513 |
| C | 3.928521 | 3.199519 | -2.112337 | C | 8.203118 | 0.115404 | -3.16482 |
| H | 4.871980 | 3.256215 | -2.649178 | H | 8.422687 | 1.010399 | -2.57423 |
| C | 3.090180 | 4.308513 | -2.064187 | H | 9.129332 | -0.37902 | -3.45212 |
| H | 3.372190 | 5.231319 | -2.565242 | H | 7.614233 | 0.357421 | -4.05518 |

Min-3 B (4+ quartet)

E= -2811.188 46 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.488412 | 0.038835 | -0.133737 | H | 4.811792 | 0.229423 | 1.690643 |
| Ru | 2.050949 | -0.080981 | 0.208246 | C | -2.717045 | 2.192762 | 2.088957 |
| N | -3.602121 | -1.070028 | 1.202480 | H | -1.975919 | 1.566746 | 2.583990 |
| O | 0.442710 | -0.976981 | -1.503731 | C | -3.186856 | 3.363052 | 2.670338 |
| O | 1.189908 | 0.102292 | -1.603319 | H | -2.815408 | 3.668950 | 3.644698 |
| C | -4.911481 | -1.359890 | 1.063164 | C | -4.142630 | 4.113845 | 1.990961 |
| H | -5.381388 | -1.031998 | 0.138746 | H | -4.537089 | 5.031681 | 2.420737 |
| N | -1.025084 | -0.569847 | 1.210604 | C | -4.602858 | 3.664087 | 0.757390 |
| C | -5.628262 | -2.033542 | 2.039429 | H | -5.361578 | 4.227996 | 0.220851 |
| H | -6.681501 | -2.247824 | 1.880571 | C | -4.102188 | 2.480228 | 0.222518 |
| N | 0.297268 | -0.361099 | 1.411921 | C | -4.575023 | 1.879806 | -1.028348 |
| C | -4.977234 | -2.419242 | 3.211656 | C | -5.558624 | 2.391303 | -1.873584 |
| H | -5.516135 | -2.944032 | 3.996826 | H | -6.038093 | 3.342669 | -1.659075 |
| N | 2.851391 | -0.246443 | 2.158456 | C | -5.932516 | 1.658861 | -2.998547 |
| C | -3.628224 | -2.127088 | 3.360481 | H | -6.699806 | 2.044317 | -3.665638 |
| H | -3.091014 | -2.422002 | 4.258626 | C | -5.338707 | 0.426916 | -3.260250 |
| N | -3.148591 | 1.759927 | 0.890712 | H | -5.643341 | -0.154854 | -4.126296 |
| C | -2.952957 | -1.455129 | 2.341095 | C | -4.357576 | -0.048925 | -2.390587 |
| N | -3.997856 | 0.688186 | -1.312804 | C | -3.651610 | -1.327392 | -2.477891 |
| C | -1.547042 | -1.126517 | 2.359796 | C | -3.906706 | -2.304382 | -3.435664 |
| N | -2.716740 | -1.533453 | -1.498791 | H | -4.654549 | -2.131481 | -4.205503 |
| C | -0.552201 | -1.245146 | 3.318216 | C | -3.212475 | -3.508859 | -3.391343 |
| H | -0.639069 | -1.638426 | 4.323683 | H | -3.411194 | -4.282683 | -4.129153 |
| N | 2.731765 | -2.054680 | -0.082262 | C | -2.274599 | -3.712561 | -2.381726 |
| C | 0.593523 | -0.753954 | 2.684964 | H | -1.721411 | -4.644467 | -2.305988 |
| N | 3.807850 | 0.217556 | -0.695142 | C | -2.058499 | -2.705233 | -1.452130 |
| C | 1.965709 | -0.625312 | 3.126745 | H | -1.336822 | -2.807685 | -0.645122 |
| N | 2.208243 | 2.033381 | 0.277692 | C | 2.120858 | -3.179725 | 0.323457 |
| C | 2.382694 | -0.849119 | 4.439403 | H | 1.170553 | -3.041614 | 0.837366 |
| H | 1.657921 | -1.150721 | 5.191793 | C | 2.659752 | -4.440391 | 0.105382 |
| C | 3.719037 | -0.673488 | 4.774478 | H | 2.134033 | -5.323484 | 0.458130 |
| H | 4.058045 | -0.842373 | 5.793705 | C | 3.877482 | -4.542827 | -0.562491 |
| C | 4.614437 | -0.273146 | 3.784034 | H | 4.329023 | -5.514420 | -0.748504 |
| H | 5.667744 | -0.120301 | 4.002459 | C | 4.516247 | -3.381697 | -0.984541 |
| C | 4.143660 | -0.073580 | 2.494133 | H | 5.470705 | -3.440356 | -1.501496 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.933012 | -2.142694 | -0.732035 | H | 0.867064 | 4.938784 | 1.332321 |
| C | 4.539213 | -0.856771 | -1.098867 | C | 1.368514 | 2.902230 | 0.865051 |
| C | 5.732807 | -0.674870 | -1.767359 | H | 0.515213 | 2.455704 | 1.373552 |
| H | 6.342523 | -1.508184 | -2.105481 | O | -1.319656 | 1.349819 | -1.387149 |
| C | 6.188524 | 0.636169 | -2.030303 | H | -1.394422 | 1.101189 | -2.358559 |
| C | 5.416404 | 1.731643 | -1.586962 | H | -0.362997 | 1.278535 | -1.216802 |
| H | 5.755686 | 2.748034 | -1.760962 | H | -0.751219 | -0.158305 | -4.083258 |
| C | 4.222799 | 1.487113 | -0.922073 | O | -1.476304 | 0.456134 | -3.891372 |
| C | 3.323383 | 2.510668 | -0.362162 | H | -1.505289 | 1.052836 | -4.655769 |
| C | 3.573348 | 3.878996 | -0.421517 | O | 7.330568 | 0.723867 | -2.675871 |
| H | 4.460104 | 4.251066 | -0.927917 | C | 7.885238 | 2.016897 | -2.99339 |
| C | 2.692007 | 4.772528 | 0.179172 | H | 8.10261 | 2.570504 | -2.07412 |
| H | 2.886258 | 5.841762 | 0.140903 | H | 8.810471 | 1.804189 | -3.52616 |
| C | 1.571066 | 4.275465 | 0.837674 | H | 7.199826 | 2.573174 | -3.64106 |

TS-3 A (4+ doublet)

E= -2887.587 09 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.098876 | -0.117453 | 0.191667 | C | -1.471809 | 2.806982 | 1.065563 |
| Ru | 2.451882 | -0.148510 | -0.236555 | H | -0.616931 | 2.335669 | 1.547242 |
| N | -2.875700 | -0.415290 | 2.078162 | C | -1.702893 | 4.173414 | 1.146746 |
| O | -0.124172 | -1.734014 | -0.977768 | H | -1.022037 | 4.808083 | 1.708358 |
| O | 0.913957 | -1.182182 | -1.463637 | C | -2.832633 | 4.698026 | 0.522622 |
| C | -4.197220 | -0.433095 | 2.351594 | H | -3.058681 | 5.760349 | 0.579563 |
| H | -4.864362 | -0.304733 | 1.503633 | C | -3.685422 | 3.837352 | -0.160411 |
| N | -0.319621 | -0.367308 | 1.393497 | H | -4.579819 | 4.226000 | -0.640501 |
| C | -4.692203 | -0.600262 | 3.635352 | C | -3.403080 | 2.473812 | -0.209271 |
| H | -5.766274 | -0.605733 | 3.798641 | C | -4.271854 | 1.483738 | -0.863586 |
| N | 1.019026 | -0.485710 | 1.250669 | C | -5.437456 | 1.757865 | -1.549132 |
| C | -3.796445 | -0.756751 | 4.691680 | H | -5.809073 | 2.769518 | -1.685976 |
| H | -4.154453 | -0.888067 | 5.709788 | C | -6.189432 | 0.694249 | -2.098884 |
| N | 3.630152 | -0.704033 | 1.342962 | C | -5.734522 | -0.625765 | -1.920395 |
| C | -2.435566 | -0.744161 | 4.419347 | H | -6.293609 | -1.462724 | -2.327275 |
| H | -1.708787 | -0.866712 | 5.218721 | C | -4.554813 | -0.839854 | -1.215877 |
| N | -2.287097 | 1.968872 | 0.404504 | C | -3.956507 | -2.143209 | -0.900275 |
| C | -1.994436 | -0.574332 | 3.106897 | C | -4.555362 | -3.366159 | -1.191117 |
| N | -3.850853 | 0.199428 | -0.708270 | H | -5.500074 | -3.396875 | -1.727955 |
| C | -0.604840 | -0.576821 | 2.713902 | C | -3.953595 | -4.547565 | -0.771331 |
| N | -2.761773 | -2.083833 | -0.230041 | H | -4.418337 | -5.506810 | -0.985778 |
| C | 0.561658 | -0.820324 | 3.438229 | C | -2.760443 | -4.476463 | -0.058921 |
| H | 0.657869 | -1.031951 | 4.495951 | H | -2.268075 | -5.373184 | 0.307004 |
| N | 3.220491 | -1.981772 | -1.044366 | C | -2.198764 | -3.230523 | 0.187480 |
| C | 1.564938 | -0.755689 | 2.482917 | H | -1.261367 | -3.121954 | 0.728777 |
| N | 3.950773 | 0.432210 | -1.483013 | C | 2.853622 | -3.207033 | -0.643465 |
| C | 2.993052 | -0.909917 | 2.534741 | H | 2.122501 | -3.246669 | 0.162041 |
| N | 2.809367 | 1.846839 | 0.398779 | C | 3.360547 | -4.358179 | -1.234017 |
| C | 3.721663 | -1.257065 | 3.675713 | H | 3.043410 | -5.333067 | -0.873986 |
| H | 3.195608 | -1.418489 | 4.613417 | C | 4.263766 | -4.233792 | -2.286687 |
| C | 5.097811 | -1.400465 | 3.597958 | H | 4.670708 | -5.115425 | -2.776170 |
| H | 5.673322 | -1.671418 | 4.479933 | C | 4.650162 | -2.962869 | -2.698968 |
| C | 5.733440 | -1.198222 | 2.370006 | H | 5.368054 | -2.843512 | -3.506779 |
| H | 6.809649 | -1.303150 | 2.264291 | C | 4.124492 | -1.843495 | -2.055643 |
| C | 4.971393 | -0.854928 | 1.268381 | C | 4.537807 | -0.465105 | -2.313515 |
| H | 5.423969 | -0.687257 | 0.294863 | C | 5.500558 | -0.043455 | -3.232059 |

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|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | 5.969660 | -0.752301 | -3.909447 | H | -1.477965 | -0.277996 | -2.449503 |
| C | 5.869433 | 1.297764 | -3.253713 | H | -0.477985 | 0.751755 | -1.844556 |
| C | 5.308312 | 2.189640 | -2.340158 | H | 1.446005 | 1.202881 | -2.823033 |
| H | 5.637185 | 3.225352 | -2.322922 | O | 1.165692 | 1.396474 | -1.913604 |
| C | 4.344168 | 1.730887 | -1.444174 | H | 1.150802 | 2.394102 | -1.848220 |
| C | 3.731525 | 2.512223 | -0.363509 | H | 1.491884 | 4.660638 | -2.319100 |
| C | 4.097430 | 3.819697 | -0.052929 | O | 1.045921 | 4.095113 | -1.669974 |
| H | 4.844551 | 4.334584 | -0.651908 | H | 0.15237 | 4.464375 | -1.61783 |
| C | 3.531342 | 4.455229 | 1.047819 | H | 6.618977 | 1.644643 | -3.96101 |
| H | 3.827031 | 5.469497 | 1.306112 | O | -7.2837 | 1.045119 | -2.74274 |
| C | 2.606018 | 3.763035 | 1.823026 | C | -8.12554 | 0.031677 | -3.32659 |
| H | 2.162954 | 4.210412 | 2.709118 | H | -8.94709 | 0.576562 | -3.78845 |
| C | 2.275892 | 2.461654 | 1.468053 | H | -7.57258 | -0.52749 | -4.08862 |
| H | 1.577758 | 1.868731 | 2.055713 | H | -8.51076 | -0.63519 | -2.54813 |
| O | -1.427306 | 0.471197 | -1.833720 | | | | |

TS-3 A (4+ quartet)

E= -2887.596 09 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.086815 | -0.362060 | 0.097491 | H | 5.265032 | 0.233982 | 1.088140 |
| Ru | 2.452713 | 0.090933 | -0.110583 | C | -1.873756 | 0.498894 | 3.068428 |
| N | -2.919268 | -2.033482 | 0.949402 | H | -1.058193 | -0.222953 | 3.070184 |
| O | 0.661656 | -1.604222 | -2.307759 | C | -2.218429 | 1.209147 | 4.210201 |
| O | 0.850327 | -0.436319 | -1.904807 | H | -1.670076 | 1.044849 | 5.134085 |
| C | -4.232969 | -2.337974 | 0.919764 | C | -3.282233 | 2.106073 | 4.147932 |
| H | -4.871575 | -1.653460 | 0.366146 | H | -3.586361 | 2.670257 | 5.026582 |
| N | -0.397475 | -1.351112 | 0.752259 | C | -3.968966 | 2.255773 | 2.947752 |
| C | -4.745626 | -3.455452 | 1.557878 | H | -4.816116 | 2.933990 | 2.884457 |
| H | -5.810739 | -3.662917 | 1.504821 | C | -3.583363 | 1.515708 | 1.832851 |
| N | 0.922823 | -1.067838 | 0.865970 | C | -4.284313 | 1.543633 | 0.543312 |
| C | -3.876209 | -4.292875 | 2.258811 | C | -5.378476 | 2.324042 | 0.228131 |
| H | -4.251629 | -5.176122 | 2.769971 | H | -5.811321 | 3.028737 | 0.932840 |
| N | 3.493230 | -0.801500 | 1.393281 | C | -5.979316 | 2.201013 | -1.046001 |
| C | -2.523438 | -3.985127 | 2.292108 | C | -5.451100 | 1.266303 | -1.959654 |
| H | -1.819951 | -4.621653 | 2.823331 | H | -5.907560 | 1.129335 | -2.935297 |
| N | -2.523861 | 0.651854 | 1.900062 | C | -4.349019 | 0.508195 | -1.582942 |
| C | -2.058333 | -2.849418 | 1.627399 | C | -3.724457 | -0.563037 | -2.366859 |
| N | -3.779139 | 0.662024 | -0.362781 | C | -4.190508 | -1.012904 | -3.597705 |
| C | -0.681543 | -2.421888 | 1.578174 | H | -5.023474 | -0.509866 | -4.082160 |
| N | -2.670970 | -1.186103 | -1.746748 | C | -3.606977 | -2.128469 | -4.191972 |
| C | 0.466101 | -2.816577 | 2.243603 | H | -3.969280 | -2.490748 | -5.151170 |
| H | 0.576958 | -3.615772 | 2.966217 | C | -2.580692 | -2.788751 | -3.523881 |
| N | 3.401873 | -1.356776 | -1.335740 | H | -2.120905 | -3.683271 | -3.934735 |
| C | 1.448036 | -1.935190 | 1.775712 | C | -2.145805 | -2.293247 | -2.301263 |
| N | 3.981361 | 1.117753 | -0.845933 | H | -1.352377 | -2.775752 | -1.738551 |
| C | 2.844637 | -1.776733 | 2.101180 | C | 3.104993 | -2.661203 | -1.440304 |
| N | 2.262962 | 1.876069 | 0.971137 | H | 2.245325 | -2.997734 | -0.864755 |
| C | 3.509758 | -2.515483 | 3.080278 | C | 3.835825 | -3.536644 | -2.236095 |
| H | 2.970693 | -3.287371 | 3.624293 | H | 3.558917 | -4.586312 | -2.280592 |
| C | 4.845041 | -2.255605 | 3.355481 | C | 4.916104 | -3.043126 | -2.959115 |
| H | 5.373036 | -2.825189 | 4.116181 | H | 5.505993 | -3.698035 | -3.595733 |
| C | 5.491777 | -1.248340 | 2.641662 | C | 5.245332 | -1.695887 | -2.842033 |
| H | 6.533580 | -1.001535 | 2.826869 | H | 6.098982 | -1.294486 | -3.382406 |
| C | 4.790312 | -0.550542 | 1.670325 | C | 4.487503 | -0.870120 | -2.016046 |

| | | | | | | | |
|---|----------|----------|-----------|---|-----------|----------|-----------|
| C | 4.804079 | 0.537620 | -1.755557 | O | -1.121001 | 1.455935 | -0.614186 |
| C | 5.858809 | 1.272290 | -2.298365 | H | -1.697518 | 2.056208 | -1.112424 |
| H | 6.528991 | 0.826644 | -3.028810 | H | -0.220761 | 1.534332 | -1.036976 |
| C | 6.051848 | 2.587247 | -1.882721 | H | 1.338123 | 1.660209 | -2.654073 |
| C | 5.206267 | 3.153516 | -0.929976 | O | 1.283648 | 1.998486 | -1.746998 |
| H | 5.366521 | 4.175614 | -0.597255 | H | 1.599479 | 2.941989 | -1.796807 |
| C | 4.162265 | 2.390887 | -0.410516 | H | 2.696234 | 4.782367 | -2.801322 |
| C | 3.214143 | 2.804438 | 0.632049 | O | 2.278587 | 4.543684 | -1.959915 |
| C | 3.270766 | 4.035425 | 1.281977 | H | 1.75514 | 5.325742 | -1.73036 |
| H | 4.030552 | 4.761977 | 1.005452 | H | 6.873672 | 3.169104 | -2.29278 |
| C | 2.364720 | 4.326597 | 2.296001 | O | -7.01388 | 2.981668 | -1.26587 |
| H | 2.413728 | 5.279307 | 2.817846 | C | -7.71748 | 2.908888 | -2.52374 |
| C | 1.407578 | 3.374273 | 2.637389 | H | -8.51507 | 3.645519 | -2.44455 |
| H | 0.687409 | 3.556973 | 3.430670 | H | -7.04621 | 3.17087 | -3.34812 |
| C | 1.392451 | 2.167735 | 1.951901 | H | -8.14392 | 1.909794 | -2.65958 |
| H | 0.667676 | 1.386209 | 2.173006 | | | | |

TS-3 B (4+ doublet)

E= -2887.589 90 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.605483 | 0.044831 | -0.201517 | H | 5.680621 | -1.818899 | 3.425791 |
| Ru | 2.034076 | -0.303735 | 0.148471 | C | 4.122189 | -1.196777 | 2.099929 |
| N | -3.751665 | -0.473815 | 1.416886 | H | 4.788638 | -0.912053 | 1.290865 |
| O | -0.044920 | -2.008330 | -1.559263 | C | -2.227044 | 2.707862 | 1.330430 |
| O | 0.671971 | -0.982724 | -1.624952 | H | -1.554802 | 2.102960 | 1.935700 |
| C | -5.098131 | -0.397248 | 1.457996 | C | -2.454738 | 4.049266 | 1.603465 |
| H | -5.586362 | -0.027129 | 0.559966 | H | -1.958018 | 4.523492 | 2.445686 |
| N | -1.104672 | -0.576252 | 1.161488 | C | -3.345679 | 4.755784 | 0.800126 |
| C | -5.828792 | -0.764665 | 2.576653 | H | -3.557468 | 5.804989 | 0.992184 |
| H | -6.912184 | -0.684502 | 2.559213 | C | -3.989575 | 4.091191 | -0.238411 |
| N | 0.237426 | -0.714235 | 1.254285 | H | -4.711349 | 4.617712 | -0.857756 |
| C | -5.152829 | -1.231084 | 3.704522 | C | -3.731442 | 2.740941 | -0.461176 |
| H | -5.700227 | -1.527242 | 4.595992 | C | -4.426642 | 1.926758 | -1.462947 |
| N | 2.800784 | -1.020035 | 1.877227 | C | -5.379510 | 2.368857 | -2.379851 |
| C | -3.768313 | -1.311261 | 3.670171 | H | -5.662620 | 3.417028 | -2.428085 |
| H | -3.211646 | -1.671352 | 4.531862 | C | -5.972573 | 1.445584 | -3.238329 |
| N | -2.830105 | 2.062736 | 0.317534 | H | -6.717204 | 1.775070 | -3.958684 |
| C | -3.082751 | -0.928017 | 2.515711 | C | -5.617254 | 0.100826 | -3.172262 |
| N | -4.098664 | 0.613665 | -1.414843 | H | -6.081275 | -0.620321 | -3.840010 |
| C | -1.648981 | -0.972552 | 2.370691 | C | -4.660159 | -0.301908 | -2.240258 |
| N | -3.182708 | -1.782205 | -1.074836 | C | -4.177111 | -1.667366 | -2.013077 |
| C | -0.646787 | -1.356448 | 3.245913 | C | -4.696507 | -2.793317 | -2.646412 |
| H | -0.749591 | -1.712378 | 4.263402 | H | -5.483336 | -2.687873 | -3.389080 |
| N | 2.740473 | -2.161245 | -0.635156 | C | -4.220368 | -4.055935 | -2.307508 |
| C | 0.524090 | -1.177311 | 2.512257 | H | -4.626473 | -4.942007 | -2.789517 |
| N | 3.758056 | 0.205660 | -0.716756 | C | -3.231819 | -4.164322 | -1.333395 |
| C | 1.908319 | -1.370165 | 2.853824 | H | -2.844702 | -5.132630 | -1.028579 |
| N | 2.311354 | 1.647160 | 0.909288 | C | -2.740999 | -3.008355 | -0.741442 |
| C | 2.351927 | -1.884262 | 4.075204 | H | -1.959104 | -3.038047 | 0.014292 |
| H | 1.623018 | -2.155600 | 4.834901 | C | 2.208745 | -3.373087 | -0.419120 |
| C | 3.708905 | -2.052230 | 4.302302 | H | 1.313373 | -3.393403 | 0.198965 |
| H | 4.064620 | -2.453233 | 5.248195 | C | 2.753616 | -4.532576 | -0.958267 |
| C | 4.608403 | -1.703192 | 3.293174 | H | 2.294690 | -5.494691 | -0.748094 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|----------|-----------|
| C | 3.886778 | -4.431875 | -1.759638 | H | 1.341729 | 3.969419 | 3.152766 |
| H | 4.334877 | -5.318035 | -2.202592 | C | 1.601058 | 2.265945 | 1.867042 |
| C | 4.452416 | -3.179095 | -1.974064 | H | 0.745546 | 1.708907 | 2.245140 |
| H | 5.349585 | -3.080673 | -2.580123 | O | -1.456985 | 0.704833 | -1.941038 |
| C | 3.873443 | -2.053769 | -1.392890 | H | -1.429097 | 0.022876 | -2.632287 |
| C | 4.443584 | -0.703932 | -1.465069 | H | -0.503017 | 0.941472 | -1.788067 |
| C | 5.592323 | -0.334696 | -2.137298 | H | 1.563495 | 1.469389 | -2.537029 |
| H | 6.157068 | -1.034839 | -2.746927 | O | 1.145095 | 1.497686 | -1.661760 |
| C | 6.069025 | 0.988914 | -2.024543 | H | 1.061648 | 2.459956 | -1.426190 |
| C | 5.372135 | 1.897012 | -1.198621 | H | 0.996787 | 4.703564 | -0.527189 |
| H | 5.742816 | 2.908293 | -1.061886 | O | 0.486937 | 4.055342 | -1.03335 |
| C | 4.219425 | 1.470653 | -0.551086 | H | 0.157966 | 4.557666 | -1.79437 |
| C | 3.430870 | 2.262348 | 0.407345 | O | 7.165187 | 1.261779 | -2.70046 |
| C | 3.805454 | 3.526588 | 0.858188 | C | 7.752271 | 2.575354 | -2.62408 |
| H | 4.700525 | 4.002698 | 0.465790 | H | 8.057334 | 2.794501 | -1.59549 |
| C | 3.056808 | 4.164513 | 1.843380 | H | 8.628386 | 2.53202 | -3.26892 |
| H | 3.361272 | 5.139641 | 2.217189 | H | 7.049926 | 3.32736 | -2.9989 |
| C | 1.935592 | 3.520204 | 2.360867 | | | | |

TS-3 B (4+ quartet)

E= -2887.589 14 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.608359 | 0.053703 | -0.200284 | C | 4.595858 | -1.430334 | 3.443840 |
| Ru | 2.043754 | -0.262691 | 0.183175 | H | 5.668115 | -1.494415 | 3.607517 |
| N | -3.764758 | -0.544787 | 1.382724 | C | 4.119916 | -0.983672 | 2.221191 |
| O | -0.082085 | -2.017538 | -1.567150 | H | 4.795212 | -0.696724 | 1.420174 |
| O | 0.617690 | -0.984994 | -1.670712 | C | -2.288315 | 2.650487 | 1.451495 |
| C | -5.113789 | -0.514589 | 1.400615 | H | -1.619001 | 2.026818 | 2.040895 |
| H | -5.598907 | -0.141010 | 0.502301 | C | -2.530283 | 3.978474 | 1.774200 |
| N | -1.112124 | -0.569422 | 1.162873 | H | -2.047317 | 4.422407 | 2.640555 |
| C | -5.850049 | -0.929948 | 2.498144 | C | -3.417115 | 4.709497 | 0.988093 |
| H | -6.935090 | -0.885340 | 2.463838 | H | -3.639096 | 5.748680 | 1.219181 |
| N | 0.234136 | -0.637691 | 1.283868 | C | -4.041741 | 4.083025 | -0.085510 |
| C | -5.177191 | -1.397300 | 3.628130 | H | -4.758587 | 4.629229 | -0.693394 |
| H | -5.729381 | -1.729775 | 4.503756 | C | -3.767741 | 2.745724 | -0.360162 |
| N | 2.800158 | -0.883625 | 1.954477 | C | -4.438031 | 1.967806 | -1.406882 |
| C | -3.790757 | -1.431710 | 3.616531 | C | -5.382873 | 2.438769 | -2.317465 |
| H | -3.236934 | -1.791971 | 4.479950 | H | -5.676868 | 3.485053 | -2.324738 |
| N | -2.872683 | 2.044128 | 0.403940 | C | -5.954902 | 1.546576 | -3.222343 |
| C | -3.098329 | -1.001740 | 2.482199 | H | -6.692840 | 1.899186 | -3.938715 |
| N | -4.096055 | 0.657469 | -1.410645 | C | -5.589789 | 0.203056 | -3.205603 |
| C | -1.662801 | -0.995680 | 2.360394 | H | -6.040804 | -0.494846 | -3.906180 |
| N | -3.185170 | -1.743646 | -1.133777 | C | -4.641550 | -0.229251 | -2.277406 |
| C | -0.661687 | -1.335304 | 3.253705 | C | -4.160385 | -1.600461 | -2.087476 |
| H | -0.767788 | -1.699454 | 4.267937 | C | -4.669369 | -2.708011 | -2.760566 |
| N | 2.648261 | -2.182263 | -0.506457 | H | -5.440295 | -2.581202 | -3.516489 |
| C | 0.514262 | -1.096315 | 2.544971 | C | -4.204294 | -3.980263 | -2.442793 |
| N | 3.773861 | 0.133936 | -0.721968 | H | -4.602149 | -4.852614 | -2.955793 |
| C | 1.898555 | -1.236924 | 2.919862 | C | -3.239871 | -4.117322 | -1.448057 |
| N | 2.395912 | 1.724139 | 0.811837 | H | -2.864283 | -5.094653 | -1.158012 |
| C | 2.328792 | -1.693348 | 4.167594 | C | -2.757837 | -2.978583 | -0.816921 |
| H | 1.592113 | -1.969266 | 4.918122 | H | -1.992647 | -3.029323 | -0.045328 |
| C | 3.686011 | -1.792831 | 4.436877 | C | 2.065909 | -3.358890 | -0.230282 |
| H | 4.032033 | -2.149150 | 5.403962 | H | 1.172514 | -3.309435 | 0.389234 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|----------|-----------|
| C | 2.558156 | -4.566966 | -0.709412 | C | 2.105937 | 3.690807 | 2.156351 |
| H | 2.058959 | -5.496358 | -0.449653 | H | 1.534503 | 4.209261 | 2.921811 |
| C | 3.692632 | -4.557138 | -1.514799 | C | 1.717409 | 2.425818 | 1.734378 |
| H | 4.101636 | -5.483425 | -1.910977 | H | 0.840859 | 1.927445 | 2.144350 |
| C | 4.310332 | -3.342272 | -1.794094 | O | -1.442881 | 0.792979 | -1.888251 |
| H | 5.209045 | -3.313963 | -2.405049 | H | -1.458425 | 0.172332 | -2.635404 |
| C | 3.782716 | -2.164596 | -1.271208 | H | -0.474588 | 0.991144 | -1.754223 |
| C | 4.409827 | -0.845997 | -1.422857 | H | 1.571618 | 1.367930 | -2.607271 |
| C | 5.563641 | -0.564309 | -2.128465 | O | 1.181119 | 1.475627 | -1.725542 |
| H | 6.091873 | -1.321634 | -2.701264 | H | 1.155480 | 2.454026 | -1.550648 |
| C | 6.094610 | 0.743016 | -2.101228 | H | 1.204352 | 4.743507 | -0.767535 |
| C | 5.445154 | 1.727629 | -1.327212 | O | 0.665371 | 4.089382 | -1.23398 |
| H | 5.854870 | 2.730884 | -1.260713 | H | 0.327711 | 4.569701 | -2.00506 |
| C | 4.285186 | 1.387483 | -0.641842 | O | 7.192754 | 0.928867 | -2.80466 |
| C | 3.536051 | 2.264641 | 0.272237 | C | 7.831882 | 2.21938 | -2.81225 |
| C | 3.965384 | 3.535708 | 0.649548 | H | 8.155604 | 2.488117 | -1.80121 |
| H | 4.877177 | 3.950708 | 0.227301 | H | 8.699238 | 2.10276 | -3.45986 |
| C | 3.249774 | 4.258127 | 1.599991 | H | 7.15647 | 2.975596 | -3.22631 |
| H | 3.595940 | 5.239410 | 1.916987 | | | | |

Structures for complex 22³⁺

Min-1 (3+ unrestricted singlet)

E= -2748.788 55 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.514329 | -0.387825 | 0.077221 | C | 4.234705 | -2.497604 | 1.046231 |
| N | 3.687540 | 1.292785 | 0.966165 | C | 5.309292 | -3.385342 | 1.020580 |
| O | 1.376360 | -1.436868 | -0.760585 | H | 5.477088 | -4.082879 | 1.836539 |
| O | -1.007769 | -1.112813 | 0.782042 | C | 6.172261 | -3.367089 | -0.072752 |
| C | 4.940529 | 1.234132 | 1.449476 | H | 7.012738 | -4.055717 | -0.107812 |
| H | 5.375540 | 0.238147 | 1.531043 | C | 5.971715 | -2.468183 | -1.118572 |
| Ru | -1.838231 | 0.178879 | -0.075510 | H | 6.654690 | -2.454698 | -1.963412 |
| N | 1.148774 | 1.240982 | 0.222502 | C | 4.886786 | -1.595374 | -1.059256 |
| C | 5.655888 | 2.359468 | 1.830662 | C | 4.531682 | -0.570316 | -2.051534 |
| H | 6.663986 | 2.256647 | 2.221928 | C | 5.255864 | -0.350636 | -3.220975 |
| N | -0.107472 | 1.405434 | -0.212522 | H | 6.126798 | -0.959933 | -3.448049 |
| C | 5.051924 | 3.608801 | 1.698041 | C | 4.859739 | 0.653031 | -4.098840 |
| H | 5.584349 | 4.513437 | 1.981752 | H | 5.419893 | 0.831820 | -5.013401 |
| N | -2.539183 | 2.097712 | -0.980956 | C | 3.742076 | 1.421000 | -3.788136 |
| C | 3.755506 | 3.683868 | 1.206001 | H | 3.401340 | 2.215571 | -4.446111 |
| H | 3.254622 | 4.643709 | 1.104436 | C | 3.057679 | 1.156839 | -2.607543 |
| N | 2.302602 | -1.369944 | 1.928376 | H | 2.177463 | 1.728178 | -2.315335 |
| C | 3.087938 | 2.511206 | 0.851456 | C | -0.880016 | -0.875790 | -2.840768 |
| N | 4.058113 | -1.643481 | 0.010519 | H | 0.010494 | -0.298771 | -2.606861 |
| C | 1.718562 | 2.472226 | 0.370097 | C | -0.993600 | -1.627804 | -4.004938 |
| N | 3.433347 | 0.191515 | -1.757224 | H | -0.179980 | -1.633619 | -4.724511 |
| C | 0.799620 | 3.456214 | 0.000097 | C | -2.152089 | -2.364882 | -4.221177 |
| H | 0.941131 | 4.530092 | -0.003979 | H | -2.271193 | -2.964029 | -5.120484 |
| N | -1.851302 | -0.833808 | -1.920263 | C | -3.164283 | -2.329164 | -3.266241 |
| C | -0.341835 | 2.741116 | -0.366486 | H | -4.076626 | -2.901365 | -3.414146 |
| N | -3.642674 | -0.656655 | -0.025410 | C | -2.996751 | -1.559543 | -2.119706 |
| C | -1.652296 | 3.125631 | -0.857575 | C | -4.008427 | -1.450623 | -1.061821 |
| N | -2.607324 | 0.980943 | 1.744871 | C | -5.264128 | -2.053700 | -1.049614 |
| C | -1.999656 | 4.428709 | -1.215723 | H | -5.622859 | -2.703112 | -1.843635 |
| H | -1.274063 | 5.231264 | -1.106655 | C | -6.084123 | -1.802702 | 0.040689 |
| C | -3.267862 | 4.682773 | -1.721041 | C | -5.709266 | -0.979435 | 1.092917 |
| H | -3.552125 | 5.692398 | -2.007797 | H | -6.404886 | -0.820632 | 1.912468 |
| C | -4.166017 | 3.626001 | -1.863423 | C | -4.444603 | -0.399214 | 1.036674 |
| H | -5.163126 | 3.780209 | -2.265777 | C | -3.862477 | 0.515153 | 2.028498 |
| C | -3.761403 | 2.357107 | -1.477252 | C | -4.527832 | 0.914269 | 3.184799 |
| H | -4.432554 | 1.503183 | -1.567007 | H | -5.524586 | 0.538237 | 3.401010 |
| C | 1.361174 | -1.173410 | 2.860346 | C | -3.909187 | 1.798790 | 4.062813 |
| H | 0.635298 | -0.397225 | 2.633817 | H | -4.420371 | 2.117544 | 4.967904 |
| C | 1.300961 | -1.927937 | 4.026162 | C | -2.633762 | 2.266640 | 3.763876 |
| H | 0.519016 | -1.734381 | 4.754765 | H | -2.117247 | 2.959285 | 4.422578 |
| C | 2.247981 | -2.924618 | 4.231901 | C | -2.018057 | 1.832424 | 2.595030 |
| H | 2.228170 | -3.533535 | 5.132324 | H | -1.020368 | 2.166847 | 2.313921 |
| C | 3.226038 | -3.137519 | 3.265234 | N | -7.431228 | -2.438633 | 0.080645 |
| H | 3.972016 | -3.915420 | 3.405658 | O | -7.716087 | -3.153794 | -0.867459 |
| C | 3.239304 | -2.352741 | 2.116464 | O | -8.117332 | -2.181049 | 1.057825 |

Min-1 (3+ quintet)

E= -2748.788 61 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.521182 | -0.391859 | 0.067006 | C | 4.251269 | -2.519077 | 0.978667 |
| N | 3.678780 | 1.268171 | 1.011368 | C | 5.330986 | -3.399619 | 0.930556 |
| O | 1.396696 | -1.421600 | -0.814145 | H | 5.498821 | -4.121666 | 1.724885 |
| O | -1.018844 | -1.129661 | 0.776885 | C | 6.199373 | -3.342132 | -0.157079 |
| C | 4.927739 | 1.202129 | 1.504057 | H | 7.043917 | -4.024668 | -0.209461 |
| H | 5.364777 | 0.205719 | 1.567420 | C | 5.999221 | -2.411455 | -1.174874 |
| Ru | -1.842505 | 0.172358 | -0.073266 | H | 6.686382 | -2.366856 | -2.015288 |
| N | 1.145315 | 1.225477 | 0.249528 | C | 4.908769 | -1.547271 | -1.093828 |
| C | 5.636690 | 2.320753 | 1.915755 | C | 4.551840 | -0.493995 | -2.055221 |
| H | 6.641606 | 2.211976 | 2.313556 | C | 5.279179 | -0.232348 | -3.214029 |
| N | -0.107287 | 1.396159 | -0.194745 | H | 6.155983 | -0.827470 | -3.455771 |
| C | 5.030676 | 3.571246 | 1.804679 | C | 4.878169 | 0.794692 | -4.062379 |
| H | 5.558289 | 4.470831 | 2.112427 | H | 5.440677 | 1.006044 | -4.968506 |
| N | -2.535877 | 2.100582 | -0.961901 | C | 3.752382 | 1.542982 | -3.733648 |
| C | 3.738359 | 3.653720 | 1.303164 | H | 3.407176 | 2.353792 | -4.369068 |
| H | 3.235768 | 4.614274 | 1.218038 | C | 3.065523 | 1.237173 | -2.564652 |
| N | 2.308750 | -1.430670 | 1.887332 | H | 2.178630 | 1.790834 | -2.259244 |
| C | 3.076835 | 2.487235 | 0.918231 | C | -0.892812 | -0.860441 | -2.850029 |
| N | 4.074590 | -1.634202 | -0.030680 | H | 0.001392 | -0.291444 | -2.610924 |
| C | 1.711453 | 2.454878 | 0.425284 | C | -1.011923 | -1.599733 | -4.021797 |
| N | 3.446539 | 0.250044 | -1.742449 | H | -0.199077 | -1.602303 | -4.742249 |
| C | 0.794589 | 3.444292 | 0.064677 | C | -2.174316 | -2.328781 | -4.244026 |
| H | 0.934367 | 4.518279 | 0.081848 | H | -2.297579 | -2.918149 | -5.149212 |
| N | -1.862516 | -0.823204 | -1.927564 | C | -3.185030 | -2.297695 | -3.287362 |
| C | -0.342126 | 2.734389 | -0.325899 | H | -4.100568 | -2.863551 | -3.439870 |
| N | -3.651657 | -0.654118 | -0.030179 | C | -3.012040 | -1.540808 | -2.133205 |
| C | -1.649505 | 3.126392 | -0.819193 | C | -4.022330 | -1.436366 | -1.073713 |
| N | -2.607825 | 0.963030 | 1.753743 | C | -5.281899 | -2.031519 | -1.067122 |
| C | -1.994340 | 4.434438 | -1.161381 | H | -5.644493 | -2.671407 | -1.867087 |
| H | -1.269190 | 5.235150 | -1.036845 | C | -6.100795 | -1.784550 | 0.024852 |
| C | -3.259153 | 4.695683 | -1.671419 | C | -5.721145 | -0.972639 | 1.084139 |
| H | -3.541355 | 5.709147 | -1.946419 | H | -6.416293 | -0.815844 | 1.904465 |
| C | -4.156573 | 3.641135 | -1.834054 | C | -4.452627 | -0.400404 | 1.033523 |
| H | -5.150989 | 3.801137 | -2.240791 | C | -3.865205 | 0.501317 | 2.033703 |
| C | -3.754894 | 2.367003 | -1.462436 | C | -4.527232 | 0.892067 | 3.194724 |
| H | -4.425738 | 1.514594 | -1.567701 | H | -5.525908 | 0.519480 | 3.408000 |
| C | 1.364230 | -1.267273 | 2.822886 | C | -3.902483 | 1.763416 | 4.081592 |
| H | 0.633615 | -0.489527 | 2.617972 | H | -4.410972 | 2.075479 | 4.990522 |
| C | 1.306031 | -2.056776 | 3.965473 | C | -2.624372 | 2.226388 | 3.786761 |
| H | 0.521123 | -1.889507 | 4.697389 | H | -2.102899 | 2.908326 | 4.452678 |
| C | 2.258203 | -3.053789 | 4.143662 | C | -2.012308 | 1.801219 | 2.612655 |
| H | 2.239714 | -3.689676 | 5.025265 | H | -1.012889 | 2.132633 | 2.334263 |
| C | 3.239740 | -3.231670 | 3.173611 | N | -7.452296 | -2.411588 | 0.058565 |
| H | 3.990155 | -4.008801 | 3.292795 | O | -7.741606 | -3.116353 | -0.895952 |
| C | 3.251030 | -2.412848 | 2.048919 | O | -8.137109 | -2.157972 | 1.037695 |

Min-1 (4+ quartet)

E= -2748.291 22 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|----|-----------|-----------|-----------|
| Ru | -2.473604 | -0.421810 | 0.014968 | H | -5.364917 | -0.146786 | -1.455843 |
| N | -3.695664 | 1.039665 | -1.134472 | Ru | 1.820820 | 0.217476 | 0.056039 |
| O | -1.254720 | -1.241152 | 0.912444 | N | -1.158908 | 1.187912 | -0.442959 |
| O | 0.921184 | -1.173855 | -0.429573 | C | -5.697926 | 1.863938 | -2.170197 |
| C | -4.952569 | 0.853605 | -1.581338 | H | -6.707033 | 1.661802 | -2.518599 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| N | 0.094148 | 1.450247 | -0.041863 | C | -5.790539 | -2.420283 | 1.676554 |
| C | -5.125217 | 3.128885 | -2.299137 | H | -6.445324 | -2.298817 | 2.535391 |
| H | -5.683674 | 3.945263 | -2.751510 | C | -4.775047 | -1.503888 | 1.411748 |
| N | 2.533887 | 2.274642 | 0.511816 | C | -4.468848 | -0.285572 | 2.172987 |
| C | -3.825010 | 3.332721 | -1.849317 | C | -5.190306 | 0.131156 | 3.287951 |
| H | -3.350084 | 4.305631 | -1.951376 | H | -6.017121 | -0.467993 | 3.660825 |
| N | -2.343978 | -1.626016 | -1.694974 | C | -4.854922 | 1.325542 | 3.920662 |
| C | -3.124807 | 2.273135 | -1.275986 | H | -5.418480 | 1.660691 | 4.788543 |
| N | -3.979539 | -1.696519 | 0.331707 | C | -3.798370 | 2.083611 | 3.423303 |
| C | -1.747771 | 2.358296 | -0.817573 | H | -3.510954 | 3.024069 | 3.885664 |
| N | -3.425203 | 0.467251 | 1.698928 | C | -3.108033 | 1.620223 | 2.310097 |
| C | -0.838018 | 3.406015 | -0.651228 | H | -2.275578 | 2.174826 | 1.879724 |
| H | -0.992225 | 4.458280 | -0.857755 | C | 1.031376 | 0.017926 | 3.051001 |
| N | 1.927983 | -0.269197 | 2.095677 | H | 0.165730 | 0.589843 | 2.725711 |
| C | 0.315469 | 2.789603 | -0.158917 | C | 1.193037 | -0.400461 | 4.366163 |
| N | 3.622411 | -0.646439 | 0.146440 | H | 0.444842 | -0.143988 | 5.110825 |
| C | 1.637020 | 3.263500 | 0.220073 | C | 2.318807 | -1.146069 | 4.703893 |
| N | 2.584625 | 0.635582 | -1.890611 | H | 2.473086 | -1.488912 | 5.724431 |
| C | 1.985571 | 4.608802 | 0.319757 | C | 3.255356 | -1.444141 | 3.717199 |
| H | 1.254654 | 5.378253 | 0.082592 | H | 4.144836 | -2.018565 | 3.964013 |
| C | 3.267113 | 4.953929 | 0.736083 | C | 3.049078 | -0.994584 | 2.417049 |
| H | 3.553634 | 5.999693 | 0.821032 | C | 3.999287 | -1.208044 | 1.322014 |
| C | 4.174192 | 3.942643 | 1.050506 | C | 5.219949 | -1.876364 | 1.397097 |
| H | 5.180872 | 4.171035 | 1.389662 | H | 5.588812 | -2.355019 | 2.301510 |
| C | 3.768891 | 2.622551 | 0.921188 | C | 5.994019 | -1.923789 | 0.247121 |
| H | 4.448199 | 1.802812 | 1.151707 | C | 5.615117 | -1.322995 | -0.945558 |
| C | -1.499779 | -1.478519 | -2.727068 | H | 6.281198 | -1.388193 | -1.802929 |
| H | -0.834634 | -0.620410 | -2.670259 | C | 4.386891 | -0.666518 | -0.973237 |
| C | -1.469193 | -2.373532 | -3.788601 | C | 3.811045 | 0.062792 | -2.109934 |
| H | -0.771962 | -2.218595 | -4.607070 | C | 4.456730 | 0.213696 | -3.333681 |
| C | -2.338760 | -3.460561 | -3.778849 | H | 5.429580 | -0.242278 | -3.500273 |
| H | -2.337898 | -4.179918 | -4.594536 | C | 3.854046 | 0.961450 | -4.342720 |
| C | -3.220218 | -3.615401 | -2.712091 | H | 4.354064 | 1.090362 | -5.300052 |
| H | -3.911422 | -4.454200 | -2.692934 | C | 2.612393 | 1.543938 | -4.104541 |
| C | -3.216593 | -2.686905 | -1.675951 | H | 2.113367 | 2.139535 | -4.864265 |
| C | -4.138025 | -2.726134 | -0.536587 | C | 2.010306 | 1.357439 | -2.865461 |
| C | -5.143462 | -3.663150 | -0.300998 | H | 1.040423 | 1.792447 | -2.628618 |
| H | -5.295953 | -4.501942 | -0.975053 | N | 7.306301 | -2.645394 | 0.298093 |
| C | -5.960399 | -3.507159 | 0.817825 | O | 7.593466 | -3.142370 | 1.373478 |
| H | -6.745951 | -4.232741 | 1.016661 | O | 7.942403 | -2.657077 | -0.741827 |

TS-1 (3+ unrestricted singlet)

E= -2748.765 75 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.271816 | -0.287042 | -0.192766 | N | 0.016265 | 1.689367 | 0.446497 |
| N | -3.798300 | 1.297216 | -0.273707 | C | -5.592424 | 3.429702 | -0.217077 |
| O | -0.769456 | -1.242610 | 0.256885 | H | -6.291996 | 4.261804 | -0.195208 |
| O | 0.597001 | -0.784249 | -0.678360 | N | 2.454670 | 2.332960 | 0.987694 |
| C | -5.099992 | 1.114926 | -0.559720 | C | -4.252235 | 3.633532 | 0.083342 |
| H | -5.395125 | 0.096370 | -0.809486 | H | -3.883806 | 4.623527 | 0.341551 |
| Ru | 1.647057 | 0.441140 | 0.207855 | N | -2.097929 | -0.421682 | -2.287754 |
| N | -1.264387 | 1.479666 | 0.177486 | C | -3.367293 | 2.556024 | 0.049252 |
| C | -6.026218 | 2.146867 | -0.547731 | N | -3.388743 | -1.899099 | -0.566570 |
| H | -7.065220 | 1.945407 | -0.792202 | C | -1.947190 | 2.646851 | 0.331470 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| N | -3.048089 | -0.711077 | 1.732235 | H | -5.034574 | -3.163299 | 2.952437 |
| C | -1.049754 | 3.645429 | 0.729895 | C | -4.267846 | -1.514574 | 4.102576 |
| H | -1.264565 | 4.685844 | 0.940700 | H | -4.745012 | -1.830660 | 5.026897 |
| N | 1.708815 | -0.509632 | 2.086752 | C | -3.505952 | -0.350310 | 4.056134 |
| C | 0.188342 | 2.994610 | 0.794012 | H | -3.375998 | 0.275631 | 4.934972 |
| N | 3.305960 | -0.648263 | 0.030324 | C | -2.915239 | 0.013494 | 2.852827 |
| C | 1.553156 | 3.353887 | 1.128768 | H | -2.317224 | 0.919280 | 2.758547 |
| N | 2.370749 | 1.092945 | -1.671761 | C | 0.863796 | -0.350038 | 3.114221 |
| C | 1.956986 | 4.615105 | 1.566960 | H | 0.066831 | 0.372247 | 2.951734 |
| H | 1.220807 | 5.408504 | 1.671988 | C | 0.994460 | -1.051783 | 4.305315 |
| C | 3.293611 | 4.841207 | 1.867256 | H | 0.290441 | -0.881591 | 5.115342 |
| H | 3.620525 | 5.819704 | 2.210695 | C | 2.043184 | -1.956656 | 4.438384 |
| C | 4.207493 | 3.798300 | 1.723628 | H | 2.178722 | -2.520565 | 5.357959 |
| H | 5.261271 | 3.932674 | 1.950314 | C | 2.928474 | -2.125775 | 3.378150 |
| C | 3.746632 | 2.568288 | 1.279587 | H | 3.758555 | -2.822293 | 3.464666 |
| H | 4.425820 | 1.726277 | 1.150559 | C | 2.748796 | -1.392232 | 2.209050 |
| C | -1.439683 | 0.406241 | -3.110355 | C | 3.642622 | -1.481653 | 1.046293 |
| H | -0.957899 | 1.253349 | -2.627116 | C | 4.753812 | -2.308746 | 0.918105 |
| C | -1.376503 | 0.203623 | -4.482233 | H | 5.076860 | -3.000722 | 1.691210 |
| H | -0.838345 | 0.907690 | -5.111081 | C | 5.469394 | -2.241382 | -0.270407 |
| C | -2.022156 | -0.903085 | -5.025166 | C | 5.125540 | -1.387627 | -1.306676 |
| H | -1.997432 | -1.092124 | -6.095525 | H | 5.729211 | -1.383126 | -2.210263 |
| C | -2.711636 | -1.765666 | -4.178980 | C | 4.007077 | -0.575173 | -1.127805 |
| H | -3.227096 | -2.631939 | -4.585435 | C | 3.496211 | 0.422915 | -2.072117 |
| C | -2.743037 | -1.511089 | -2.810723 | C | 4.124590 | 0.734275 | -3.276686 |
| C | -3.462456 | -2.350849 | -1.841279 | H | 5.017437 | 0.194376 | -3.581865 |
| C | -4.184562 | -3.509412 | -2.116098 | C | 3.614920 | 1.750664 | -4.076064 |
| H | -4.260740 | -3.894397 | -3.129350 | H | 4.101875 | 2.005911 | -5.013973 |
| C | -4.808408 | -4.180291 | -1.064463 | C | 2.486487 | 2.444275 | -3.646848 |
| H | -5.370990 | -5.089045 | -1.263004 | H | 2.069479 | 3.260712 | -4.230468 |
| C | -4.717944 | -3.693633 | 0.236745 | C | 1.896990 | 2.083907 | -2.441597 |
| H | -5.207932 | -4.220264 | 1.051181 | H | 1.018129 | 2.599651 | -2.056335 |
| C | -3.990195 | -2.526740 | 0.471744 | O | 7.248459 | -3.031722 | -1.503242 |
| C | -3.817400 | -1.844073 | 1.759688 | N | 6.656144 | -3.124291 | -0.438775 |
| C | -4.426500 | -2.262397 | 2.941705 | O | 6.920695 | -3.855374 | 0.503620 |

TS-1 (3+ triplet)

E= -2748.764 44 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.273753 | -0.269521 | -0.211858 | H | -3.889236 | 4.572967 | 0.748997 |
| N | -3.808639 | 1.311967 | -0.152902 | N | -2.071541 | -0.205899 | -2.303573 |
| O | -0.800971 | -1.299447 | 0.126194 | C | -3.374999 | 2.538633 | 0.274332 |
| O | 0.642912 | -0.777422 | -0.715763 | N | -3.387671 | -1.838462 | -0.747809 |
| C | -5.113056 | 1.154437 | -0.441772 | C | -1.952345 | 2.608669 | 0.548973 |
| H | -5.409907 | 0.161162 | -0.776814 | N | -3.081809 | -0.870281 | 1.655553 |
| Ru | 1.646964 | 0.428285 | 0.232866 | C | -1.049834 | 3.582826 | 0.992957 |
| N | -1.268801 | 1.456740 | 0.304585 | H | -1.264031 | 4.605461 | 1.278256 |
| C | -6.039096 | 2.180595 | -0.332745 | N | 1.681330 | -0.626204 | 2.052728 |
| H | -7.080205 | 2.000678 | -0.584963 | C | 0.192256 | 2.936930 | 0.984187 |
| N | 0.018542 | 1.657550 | 0.549633 | N | 3.305280 | -0.653738 | 0.011582 |
| C | -5.602226 | 3.430554 | 0.103748 | C | 1.558742 | 3.279207 | 1.329202 |
| H | -6.301611 | 4.257101 | 0.203818 | N | 2.401508 | 1.189682 | -1.597040 |
| N | 2.462403 | 2.271019 | 1.123552 | C | 1.961219 | 4.514023 | 1.838732 |
| C | -4.259647 | 3.608791 | 0.408957 | H | 1.223457 | 5.297616 | 1.994214 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.298757 | 4.726374 | 2.144238 | C | -2.970088 | -0.251805 | 2.840257 |
| H | 3.624772 | 5.684110 | 2.542715 | H | -2.375998 | 0.661240 | 2.839294 |
| C | 4.215195 | 3.696675 | 1.934239 | C | 0.820495 | -0.523827 | 3.074183 |
| H | 5.269751 | 3.821252 | 2.162904 | H | 0.030506 | 0.212487 | 2.942658 |
| C | 3.755443 | 2.493649 | 1.421197 | C | 0.929609 | -1.296951 | 4.222541 |
| H | 4.436041 | 1.662706 | 1.238931 | H | 0.214560 | -1.172489 | 5.031191 |
| C | -1.395517 | 0.691943 | -3.032885 | C | 1.972473 | -2.213483 | 4.315953 |
| H | -0.928754 | 1.493594 | -2.464523 | H | 2.091645 | -2.832302 | 5.201915 |
| C | -1.299201 | 0.611684 | -4.415382 | C | 2.873006 | -2.324304 | 3.260631 |
| H | -0.746253 | 1.368004 | -4.965849 | H | 3.697714 | -3.030176 | 3.317555 |
| C | -1.930929 | -0.442108 | -5.068719 | C | 2.714752 | -1.521434 | 2.135008 |
| H | -1.881262 | -0.535438 | -6.150802 | C | 3.623252 | -1.547990 | 0.980498 |
| C | -2.638556 | -1.376608 | -4.319067 | C | 4.729833 | -2.374962 | 0.817528 |
| H | -3.142339 | -2.203132 | -4.813398 | H | 5.038301 | -3.113386 | 1.552599 |
| C | -2.701744 | -1.245782 | -2.934725 | C | 5.460126 | -2.244825 | -0.356830 |
| C | -3.437733 | -2.170759 | -2.059563 | C | 5.133675 | -1.330661 | -1.345930 |
| C | -4.151576 | -3.299815 | -2.452985 | H | 5.747403 | -1.279639 | -2.241320 |
| H | -4.209900 | -3.589104 | -3.498757 | C | 4.018629 | -0.521543 | -1.132969 |
| C | -4.790261 | -4.066679 | -1.478587 | C | 3.525062 | 0.532504 | -2.023770 |
| H | -5.346935 | -4.953764 | -1.769858 | C | 4.168763 | 0.905333 | -3.202542 |
| C | -4.720735 | -3.703830 | -0.136482 | H | 5.059627 | 0.374751 | -3.529050 |
| H | -5.220610 | -4.305872 | 0.617456 | C | 3.677119 | 1.970034 | -3.948145 |
| C | -4.000210 | -2.562482 | 0.217642 | H | 4.175704 | 2.272728 | -4.865613 |
| C | -3.847406 | -2.002837 | 1.565828 | C | 2.551976 | 2.650878 | -3.490332 |
| C | -4.471975 | -2.530766 | 2.694726 | H | 2.149586 | 3.504176 | -4.029901 |
| H | -5.076686 | -3.430259 | 2.612552 | C | 1.946874 | 2.228894 | -2.313317 |
| C | -4.333520 | -1.893595 | 3.922200 | H | 1.070765 | 2.732887 | -1.907114 |
| H | -4.822470 | -2.295807 | 4.806035 | O | 7.250976 | -2.972918 | -1.610495 |
| C | -3.577133 | -0.727094 | 3.995424 | N | 6.642165 | -3.125545 | -0.562325 |
| H | -3.463305 | -0.184862 | 4.930300 | O | 6.887364 | -3.915342 | 0.337030 |

TS-1 (4+ doublet)

E= -2748.268 56 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.279789 | 0.309654 | 0.159930 | N | -3.024524 | 0.746567 | -1.784785 |
| N | -3.796582 | -1.241917 | 0.163499 | C | -1.033138 | -3.657077 | -0.619532 |
| O | -0.765645 | 1.200951 | -0.327867 | H | -1.252080 | -4.701916 | -0.803344 |
| O | 0.546804 | 0.793524 | 0.585347 | N | 1.842524 | 0.272690 | -2.111284 |
| C | -5.112476 | -1.029938 | 0.353317 | C | 0.212840 | -3.025156 | -0.648065 |
| H | -5.410062 | -0.002881 | 0.558531 | N | 3.334738 | 0.659958 | -0.010247 |
| Ru | 1.677094 | -0.470706 | -0.152126 | C | 1.585569 | -3.408525 | -0.911074 |
| N | -1.247021 | -1.464493 | -0.150140 | N | 2.393264 | -0.970555 | 1.785548 |
| C | -6.049556 | -2.052965 | 0.308590 | C | 1.991947 | -4.688532 | -1.287547 |
| H | -7.099000 | -1.830289 | 0.481977 | H | 1.254155 | -5.481225 | -1.387219 |
| N | 0.040499 | -1.698984 | -0.351054 | C | 3.336607 | -4.935344 | -1.537811 |
| C | -5.617241 | -3.352928 | 0.044605 | H | 3.667277 | -5.928588 | -1.832607 |
| H | -6.328686 | -4.174337 | 0.000147 | C | 4.252621 | -3.892251 | -1.406755 |
| N | 2.493261 | -2.387317 | -0.777245 | H | 5.312646 | -4.043326 | -1.592348 |
| C | -4.263281 | -3.584766 | -0.162015 | C | 3.791861 | -2.639677 | -1.023785 |
| H | -3.896762 | -4.586834 | -0.372066 | H | 4.476400 | -1.801462 | -0.903291 |
| N | -2.308953 | 0.374607 | 2.255104 | C | -1.806947 | -0.545462 | 3.097414 |
| C | -3.364853 | -2.519008 | -0.099731 | H | -1.373717 | -1.425761 | 2.627201 |
| N | -3.382893 | 1.953103 | 0.494553 | C | -1.845777 | -0.389205 | 4.475168 |
| C | -1.935988 | -2.634697 | -0.299255 | H | -1.438467 | -1.162976 | 5.120337 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|----------|-----------|-----------|
| C | -2.429314 | 0.759989 | 5.004260 | H | 0.638674 | 0.209749 | -5.253964 |
| H | -2.482976 | 0.910960 | 6.080060 | C | 2.287002 | 1.448606 | -4.592570 |
| C | -2.964096 | 1.710251 | 4.138090 | H | 2.466626 | 1.905615 | -5.563006 |
| H | -3.437597 | 2.604371 | 4.535637 | C | 3.087939 | 1.782629 | -3.503465 |
| C | -2.905726 | 1.501175 | 2.763934 | H | 3.896950 | 2.499342 | -3.620888 |
| C | -3.498627 | 2.401820 | 1.768402 | C | 2.858005 | 1.181217 | -2.269970 |
| C | -4.165260 | 3.598524 | 2.017135 | C | 3.684433 | 1.415848 | -1.080757 |
| H | -4.273001 | 3.980477 | 3.028903 | C | 4.762763 | 2.291144 | -0.981534 |
| C | -4.699426 | 4.309185 | 0.940984 | H | 5.097666 | 2.927326 | -1.797614 |
| H | -5.218635 | 5.248141 | 1.118731 | C | 5.433686 | 2.345263 | 0.232195 |
| C | -4.583427 | 3.817134 | -0.356675 | C | 5.084934 | 1.560386 | 1.320510 |
| H | -5.014149 | 4.368319 | -1.188407 | H | 5.661256 | 1.646033 | 2.238923 |
| C | -3.911368 | 2.612041 | -0.565528 | C | 4.000027 | 0.697829 | 1.170345 |
| C | -3.735937 | 1.915926 | -1.843127 | C | 3.489073 | -0.243592 | 2.170476 |
| C | -4.297002 | 2.345657 | -3.044370 | C | 4.086026 | -0.455061 | 3.410972 |
| H | -4.862251 | 3.273463 | -3.082391 | H | 4.956637 | 0.125949 | 3.705335 |
| C | -4.151644 | 1.570711 | -4.190425 | C | 3.575643 | -1.430109 | 4.263217 |
| H | -4.595012 | 1.893834 | -5.129486 | H | 4.041734 | -1.610607 | 5.229165 |
| C | -3.448522 | 0.371221 | -4.110532 | C | 2.476623 | -2.179186 | 3.851160 |
| H | -3.330628 | -0.272977 | -4.977968 | H | 2.063065 | -2.965421 | 4.477362 |
| C | -2.899637 | -0.003338 | -2.890320 | C | 1.915370 | -1.918527 | 2.606900 |
| H | -2.343610 | -0.932120 | -2.773702 | H | 1.060758 | -2.481682 | 2.235670 |
| C | 1.081813 | -0.053119 | -3.169025 | O | 7.134164 | 3.299162 | 1.460262 |
| H | 0.309211 | -0.795911 | -2.981340 | N | 6.588210 | 3.288348 | 0.370159 |
| C | 1.270654 | 0.511936 | -4.423162 | O | 6.855595 | 3.944718 | -0.622034 |

TS-1 (4+ quartet)

E= -2748.268 52 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.260703 | -0.322876 | -0.112455 | N | 3.322349 | -0.625530 | 0.095957 |
| N | -3.777045 | 1.178614 | -0.559179 | C | 1.549513 | 3.485882 | 0.477774 |
| O | -0.710552 | -1.161666 | 0.495521 | N | 2.314113 | 0.771523 | -1.866890 |
| O | 0.543581 | -0.921440 | -0.460144 | C | 1.952681 | 4.805428 | 0.681526 |
| C | -5.069564 | 0.928820 | -0.837584 | H | 1.220275 | 5.607538 | 0.627722 |
| H | -5.365327 | -0.119013 | -0.852957 | C | 3.286299 | 5.079478 | 0.960470 |
| Ru | 1.639528 | 0.468767 | 0.127667 | H | 3.614530 | 6.103362 | 1.123863 |
| N | -1.252453 | 1.459315 | -0.142739 | C | 4.194004 | 4.023269 | 1.030215 |
| C | -5.990580 | 1.937062 | -1.089840 | H | 5.245028 | 4.194154 | 1.247279 |
| H | -7.023535 | 1.680674 | -1.309298 | C | 3.737879 | 2.730408 | 0.808514 |
| N | 0.013772 | 1.718763 | 0.144774 | H | 4.418463 | 1.881270 | 0.845679 |
| C | -5.565715 | 3.264436 | -1.047342 | C | -1.624120 | -0.265960 | -3.150152 |
| H | -6.264980 | 4.075882 | -1.235349 | H | -1.160356 | 0.685122 | -2.897912 |
| N | 2.450565 | 2.450002 | 0.535308 | C | -1.629256 | -0.760814 | -4.447254 |
| C | -4.233037 | 3.537543 | -0.763131 | H | -1.163528 | -0.190942 | -5.246740 |
| H | -3.870955 | 4.562449 | -0.729283 | C | -2.249374 | -1.982045 | -4.697012 |
| N | -2.193998 | -0.922289 | -2.127060 | H | -2.275772 | -2.397412 | -5.701801 |
| C | -3.350383 | 2.483907 | -0.527112 | C | -2.853985 | -2.662472 | -3.643064 |
| N | -3.395717 | -1.979731 | -0.070270 | H | -3.356972 | -3.609029 | -3.823879 |
| C | -1.936291 | 2.640211 | -0.250567 | C | -2.825272 | -2.117569 | -2.363005 |
| N | -3.021715 | -0.279615 | 1.871910 | C | -3.486608 | -2.723455 | -1.200599 |
| C | -1.044931 | 3.696407 | -0.032094 | C | -4.187773 | -3.926639 | -1.172453 |
| H | -1.258784 | 4.758269 | -0.047055 | H | -4.276358 | -4.545087 | -2.061684 |
| N | 1.807577 | -0.084023 | 2.151987 | C | -4.781028 | -4.333352 | 0.022986 |
| C | 0.186169 | 3.073313 | 0.210954 | H | -5.329988 | -5.271567 | 0.060584 |

| | | | | | | | |
|---|-----------|-----------|----------|---|----------|-----------|-----------|
| C | -4.682804 | -3.543186 | 1.167178 | C | 2.851370 | -0.940406 | 2.396517 |
| H | -5.155446 | -3.863721 | 2.091762 | C | 3.691638 | -1.260955 | 1.236082 |
| C | -3.971567 | -2.345833 | 1.100754 | C | 4.798246 | -2.105795 | 1.222116 |
| C | -3.787194 | -1.373158 | 2.183474 | H | 5.151161 | -2.650097 | 2.095110 |
| C | -4.376394 | -1.493122 | 3.439968 | C | 5.475112 | -2.253182 | 0.019129 |
| H | -4.985134 | -2.361811 | 3.677804 | C | 5.103259 | -1.592140 | -1.141782 |
| C | -4.200531 | -0.486204 | 4.384516 | H | 5.684343 | -1.749949 | -2.047499 |
| H | -4.666196 | -0.567343 | 5.364055 | C | 3.988587 | -0.757490 | -1.077474 |
| C | -3.437622 | 0.629228 | 4.048908 | C | 3.441541 | 0.053247 | -2.170535 |
| H | -3.294272 | 1.447288 | 4.750015 | C | 4.031820 | 0.148311 | -3.428578 |
| C | -2.867328 | 0.693960 | 2.783626 | H | 4.927855 | -0.423395 | -3.657529 |
| H | -2.270644 | 1.549500 | 2.469957 | C | 3.480818 | 0.995294 | -4.386057 |
| C | 1.030921 | 0.310103 | 3.172865 | H | 3.940737 | 1.084402 | -5.367622 |
| H | 0.235050 | 1.005310 | 2.914973 | C | 2.347687 | 1.735718 | -4.060060 |
| C | 1.230887 | -0.130601 | 4.474898 | H | 1.899771 | 2.424530 | -4.771606 |
| H | 0.582932 | 0.223366 | 5.272224 | C | 1.796762 | 1.595267 | -2.791633 |
| C | 2.276093 | -1.013156 | 4.732317 | H | 0.916461 | 2.159814 | -2.486504 |
| H | 2.464152 | -1.374550 | 5.740734 | O | 7.214336 | -3.260883 | -1.108534 |
| C | 3.094186 | -1.418655 | 3.680146 | N | 6.662446 | -3.165137 | -0.025676 |
| H | 3.924746 | -2.095420 | 3.865052 | O | 6.946446 | -3.713840 | 1.025416 |

Min-2 (3+ unrestricted singlet)

E= -2748.774 93 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.270385 | -0.302598 | -0.103691 | C | 3.305266 | 5.133109 | 0.814106 |
| N | -3.811549 | 1.191403 | -0.273641 | H | 3.642364 | 6.156286 | 0.961163 |
| O | -0.572423 | -1.093613 | 0.421561 | C | 4.219950 | 4.081288 | 0.791010 |
| O | 0.421762 | -0.849060 | -0.510330 | H | 5.284994 | 4.252634 | 0.918309 |
| C | -5.120469 | 0.920860 | -0.430804 | C | 3.747651 | 2.792261 | 0.597741 |
| H | -5.386287 | -0.133758 | -0.485755 | H | 4.425817 | 1.940717 | 0.568306 |
| Ru | 1.648614 | 0.535800 | 0.109134 | C | -1.768069 | 0.085289 | -3.156408 |
| N | -1.282148 | 1.506659 | -0.019546 | H | -1.310990 | 1.015446 | -2.824376 |
| C | -6.086029 | 1.911712 | -0.521038 | C | -1.824489 | -0.270595 | -4.497084 |
| H | -7.129287 | 1.638628 | -0.651069 | H | -1.406464 | 0.389721 | -5.252122 |
| N | 0.002688 | 1.776424 | 0.153787 | C | -2.438481 | -1.469934 | -4.845485 |
| C | -5.687395 | 3.244939 | -0.438102 | H | -2.507225 | -1.778309 | -5.885753 |
| H | -6.419403 | 4.046302 | -0.502336 | C | -2.977427 | -2.268865 | -3.842196 |
| N | 2.441223 | 2.510897 | 0.437999 | H | -3.468650 | -3.204827 | -4.095312 |
| C | -4.340714 | 3.538328 | -0.271419 | C | -2.892595 | -1.860062 | -2.514099 |
| H | -3.998847 | 4.568397 | -0.204401 | C | -3.453231 | -2.620622 | -1.387832 |
| N | -2.277798 | -0.681927 | -2.181755 | C | -4.105616 | -3.848403 | -1.455091 |
| C | -3.412483 | 2.500299 | -0.191714 | H | -4.244000 | -4.355779 | -2.405997 |
| N | -3.296568 | -2.010620 | -0.186842 | C | -4.578948 | -4.428219 | -0.277833 |
| C | -1.984320 | 2.673575 | -0.018710 | C | -4.407236 | -3.782833 | 0.942957 |
| N | -2.840698 | -0.539500 | 1.901255 | H | -4.779446 | -4.236497 | 1.857562 |
| C | -1.093126 | 3.738221 | 0.166036 | C | -3.753559 | -2.550482 | 0.969836 |
| H | -1.321867 | 4.795691 | 0.215731 | C | -3.514835 | -1.707993 | 2.144686 |
| N | 1.852994 | 0.026621 | 2.147588 | C | -3.974095 | -2.012915 | 3.425068 |
| C | 0.161187 | 3.124176 | 0.271947 | H | -4.506693 | -2.943284 | 3.605038 |
| N | 3.271574 | -0.613354 | 0.063182 | C | -3.764854 | -1.115878 | 4.465533 |
| C | 1.536393 | 3.540637 | 0.459157 | H | -4.126922 | -1.342489 | 5.465230 |
| N | 2.228667 | 0.723499 | -1.899417 | C | -3.103101 | 0.080496 | 4.201063 |
| C | 1.954955 | 4.858034 | 0.645707 | H | -2.940617 | 0.820186 | 4.980608 |
| H | 1.217389 | 5.656934 | 0.659297 | C | -2.658883 | 0.328132 | 2.909266 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -2.144268 | 1.251324 | 2.646227 | H | 5.486650 | -1.924528 | -2.133951 |
| C | 1.104686 | 0.448330 | 3.177626 | C | 3.877819 | -0.832558 | -1.131866 |
| H | 0.307982 | 1.143516 | 2.920000 | C | 3.304018 | -0.058075 | -2.233226 |
| C | 1.331425 | 0.039251 | 4.484996 | C | 3.824569 | -0.047808 | -3.526279 |
| H | 0.704452 | 0.417619 | 5.287842 | H | 4.677768 | -0.673858 | -3.775276 |
| C | 2.379397 | -0.840424 | 4.740383 | C | 3.259973 | 0.780463 | -4.488539 |
| H | 2.590167 | -1.176499 | 5.752609 | H | 3.663806 | 0.802543 | -5.497616 |
| C | 3.167142 | -1.277144 | 3.680130 | C | 2.185341 | 1.591823 | -4.132372 |
| H | 3.996812 | -1.956468 | 3.858688 | H | 1.730827 | 2.272084 | -4.847853 |
| C | 2.892871 | -0.830984 | 2.390373 | C | 1.701978 | 1.532859 | -2.832003 |
| C | 3.681858 | -1.211092 | 1.211937 | H | 0.869744 | 2.152173 | -2.500148 |
| C | 4.761929 | -2.086288 | 1.188304 | H | -5.086729 | -5.388596 | -0.315256 |
| H | 5.135874 | -2.596868 | 2.071721 | N | 6.528073 | -3.256929 | -0.089595 |
| C | 5.377233 | -2.316203 | -0.035667 | O | 7.033420 | -3.427325 | -1.188890 |
| C | 4.961753 | -1.705343 | -1.207949 | O | 6.854881 | -3.768714 | 0.970839 |

Min-2 (3+ triplet)

E= -2748.771 56 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.254154 | -0.242563 | -0.189014 | H | 4.424496 | 1.735393 | 1.078839 |
| N | -3.824973 | 1.186873 | 0.174265 | C | -1.668744 | 1.257217 | -2.853187 |
| O | -0.603917 | -1.279567 | -0.086139 | H | -1.254227 | 2.008348 | -2.182910 |
| O | 0.533015 | -0.769562 | -0.728127 | C | -1.671280 | 1.420472 | -4.231810 |
| C | -5.136018 | 0.968046 | -0.038921 | H | -1.250091 | 2.319669 | -4.673510 |
| H | -5.395237 | -0.009679 | -0.442376 | C | -2.238828 | 0.424575 | -5.020967 |
| Ru | 1.630099 | 0.504509 | 0.260865 | H | -2.266010 | 0.520671 | -6.103609 |
| N | -1.293847 | 1.425511 | 0.502079 | C | -2.787171 | -0.696124 | -4.405131 |
| C | -6.109769 | 1.917514 | 0.228838 | H | -3.244186 | -1.478594 | -5.005309 |
| H | -7.153976 | 1.690301 | 0.034107 | C | -2.757460 | -0.806336 | -3.017777 |
| N | -0.003574 | 1.665674 | 0.673211 | C | -3.334041 | -1.938561 | -2.276201 |
| C | -5.718562 | 3.151246 | 0.748242 | C | -3.934813 | -3.069518 | -2.822412 |
| H | -6.457541 | 3.917128 | 0.970763 | H | -4.018689 | -3.193547 | -3.898685 |
| N | 2.435146 | 2.298129 | 1.147455 | C | -4.424731 | -4.055215 | -1.965263 |
| C | -4.371099 | 3.389834 | 0.979836 | C | -4.317016 | -3.905386 | -0.586352 |
| H | -4.035165 | 4.341491 | 1.384755 | H | -4.697086 | -4.676523 | 0.078347 |
| N | -2.187620 | 0.176751 | -2.251809 | C | -3.712822 | -2.754269 | -0.078152 |
| C | -3.434449 | 2.397711 | 0.688416 | C | -3.537520 | -2.401704 | 1.333380 |
| N | -3.247177 | -1.812010 | -0.930306 | C | -4.031657 | -3.164723 | 2.389877 |
| C | -2.005048 | 2.524997 | 0.883841 | H | -4.542903 | -4.103094 | 2.190608 |
| N | -2.889893 | -1.215969 | 1.566362 | C | -3.886482 | -2.712376 | 3.695680 |
| C | -1.113227 | 3.501980 | 1.343855 | H | -4.275735 | -3.297769 | 4.524915 |
| H | -1.347328 | 4.488331 | 1.725038 | C | -3.254770 | -1.491803 | 3.919346 |
| N | 1.740508 | -0.569535 | 2.068887 | H | -3.143496 | -1.088985 | 4.922582 |
| C | 0.150055 | 2.914902 | 1.199359 | C | -2.773299 | -0.778495 | 2.830142 |
| N | 3.250107 | -0.612810 | -0.060429 | H | -2.280845 | 0.185312 | 2.948259 |
| C | 1.525472 | 3.269933 | 1.480877 | C | 0.956758 | -0.443985 | 3.149746 |
| N | 2.304108 | 1.254164 | -1.589582 | H | 0.184521 | 0.319942 | 3.078744 |
| C | 1.939564 | 4.478550 | 2.041784 | C | 1.124416 | -1.219220 | 4.289670 |
| H | 1.198340 | 5.231465 | 2.298984 | H | 0.472196 | -1.072632 | 5.146466 |
| C | 3.290428 | 4.704380 | 2.266063 | C | 2.148080 | -2.161682 | 4.313879 |
| H | 3.624615 | 5.642101 | 2.703315 | H | 2.313633 | -2.781057 | 5.191958 |
| C | 4.210610 | 3.714370 | 1.921979 | C | 2.971848 | -2.293699 | 3.200094 |
| H | 5.276444 | 3.851785 | 2.080207 | H | 3.784031 | -3.016192 | 3.204028 |
| C | 3.742487 | 2.534608 | 1.365277 | C | 2.757266 | -1.487832 | 2.085972 |

| | | | | | | | |
|---|----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.591153 | -1.532812 | 0.876649 | C | 3.457387 | 2.035913 | -4.005403 |
| C | 4.649452 | -2.402538 | 0.637249 | H | 3.907820 | 2.339653 | -4.947061 |
| H | 4.971164 | -3.161622 | 1.345095 | C | 2.383931 | 2.741580 | -3.467761 |
| C | 5.311604 | -2.290041 | -0.578791 | H | 1.976400 | 3.616133 | -3.968051 |
| C | 4.960405 | -1.354174 | -1.537886 | C | 1.839008 | 2.318495 | -2.262708 |
| H | 5.515978 | -1.318233 | -2.471196 | H | 1.005251 | 2.840713 | -1.796218 |
| C | 3.894971 | -0.503019 | -1.247195 | H | -4.892252 | -4.945560 | -2.377846 |
| C | 3.381126 | 0.573641 | -2.095662 | N | 6.440491 | -3.216124 | -0.864013 |
| C | 3.961314 | 0.945371 | -3.307080 | O | 6.987290 | -3.081100 | -1.948190 |
| H | 4.814831 | 0.394327 | -3.694078 | O | 6.709786 | -4.022327 | 0.013856 |

Min-2 (4+ doublet)

E= -2748.277 97 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.283559 | 0.301659 | -0.091569 | C | 2.840462 | 0.641364 | -4.931973 |
| N | 3.813265 | -1.177475 | 0.043082 | H | 2.986099 | 0.764482 | -6.002753 |
| O | 0.571348 | 1.141294 | 0.297428 | C | 3.242618 | 1.642673 | -4.052077 |
| O | -0.422304 | 0.809848 | -0.569947 | H | 3.703735 | 2.550184 | -4.433544 |
| C | 5.130330 | -0.910800 | -0.027118 | C | 3.068916 | 1.467769 | -2.682580 |
| H | 5.403838 | 0.132123 | -0.176032 | C | 3.515421 | 2.427611 | -1.666512 |
| Ru | -1.672007 | -0.541789 | 0.117425 | C | 4.128817 | 3.656009 | -1.895376 |
| N | 1.270686 | -1.472008 | 0.180298 | H | 4.305371 | 4.012879 | -2.906638 |
| C | 6.098293 | -1.902152 | 0.072337 | C | 4.521284 | 4.430894 | -0.802692 |
| H | 7.149224 | -1.635091 | -0.000267 | C | 4.314826 | 3.970527 | 0.494407 |
| N | -0.024005 | -1.741689 | 0.277393 | H | 4.632914 | 4.570153 | 1.343168 |
| C | 5.696122 | -3.223596 | 0.260999 | C | 3.699933 | 2.731942 | 0.682971 |
| H | 6.432025 | -4.019990 | 0.344007 | C | 3.442341 | 2.068416 | 1.961293 |
| N | -2.470617 | -2.483660 | 0.489103 | C | 3.854323 | 2.566536 | 3.196041 |
| C | 4.338658 | -3.509670 | 0.345200 | H | 4.356872 | 3.528614 | 3.256244 |
| H | 3.993747 | -4.529775 | 0.497157 | C | 3.641964 | 1.817120 | 4.347977 |
| N | 2.490145 | 0.326121 | -2.191480 | H | 3.970722 | 2.192791 | 5.314113 |
| C | 3.408930 | -2.475582 | 0.236239 | C | 3.020884 | 0.574945 | 4.240363 |
| N | 3.310529 | 2.005145 | -0.394074 | H | 2.855195 | -0.050162 | 5.113841 |
| C | 1.974303 | -2.636981 | 0.325014 | C | 2.619665 | 0.131508 | 2.986924 |
| N | 2.810047 | 0.855462 | 1.871666 | H | 2.133275 | -0.832533 | 2.848884 |
| C | 1.076561 | -3.691831 | 0.529012 | C | -1.363334 | -0.510631 | 3.205893 |
| H | 1.306375 | -4.739594 | 0.680127 | H | -0.600512 | -1.258709 | 2.997967 |
| N | -2.016930 | -0.028326 | 2.133794 | C | -1.647542 | -0.094284 | 4.499174 |
| C | -0.182599 | -3.086317 | 0.494430 | H | -1.103281 | -0.521385 | 5.337281 |
| N | -3.299148 | 0.641913 | -0.014926 | C | -2.650875 | 0.851729 | 4.696161 |
| C | -1.561933 | -3.504557 | 0.625702 | H | -2.906170 | 1.191477 | 5.697355 |
| N | -2.257909 | -0.806787 | -1.889144 | C | -3.342869 | 1.344314 | 3.592731 |
| C | -1.981621 | -4.813757 | 0.860267 | H | -4.141643 | 2.069333 | 3.728314 |
| H | -1.243174 | -5.605121 | 0.965817 | C | -3.019704 | 0.887882 | 2.318728 |
| C | -3.340118 | -5.092355 | 0.955136 | C | -3.729018 | 1.286206 | 1.099185 |
| H | -3.681308 | -6.108651 | 1.138021 | C | -4.772033 | 2.203200 | 1.011621 |
| C | -4.255973 | -4.051375 | 0.810087 | H | -5.161232 | 2.751633 | 1.866411 |
| H | -5.326543 | -4.225552 | 0.878017 | C | -5.333844 | 2.419158 | -0.239457 |
| C | -3.783158 | -2.766429 | 0.575460 | C | -4.909638 | 1.749020 | -1.374848 |
| H | -4.465330 | -1.926475 | 0.457134 | H | -5.401547 | 1.952674 | -2.323299 |
| C | 2.117421 | -0.643047 | -3.046317 | C | -3.862968 | 0.838087 | -1.233065 |
| H | 1.694683 | -1.536838 | -2.591246 | C | -3.294741 | -0.003065 | -2.285551 |
| C | 2.271707 | -0.522711 | -4.420016 | C | -3.788703 | -0.062770 | -3.587056 |
| H | 1.969270 | -1.336936 | -5.073159 | H | -4.613678 | 0.578386 | -3.887965 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -3.237271 | -0.964387 | -4.491344 | H | -0.936145 | -2.313851 | -2.386235 |
| H | -3.623469 | -1.027740 | -5.506025 | H | 4.999020 | 5.393983 | -0.966465 |
| C | -2.200939 | -1.794317 | -4.069865 | N | -6.447023 | 3.410376 | -0.364404 |
| H | -1.758050 | -2.527220 | -4.739196 | O | -6.902831 | 3.555373 | -1.486037 |
| C | -1.740179 | -1.684898 | -2.764110 | O | -6.776234 | 3.968577 | 0.668776 |

Min-2 (4+ quartet)

E= -2748.271 86 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.272943 | 0.265514 | -0.122115 | C | 3.377809 | 2.423946 | -1.772892 |
| N | 3.839633 | -1.194406 | -0.072530 | C | 3.951079 | 3.664094 | -2.046168 |
| O | 0.595864 | 1.269455 | 0.148419 | H | 4.044306 | 4.022557 | -3.067886 |
| O | -0.516135 | 0.890340 | -0.552971 | C | 4.406318 | 4.447316 | -0.986559 |
| C | 5.151162 | -0.943071 | -0.239422 | C | 4.293244 | 3.986849 | 0.322507 |
| H | 5.422520 | 0.096175 | -0.416242 | H | 4.654544 | 4.594302 | 1.148120 |
| Ru | -1.654709 | -0.558859 | 0.167233 | C | 3.712308 | 2.739774 | 0.552693 |
| N | 1.301130 | -1.466066 | 0.193888 | C | 3.538266 | 2.081744 | 1.847867 |
| C | 6.112936 | -1.943403 | -0.196301 | C | 4.007495 | 2.588094 | 3.057737 |
| H | 7.159634 | -1.690258 | -0.342193 | H | 4.506264 | 3.553540 | 3.087827 |
| N | -0.011271 | -1.726578 | 0.391436 | C | 3.856569 | 1.843296 | 4.222795 |
| C | 5.710213 | -3.257826 | 0.035290 | H | 4.231182 | 2.225793 | 5.169430 |
| H | 6.441585 | -4.061679 | 0.076044 | C | 3.241025 | 0.595782 | 4.152500 |
| N | -2.445132 | -2.468055 | 0.718376 | H | 3.127406 | -0.028840 | 5.034672 |
| C | 4.358300 | -3.529333 | 0.215324 | C | 2.785568 | 0.141228 | 2.922355 |
| H | 4.015573 | -4.545319 | 0.397207 | H | 2.311063 | -0.832422 | 2.813067 |
| N | 2.316551 | 0.326719 | -2.224570 | C | -1.160627 | -0.198944 | 3.209034 |
| C | 3.436838 | -2.485735 | 0.158955 | H | -0.396669 | -0.953738 | 3.032691 |
| N | 3.274336 | 1.996815 | -0.491387 | C | -1.385294 | 0.336160 | 4.470202 |
| C | 2.004364 | -2.627180 | 0.338134 | H | -0.789493 | 0.000397 | 5.314780 |
| N | 2.913656 | 0.864687 | 1.796426 | C | -2.393413 | 1.283739 | 4.628562 |
| C | 1.114122 | -3.657888 | 0.653724 | H | -2.602014 | 1.716732 | 5.604192 |
| H | 1.347088 | -4.700138 | 0.839056 | C | -3.149547 | 1.658122 | 3.521078 |
| N | -1.878568 | 0.166621 | 2.133227 | H | -3.953051 | 2.382503 | 3.628683 |
| C | -0.151874 | -3.045292 | 0.678157 | C | -2.884608 | 1.085229 | 2.280859 |
| N | -3.295163 | 0.611004 | -0.000207 | C | -3.661026 | 1.361669 | 1.068255 |
| C | -1.520295 | -3.467867 | 0.898623 | C | -4.704493 | 2.275653 | 0.948645 |
| N | -2.322073 | -0.975363 | -1.789911 | H | -5.045969 | 2.906039 | 1.766469 |
| C | -1.911602 | -4.758450 | 1.251228 | C | -5.328791 | 2.379847 | -0.286045 |
| H | -1.160225 | -5.532119 | 1.391585 | C | -4.960664 | 1.609524 | -1.376856 |
| C | -3.262109 | -5.041394 | 1.422505 | H | -5.493972 | 1.734473 | -2.316518 |
| H | -3.582949 | -6.043081 | 1.698855 | C | -3.910677 | 0.708480 | -1.203650 |
| C | -4.195873 | -4.023585 | 1.234009 | C | -3.384412 | -0.217616 | -2.206067 |
| H | -5.260408 | -4.202704 | 1.359550 | C | -3.932206 | -0.390545 | -3.475093 |
| C | -3.749257 | -2.756700 | 0.880436 | H | -4.777809 | 0.215231 | -3.791588 |
| H | -4.445844 | -1.934973 | 0.724360 | C | -3.407524 | -1.358790 | -4.325138 |
| C | 1.884758 | -0.644940 | -3.047846 | H | -3.836428 | -1.510677 | -5.312938 |
| H | 1.485213 | -1.533624 | -2.563468 | C | -2.343770 | -2.141249 | -3.881937 |
| C | 1.955086 | -0.531878 | -4.428993 | H | -1.922346 | -2.925729 | -4.505122 |
| H | 1.605430 | -1.347205 | -5.056688 | C | -1.831201 | -1.919847 | -2.610341 |
| C | 2.495152 | 0.626770 | -4.981801 | H | -1.008292 | -2.513075 | -2.215035 |
| H | 2.572524 | 0.744617 | -6.060214 | H | 4.854719 | 5.418197 | -1.183595 |
| C | 2.955168 | 1.630071 | -4.133969 | N | -6.443764 | 3.363888 | -0.445220 |
| H | 3.396989 | 2.533084 | -4.547441 | O | -6.946193 | 3.419326 | -1.554928 |
| C | 2.866404 | 1.463757 | -2.754868 | O | -6.728254 | 4.006701 | 0.551390 |

TS-2 A (3+ unrestricted singlet)

E= -2901.602 58 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.657568 | -0.168492 | 0.389873 | C | -5.785257 | 0.600774 | -1.733551 |
| Ru | 2.495185 | 0.099374 | -0.250302 | C | -5.253117 | -0.676769 | -1.784827 |
| N | -2.405293 | -0.789441 | 2.230360 | H | -5.782862 | -1.453705 | -2.329209 |
| O | -0.056630 | -0.814343 | -1.031218 | C | -4.043999 | -0.893287 | -1.128304 |
| O | 0.883610 | 0.134087 | -1.328995 | C | -3.323425 | -2.160427 | -1.022900 |
| C | -3.700980 | -1.108860 | 2.432449 | C | -3.774521 | -3.365690 | -1.555043 |
| H | -4.344413 | -1.083914 | 1.556847 | H | -4.708498 | -3.401559 | -2.110142 |
| N | 0.039156 | -0.296942 | 1.619909 | C | -3.021862 | -4.518999 | -1.369732 |
| C | -4.199173 | -1.447917 | 3.678179 | H | -3.363910 | -5.467285 | -1.776870 |
| H | -5.250860 | -1.697713 | 3.784675 | C | -1.830602 | -4.440608 | -0.652457 |
| N | 1.328232 | -0.027357 | 1.445896 | H | -1.217641 | -5.320983 | -0.479608 |
| C | -3.332426 | -1.457846 | 4.771653 | C | -1.430406 | -3.210674 | -0.148099 |
| H | -3.695611 | -1.714488 | 5.763731 | H | -0.506931 | -3.083866 | 0.411164 |
| N | 3.906525 | 0.310724 | 1.360963 | C | 2.477525 | -2.955413 | 0.365636 |
| C | -1.997326 | -1.141816 | 4.573530 | H | 1.798397 | -2.658351 | 1.163809 |
| H | -1.291866 | -1.149025 | 5.400846 | C | 2.855925 | -4.278204 | 0.177511 |
| N | -2.073397 | 1.817034 | 1.006130 | H | 2.472770 | -5.051801 | 0.837746 |
| C | -1.542680 | -0.814735 | 3.294765 | C | 3.744699 | -4.579683 | -0.850320 |
| N | -3.432191 | 0.126006 | -0.479633 | H | 4.069584 | -5.602717 | -1.023174 |
| C | -0.178884 | -0.508376 | 2.951590 | C | 4.225681 | -3.548448 | -1.650498 |
| N | -2.152257 | -2.093821 | -0.323212 | H | 4.927646 | -3.763251 | -2.452140 |
| C | 1.023984 | -0.372194 | 3.648928 | C | 3.812441 | -2.239558 | -1.414877 |
| H | 1.193814 | -0.486295 | 4.712454 | C | 4.285794 | -1.083117 | -2.191110 |
| N | 2.929758 | -1.955030 | -0.405602 | C | 5.182497 | -1.107787 | -3.256256 |
| C | 1.959129 | -0.069489 | 2.655863 | H | 5.606147 | -2.044798 | -3.607603 |
| N | 3.775697 | 0.102740 | -1.773804 | C | 5.535037 | 0.092293 | -3.873452 |
| C | 3.390191 | 0.157613 | 2.618771 | H | 6.233396 | 0.086507 | -4.706311 |
| N | 2.647409 | 2.153455 | -0.663585 | C | 5.001945 | 1.296973 | -3.424463 |
| C | 4.207900 | 0.228857 | 3.746466 | H | 5.283612 | 2.231143 | -3.903034 |
| H | 3.772009 | 0.103928 | 4.734847 | C | 4.108705 | 1.282677 | -2.352772 |
| C | 5.568052 | 0.461943 | 3.593995 | C | 3.467081 | 2.441512 | -1.725058 |
| H | 6.216207 | 0.519313 | 4.465024 | C | 3.668150 | 3.758190 | -2.135890 |
| C | 6.087330 | 0.625771 | 2.310834 | H | 4.321400 | 3.971963 | -2.978068 |
| H | 7.144554 | 0.814192 | 2.147386 | C | 3.032970 | 4.796202 | -1.464634 |
| C | 5.225037 | 0.544559 | 1.228173 | H | 3.184815 | 5.825846 | -1.778405 |
| H | 5.587026 | 0.665306 | 0.208180 | C | 2.206482 | 4.494055 | -0.385672 |
| C | -1.371529 | 2.595896 | 1.841361 | H | 1.694646 | 5.275498 | 0.169372 |
| H | -0.487354 | 2.138712 | 2.283114 | C | 2.043651 | 3.164949 | -0.019533 |
| C | -1.743195 | 3.901846 | 2.137589 | H | 1.413657 | 2.871374 | 0.818186 |
| H | -1.144458 | 4.491785 | 2.826468 | O | -1.408378 | 1.527663 | -1.615180 |
| C | -2.894282 | 4.418801 | 1.552370 | H | -1.664445 | 0.929536 | -2.358253 |
| H | -3.218724 | 5.434859 | 1.763212 | H | -0.436627 | 1.540074 | -1.677070 |
| C | -3.639708 | 3.608633 | 0.701699 | H | -1.08078 | -1.017121 | -2.739680 |
| H | -4.550884 | 3.988754 | 0.247266 | O | -1.87538 | -0.661969 | -3.181215 |
| C | -3.217201 | 2.308731 | 0.440875 | H | -1.73947 | -0.791317 | -4.130787 |
| C | -3.973070 | 1.368612 | -0.396152 | N | -7.06818 | 0.870180 | -2.436900 |
| C | -5.177498 | 1.637172 | -1.037595 | O | -7.56648 | -0.07517 | -3.02935 |
| H | -5.659314 | 2.610716 | -1.017231 | O | -7.49835 | 2.010985 | -2.35476 |

TS-2 A (3+ triplet)**E= -2901.597 46 a.u.**

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.676242 | -0.046858 | 0.414868 | C | -5.798009 | 0.153069 | -1.836806 |
| Ru | 2.511983 | 0.045451 | -0.257463 | C | -5.245856 | -1.094238 | -1.595261 |
| N | -2.433118 | -0.224183 | 2.344146 | H | -5.760923 | -1.983225 | -1.948997 |
| O | -0.011039 | -0.961129 | -0.814276 | C | -4.036915 | -1.136041 | -0.905413 |
| O | 0.904402 | -0.051462 | -1.350219 | C | -3.293721 | -2.332428 | -0.515699 |
| C | -3.728755 | -0.486506 | 2.618143 | C | -3.714018 | -3.635161 | -0.770479 |
| H | -4.374987 | -0.659837 | 1.761539 | H | -4.643319 | -3.813506 | -1.305599 |
| N | 0.022974 | 0.111002 | 1.638607 | C | -2.935442 | -4.701658 | -0.337775 |
| C | -4.223352 | -0.529789 | 3.909481 | H | -3.253124 | -5.723858 | -0.528008 |
| H | -5.275450 | -0.744617 | 4.073227 | C | -1.749361 | -4.440025 | 0.343908 |
| N | 1.318861 | 0.306568 | 1.415421 | H | -1.116149 | -5.246556 | 0.703550 |
| C | -3.353507 | -0.290689 | 4.974679 | C | -1.381747 | -3.120585 | 0.568917 |
| H | -3.714623 | -0.311884 | 5.999902 | H | -0.464318 | -2.851736 | 1.086609 |
| N | 3.912706 | 0.539636 | 1.292394 | C | 2.463884 | -2.806600 | 0.994839 |
| C | -2.018765 | -0.032621 | 4.706263 | H | 1.827368 | -2.324404 | 1.735758 |
| H | -1.310883 | 0.147215 | 5.511733 | C | 2.794505 | -4.152587 | 1.074029 |
| N | -2.114349 | 2.024535 | 0.553731 | H | 2.419023 | -4.756853 | 1.895660 |
| C | -1.567015 | -0.009488 | 3.385021 | C | 3.628305 | -4.694333 | 0.099444 |
| N | -3.444275 | 0.014350 | -0.505606 | H | 3.915098 | -5.742548 | 0.133069 |
| C | -0.200114 | 0.197044 | 2.983848 | C | 4.105231 | -3.871805 | -0.915808 |
| N | -2.129179 | -2.086968 | 0.155038 | H | 4.765195 | -4.275287 | -1.679457 |
| C | 1.005138 | 0.452610 | 3.642760 | C | 3.742303 | -2.527351 | -0.943499 |
| H | 1.172655 | 0.563441 | 4.706992 | C | 4.215538 | -1.571974 | -1.955333 |
| N | 2.912442 | -2.008287 | 0.014213 | C | 5.058579 | -1.848596 | -3.028346 |
| C | 1.946782 | 0.511221 | 2.613448 | H | 5.434599 | -2.854216 | -3.196603 |
| N | 3.763954 | -0.306622 | -1.765471 | C | 5.417799 | -0.814857 | -3.893057 |
| C | 3.382870 | 0.683753 | 2.545273 | H | 6.073426 | -1.017933 | -4.735784 |
| N | 2.762358 | 1.970225 | -1.054132 | C | 4.944838 | 0.475537 | -3.677143 |
| C | 4.194673 | 0.981095 | 3.640890 | H | 5.230554 | 1.281763 | -4.347537 |
| H | 3.748261 | 1.090893 | 4.626345 | C | 4.106035 | 0.715514 | -2.588025 |
| C | 5.560989 | 1.139750 | 3.458111 | C | 3.542697 | 2.004211 | -2.180912 |
| H | 6.204668 | 1.371861 | 4.303030 | C | 3.787812 | 3.206265 | -2.843006 |
| C | 6.094025 | 1.002685 | 2.176455 | H | 4.408087 | 3.219293 | -3.735614 |
| H | 7.157594 | 1.121313 | 1.990049 | C | 3.242321 | 4.386962 | -2.354415 |
| C | 5.238338 | 0.706442 | 1.127336 | H | 3.429921 | 5.328992 | -2.863456 |
| H | 5.609670 | 0.587291 | 0.110652 | C | 2.461681 | 4.342936 | -1.201887 |
| C | -1.425885 | 2.986073 | 1.184158 | H | 2.024808 | 5.244871 | -0.782207 |
| H | -0.533698 | 2.656721 | 1.714641 | C | 2.247735 | 3.118341 | -0.584880 |
| C | -1.819441 | 4.318859 | 1.172839 | H | 1.648910 | 3.024537 | 0.318989 |
| H | -1.231594 | 5.061994 | 1.704836 | O | -1.424395 | 1.137649 | -1.907550 |
| C | -2.976859 | 4.668061 | 0.485191 | H | -1.655650 | 0.374426 | -2.491197 |
| H | -3.317395 | 5.700164 | 0.455709 | H | -0.449946 | 1.148625 | -1.949807 |
| C | -3.706572 | 3.672218 | -0.156274 | H | -1.00356 | -1.555626 | -2.371783 |
| H | -4.621286 | 3.923648 | -0.686624 | O | -1.80221 | -1.373850 | -2.907895 |
| C | -3.263638 | 2.353895 | -0.110390 | H | -1.61814 | -1.710587 | -3.796209 |
| C | -4.002782 | 1.235193 | -0.709753 | N | -7.08179 | 0.234010 | -2.583178 |
| C | -5.208708 | 1.330615 | -1.396088 | O | -7.56279 | -0.82962 | -2.94465 |
| H | -5.704973 | 2.275496 | -1.599318 | O | -7.531 | 1.356169 | -2.7635 |

TS-2 B (3+ unrestricted singlet)**E= -2901.603 11 a.u.**

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.307218 | -0.165155 | 0.128780 | C | 5.622705 | -1.635985 | 3.182840 |
| Ru | -1.843987 | 0.344022 | -0.309490 | H | 6.365402 | -1.969473 | 3.903116 |
| N | 3.612303 | 0.421238 | -1.388987 | C | 5.127817 | -2.524449 | 2.234309 |
| O | 0.398575 | -1.260737 | 0.304792 | H | 5.482816 | -3.551033 | 2.204382 |
| O | -0.621313 | -0.571911 | 0.899792 | C | 4.170188 | -2.073355 | 1.326882 |
| C | 4.921190 | 0.092477 | -1.406810 | C | 3.563203 | -2.837015 | 0.237368 |
| H | 5.264856 | -0.556513 | -0.605616 | C | 3.881490 | -4.157671 | -0.070215 |
| N | 1.078319 | 0.817830 | -1.264795 | H | 4.607159 | -4.697540 | 0.532640 |
| C | 5.790895 | 0.550336 | -2.381127 | C | 3.266545 | -4.777687 | -1.150902 |
| H | 6.835285 | 0.253736 | -2.348733 | H | 3.509423 | -5.807164 | -1.402295 |
| N | -0.213762 | 1.122204 | -1.303463 | C | 2.342464 | -4.060133 | -1.906550 |
| C | 5.301001 | 1.387300 | -3.384337 | H | 1.846257 | -4.506730 | -2.763806 |
| H | 5.961153 | 1.767052 | -4.160211 | C | 2.061785 | -2.748138 | -1.551654 |
| N | -2.708118 | 1.744287 | -1.693901 | H | 1.343739 | -2.139204 | -2.095375 |
| C | 3.956061 | 1.722744 | -3.381562 | C | -1.530095 | -1.596768 | -2.729643 |
| H | 3.537751 | 2.364839 | -4.152851 | H | -0.662586 | -0.976821 | -2.952437 |
| N | 2.806423 | 1.650547 | 1.110338 | C | -1.900083 | -2.660855 | -3.542064 |
| C | 3.118531 | 1.227569 | -2.380468 | H | -1.317230 | -2.893446 | -4.429440 |
| N | 3.735127 | -0.794097 | 1.386700 | C | -3.033478 | -3.397303 | -3.208673 |
| C | 1.702379 | 1.467681 | -2.291049 | H | -3.357185 | -4.231644 | -3.825953 |
| N | 2.651747 | -2.144780 | -0.508651 | C | -3.758818 | -3.041272 | -2.076568 |
| C | 0.764472 | 2.210850 | -3.012240 | H | -4.652938 | -3.596382 | -1.804127 |
| H | 0.933141 | 2.828019 | -3.886078 | C | -3.340678 | -1.963366 | -1.300378 |
| N | -2.218193 | -1.249481 | -1.630948 | C | -4.057315 | -1.498503 | -0.105408 |
| C | -0.443121 | 1.961651 | -2.354920 | C | -5.208316 | -2.060374 | 0.436106 |
| N | -3.500791 | -0.404494 | 0.479181 | H | -5.699490 | -2.934553 | 0.017311 |
| C | -1.827382 | 2.342845 | -2.553357 | C | -5.744100 | -1.466427 | 1.571688 |
| N | -2.192602 | 1.683081 | 1.272276 | C | -5.181040 | -0.347391 | 2.165618 |
| C | -2.266878 | 3.245654 | -3.521429 | H | -5.650140 | 0.075079 | 3.050163 |
| H | -1.545692 | 3.707342 | -4.191656 | C | -4.029598 | 0.180679 | 1.585721 |
| C | -3.618901 | 3.546970 | -3.615582 | C | -3.290035 | 1.363430 | 2.030223 |
| H | -3.974148 | 4.248773 | -4.366151 | C | -3.661499 | 2.145385 | 3.122736 |
| C | -4.510585 | 2.940854 | -2.732120 | H | -4.535542 | 1.878687 | 3.711794 |
| H | -5.575617 | 3.151502 | -2.768304 | C | -2.912786 | 3.269204 | 3.451484 |
| C | -4.014693 | 2.051740 | -1.790931 | H | -3.194980 | 3.886625 | 4.300491 |
| H | -4.675081 | 1.555589 | -1.081338 | C | -1.804406 | 3.590786 | 2.672136 |
| C | 2.343851 | 2.883626 | 0.861190 | H | -1.196255 | 4.464522 | 2.890354 |
| H | 1.653689 | 2.968159 | 0.023020 | C | -1.482203 | 2.775180 | 1.595709 |
| C | 2.720591 | 3.990386 | 1.611758 | H | -0.631282 | 2.982903 | 0.949779 |
| H | 2.322865 | 4.971842 | 1.367524 | O | 1.413579 | -0.138107 | 2.618298 |
| C | 3.622030 | 3.812356 | 2.655946 | H | 1.452616 | -1.107379 | 2.803307 |
| H | 3.943495 | 4.654560 | 3.263802 | H | 0.469722 | 0.005976 | 2.427950 |
| C | 4.123653 | 2.538842 | 2.904411 | H | 0.834441 | -2.718426 | 1.639091 |
| H | 4.840373 | 2.384517 | 3.706495 | O | 1.444819 | -2.864445 | 2.385022 |
| C | 3.708525 | 1.466134 | 2.120941 | H | 1.034361 | -3.541047 | 2.942289 |
| C | 4.227508 | 0.100219 | 2.278457 | N | -6.96946 | -2.053530 | 2.172271 |
| C | 5.184181 | -0.312240 | 3.202028 | O | -7.40395 | -1.49414 | 3.168362 |
| H | 5.592006 | 0.383975 | 3.929511 | O | -7.42444 | -3.04089 | 1.613116 |

TS-2 B (3+ triplet)

E= -2901.597 59 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|----------|-----------|-----------|
| Ru | 2.331084 | 0.169846 | -0.130579 | N | 3.643180 | -0.529372 | 1.326264 |
| Ru | -1.855679 | -0.394637 | 0.278405 | O | 0.336582 | 1.211676 | -0.230710 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| O | -0.658059 | 0.536306 | -0.938488 | C | 5.093226 | 2.771852 | -2.004635 |
| C | 4.951703 | -0.201334 | 1.377252 | H | 5.420287 | 3.801268 | -1.885987 |
| H | 5.297835 | 0.507452 | 0.629357 | C | 4.141917 | 2.220909 | -1.147212 |
| N | 1.098659 | -0.930066 | 1.167700 | C | 3.501509 | 2.873953 | -0.006116 |
| C | 5.817191 | -0.733499 | 2.316696 | C | 3.768222 | 4.177431 | 0.405256 |
| H | 6.861704 | -0.435417 | 2.312067 | H | 4.481703 | 4.786302 | -0.144027 |
| N | -0.195495 | -1.233838 | 1.195349 | C | 3.115418 | 4.693268 | 1.517916 |
| C | 5.324327 | -1.647948 | 3.248753 | H | 3.317078 | 5.709082 | 1.848766 |
| H | 5.981767 | -2.087167 | 3.994940 | C | 2.206680 | 3.889350 | 2.201907 |
| N | -2.691642 | -1.865442 | 1.602424 | H | 1.681482 | 4.253297 | 3.080827 |
| C | 3.980187 | -1.983291 | 3.213423 | C | 1.980911 | 2.598124 | 1.746875 |
| H | 3.559794 | -2.684276 | 3.930435 | H | 1.278618 | 1.924710 | 2.232266 |
| N | 2.861633 | -1.541645 | -1.269754 | C | -1.519061 | 1.364994 | 2.825384 |
| C | 3.146075 | -1.411054 | 2.250890 | H | -0.670876 | 0.706129 | 3.006381 |
| N | 3.741909 | 0.940342 | -1.318854 | C | -1.856694 | 2.387056 | 3.702484 |
| C | 1.728974 | -1.644248 | 2.146741 | H | -1.269791 | 2.544591 | 4.603636 |
| N | 2.606501 | 2.095007 | 0.672268 | C | -2.965680 | 3.178426 | 3.414634 |
| C | 0.795505 | -2.428991 | 2.828849 | H | -3.264228 | 3.982468 | 4.082836 |
| H | 0.968664 | -3.096673 | 3.663802 | C | -3.701052 | 2.917823 | 2.262891 |
| N | -2.217122 | 1.111980 | 1.707901 | H | -4.576414 | 3.517197 | 2.025558 |
| C | -0.415645 | -2.136741 | 2.198844 | C | -3.315978 | 1.876944 | 1.421416 |
| N | -3.511552 | 0.426557 | -0.442579 | C | -4.040227 | 1.502046 | 0.200639 |
| C | -1.796164 | -2.523187 | 2.400336 | C | -5.172145 | 2.126442 | -0.310915 |
| N | -2.276038 | -1.661329 | -1.344125 | H | -5.639596 | 2.988511 | 0.157199 |
| C | -2.220638 | -3.486690 | 3.316663 | C | -5.718787 | 1.615353 | -1.481394 |
| H | -1.488228 | -3.995157 | 3.939126 | C | -5.185249 | 0.516285 | -2.135155 |
| C | -3.571157 | -3.788779 | 3.417414 | H | -5.661926 | 0.158053 | -3.043771 |
| H | -3.914985 | -4.537355 | 4.127023 | C | -4.053024 | -0.078149 | -1.581555 |
| C | -4.478225 | -3.123336 | 2.592757 | C | -3.357736 | -1.262255 | -2.085410 |
| H | -5.543331 | -3.331926 | 2.637890 | C | -3.761945 | -1.979745 | -3.209892 |
| C | -3.997832 | -2.176121 | 1.702662 | H | -4.621955 | -1.649623 | -3.787185 |
| H | -4.669286 | -1.630739 | 1.041306 | C | -3.065555 | -3.122395 | -3.583251 |
| C | 2.424026 | -2.801417 | -1.138036 | H | -3.373721 | -3.691173 | -4.456881 |
| H | 1.719188 | -2.972411 | -0.325696 | C | -1.976612 | -3.528636 | -2.815753 |
| C | 2.841034 | -3.830719 | -1.972873 | H | -1.411978 | -4.422091 | -3.067682 |
| H | 2.463650 | -4.838541 | -1.822302 | C | -1.616319 | -2.772742 | -1.708400 |
| C | 3.753853 | -3.541900 | -2.981652 | H | -0.776054 | -3.045455 | -1.072985 |
| H | 4.105734 | -4.320744 | -3.653728 | O | 1.437437 | 0.339895 | -2.609457 |
| C | 4.225506 | -2.239824 | -3.112515 | H | 1.441832 | 1.323857 | -2.696435 |
| H | 4.949129 | -2.000081 | -3.886943 | H | 0.499495 | 0.144818 | -2.431940 |
| C | 3.772846 | -1.248555 | -2.246783 | H | 0.766845 | 2.733642 | -1.368073 |
| C | 4.260779 | 0.137897 | -2.280636 | O | 1.362991 | 3.024525 | -2.086787 |
| C | 5.212812 | 0.652115 | -3.156932 | H | 0.894399 | 3.723792 | -2.563922 |
| H | 5.642095 | 0.032116 | -3.939011 | N | -6.92324 | 2.272093 | -2.051808 |
| C | 5.617481 | 1.979676 | -3.020509 | O | -7.36787 | 1.784562 | -3.08054 |
| H | 6.355835 | 2.391792 | -3.703550 | O | -7.35195 | 3.238061 | -1.43746 |

TS-2 A (4+ doublet)

E= -2901.123 02 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.574768 | -0.279013 | 0.336872 | O | 0.767821 | 0.660245 | -0.999661 |
| Ru | 2.506066 | 0.152316 | -0.213597 | C | -3.593666 | -1.769038 | 2.082914 |
| N | -2.301181 | -1.393676 | 1.971133 | H | -4.250972 | -1.501794 | 1.260341 |
| O | -0.156239 | -0.330397 | -1.090705 | N | 0.129784 | -0.752982 | 1.501708 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -4.077243 | -2.449051 | 3.188646 | C | -3.221647 | -1.858662 | -1.540743 |
| H | -5.128776 | -2.719890 | 3.230825 | C | -3.652521 | -2.888252 | -2.375272 |
| N | 1.425980 | -0.487465 | 1.378312 | H | -4.580879 | -2.789088 | -2.932497 |
| C | -3.201712 | -2.765418 | 4.228179 | C | -2.894619 | -4.049829 | -2.477879 |
| H | -3.555854 | -3.294897 | 5.109605 | H | -3.223662 | -4.863473 | -3.119979 |
| N | 3.992630 | -0.230868 | 1.268798 | C | -1.719267 | -4.156950 | -1.738229 |
| C | -1.867680 | -2.401802 | 4.114355 | H | -1.107443 | -5.054007 | -1.780958 |
| H | -1.153501 | -2.645637 | 4.897241 | C | -1.332377 | -3.093992 | -0.931817 |
| N | -2.065804 | 1.430165 | 1.503688 | H | -0.420049 | -3.117353 | -0.340400 |
| C | -1.429434 | -1.722983 | 2.976677 | C | 2.610738 | -2.933741 | -0.574700 |
| N | -3.391735 | 0.189563 | -0.383326 | H | 2.082872 | -2.924056 | 0.378053 |
| C | -0.065095 | -1.348430 | 2.710984 | C | 2.941317 | -4.120327 | -1.214138 |
| N | -2.056295 | -1.969810 | -0.833610 | H | 2.677095 | -5.072285 | -0.761005 |
| C | 1.160375 | -1.473314 | 3.379217 | C | 3.638060 | -4.061002 | -2.418948 |
| H | 1.344385 | -1.913704 | 4.351582 | H | 3.924354 | -4.971016 | -2.941161 |
| N | 2.931015 | -1.728409 | -1.077815 | C | 3.986242 | -2.817678 | -2.938403 |
| C | 2.087059 | -0.918373 | 2.497754 | H | 4.546784 | -2.753677 | -3.867545 |
| N | 3.635154 | 0.662831 | -1.807150 | C | 3.633721 | -1.658591 | -2.252421 |
| C | 3.525862 | -0.741661 | 2.453134 | C | 4.014852 | -0.305774 | -2.676002 |
| N | 2.836609 | 2.205192 | 0.108458 | C | 4.731796 | 0.034410 | -3.820575 |
| C | 4.396796 | -1.043787 | 3.498652 | H | 5.049600 | -0.727015 | -4.527909 |
| H | 4.003418 | -1.447212 | 4.428777 | C | 5.046846 | 1.374182 | -4.048920 |
| C | 5.759575 | -0.819744 | 3.342145 | H | 5.605170 | 1.654763 | -4.938787 |
| H | 6.450218 | -1.050193 | 4.149899 | C | 4.663689 | 2.349869 | -3.133382 |
| C | 6.225755 | -0.293026 | 2.138520 | H | 4.926649 | 3.390658 | -3.303064 |
| H | 7.283206 | -0.102998 | 1.976022 | C | 3.950131 | 1.967422 | -1.996444 |
| C | 5.313566 | -0.011181 | 1.131358 | C | 3.514474 | 2.836961 | -0.902482 |
| H | 5.635038 | 0.397466 | 0.175068 | C | 3.805600 | 4.197371 | -0.822336 |
| C | -1.350986 | 1.970493 | 2.501307 | H | 4.346087 | 4.687652 | -1.628114 |
| H | -0.432463 | 1.449598 | 2.764143 | C | 3.422105 | 4.920613 | 0.301727 |
| C | -1.757363 | 3.118258 | 3.171881 | H | 3.653620 | 5.980469 | 0.376611 |
| H | -1.151724 | 3.515379 | 3.982036 | C | 2.756243 | 4.262403 | 1.332859 |
| C | -2.953563 | 3.723103 | 2.800547 | H | 2.456666 | 4.787441 | 2.235752 |
| H | -3.307697 | 4.616537 | 3.309644 | C | 2.483503 | 2.907741 | 1.198188 |
| C | -3.705454 | 3.158342 | 1.772718 | H | 1.972704 | 2.345374 | 1.977029 |
| H | -4.648827 | 3.610481 | 1.477234 | O | -1.556378 | 2.083089 | -1.126377 |
| C | -3.246170 | 2.011501 | 1.134777 | H | -2.061175 | 2.066311 | -1.977636 |
| C | -3.989005 | 1.318386 | 0.075804 | H | -0.624690 | 2.160207 | -1.381957 |
| C | -5.229567 | 1.691042 | -0.431337 | H | -3.08108 | 1.776846 | -4.166649 |
| H | -5.761684 | 2.582672 | -0.108686 | O | -3.28843 | 2.091907 | -3.274471 |
| C | -5.808477 | 0.871890 | -1.390917 | H | -3.64549 | 2.980619 | -3.425677 |
| C | -5.218964 | -0.301693 | -1.826880 | N | -7.12754 | 1.268638 | -1.969102 |
| H | -5.738347 | -0.918455 | -2.556486 | O | -7.60437 | 0.496639 | -2.78443 |
| C | -3.977822 | -0.634638 | -1.286919 | O | -7.58428 | 2.328067 | -1.5712 |

TS-2 A (4+ quartet)

E= -2901.106 90 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|----------|
| Ru | -1.664579 | -0.611605 | 0.201430 | H | -4.338977 | -2.049991 | 0.657608 |
| Ru | 2.513658 | 0.276412 | -0.166896 | N | 0.073060 | -1.422836 | 0.951918 |
| N | -2.353172 | -2.269217 | 1.214021 | C | -4.073344 | -3.759364 | 1.955923 |
| O | -0.193560 | 0.073611 | -1.412199 | H | -5.125125 | -4.031927 | 1.942695 |
| O | 0.868480 | 0.770388 | -1.098942 | N | 1.355238 | -1.044998 | 0.970722 |
| C | -3.645746 | -2.655379 | 1.236177 | C | -3.139451 | -4.496396 | 2.684839 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -3.448396 | -5.365665 | 3.260578 | H | -4.588265 | -1.238721 | -3.938040 |
| N | 3.923231 | -0.621928 | 1.101170 | C | -3.035513 | -2.732076 | -3.984269 |
| C | -1.806774 | -4.107378 | 2.661901 | H | -3.367134 | -3.167830 | -4.923824 |
| H | -1.054111 | -4.664701 | 3.214476 | C | -1.937259 | -3.255134 | -3.305863 |
| N | -2.130867 | 0.474367 | 1.954543 | H | -1.391112 | -4.110460 | -3.693992 |
| C | -1.424228 | -2.991877 | 1.917313 | C | -1.546488 | -2.670622 | -2.108181 |
| N | -3.423267 | 0.234831 | -0.300791 | H | -0.694593 | -3.036191 | -1.538748 |
| C | -0.073346 | -2.497070 | 1.792942 | C | 2.732001 | -2.359615 | -1.825743 |
| N | -2.194749 | -1.622093 | -1.577250 | H | 2.062405 | -2.752296 | -1.061869 |
| C | 1.159962 | -2.818860 | 2.353529 | C | 3.202960 | -3.153354 | -2.864852 |
| H | 1.386704 | -3.611581 | 3.056043 | H | 2.905724 | -4.196616 | -2.928588 |
| N | 3.079480 | -1.070946 | -1.687495 | C | 4.065977 | -2.590352 | -3.799911 |
| C | 2.040275 | -1.880097 | 1.803311 | H | 4.457578 | -3.182945 | -4.623386 |
| N | 3.758325 | 1.417446 | -1.220999 | C | 4.434480 | -1.254715 | -3.661921 |
| C | 3.460714 | -1.629971 | 1.907507 | H | 5.115441 | -0.802621 | -4.378522 |
| N | 2.548780 | 2.035285 | 1.004415 | C | 3.938302 | -0.507191 | -2.597555 |
| C | 4.326495 | -2.318314 | 2.756973 | C | 4.306024 | 0.893804 | -2.347102 |
| H | 3.938595 | -3.116525 | 3.385203 | C | 5.150758 | 1.685578 | -3.123211 |
| C | 5.671252 | -1.973655 | 2.796993 | H | 5.604059 | 1.298425 | -4.031822 |
| H | 6.355164 | -2.503609 | 3.455819 | C | 5.413100 | 2.993394 | -2.716369 |
| C | 6.129333 | -0.937886 | 1.982740 | H | 6.071370 | 3.621153 | -3.312548 |
| H | 7.173014 | -0.635428 | 1.983794 | C | 4.845002 | 3.501725 | -1.547935 |
| C | 5.230290 | -0.289963 | 1.150347 | H | 5.061880 | 4.519963 | -1.235980 |
| H | 5.549254 | 0.515620 | 0.492889 | C | 4.003738 | 2.683172 | -0.797189 |
| C | -1.464336 | 0.462577 | 3.120239 | C | 3.332442 | 3.024782 | 0.464399 |
| H | -0.585158 | -0.178645 | 3.160642 | C | 3.475403 | 4.249831 | 1.109955 |
| C | -1.868584 | 1.210152 | 4.218885 | H | 4.101007 | 5.026722 | 0.677560 |
| H | -1.303336 | 1.158390 | 5.145776 | C | 2.821420 | 4.474034 | 2.318889 |
| C | -3.015102 | 1.992581 | 4.113324 | H | 2.934497 | 5.425649 | 2.832943 |
| H | -3.368901 | 2.579188 | 4.958005 | C | 2.033900 | 3.461795 | 2.858761 |
| C | -3.718853 | 1.997137 | 2.912815 | H | 1.515108 | 3.594532 | 3.804196 |
| H | -4.629452 | 2.583326 | 2.817513 | C | 1.926332 | 2.258979 | 2.171805 |
| C | -3.264945 | 1.230478 | 1.843761 | H | 1.331708 | 1.430675 | 2.551077 |
| C | -3.968510 | 1.126838 | 0.562897 | O | -1.366886 | 2.282194 | -0.143528 |
| C | -5.101431 | 1.841101 | 0.191163 | H | -2.029616 | 2.836412 | -0.623166 |
| H | -5.566789 | 2.591682 | 0.825067 | H | -0.555535 | 2.400429 | -0.656342 |
| C | -5.630180 | 1.601347 | -1.068414 | H | -3.17346 | 3.993843 | -2.458359 |
| C | -5.111807 | 0.648116 | -1.926902 | O | -3.33048 | 3.750882 | -1.533836 |
| H | -5.591330 | 0.478442 | -2.888007 | H | -3.65702 | 4.572892 | -1.137022 |
| C | -3.974797 | -0.040791 | -1.505900 | N | -6.77009 | 2.439208 | -1.532047 |
| C | -3.287698 | -1.113028 | -2.223977 | O | -7.29214 | 2.102783 | -2.58164 |
| C | -3.717026 | -1.650864 | -3.434708 | O | -7.04603 | 3.395421 | -0.82273 |

TS-2 B (4+ doublet)

E= -2901.122 81 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|----------|-----------|
| Ru | 2.211662 | -0.173068 | -0.024544 | C | 5.749852 | 2.065378 | -1.305148 |
| Ru | -1.850021 | 0.553768 | -0.053107 | H | 6.798210 | 1.817962 | -1.448642 |
| N | 3.553616 | 1.315867 | -0.699576 | N | -0.278811 | 1.796134 | -0.311317 |
| O | 0.478406 | -1.038760 | -0.445733 | C | 5.274210 | 3.361569 | -1.504778 |
| O | -0.499862 | -0.803174 | 0.471278 | H | 5.947065 | 4.158311 | -1.813179 |
| C | 4.865622 | 1.074883 | -0.908455 | N | -2.772825 | 2.458076 | -0.336999 |
| H | 5.207289 | 0.057983 | -0.737609 | C | 3.923895 | 3.615705 | -1.312091 |
| N | 1.022730 | 1.544450 | -0.408421 | H | 3.514164 | 4.610010 | -1.472844 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| N | 2.750919 | 0.450155 | 1.933899 | C | 3.178501 | -2.548363 | -4.180693 |
| C | 3.074608 | 2.581734 | -0.916461 | H | 3.418988 | -3.108329 | -5.081321 |
| N | 3.648465 | -1.496582 | 0.433720 | C | 2.294881 | -1.472543 | -4.226066 |
| C | 1.650293 | 2.703858 | -0.744592 | H | 1.830734 | -1.164175 | -5.158976 |
| N | 2.566325 | -1.118985 | -1.877197 | C | 2.012176 | -0.786875 | -3.052192 |
| C | 0.706689 | 3.733543 | -0.873982 | H | 1.324214 | 0.055069 | -3.024372 |
| H | 0.885762 | 4.767601 | -1.142299 | C | -1.665792 | 0.637707 | -3.152627 |
| N | -2.258574 | 0.096856 | -2.073559 | H | -0.904647 | 1.389505 | -2.948266 |
| C | -0.511239 | 3.116923 | -0.595206 | C | -2.007192 | 0.277522 | -4.449204 |
| N | -3.432037 | -0.691607 | 0.101392 | H | -1.512478 | 0.754288 | -5.291466 |
| C | -1.910914 | 3.497208 | -0.581217 | C | -3.006687 | -0.673553 | -4.641487 |
| N | -2.352362 | 0.710386 | 1.985012 | H | -3.307858 | -0.969458 | -5.643789 |
| C | -2.386006 | 4.791176 | -0.788855 | C | -3.635907 | -1.226923 | -3.529978 |
| H | -1.683761 | 5.599242 | -0.980041 | H | -4.432279 | -1.955568 | -3.660053 |
| C | -3.753782 | 5.034918 | -0.744385 | C | -3.256189 | -0.825182 | -2.252490 |
| H | -4.137945 | 6.039572 | -0.904511 | C | -3.903039 | -1.290162 | -1.021365 |
| C | -4.622917 | 3.975338 | -0.488985 | C | -4.930686 | -2.224542 | -0.931836 |
| H | -5.698521 | 4.123563 | -0.445677 | H | -5.350423 | -2.737941 | -1.793707 |
| C | -4.094529 | 2.707554 | -0.289419 | C | -5.436712 | -2.504223 | 0.330110 |
| H | -4.737232 | 1.852008 | -0.089755 | C | -4.973637 | -1.878089 | 1.475529 |
| C | 2.271902 | 1.501302 | 2.615517 | H | -5.425139 | -2.126617 | 2.433211 |
| H | 1.558802 | 2.127096 | 2.082444 | C | -3.944953 | -0.947421 | 1.330591 |
| C | 2.665871 | 1.786392 | 3.916964 | C | -3.349695 | -0.137344 | 2.392984 |
| H | 2.259367 | 2.654586 | 4.428708 | C | -3.784631 | -0.145744 | 3.716560 |
| C | 3.599072 | 0.956575 | 4.530087 | H | -4.578877 | -0.820839 | 4.025773 |
| H | 3.938120 | 1.154521 | 5.544285 | C | -3.214252 | 0.730265 | 4.634098 |
| C | 4.108947 | -0.127763 | 3.820498 | H | -3.553321 | 0.738767 | 5.667324 |
| H | 4.846350 | -0.779375 | 4.281841 | C | -2.221225 | 1.606413 | 4.202609 |
| C | 3.673819 | -0.368157 | 2.522032 | H | -1.766058 | 2.321152 | 4.882935 |
| C | 4.183225 | -1.457338 | 1.679385 | C | -1.819908 | 1.566186 | 2.873712 |
| C | 5.172036 | -2.373328 | 2.026343 | H | -1.055567 | 2.235859 | 2.485296 |
| H | 5.623540 | -2.355947 | 3.014702 | O | 1.439602 | -1.987571 | 2.013083 |
| C | 5.596127 | -3.308829 | 1.081899 | H | 1.637510 | -2.933952 | 1.802405 |
| H | 6.371310 | -4.025994 | 1.341877 | H | 0.473712 | -1.918885 | 1.993014 |
| C | 5.053933 | -3.308230 | -0.198853 | H | 1.841013 | -5.209400 | 0.998540 |
| H | 5.405238 | -4.017744 | -0.943310 | O | 2.340157 | -4.540695 | 1.489937 |
| C | 4.069553 | -2.371836 | -0.513055 | H | 2.592775 | -5.000031 | 2.305215 |
| C | 3.451858 | -2.160164 | -1.820865 | N | -6.52968 | -3.515283 | 0.456346 |
| C | 3.762420 | -2.891536 | -2.966254 | O | -6.93726 | -3.71745 | 1.588106 |
| H | 4.465959 | -3.718585 | -2.912709 | O | -6.8948 | -4.03427 | -0.58564 |

TS-2 B (4+ quartet)

E= -2901.108 88 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.246466 | -0.161909 | -0.108303 | N | -0.214862 | 1.777276 | -0.243045 |
| Ru | -1.788614 | 0.577036 | -0.048473 | C | 5.359565 | 3.341300 | -1.419520 |
| N | 3.619038 | 1.276318 | -0.717374 | H | 6.041080 | 4.144018 | -1.690943 |
| O | 0.436843 | -1.266226 | -0.649886 | N | -2.674769 | 2.515538 | -0.033636 |
| O | -0.787706 | -1.171518 | -0.133865 | C | 4.009154 | 3.600323 | -1.225970 |
| C | 4.930132 | 1.034480 | -0.915694 | H | 3.611730 | 4.605507 | -1.345908 |
| H | 5.256453 | 0.006256 | -0.781292 | N | 2.717096 | 0.407628 | 1.890333 |
| N | 1.089436 | 1.511248 | -0.434475 | C | 3.149072 | 2.557693 | -0.881052 |
| C | 5.824569 | 2.034986 | -1.266896 | N | 3.577216 | -1.584426 | 0.408337 |
| H | 6.872122 | 1.786777 | -1.415393 | C | 1.726073 | 2.682091 | -0.685427 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| N | 2.627094 | -1.147658 | -1.942551 | C | 2.438887 | -1.491086 | -4.302377 |
| C | 0.796502 | 3.740997 | -0.662793 | H | 2.033547 | -1.159262 | -5.254202 |
| H | 0.989440 | 4.793159 | -0.836055 | C | 2.140618 | -0.790762 | -3.141197 |
| N | -2.385928 | 0.393007 | -2.059013 | H | 1.497237 | 0.086685 | -3.146040 |
| C | -0.420040 | 3.131708 | -0.381280 | C | -1.837695 | 1.039242 | -3.103098 |
| N | -3.435970 | -0.615079 | 0.080922 | H | -1.011766 | 1.709499 | -2.871455 |
| C | -1.800641 | 3.551719 | -0.238845 | C | -2.298090 | 0.872640 | -4.402889 |
| N | -2.100602 | 0.429224 | 2.031291 | H | -1.831410 | 1.424493 | -5.214525 |
| C | -2.245907 | 4.870856 | -0.295910 | C | -3.364952 | 0.008617 | -4.634833 |
| H | -1.533884 | 5.676224 | -0.460919 | H | -3.754149 | -0.137667 | -5.639777 |
| C | -3.600641 | 5.142321 | -0.138881 | C | -3.941564 | -0.656162 | -3.556683 |
| H | -3.963468 | 6.166673 | -0.180160 | H | -4.786291 | -1.322441 | -3.713486 |
| C | -4.483919 | 4.084729 | 0.072844 | C | -3.444850 | -0.448217 | -2.273041 |
| H | -5.549131 | 4.255335 | 0.203277 | C | -4.018284 | -1.043145 | -1.064179 |
| C | -3.983494 | 2.790770 | 0.116510 | C | -5.081044 | -1.943415 | -1.011322 |
| H | -4.637924 | 1.936078 | 0.277457 | H | -5.590927 | -2.321052 | -1.894662 |
| C | 2.314225 | 1.501430 | 2.554636 | C | -5.497628 | -2.370521 | 0.239772 |
| H | 1.671925 | 2.184536 | 2.000809 | C | -4.908478 | -1.927890 | 1.413650 |
| C | 2.697679 | 1.769730 | 3.862344 | H | -5.288117 | -2.292088 | 2.365512 |
| H | 2.356053 | 2.677516 | 4.353026 | C | -3.850255 | -1.027572 | 1.302648 |
| C | 3.541651 | 0.870965 | 4.507595 | C | -3.113280 | -0.413773 | 2.408565 |
| H | 3.870863 | 1.049997 | 5.528501 | C | -3.418957 | -0.603749 | 3.753727 |
| C | 3.979131 | -0.255448 | 3.817872 | H | -4.229140 | -1.270109 | 4.039738 |
| H | 4.654676 | -0.956657 | 4.300374 | C | -2.696733 | 0.078308 | 4.728228 |
| C | 3.562147 | -0.472855 | 2.507847 | H | -2.934388 | -0.056957 | 5.780817 |
| C | 4.030048 | -1.596373 | 1.686325 | C | -1.683116 | 0.947451 | 4.332219 |
| C | 4.915776 | -2.593018 | 2.089189 | H | -1.108849 | 1.513733 | 5.060570 |
| H | 5.292501 | -2.624769 | 3.107848 | C | -1.419325 | 1.099506 | 2.977669 |
| C | 5.334866 | -3.547972 | 1.162799 | H | -0.648628 | 1.776140 | 2.615399 |
| H | 6.032144 | -4.325520 | 1.465855 | O | 1.176030 | -1.871834 | 1.880344 |
| C | 4.883502 | -3.492948 | -0.151292 | H | 1.290579 | -2.770113 | 1.479135 |
| H | 5.227664 | -4.221381 | -0.880665 | H | 0.214840 | -1.760170 | 1.909063 |
| C | 3.989844 | -2.485555 | -0.513388 | H | 1.045102 | -4.658797 | 0.049896 |
| C | 3.449793 | -2.235976 | -1.849023 | O | 1.686973 | -4.302400 | 0.680942 |
| C | 3.769275 | -2.985503 | -2.979710 | H | 1.867971 | -5.046046 | 1.276093 |
| H | 4.423000 | -3.849942 | -2.894511 | N | -6.62782 | -3.345324 | 0.326670 |
| C | 3.260776 | -2.612421 | -4.218977 | O | -6.94698 | -3.68696 | 1.453278 |
| H | 3.511069 | -3.185108 | -5.108890 | O | -7.10682 | -3.69724 | -0.73825 |

Min-3 A (3+ unrestricted singlet)

E= -2901.610 74 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.801258 | -0.248959 | 0.313941 | H | -3.557086 | -3.637474 | 4.858326 |
| Ru | 2.560227 | 0.202572 | -0.250990 | N | 3.821064 | 0.259088 | 1.496572 |
| N | -2.445435 | -1.536827 | 1.800567 | C | -1.947918 | -2.563174 | 3.916381 |
| O | 0.314528 | -0.856485 | -1.488444 | H | -1.224941 | -2.763681 | 4.703404 |
| O | 1.180168 | 0.155402 | -1.591112 | N | -2.279328 | 1.387519 | 1.559034 |
| C | -3.699524 | -2.024649 | 1.884891 | C | -1.560068 | -1.811743 | 2.805930 |
| H | -4.361712 | -1.784222 | 1.056076 | N | -3.587118 | 0.262909 | -0.406619 |
| N | -0.025569 | -0.696717 | 1.366102 | C | -0.234462 | -1.289893 | 2.581717 |
| C | -4.134193 | -2.783694 | 2.958092 | N | -2.216193 | -1.821194 | -1.031935 |
| H | -5.155048 | -3.154224 | 2.976213 | C | 0.939017 | -1.246816 | 3.335099 |
| N | 1.247393 | -0.289372 | 1.315957 | H | 1.104027 | -1.632047 | 4.333823 |
| C | -3.243569 | -3.051068 | 3.998229 | N | 3.195278 | -1.773387 | -0.641373 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 1.853951 | -0.604329 | 2.500309 | H | -0.558671 | -2.978635 | -0.652657 |
| N | 3.991372 | 0.533056 | -1.588519 | C | 2.725022 | -2.913894 | -0.116486 |
| C | 3.253494 | -0.249290 | 2.629735 | H | 1.920454 | -2.798858 | 0.607957 |
| N | 2.560883 | 2.298761 | -0.339751 | C | 3.231443 | -4.161048 | -0.461398 |
| C | 3.990356 | -0.381968 | 3.806647 | H | 2.827288 | -5.057775 | 0.000182 |
| H | 3.515691 | -0.789027 | 4.696249 | C | 4.264567 | -4.229144 | -1.390385 |
| C | 5.321081 | 0.014358 | 3.830377 | H | 4.689900 | -5.186972 | -1.679889 |
| H | 5.906468 | -0.083323 | 4.741418 | C | 4.752578 | -3.050712 | -1.947068 |
| C | 5.891623 | 0.544090 | 2.674114 | H | 5.556725 | -3.085678 | -2.677493 |
| H | 6.926446 | 0.873618 | 2.652540 | C | 4.207752 | -1.828827 | -1.562595 |
| C | 5.108575 | 0.647158 | 1.534540 | C | 4.656798 | -0.532979 | -2.097802 |
| H | 5.511909 | 1.051599 | 0.607190 | C | 5.662084 | -0.326661 | -3.039082 |
| C | -1.594680 | 1.860698 | 2.612546 | H | 6.211171 | -1.163801 | -3.461654 |
| H | -0.692623 | 1.311163 | 2.876836 | C | 5.957978 | 0.976126 | -3.440523 |
| C | -2.004729 | 2.975893 | 3.332760 | H | 6.738678 | 1.150124 | -4.176511 |
| H | -1.419558 | 3.314323 | 4.183494 | C | 5.262709 | 2.053587 | -2.900500 |
| C | -3.171491 | 3.630203 | 2.950482 | H | 5.499905 | 3.067688 | -3.210902 |
| H | -3.524591 | 4.503373 | 3.493580 | C | 4.264881 | 1.808467 | -1.955874 |
| C | -3.892294 | 3.141396 | 1.866182 | C | 3.458305 | 2.805817 | -1.247150 |
| H | -4.813857 | 3.628853 | 1.558643 | C | 3.593368 | 4.181160 | -1.427509 |
| C | -3.435545 | 2.016324 | 1.184661 | H | 4.308183 | 4.567325 | -2.149779 |
| C | -4.161831 | 1.396865 | 0.070065 | C | 2.817859 | 5.056593 | -0.677101 |
| C | -5.359567 | 1.847973 | -0.476180 | H | 2.917972 | 6.130660 | -0.811279 |
| H | -5.864908 | 2.749558 | -0.141067 | C | 1.921582 | 4.534372 | 0.251737 |
| C | -5.924281 | 1.099705 | -1.499551 | H | 1.303374 | 5.183569 | 0.865410 |
| C | -5.350855 | -0.069908 | -1.971277 | C | 1.826042 | 3.156501 | 0.389327 |
| H | -5.842256 | -0.619976 | -2.769243 | H | 1.145720 | 2.695442 | 1.103953 |
| C | -4.151724 | -0.478677 | -1.391880 | H | -0.853046 | -0.458105 | -2.985625 |
| C | -3.398509 | -1.690851 | -1.706588 | O | -1.607047 | 0.099392 | -3.276355 |
| C | -3.840177 | -2.671528 | -2.590065 | H | -1.398574 | 0.399738 | -4.172848 |
| H | -4.781865 | -2.545334 | -3.118321 | O | -1.19685 | 1.396881 | -1.013313 |
| C | -3.073515 | -3.814337 | -2.782571 | H | -1.45209 | 1.112248 | -1.941724 |
| H | -3.407493 | -4.590526 | -3.466536 | H | -0.22276 | 1.419902 | -1.069887 |
| C | -1.881552 | -3.950027 | -2.076684 | N | -7.19761 | 1.568309 | -2.107957 |
| H | -1.258690 | -4.833232 | -2.187949 | O | -7.65817 | 0.87005 | -2.99869 |
| C | -1.488589 | -2.935325 | -1.213656 | O | -7.65936 | 2.607166 | -1.6593 |

Min-3 A (3+ triplet)

E= -2901.607 29 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.876897 | -0.160821 | 0.370048 | C | -1.960898 | -1.620518 | 4.383318 |
| Ru | 2.620536 | 0.143950 | -0.259120 | H | -1.216027 | -1.664896 | 5.174147 |
| N | -2.509936 | -1.055202 | 2.109837 | N | -2.363705 | 1.718833 | 1.175787 |
| O | 0.572096 | -1.213979 | -1.397700 | C | -1.599094 | -1.130662 | 3.126495 |
| O | 1.217317 | -0.076559 | -1.671290 | N | -3.654433 | 0.137313 | -0.447791 |
| C | -3.767682 | -1.488839 | 2.332831 | C | -0.271041 | -0.698922 | 2.769890 |
| H | -4.453427 | -1.415996 | 1.491903 | N | -2.212829 | -1.995314 | -0.599979 |
| N | -0.053565 | -0.379421 | 1.451242 | C | 0.903143 | -0.535847 | 3.502040 |
| C | -4.177514 | -1.993532 | 3.555277 | H | 1.057598 | -0.706722 | 4.560211 |
| H | -5.202716 | -2.330172 | 3.680351 | N | 3.340721 | -1.836519 | -0.317111 |
| N | 1.236805 | -0.036057 | 1.321113 | C | 1.833656 | -0.113063 | 2.557208 |
| C | -3.259146 | -2.053431 | 4.604296 | N | 4.037881 | 0.273049 | -1.649402 |
| H | -3.553769 | -2.437967 | 5.577456 | C | 3.237072 | 0.223494 | 2.639079 |
| N | 3.840692 | 0.462055 | 1.437635 | N | 2.594818 | 2.194443 | -0.677193 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 3.948180 | 0.327058 | 3.836669 | H | 2.133248 | -2.648854 | 1.143225 |
| H | 3.443418 | 0.134417 | 4.780323 | C | 3.468654 | -4.143372 | 0.309812 |
| C | 5.287447 | 0.686902 | 3.808778 | H | 3.107746 | -4.948564 | 0.943763 |
| H | 5.853083 | 0.772514 | 4.733248 | C | 4.478528 | -4.356046 | -0.624633 |
| C | 5.893864 | 0.942980 | 2.578731 | H | 4.928358 | -5.338750 | -0.742779 |
| H | 6.939211 | 1.230914 | 2.512421 | C | 4.910087 | -3.290514 | -1.406499 |
| C | 5.138633 | 0.819389 | 1.423414 | H | 5.696858 | -3.435993 | -2.142245 |
| H | 5.571313 | 1.002026 | 0.441252 | C | 4.332284 | -2.034208 | -1.239040 |
| C | -1.687341 | 2.438666 | 2.085701 | C | 4.721664 | -0.843405 | -2.002032 |
| H | -0.774285 | 1.980759 | 2.464076 | C | 5.691511 | -0.773711 | -3.000273 |
| C | -2.117830 | 3.682842 | 2.528967 | H | 6.251570 | -1.657851 | -3.292905 |
| H | -1.538828 | 4.221579 | 3.274165 | C | 5.936067 | 0.447533 | -3.624224 |
| C | -3.298196 | 4.208015 | 2.011683 | H | 6.688309 | 0.516021 | -4.405626 |
| H | -3.667030 | 5.177233 | 2.338060 | C | 5.222845 | 1.581222 | -3.245191 |
| C | -4.012046 | 3.465737 | 1.077183 | H | 5.417979 | 2.535558 | -3.727013 |
| H | -4.944410 | 3.849998 | 0.671329 | C | 4.262746 | 1.473545 | -2.239479 |
| C | -3.535161 | 2.220912 | 0.674686 | C | 3.447316 | 2.558916 | -1.688268 |
| C | -4.250322 | 1.342801 | -0.257973 | C | 3.528563 | 3.885322 | -2.107543 |
| C | -5.449850 | 1.630055 | -0.902395 | H | 4.208142 | 4.161888 | -2.909596 |
| H | -5.973007 | 2.576073 | -0.793162 | C | 2.743184 | 4.853606 | -1.493557 |
| C | -5.990446 | 0.652003 | -1.725241 | H | 2.802352 | 5.890641 | -1.814145 |
| C | -5.387619 | -0.582119 | -1.912572 | C | 1.891007 | 4.475186 | -0.459046 |
| H | -5.857586 | -1.309108 | -2.569415 | H | 1.268118 | 5.202930 | 0.053586 |
| C | -4.188467 | -0.822569 | -1.245958 | C | 1.849191 | 3.140876 | -0.081072 |
| C | -3.395675 | -2.051227 | -1.285850 | H | 1.207548 | 2.788411 | 0.724728 |
| C | -3.795440 | -3.209783 | -1.945846 | H | -0.715434 | -1.229267 | -2.910576 |
| H | -4.738466 | -3.232012 | -2.486231 | O | -1.512952 | -0.791191 | -3.272478 |
| C | -2.983985 | -4.336718 | -1.902462 | H | -1.335834 | -0.646509 | -4.213386 |
| H | -3.284287 | -5.249141 | -2.411420 | O | -1.2409 | 1.016004 | -1.348089 |
| C | -1.789349 | -4.277386 | -1.189682 | H | -1.4752 | 0.496860 | -2.173457 |
| H | -1.130567 | -5.138736 | -1.122689 | H | -0.26237 | 1.018131 | -1.395871 |
| C | -1.442066 | -3.093864 | -0.552253 | N | -7.26512 | 0.939680 | -2.433207 |
| H | -0.512997 | -2.985869 | 0.002605 | O | -7.70103 | 0.046058 | -3.14387 |
| C | 2.926562 | -2.870988 | 0.430961 | O | -7.75407 | 2.042766 | -2.23773 |

Min-3 B (3+ unrestricted singlet)

E= -2901.611 14 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.453492 | 0.133937 | -0.164213 | N | 3.054982 | -1.817494 | -0.722789 |
| Ru | -1.900683 | -0.267917 | 0.240475 | C | 3.052054 | -0.711843 | 2.602602 |
| N | 3.607154 | -0.040657 | 1.548011 | N | 3.934859 | 0.535151 | -1.455061 |
| O | 0.101027 | 1.592438 | -0.291176 | C | 1.662384 | -1.046456 | 2.418737 |
| O | -0.886962 | 0.925481 | -0.901417 | N | 2.720863 | 2.214248 | 0.063820 |
| C | 4.889215 | 0.367439 | 1.635915 | C | 0.718690 | -1.760144 | 3.157785 |
| H | 5.280071 | 0.902302 | 0.773136 | H | 0.856309 | -2.258404 | 4.109569 |
| N | 1.084972 | -0.567549 | 1.273551 | N | -2.402762 | 1.277360 | 1.584371 |
| C | 5.674086 | 0.123272 | 2.749863 | C | -0.446641 | -1.671357 | 2.394673 |
| H | 6.701228 | 0.475755 | 2.771593 | N | -3.623646 | 0.328256 | -0.522993 |
| N | -0.198346 | -0.940277 | 1.266878 | C | -1.802976 | -2.154526 | 2.568044 |
| C | 5.121923 | -0.578188 | 3.822419 | N | -2.124118 | -1.613278 | -1.351241 |
| H | 5.715307 | -0.792049 | 4.707937 | C | -2.205709 | -3.008560 | 3.594449 |
| N | -2.688298 | -1.722238 | 1.622120 | H | -1.481620 | -3.339066 | 4.335339 |
| C | 3.801437 | -0.994395 | 3.746020 | C | -3.526935 | -3.432494 | 3.655199 |
| H | 3.336926 | -1.533316 | 4.568247 | H | -3.853690 | -4.098067 | 4.450453 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -4.423310 | -2.997900 | 2.680623 | C | -2.161881 | 2.744666 | 3.461780 |
| H | -5.463196 | -3.311868 | 2.686340 | H | -1.574601 | 3.052346 | 4.322623 |
| C | -3.963063 | -2.146474 | 1.687293 | C | -3.372222 | 3.359152 | 3.156592 |
| H | -4.627893 | -1.779925 | 0.906430 | H | -3.756971 | 4.167534 | 3.773443 |
| C | 2.609333 | -2.989424 | -0.242788 | C | -4.091014 | 2.922734 | 2.047914 |
| H | 1.881073 | -2.925197 | 0.564103 | H | -5.037470 | 3.391884 | 1.791383 |
| C | 3.046719 | -4.213624 | -0.732419 | C | -3.592386 | 1.880174 | 1.272099 |
| H | 2.662596 | -5.135433 | -0.304203 | C | -4.279390 | 1.351848 | 0.084487 |
| C | 3.984299 | -4.227225 | -1.760178 | C | -5.488392 | 1.800842 | -0.435674 |
| H | 4.352591 | -5.166463 | -2.165569 | H | -6.060359 | 2.614713 | 0.001735 |
| C | 4.457660 | -3.017357 | -2.256080 | C | -5.974473 | 1.172122 | -1.575181 |
| H | 5.199811 | -3.007633 | -3.049953 | C | -5.307939 | 0.125503 | -2.192996 |
| C | 3.987512 | -1.819385 | -1.723959 | H | -5.742310 | -0.328939 | -3.079439 |
| C | 4.474599 | -0.499273 | -2.144152 | C | -4.101877 | -0.291746 | -1.633071 |
| C | 5.436482 | -0.249687 | -3.120479 | C | -3.257508 | -1.394947 | -2.095187 |
| H | 5.881479 | -1.064526 | -3.684796 | C | -3.571225 | -2.208551 | -3.182466 |
| C | 5.828543 | 1.064966 | -3.366649 | H | -4.473570 | -2.021460 | -3.759415 |
| H | 6.574414 | 1.273348 | -4.129408 | C | -2.731620 | -3.263507 | -3.518993 |
| C | 5.277959 | 2.108256 | -2.629835 | H | -2.969197 | -3.904817 | -4.363906 |
| H | 5.590359 | 3.133205 | -2.810682 | C | -1.591670 | -3.487607 | -2.750992 |
| C | 4.318295 | 1.816998 | -1.660546 | H | -0.914082 | -4.307068 | -2.974174 |
| C | 3.663006 | 2.764478 | -0.760127 | C | -1.326979 | -2.644450 | -1.680831 |
| C | 3.976535 | 4.118857 | -0.690006 | H | -0.452731 | -2.777176 | -1.045126 |
| H | 4.726037 | 4.539665 | -1.355341 | O | 1.367860 | -0.059802 | -2.066201 |
| C | 3.332656 | 4.924599 | 0.240981 | H | 1.421604 | 0.842996 | -2.502013 |
| H | 3.570939 | 5.983160 | 0.308405 | H | 0.412516 | -0.132400 | -1.875028 |
| C | 2.390084 | 4.351213 | 1.089824 | H | 0.768289 | 2.583449 | -1.814240 |
| H | 1.873397 | 4.943077 | 1.840140 | O | 1.345236 | 2.525931 | -2.606818 |
| C | 2.112486 | 2.996071 | 0.970737 | H | 0.871792 | 2.970369 | -3.324881 |
| H | 1.372082 | 2.497962 | 1.591560 | N | -7.26107 | 1.638659 | -2.153464 |
| C | -1.712934 | 1.710137 | 2.649571 | O | -7.64633 | 1.053418 | -3.15503 |
| H | -0.776040 | 1.189932 | 2.842870 | O | -7.8103 | 2.563374 | -1.57249 |

Min-3 B (3+ triplet)

E= -2901.607 97 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | 2.536413 | 0.115391 | -0.169708 | N | 4.027337 | 0.465591 | -1.455525 |
| Ru | -1.954089 | -0.251846 | 0.254088 | C | 1.669024 | -0.873291 | 2.450797 |
| N | 3.660977 | 0.015087 | 1.554482 | N | 2.752176 | 2.203236 | -0.048825 |
| O | -0.115501 | 1.689011 | -0.382648 | C | 0.720283 | -1.526504 | 3.230164 |
| O | -0.917516 | 0.837184 | -1.045580 | H | 0.850918 | -1.963846 | 4.212260 |
| C | 4.952091 | 0.393672 | 1.646124 | N | -2.500691 | 1.355517 | 1.503344 |
| H | 5.380222 | 0.849146 | 0.756081 | C | -0.441310 | -1.480432 | 2.458403 |
| N | 1.100960 | -0.465103 | 1.264845 | N | -3.686393 | 0.262592 | -0.533021 |
| C | 5.700633 | 0.213372 | 2.796676 | C | -1.787691 | -1.962053 | 2.676016 |
| H | 6.737034 | 0.537825 | 2.819657 | N | -2.143255 | -1.690311 | -1.253503 |
| N | -0.190552 | -0.826855 | 1.279819 | C | -2.164807 | -2.767137 | 3.752843 |
| C | 5.102177 | -0.388651 | 3.904662 | H | -1.426251 | -3.046511 | 4.500408 |
| H | 5.666819 | -0.549381 | 4.819643 | C | -3.475227 | -3.212069 | 3.849464 |
| N | -2.690527 | -1.592744 | 1.719594 | H | -3.782916 | -3.840136 | 4.681795 |
| C | 3.773024 | -0.773813 | 3.823548 | C | -4.387626 | -2.847464 | 2.859329 |
| H | 3.272842 | -1.235077 | 4.671621 | H | -5.421957 | -3.177839 | 2.893684 |
| N | 3.139148 | -1.848163 | -0.644352 | C | -3.956158 | -2.041126 | 1.817911 |
| C | 3.061856 | -0.557809 | 2.641057 | H | -4.635822 | -1.725136 | 1.028424 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | 2.683631 | -2.998376 | -0.121401 | C | -3.521436 | 3.487973 | 2.973967 |
| H | 1.939003 | -2.897947 | 0.666870 | H | -3.925014 | 4.316293 | 3.550961 |
| C | 3.129874 | -4.242454 | -0.548031 | C | -4.229111 | 2.980439 | 1.889705 |
| H | 2.736818 | -5.144799 | -0.087670 | H | -5.186800 | 3.412314 | 1.610203 |
| C | 4.087598 | -4.301147 | -1.555832 | C | -3.704763 | 1.912390 | 1.165903 |
| H | 4.462872 | -5.257386 | -1.911962 | C | -4.371811 | 1.305258 | 0.008818 |
| C | 4.571441 | -3.114437 | -2.095557 | C | -5.585570 | 1.697716 | -0.545566 |
| H | 5.328934 | -3.139095 | -2.874554 | H | -6.177717 | 2.521525 | -0.156358 |
| C | 4.091771 | -1.894294 | -1.626131 | C | -6.047669 | 0.998618 | -1.652721 |
| C | 4.582667 | -0.592415 | -2.094171 | C | -5.350345 | -0.063903 | -2.206549 |
| C | 5.554173 | -0.376491 | -3.069311 | H | -5.764609 | -0.574898 | -3.071534 |
| H | 6.013036 | -1.211120 | -3.592227 | C | -4.142454 | -0.424072 | -1.614648 |
| C | 5.934943 | 0.930073 | -3.369181 | C | -3.271077 | -1.528221 | -2.018205 |
| H | 6.688454 | 1.112830 | -4.130964 | C | -3.551357 | -2.389878 | -3.076932 |
| C | 5.359778 | 1.999895 | -2.690652 | H | -4.449867 | -2.246863 | -3.672012 |
| H | 5.660036 | 3.019122 | -2.918312 | C | -2.681182 | -3.434177 | -3.363969 |
| C | 4.391767 | 1.743023 | -1.719815 | H | -2.892221 | -4.113189 | -4.186156 |
| C | 3.700249 | 2.725258 | -0.884823 | C | -1.542817 | -3.597291 | -2.578092 |
| C | 3.977379 | 4.089294 | -0.893509 | H | -0.839940 | -4.404390 | -2.765180 |
| H | 4.732807 | 4.487764 | -1.565810 | C | -1.312538 | -2.708493 | -1.537452 |
| C | 3.286317 | 4.934813 | -0.034765 | H | -0.439019 | -2.789115 | -0.892169 |
| H | 3.493652 | 6.001991 | -0.031197 | O | 1.420392 | -0.058959 | -2.027733 |
| C | 2.334321 | 4.391417 | 0.823875 | H | 1.478896 | 0.830610 | -2.488473 |
| H | 1.777851 | 5.016553 | 1.516525 | H | 0.462963 | -0.094005 | -1.812883 |
| C | 2.098993 | 3.023931 | 0.789677 | H | 0.686032 | 2.580153 | -1.909941 |
| H | 1.352708 | 2.547642 | 1.421213 | O | 1.310505 | 2.508408 | -2.664318 |
| C | -1.821171 | 1.858009 | 2.545090 | H | 0.850075 | 2.879435 | -3.430980 |
| H | -0.867682 | 1.377221 | 2.758463 | N | -7.33749 | 1.403423 | -2.266021 |
| C | -2.295497 | 2.918484 | 3.306197 | O | -7.69852 | 0.758499 | -3.23994 |
| H | -1.714598 | 3.283587 | 4.148721 | O | -7.91509 | 2.343234 | -1.73905 |

Min-3 A (4+ doublet)

E= -2901.130 99 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.872018 | -0.346828 | 0.248994 | N | -2.268999 | -1.428447 | -1.507138 |
| Ru | 2.615219 | 0.279820 | -0.192161 | C | 0.899070 | -2.176937 | 2.755314 |
| N | -2.504095 | -2.024576 | 1.270922 | H | 1.071902 | -2.843152 | 3.591743 |
| O | 0.501824 | -0.318401 | -1.869823 | N | 3.334715 | -1.518924 | -1.061681 |
| O | 1.303615 | 0.669094 | -1.556761 | C | 1.801723 | -1.286424 | 2.167247 |
| C | -3.758942 | -2.516230 | 1.238417 | N | 4.097912 | 0.968096 | -1.341359 |
| H | -4.451135 | -2.024749 | 0.558720 | C | 3.188540 | -0.974285 | 2.448580 |
| N | -0.075497 | -1.061355 | 1.043245 | N | 2.645901 | 2.312086 | 0.339626 |
| C | -4.155364 | -3.585349 | 2.026449 | C | 3.882627 | -1.441987 | 3.564375 |
| H | -5.177311 | -3.949105 | 1.963221 | H | 3.390891 | -2.106630 | 4.270647 |
| N | 1.200968 | -0.628368 | 1.129128 | C | 5.197835 | -1.041139 | 3.768460 |
| C | -3.228346 | -4.169611 | 2.890270 | H | 5.752481 | -1.396036 | 4.633947 |
| H | -3.513747 | -5.005419 | 3.524701 | C | 5.790805 | -0.171972 | 2.853251 |
| N | 3.782067 | -0.139957 | 1.544639 | H | 6.813860 | 0.171214 | 2.981030 |
| C | -1.932765 | -3.671056 | 2.925534 | C | 5.051586 | 0.253052 | 1.758505 |
| H | -1.185110 | -4.110977 | 3.581162 | H | 5.478259 | 0.923524 | 1.014700 |
| N | -2.454592 | 0.796975 | 1.929716 | C | -1.805233 | 0.894162 | 3.103397 |
| C | -1.585113 | -2.599358 | 2.102721 | H | -0.908954 | 0.284755 | 3.206804 |
| N | -3.673524 | 0.370939 | -0.325448 | C | -2.246501 | 1.717582 | 4.131719 |
| C | -0.267795 | -2.013401 | 2.021605 | H | -1.693688 | 1.756319 | 5.066512 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -3.403104 | 2.469039 | 3.943458 | H | 5.755444 | -2.204100 | -3.325078 |
| H | -3.780029 | 3.117714 | 4.730878 | C | 4.358038 | -1.309519 | -1.949625 |
| C | -4.083577 | 2.368087 | 2.733397 | C | 4.780458 | 0.089628 | -2.115573 |
| H | -4.996167 | 2.936293 | 2.571510 | C | 5.785565 | 0.558407 | -2.958310 |
| C | -3.599188 | 1.523222 | 1.739087 | H | 6.351024 | -0.123930 | -3.587326 |
| C | -4.277547 | 1.294790 | 0.461007 | C | 6.062069 | 1.925840 | -2.989655 |
| C | -5.460965 | 1.896816 | 0.039668 | H | 6.841872 | 2.304208 | -3.646290 |
| H | -5.993982 | 2.642617 | 0.624692 | C | 5.351463 | 2.805877 | -2.178735 |
| C | -5.976281 | 1.512312 | -1.189190 | H | 5.577012 | 3.868815 | -2.198179 |
| C | -5.372679 | 0.551152 | -1.983367 | C | 4.355784 | 2.298945 | -1.341975 |
| H | -5.834301 | 0.278054 | -2.929475 | C | 3.545807 | 3.055379 | -0.384463 |
| C | -4.190666 | -0.020755 | -1.515295 | C | 3.692249 | 4.421572 | -0.152057 |
| C | -3.414921 | -1.073725 | -2.166252 | H | 4.407755 | 5.000110 | -0.730985 |
| C | -3.799299 | -1.720920 | -3.336259 | C | 2.932102 | 5.040200 | 0.834341 |
| H | -4.713825 | -1.429595 | -3.846922 | H | 3.044046 | 6.104863 | 1.025245 |
| C | -3.013310 | -2.753058 | -3.837868 | C | 2.041358 | 4.272288 | 1.581012 |
| H | -3.306210 | -3.272426 | -4.747372 | H | 1.442194 | 4.715364 | 2.371620 |
| C | -1.858789 | -3.118690 | -3.149514 | C | 1.929779 | 2.916318 | 1.304759 |
| H | -1.225957 | -3.928459 | -3.501933 | H | 1.255160 | 2.268941 | 1.864212 |
| C | -1.522008 | -2.438490 | -1.986906 | H | -0.824657 | 0.669289 | -3.343334 |
| H | -0.627137 | -2.675629 | -1.416581 | O | -1.610413 | 1.212859 | -3.158803 |
| C | 2.899202 | -2.770935 | -0.846641 | H | -1.643150 | 1.888423 | -3.854305 |
| H | 2.087103 | -2.872008 | -0.128304 | O | -1.22576 | 1.544579 | -0.583769 |
| C | 3.448027 | -3.873499 | -1.489002 | H | -1.42378 | 1.570135 | -1.574812 |
| H | 3.071822 | -4.870122 | -1.274899 | H | -0.26189 | 1.666985 | -0.545708 |
| C | 4.488901 | -3.672736 | -2.390898 | N | -7.2385 | 2.153705 | -1.670653 |
| H | 4.948292 | -4.513276 | -2.906003 | O | -7.6425 | 1.776968 | -2.75801 |
| C | 4.943146 | -2.376905 | -2.623786 | O | -7.72625 | 2.987274 | -0.92593 |

Min-3 A (4+ quartet)

E= -2901.129 15 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.883114 | -0.366815 | 0.264172 | H | 1.089375 | -2.907363 | 3.537465 |
| Ru | 2.651269 | 0.291312 | -0.179919 | N | 3.357575 | -1.455646 | -1.123152 |
| N | -2.532203 | -2.007480 | 1.329125 | C | 1.811014 | -1.348458 | 2.109322 |
| O | 0.595670 | -0.416462 | -2.244244 | N | 4.134826 | 1.038997 | -1.265551 |
| O | 1.338783 | 0.442300 | -1.653260 | C | 3.207090 | -1.065526 | 2.368211 |
| C | -3.798273 | -2.471499 | 1.341747 | N | 2.598241 | 2.318541 | 0.410130 |
| H | -4.504048 | -1.962067 | 0.689725 | C | 3.913786 | -1.570284 | 3.459671 |
| N | -0.085217 | -1.079912 | 1.034184 | H | 3.417463 | -2.236338 | 4.161268 |
| C | -4.188660 | -3.534891 | 2.139881 | C | 5.242508 | -1.209356 | 3.646384 |
| H | -5.220162 | -3.875486 | 2.114156 | H | 5.803910 | -1.595812 | 4.493689 |
| N | 1.203186 | -0.666597 | 1.094653 | C | 5.840536 | -0.341607 | 2.733824 |
| C | -3.242490 | -4.144298 | 2.965061 | H | 6.874266 | -0.026133 | 2.846047 |
| H | -3.521932 | -4.977732 | 3.605208 | C | 5.095809 | 0.120284 | 1.658698 |
| N | 3.807489 | -0.228346 | 1.469025 | H | 5.528448 | 0.788812 | 0.918117 |
| C | -1.936367 | -3.673884 | 2.954553 | C | -1.793658 | 0.918280 | 3.090393 |
| H | -1.174850 | -4.133574 | 3.579919 | H | -0.900157 | 0.305074 | 3.195831 |
| N | -2.444927 | 0.816726 | 1.918082 | C | -2.229586 | 1.751022 | 4.113433 |
| C | -1.595834 | -2.604912 | 2.124736 | H | -1.675095 | 1.793730 | 5.047094 |
| N | -3.674481 | 0.363337 | -0.320895 | C | -3.383582 | 2.506017 | 3.922282 |
| C | -0.271232 | -2.041859 | 2.008165 | H | -3.756122 | 3.161664 | 4.705995 |
| N | -2.285307 | -1.469048 | -1.476674 | C | -4.068076 | 2.397961 | 2.715176 |
| C | 0.908138 | -2.231289 | 2.710815 | H | -4.980332 | 2.966449 | 2.552110 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|----------|-----------|
| C | -3.589247 | 1.543504 | 1.726157 | C | 4.828824 | 0.197140 | -2.069619 |
| C | -4.273367 | 1.301431 | 0.453885 | C | 5.850934 | 0.706622 | -2.870805 |
| C | -5.455781 | 1.901789 | 0.027069 | H | 6.424714 | 0.056170 | -3.525528 |
| H | -5.984924 | 2.656956 | 0.603576 | C | 6.130762 | 2.070670 | -2.824062 |
| C | -5.975855 | 1.500595 | -1.194544 | H | 6.924189 | 2.480992 | -3.444082 |
| C | -5.376954 | 0.526543 | -1.976840 | C | 5.402523 | 2.912829 | -1.984486 |
| H | -5.842911 | 0.240664 | -2.917021 | H | 5.628143 | 3.975452 | -1.951377 |
| C | -4.195958 | -0.042866 | -1.503929 | C | 4.388819 | 2.368916 | -1.197164 |
| C | -3.425507 | -1.107693 | -2.143727 | C | 3.538036 | 3.084769 | -0.236765 |
| C | -3.813953 | -1.764802 | -3.307091 | C | 3.668798 | 4.441619 | 0.046834 |
| H | -4.723225 | -1.468641 | -3.824440 | H | 4.416336 | 5.038495 | -0.469580 |
| C | -3.042601 | -2.817204 | -3.790406 | C | 2.847714 | 5.030870 | 1.003783 |
| H | -3.340999 | -3.345684 | -4.692886 | H | 2.949234 | 6.088567 | 1.235181 |
| C | -1.898039 | -3.192721 | -3.091150 | C | 1.908325 | 4.243869 | 1.664286 |
| H | -1.278528 | -4.019465 | -3.427365 | H | 1.258251 | 4.664043 | 2.426559 |
| C | -1.554737 | -2.499602 | -1.938166 | C | 1.817990 | 2.896908 | 1.340000 |
| H | -0.669182 | -2.748140 | -1.358434 | H | 1.107305 | 2.233667 | 1.831068 |
| C | 2.922320 | -2.716719 | -0.976210 | H | -1.369580 | 1.149044 | -3.818156 |
| H | 2.096532 | -2.852827 | -0.279140 | O | -1.982156 | 1.542893 | -3.177955 |
| C | 3.489002 | -3.788641 | -1.654730 | H | -2.260217 | 2.379080 | -3.584583 |
| H | 3.110665 | -4.794402 | -1.493662 | O | -1.12414 | 1.419891 | -0.663738 |
| C | 4.546808 | -3.546273 | -2.525838 | H | -1.44778 | 1.543419 | -1.608963 |
| H | 5.017129 | -4.361585 | -3.070497 | H | -0.15334 | 1.399175 | -0.746019 |
| C | 5.002360 | -2.241347 | -2.688399 | N | -7.2366 | 2.139298 | -1.682123 |
| H | 5.829323 | -2.034689 | -3.362894 | O | -7.63997 | 1.754869 | -2.76729 |
| C | 4.400741 | -1.205268 | -1.978749 | O | -7.72411 | 2.979975 | -0.94517 |

Min-3 B (4+ doublet)

E= -2901.131 06 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.556898 | -0.168812 | -0.123895 | C | 0.424744 | 2.151572 | 1.849329 |
| Ru | 1.961989 | 0.314911 | 0.139666 | N | 3.735057 | -0.423232 | -0.416206 |
| N | -3.664824 | 0.397603 | 1.522401 | C | 1.757244 | 2.719691 | 1.883613 |
| O | 0.157299 | -1.775192 | 0.016326 | N | 2.231742 | 1.234791 | -1.728476 |
| O | 1.041752 | -1.157116 | -0.725257 | C | 2.114361 | 3.827073 | 2.653052 |
| C | -4.952067 | 0.056310 | 1.731926 | H | 1.377917 | 4.300006 | 3.298316 |
| H | -5.391788 | -0.628831 | 1.010868 | C | 3.410354 | 4.323249 | 2.576658 |
| N | -1.109708 | 0.782675 | 1.062902 | H | 3.704251 | 5.186385 | 3.169361 |
| C | -5.683667 | 0.550085 | 2.800651 | C | 4.323869 | 3.703931 | 1.723827 |
| H | -6.718106 | 0.243901 | 2.930336 | H | 5.344167 | 4.065723 | 1.629637 |
| N | 0.177328 | 1.169398 | 0.928309 | C | 3.911537 | 2.601661 | 0.989258 |
| C | -5.072248 | 1.437364 | 3.686921 | H | 4.594181 | 2.083218 | 0.318480 |
| H | -5.624365 | 1.845675 | 4.530094 | C | -2.861599 | 2.834742 | -0.881021 |
| N | 2.662332 | 2.105423 | 1.065662 | H | -2.123566 | 2.973543 | -0.092696 |
| C | -3.745002 | 1.789360 | 3.479634 | C | -3.352956 | 3.907572 | -1.612943 |
| H | -3.237955 | 2.471152 | 4.158162 | H | -3.002952 | 4.913649 | -1.398123 |
| N | -3.267150 | 1.570188 | -1.095250 | C | -4.301212 | 3.666883 | -2.603640 |
| C | -3.052755 | 1.253950 | 2.393208 | H | -4.712303 | 4.484975 | -3.190627 |
| N | -4.057962 | -0.898250 | -1.266040 | C | -4.730604 | 2.361883 | -2.824543 |
| C | -1.664801 | 1.513497 | 2.089707 | H | -5.480575 | 2.156898 | -3.584176 |
| N | -2.771249 | -2.133302 | 0.581925 | C | -4.209337 | 1.323510 | -2.057641 |
| C | -0.722957 | 2.393729 | 2.607187 | C | -4.647130 | -0.071326 | -2.162109 |
| H | -0.848882 | 3.104575 | 3.414729 | C | -5.610491 | -0.572903 | -3.035872 |
| N | 2.533813 | -0.752609 | 1.883599 | H | -6.098787 | 0.075400 | -3.758502 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| C | -5.951610 | -1.922525 | -2.967264 | C | 5.607674 | -1.804720 | 0.059581 |
| H | -6.700622 | -2.327162 | -3.643776 | H | 6.191590 | -2.462323 | 0.699262 |
| C | -5.348471 | -2.748417 | -2.023011 | C | 6.078771 | -1.515228 | -1.214054 |
| H | -5.627466 | -3.796552 | -1.954108 | C | 5.406181 | -0.679143 | -2.089850 |
| C | -4.389174 | -2.207531 | -1.166808 | H | 5.836303 | -0.483809 | -3.069454 |
| C | -3.684999 | -2.900263 | -0.089668 | C | 4.201822 | -0.125555 | -1.654681 |
| C | -3.926584 | -4.217502 | 0.289125 | C | 3.361834 | 0.821221 | -2.389936 |
| H | -4.656364 | -4.815652 | -0.250668 | C | 3.686673 | 1.336394 | -3.642999 |
| C | -3.241190 | -4.757598 | 1.371867 | H | 4.584975 | 1.000742 | -4.155458 |
| H | -3.427378 | -5.783348 | 1.681573 | C | 2.865649 | 2.295029 | -4.227574 |
| C | -2.328870 | -3.960890 | 2.060453 | H | 3.113780 | 2.707239 | -5.202799 |
| H | -1.784799 | -4.342179 | 2.920072 | C | 1.735519 | 2.727357 | -3.537392 |
| C | -2.125007 | -2.654132 | 1.640374 | H | 1.078897 | 3.486561 | -3.953221 |
| H | -1.418577 | -1.991087 | 2.134191 | C | 1.455180 | 2.176115 | -2.293948 |
| C | 1.864041 | -0.855169 | 3.042966 | H | 0.589110 | 2.484430 | -1.709543 |
| H | 0.922198 | -0.311261 | 3.095061 | O | -1.449012 | -0.515071 | -1.951791 |
| C | 2.338709 | -1.600320 | 4.115609 | H | -1.440622 | -1.502148 | -2.166694 |
| H | 1.768643 | -1.645183 | 5.039604 | H | -0.504739 | -0.297907 | -1.870141 |
| C | 3.553874 | -2.265978 | 3.984363 | H | -0.65059 | -3.312012 | -1.465056 |
| H | 3.959738 | -2.850746 | 4.806693 | O | -1.35546 | -3.137098 | -2.111035 |
| C | 4.252441 | -2.169706 | 2.782866 | H | -1.15196 | -3.682502 | -2.887007 |
| H | 5.203197 | -2.683139 | 2.663294 | N | 7.369631 | -2.127201 | -1.656134 |
| C | 3.729516 | -1.407412 | 1.743272 | O | 7.738019 | -1.83252 | -2.78088 |
| C | 4.398833 | -1.232968 | 0.446365 | O | 7.914884 | -2.85705 | -0.84507 |

Min-3 B (4+ quartet)

E= -2901.13082 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.561088 | 0.126155 | -0.149500 | C | 1.806400 | -2.797840 | 1.721679 |
| Ru | 1.995986 | -0.282602 | 0.181197 | N | 2.126211 | 1.072281 | 1.795052 |
| N | -3.664218 | -1.614191 | -0.184916 | C | 2.176055 | -3.921374 | 2.461675 |
| O | 0.520936 | 0.381890 | -1.741307 | H | 1.431376 | -4.674677 | 2.707417 |
| O | 1.111910 | 1.195731 | -0.903239 | C | 3.490991 | -4.060477 | 2.888266 |
| C | -4.954958 | -1.701058 | -0.566107 | H | 3.792559 | -4.929488 | 3.468151 |
| H | -5.406041 | -0.789677 | -0.951416 | C | 4.413697 | -3.066562 | 2.565639 |
| N | -1.101267 | -1.298706 | 0.329114 | H | 5.450955 | -3.133010 | 2.882447 |
| C | -5.675363 | -2.881237 | -0.475455 | C | 3.991268 | -1.976302 | 1.818695 |
| H | -6.711968 | -2.903861 | -0.800284 | H | 4.681724 | -1.183931 | 1.537164 |
| N | 0.204425 | -1.326268 | 0.690356 | C | -2.977998 | -0.196820 | 2.906313 |
| C | -5.049318 | -4.018473 | 0.036219 | H | -2.190471 | -0.940434 | 2.795767 |
| H | -5.591996 | -4.956661 | 0.123963 | C | -3.550887 | 0.078634 | 4.141095 |
| N | 2.720321 | -1.835954 | 1.397109 | H | -3.214271 | -0.457634 | 5.024281 |
| C | -3.719850 | -3.936778 | 0.427368 | C | -4.560670 | 1.034401 | 4.215863 |
| H | -3.201650 | -4.808024 | 0.820640 | H | -5.035680 | 1.268254 | 5.165860 |
| N | -3.360173 | 0.429837 | 1.779605 | C | -4.967681 | 1.678788 | 3.051747 |
| C | -3.038803 | -2.725109 | 0.304767 | H | -5.765578 | 2.416241 | 3.087835 |
| N | -4.073549 | 1.419363 | -0.503515 | C | -4.362522 | 1.361114 | 1.838392 |
| C | -1.649386 | -2.524591 | 0.642489 | C | -4.761185 | 1.926858 | 0.546911 |
| N | -2.659536 | 0.146913 | -2.240898 | C | -5.773825 | 2.860332 | 0.326596 |
| C | -0.693970 | -3.331398 | 1.242690 | H | -6.344775 | 3.268414 | 1.156541 |
| H | -0.810954 | -4.344592 | 1.607366 | C | -6.062656 | 3.250530 | -0.978896 |
| N | 2.731202 | -1.421852 | -1.444158 | H | -6.855017 | 3.971107 | -1.167056 |
| C | 0.459133 | -2.542480 | 1.256400 | C | -5.354186 | 2.702155 | -2.044778 |
| N | 3.758071 | 0.594786 | -0.186899 | H | -5.596858 | 2.985383 | -3.065752 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|----------|-----------|
| C | -4.347862 | 1.773209 | -1.781912 | C | 6.074127 | 1.884005 | -0.750543 |
| C | -3.546993 | 1.048046 | -2.769860 | C | 5.327592 | 2.301564 | 0.341888 |
| C | -3.689929 | 1.179651 | -4.148163 | H | 5.690611 | 3.133283 | 0.940825 |
| H | -4.396992 | 1.896402 | -4.558403 | C | 4.142201 | 1.622382 | 0.612227 |
| C | -2.938513 | 0.373725 | -4.998421 | C | 3.234925 | 1.877023 | 1.737681 |
| H | -3.049219 | 0.463094 | -6.076578 | C | 3.476975 | 2.829652 | 2.723779 |
| C | -2.062659 | -0.558238 | -4.448029 | H | 4.361859 | 3.459086 | 2.671561 |
| H | -1.473280 | -1.218140 | -5.078324 | C | 2.588338 | 2.961139 | 3.787173 |
| C | -1.953155 | -0.644965 | -3.066908 | H | 2.775419 | 3.694877 | 4.567740 |
| H | -1.280777 | -1.350065 | -2.583565 | C | 1.471348 | 2.132241 | 3.840661 |
| C | 2.154231 | -2.500162 | -1.997482 | H | 0.763554 | 2.194537 | 4.662545 |
| H | 1.203744 | -2.805262 | -1.561146 | C | 1.277012 | 1.202486 | 2.827183 |
| C | 2.724769 | -3.186570 | -3.062338 | H | 0.424622 | 0.525886 | 2.819574 |
| H | 2.224933 | -4.059506 | -3.473475 | O | -1.374717 | 1.893933 | 0.129661 |
| C | 3.937293 | -2.738347 | -3.580216 | H | -1.761236 | 2.776695 | -0.149026 |
| H | 4.411335 | -3.253871 | -4.412139 | H | -0.465911 | 1.864087 | -0.230477 |
| C | 4.540884 | -1.620757 | -3.012847 | H | -2.13843 | 4.699845 | -1.397853 |
| H | 5.490423 | -1.257590 | -3.398163 | O | -2.45093 | 4.242187 | -0.602467 |
| C | 3.926160 | -0.978304 | -1.940876 | H | -2.50858 | 4.941928 | 0.066150 |
| C | 4.496771 | 0.175416 | -1.243037 | N | 7.345042 | 2.603294 | -1.067024 |
| C | 5.691854 | 0.822582 | -1.554299 | O | 7.6271 | 3.532165 | -0.32785 |
| H | 6.327344 | 0.535017 | -2.388632 | O | 7.964459 | 2.186699 | -2.0316 |

TS-3 A (3+ unrestricted singlet)

E= -2977.993 72 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.070572 | -0.165511 | 0.258466 | C | 3.837597 | -1.791090 | 3.422863 |
| Ru | 2.599240 | -0.051599 | -0.250940 | H | 3.300169 | -2.152729 | 4.295951 |
| N | -2.761338 | -0.531294 | 2.156860 | C | 5.219643 | -1.852878 | 3.361618 |
| O | 0.436968 | -2.120072 | -1.513659 | H | 5.789196 | -2.262237 | 4.192228 |
| O | 0.981186 | -1.002614 | -1.772966 | C | 5.868962 | -1.387185 | 2.215865 |
| C | -4.054350 | -0.438387 | 2.533801 | H | 6.950625 | -1.420224 | 2.123126 |
| H | -4.751138 | -0.102521 | 1.770124 | C | 5.111079 | -0.874507 | 1.179643 |
| N | -0.212010 | -0.585311 | 1.320246 | H | 5.571573 | -0.501968 | 0.268367 |
| C | -4.487106 | -0.748147 | 3.812124 | C | -1.393626 | 2.758137 | 1.064663 |
| H | -5.540712 | -0.653653 | 4.058980 | H | -0.486577 | 2.305797 | 1.461813 |
| N | 1.122590 | -0.696944 | 1.135453 | C | -1.641380 | 4.120475 | 1.165882 |
| C | -3.554332 | -1.178919 | 4.754363 | H | -0.918117 | 4.766244 | 1.658410 |
| H | -3.862138 | -1.434982 | 5.764920 | C | -2.828033 | 4.629404 | 0.641442 |
| N | 3.763038 | -0.805504 | 1.236818 | H | -3.063811 | 5.688169 | 0.715398 |
| C | -2.222806 | -1.271784 | 4.378915 | C | -3.718320 | 3.754232 | 0.030166 |
| H | -1.467333 | -1.599282 | 5.088897 | H | -4.654261 | 4.124710 | -0.380795 |
| N | -2.245811 | 1.899318 | 0.479258 | C | -3.415035 | 2.396000 | -0.043244 |
| C | -1.842757 | -0.940319 | 3.077141 | C | -4.297681 | 1.397381 | -0.648820 |
| N | -3.826323 | 0.124733 | -0.542102 | C | -5.515461 | 1.638931 | -1.275916 |
| C | -0.477307 | -0.979818 | 2.607638 | H | -5.939631 | 2.632919 | -1.388747 |
| N | -2.581966 | -2.131753 | -0.255557 | C | -6.207447 | 0.549280 | -1.785500 |
| C | 0.695219 | -1.349415 | 3.258554 | C | -5.723142 | -0.747848 | -1.690948 |
| H | 0.811368 | -1.699522 | 4.276635 | H | -6.302218 | -1.561243 | -2.119689 |
| N | 3.374213 | -1.736632 | -1.323591 | C | -4.501033 | -0.941466 | -1.054153 |
| C | 1.682473 | -1.151992 | 2.302155 | C | -3.815096 | -2.220467 | -0.851675 |
| N | 4.047842 | 0.739842 | -1.374266 | C | -4.357046 | -3.452118 | -1.210356 |
| C | 3.114548 | -1.265645 | 2.347711 | H | -5.334531 | -3.500749 | -1.683814 |
| N | 2.780159 | 1.839414 | 0.627771 | C | -3.647497 | -4.618332 | -0.946603 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -4.063176 | -5.585803 | -1.216520 | C | 3.695099 | 2.642371 | -0.006015 |
| C | -2.405823 | -4.522876 | -0.325662 | C | 3.994754 | 3.909676 | 0.490796 |
| H | -1.823477 | -5.409910 | -0.092406 | H | 4.734920 | 4.528587 | -0.010837 |
| C | -1.910177 | -3.267119 | 0.000694 | C | 3.373455 | 4.366485 | 1.646965 |
| H | -0.939517 | -3.136353 | 0.474589 | H | 3.613608 | 5.348439 | 2.047151 |
| C | 3.059516 | -3.022160 | -1.116457 | C | 2.466019 | 3.533273 | 2.296675 |
| H | 2.334819 | -3.210077 | -0.328382 | H | 1.980325 | 3.836866 | 3.220583 |
| C | 3.604092 | -4.050390 | -1.878014 | C | 2.203799 | 2.280876 | 1.760197 |
| H | 3.323694 | -5.079737 | -1.672897 | H | 1.520173 | 1.582355 | 2.240213 |
| C | 4.502312 | -3.734721 | -2.892211 | O | -1.357755 | 0.260511 | -1.763686 |
| H | 4.938827 | -4.515025 | -3.510592 | H | -1.202062 | -0.583658 | -2.221234 |
| C | 4.851968 | -2.403789 | -3.093783 | H | -0.455976 | 0.659058 | -1.715341 |
| H | 5.570442 | -2.135914 | -3.864525 | H | 1.425049 | 1.345669 | -2.658514 |
| C | 4.287520 | -1.417755 | -2.287692 | O | 1.188565 | 1.456137 | -1.723552 |
| C | 4.662209 | -0.004088 | -2.329403 | H | 1.187898 | 2.437566 | -1.557706 |
| C | 5.598523 | 0.588799 | -3.177194 | H | 1.535442 | 4.773673 | -1.750559 |
| H | 6.088968 | 0.006993 | -3.953204 | O | 1.022289 | 4.135942 | -1.23301 |
| C | 5.906553 | 1.935394 | -3.009033 | H | 0.111113 | 4.455577 | -1.30097 |
| H | 6.634849 | 2.411390 | -3.660487 | O | -8.07302 | -0.20895 | -2.90097 |
| C | 5.301975 | 2.668237 | -1.988908 | O | -7.88257 | 1.943362 | -2.52663 |
| H | 5.569574 | 3.710643 | -1.836568 | N | -7.50353 | 0.781597 | -2.46479 |
| C | 4.366018 | 2.045424 | -1.165215 | | | | |

TS-3 A (3+ triplet)

E= -2978.006 06 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.060798 | -0.173606 | 0.292343 | C | 3.880546 | -1.410236 | 3.565443 |
| Ru | 2.609214 | -0.045706 | -0.243939 | H | 3.349798 | -1.731170 | 4.458322 |
| N | -2.758596 | -0.601828 | 2.174283 | C | 5.264803 | -1.406601 | 3.523566 |
| O | 0.495660 | -2.113999 | -1.667214 | H | 5.842179 | -1.723392 | 4.388502 |
| O | 0.998184 | -0.974919 | -1.824475 | C | 5.905636 | -0.994317 | 2.353305 |
| C | -4.062331 | -0.596663 | 2.525551 | H | 6.988778 | -0.977538 | 2.274398 |
| H | -4.766302 | -0.326196 | 1.742812 | C | 5.137618 | -0.599969 | 1.273395 |
| N | -0.202047 | -0.549125 | 1.365879 | H | 5.591864 | -0.272422 | 0.342147 |
| C | -4.496447 | -0.912654 | 3.801609 | C | -1.501350 | 2.730844 | 1.246000 |
| H | -5.558820 | -0.891341 | 4.027053 | H | -0.602189 | 2.285088 | 1.666449 |
| N | 1.137750 | -0.597530 | 1.194600 | C | -1.791666 | 4.080740 | 1.391466 |
| C | -3.552938 | -1.253375 | 4.769924 | H | -1.110206 | 4.724885 | 1.941616 |
| H | -3.860778 | -1.508908 | 5.780622 | C | -2.969495 | 4.578900 | 0.837988 |
| N | 3.786898 | -0.596328 | 1.310677 | H | -3.236820 | 5.627493 | 0.943100 |
| C | -2.211585 | -1.259081 | 4.419952 | C | -3.813037 | 3.704803 | 0.161914 |
| H | -1.448329 | -1.518273 | 5.149525 | H | -4.745252 | 4.065472 | -0.265977 |
| N | -2.303056 | 1.875384 | 0.588756 | C | -3.469643 | 2.358930 | 0.048690 |
| C | -1.830694 | -0.929556 | 3.117670 | C | -4.310495 | 1.358262 | -0.611056 |
| N | -3.812016 | 0.094348 | -0.527566 | C | -5.518131 | 1.588895 | -1.261725 |
| C | -0.459122 | -0.899634 | 2.667950 | H | -5.963054 | 2.575583 | -1.357799 |
| N | -2.514755 | -2.136687 | -0.283978 | C | -6.171862 | 0.498232 | -1.817679 |
| C | 0.725481 | -1.169399 | 3.344184 | C | -5.659264 | -0.789633 | -1.747213 |
| H | 0.850931 | -1.463291 | 4.378818 | H | -6.208099 | -1.603802 | -2.212749 |
| N | 3.322321 | -1.847485 | -1.120721 | C | -4.448431 | -0.972151 | -1.086176 |
| C | 1.709959 | -0.962936 | 2.385800 | C | -3.736123 | -2.239601 | -0.902606 |
| N | 4.036028 | 0.604765 | -1.461063 | C | -4.245631 | -3.474782 | -1.295698 |
| C | 3.146191 | -1.003489 | 2.447511 | H | -5.214566 | -3.533774 | -1.785347 |
| N | 2.782898 | 1.940635 | 0.398963 | C | -3.516680 | -4.631285 | -1.043321 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -3.907682 | -5.601498 | -1.338977 | C | 4.002183 | 3.974449 | 0.006297 |
| C | -2.288439 | -4.522828 | -0.397749 | H | 4.735545 | 4.528434 | -0.575017 |
| H | -1.693241 | -5.402636 | -0.169529 | C | 3.406899 | 4.560725 | 1.117942 |
| C | -1.825344 | -3.264129 | -0.037761 | H | 3.660111 | 5.579304 | 1.401857 |
| H | -0.867928 | -3.123973 | 0.460301 | C | 2.511212 | 3.811272 | 1.874853 |
| C | 2.984484 | -3.098744 | -0.780319 | H | 2.048967 | 4.218545 | 2.770426 |
| H | 2.245158 | -3.187094 | 0.013021 | C | 2.230890 | 2.509348 | 1.483123 |
| C | 3.531893 | -4.215048 | -1.403047 | H | 1.555700 | 1.869567 | 2.049848 |
| H | 3.234553 | -5.210835 | -1.086354 | O | -1.356306 | 0.354682 | -1.714189 |
| C | 4.455827 | -4.028111 | -2.425601 | H | -1.252245 | -0.441940 | -2.259191 |
| H | 4.897098 | -4.878916 | -2.938623 | H | -0.454501 | 0.765973 | -1.713424 |
| C | 4.822208 | -2.732408 | -2.774895 | H | 1.329114 | 1.461796 | -2.815360 |
| H | 5.556922 | -2.563298 | -3.558215 | O | 1.124133 | 1.541799 | -1.870601 |
| C | 4.254446 | -1.652845 | -2.102603 | H | 1.064297 | 2.516564 | -1.688198 |
| C | 4.637675 | -0.255552 | -2.321488 | H | 1.237231 | 4.883004 | -1.768127 |
| C | 5.563399 | 0.225349 | -3.247743 | O | 0.786338 | 4.189342 | -1.264926 |
| H | 6.045468 | -0.448357 | -3.951265 | H | -0.14497 | 4.451801 | -1.28351 |
| C | 5.869204 | 1.583326 | -3.255359 | H | 6.588157 | 1.973079 | -3.97132 |
| C | 5.272840 | 2.441200 | -2.332364 | O | -7.99238 | -0.27186 | -2.99754 |
| H | 5.535557 | 3.495849 | -2.321923 | O | -7.85949 | 1.873874 | -2.56486 |
| C | 4.349365 | 1.926757 | -1.424182 | N | -7.45609 | 0.719487 | -2.52263 |
| C | 3.689751 | 2.660514 | -0.336814 | | | | |

TS-3 B (3+ unrestricted singlet)

E= -2977.991 62 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.706676 | 0.134516 | -0.270774 | C | 2.099970 | -2.674375 | 3.804139 |
| Ru | 1.921207 | -0.419967 | 0.205555 | H | 1.343972 | -3.036450 | 4.496418 |
| N | -3.842119 | -0.311787 | 1.377056 | C | 3.443191 | -2.933959 | 4.017214 |
| O | -0.155080 | -2.036150 | -1.669704 | H | 3.762049 | -3.503159 | 4.886839 |
| O | 0.547805 | -0.982377 | -1.687895 | C | 4.380698 | -2.458765 | 3.096648 |
| C | -5.164673 | -0.062471 | 1.484910 | H | 5.443857 | -2.641859 | 3.222544 |
| H | -5.622232 | 0.452309 | 0.643917 | C | 3.937457 | -1.739911 | 2.002554 |
| N | -1.203259 | -0.673810 | 1.086356 | H | 4.628978 | -1.351653 | 1.259340 |
| C | -5.910230 | -0.433637 | 2.591233 | C | -1.860947 | 2.812819 | 1.052524 |
| H | -6.971937 | -0.206106 | 2.622749 | H | -1.140942 | 2.181660 | 1.570981 |
| N | 0.113481 | -0.967377 | 1.170365 | C | -1.944396 | 4.178984 | 1.286949 |
| C | -5.276826 | -1.096770 | 3.641207 | H | -1.287833 | 4.644614 | 2.019018 |
| H | -5.834784 | -1.406305 | 4.521192 | C | -2.895310 | 4.923400 | 0.589482 |
| N | 2.628555 | -1.478275 | 1.792970 | H | -3.000618 | 5.992662 | 0.755765 |
| C | -3.917497 | -1.352086 | 3.543273 | C | -3.724610 | 4.268854 | -0.313388 |
| H | -3.389384 | -1.862993 | 4.344688 | H | -4.481236 | 4.825529 | -0.860595 |
| N | -2.655991 | 2.166279 | 0.181852 | C | -3.599052 | 2.893607 | -0.504909 |
| C | -3.215144 | -0.949550 | 2.406083 | C | -4.451769 | 2.115602 | -1.406702 |
| N | -4.193162 | 0.782767 | -1.372411 | C | -5.461670 | 2.606179 | -2.232452 |
| C | -1.795546 | -1.149129 | 2.229630 | H | -5.682647 | 3.669746 | -2.268903 |
| N | -3.358084 | -1.661334 | -1.135802 | C | -6.184988 | 1.714863 | -3.020931 |
| C | -0.853802 | -1.753992 | 3.056352 | C | -5.892181 | 0.353866 | -2.983115 |
| H | -1.013073 | -2.216687 | 4.022335 | H | -6.447415 | -0.340794 | -3.607969 |
| N | 2.702553 | -2.090501 | -0.892336 | C | -4.875998 | -0.101904 | -2.144341 |
| C | 0.338897 | -1.614506 | 2.359093 | C | -4.431729 | -1.489348 | -1.974256 |
| N | 3.655181 | 0.258487 | -0.499485 | C | -5.045503 | -2.578166 | -2.588699 |
| C | 1.699747 | -1.943954 | 2.680785 | H | -5.893278 | -2.422846 | -3.251234 |
| N | 2.131724 | 1.329370 | 1.334418 | C | -4.579804 | -3.864231 | -2.339532 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|-----------|-----------|
| H | -5.056274 | -4.720680 | -2.809748 | C | 3.591243 | 3.208474 | 1.695550 |
| C | -3.503944 | -4.032451 | -1.473377 | H | 4.485459 | 3.763366 | 1.422148 |
| H | -3.115508 | -5.020420 | -1.242360 | C | 2.808793 | 3.628504 | 2.763910 |
| C | -2.923819 | -2.910571 | -0.896209 | H | 3.079198 | 4.519438 | 3.325228 |
| H | -2.072573 | -2.985572 | -0.222846 | C | 1.694299 | 2.871551 | 3.118597 |
| C | 2.204437 | -3.333846 | -0.910620 | H | 1.072071 | 3.144784 | 3.967150 |
| H | 1.309944 | -3.494150 | -0.314227 | C | 1.394468 | 1.731841 | 2.385712 |
| C | 2.779040 | -4.351219 | -1.665267 | H | 0.547620 | 1.094467 | 2.635365 |
| H | 2.344034 | -5.346561 | -1.646707 | O | -1.531903 | 0.654201 | -2.046372 |
| C | 3.905925 | -4.069983 | -2.431146 | H | -1.415759 | -0.142150 | -2.591274 |
| H | 4.372814 | -4.842062 | -3.037575 | H | -0.611495 | 0.880888 | -1.772712 |
| C | 4.442406 | -2.787321 | -2.395771 | H | 1.499847 | 1.389014 | -2.203979 |
| H | 5.336901 | -2.549021 | -2.966184 | O | 1.07233 | 1.412910 | -1.332929 |
| C | 3.833291 | -1.814255 | -1.606643 | H | 1.115335 | 2.362927 | -1.035211 |
| C | 4.368161 | -0.469831 | -1.400394 | H | 1.529296 | 4.682178 | -1.015170 |
| C | 5.519344 | 0.063974 | -1.975620 | O | 1.067324 | 4.002967 | -0.501364 |
| H | 6.116837 | -0.469946 | -2.709917 | H | 0.173159 | 4.355561 | -0.38324 |
| C | 5.907446 | 1.334628 | -1.578848 | H | -6.97464 | 2.082098 | -3.67083 |
| C | 5.211395 | 2.059576 | -0.621083 | N | 7.120093 | 1.937793 | -2.18763 |
| H | 5.582690 | 3.038314 | -0.329384 | O | 7.403435 | 3.068613 | -1.81748 |
| C | 4.066821 | 1.486439 | -0.075901 | O | 7.715097 | 1.24869 | -3.00251 |
| C | 3.246300 | 2.054335 | 0.995456 | | | | |

TS-3 B (3+ triplet)

E= -2978.003 80 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.675123 | 0.048266 | -0.254004 | C | 2.174783 | -1.966159 | 4.187228 |
| Ru | 1.957424 | -0.306583 | 0.287324 | H | 1.424856 | -2.311913 | 4.894306 |
| N | -3.854097 | -0.588533 | 1.291070 | C | 3.524203 | -2.043182 | 4.487407 |
| O | 0.111266 | -2.129435 | -1.760291 | H | 3.853633 | -2.451245 | 5.439651 |
| O | 0.630388 | -0.998268 | -1.664636 | C | 4.453513 | -1.590840 | 3.548054 |
| C | -5.203116 | -0.535267 | 1.290750 | H | 5.521773 | -1.630737 | 3.740185 |
| H | -5.662317 | -0.121942 | 0.396253 | C | 3.996291 | -1.081838 | 2.346919 |
| N | -1.189434 | -0.662219 | 1.151767 | H | 4.682777 | -0.720122 | 1.586436 |
| C | -5.970107 | -0.974584 | 2.356484 | C | -2.362365 | 2.636485 | 1.438613 |
| H | -7.052910 | -0.907888 | 2.301205 | H | -1.677579 | 2.021778 | 2.019483 |
| N | 0.146191 | -0.791078 | 1.306101 | C | -2.651355 | 3.946500 | 1.793182 |
| C | -5.329398 | -1.494547 | 3.480492 | H | -2.192595 | 4.383857 | 2.676014 |
| H | -5.902830 | -1.848455 | 4.333403 | C | -3.546048 | 4.672024 | 1.011191 |
| N | 2.680288 | -1.001138 | 2.049685 | H | -3.799035 | 5.699769 | 1.259317 |
| C | -3.944169 | -1.553124 | 3.490664 | C | -4.139960 | 4.046340 | -0.078881 |
| H | -3.411144 | -1.954387 | 4.349223 | H | -4.871062 | 4.579025 | -0.682200 |
| N | -2.907130 | 2.025820 | 0.372503 | C | -3.826176 | 2.721066 | -0.376330 |
| C | -3.220948 | -1.096284 | 2.387416 | C | -4.481574 | 1.949656 | -1.436504 |
| N | -4.119253 | 0.640752 | -1.449268 | C | -5.423908 | 2.416911 | -2.351497 |
| C | -1.779673 | -1.117554 | 2.304556 | H | -5.727044 | 3.460758 | -2.352673 |
| N | -3.106792 | -1.737752 | -1.263680 | C | -5.974650 | 1.528884 | -3.272291 |
| C | -0.814349 | -1.528347 | 3.217184 | C | -5.579479 | 0.193253 | -3.276982 |
| H | -0.964255 | -1.924587 | 4.213755 | H | -5.999104 | -0.497980 | -4.003244 |
| N | 2.699693 | -2.137188 | -0.493572 | C | -4.634472 | -0.239374 | -2.347557 |
| C | 0.386826 | -1.301150 | 2.555852 | C | -4.106089 | -1.599421 | -2.196453 |
| N | 3.677453 | 0.248905 | -0.511436 | C | -4.590028 | -2.698896 | -2.901889 |
| C | 1.759042 | -1.441353 | 2.959555 | H | -5.380290 | -2.568419 | -3.637023 |
| N | 2.092228 | 1.644727 | 1.020344 | C | -4.077399 | -3.965058 | -2.643928 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|----------|-----------|
| H | -4.454909 | -4.830326 | -3.182825 | C | 3.483419 | 3.605810 | 0.982021 |
| C | -3.089676 | -4.103415 | -1.673294 | H | 4.366894 | 4.119612 | 0.610538 |
| H | -2.676255 | -5.077053 | -1.425238 | C | 2.655583 | 4.223513 | 1.914847 |
| C | -2.634394 | -2.971243 | -1.011470 | H | 2.883418 | 5.225977 | 2.269058 |
| H | -1.858916 | -3.024193 | -0.250052 | C | 1.555068 | 3.526212 | 2.404213 |
| C | 2.182762 | -3.362380 | -0.325532 | H | 0.899359 | 3.961158 | 3.153974 |
| H | 1.259942 | -3.409429 | 0.248856 | C | 1.311062 | 2.242964 | 1.932557 |
| C | 2.776937 | -4.503343 | -0.854699 | H | 0.472295 | 1.645439 | 2.284517 |
| H | 2.325159 | -5.476364 | -0.682999 | O | -1.443252 | 0.815857 | -1.920968 |
| C | 3.946100 | -4.370968 | -1.595799 | H | -1.478590 | 0.185747 | -2.658900 |
| H | 4.432175 | -5.241629 | -2.028738 | H | -0.474872 | 0.914415 | -1.737597 |
| C | 4.497519 | -3.104689 | -1.764194 | H | 1.564313 | 1.478139 | -2.541828 |
| H | 5.420767 | -2.978565 | -2.324411 | O | 1.198723 | 1.476959 | -1.644145 |
| C | 3.866761 | -2.001529 | -1.195028 | H | 0.979775 | 2.418823 | -1.424296 |
| C | 4.405500 | -0.640148 | -1.237094 | H | 0.414755 | 4.713405 | -0.949902 |
| C | 5.563819 | -0.221815 | -1.888564 | O | 0.049852 | 3.816396 | -0.937883 |
| H | 6.178019 | -0.884836 | -2.492150 | H | -0.75615 | 3.877575 | -1.47161 |
| C | 5.935687 | 1.106963 | -1.749304 | H | -6.71031 | 1.879437 | -3.99122 |
| C | 5.212471 | 2.007916 | -0.978938 | O | 7.440023 | 2.764945 | -2.29043 |
| H | 5.567642 | 3.031433 | -0.893294 | O | 7.767468 | 0.752722 | -3.10001 |
| C | 4.061070 | 1.544867 | -0.349941 | N | 7.159917 | 1.584304 | -2.44235 |
| C | 3.196276 | 2.312152 | 0.553094 | | | | |

TS-3 A (4+ doublet)

E= -2977.537 41 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -1.993274 | -0.476133 | 0.094680 | C | 3.688140 | -2.514358 | 3.018035 |
| Ru | 2.529782 | 0.146992 | -0.089465 | H | 3.175615 | -3.313453 | 3.548245 |
| N | -2.747264 | -2.230310 | 0.837921 | C | 5.018686 | -2.226676 | 3.283784 |
| O | 0.892687 | -1.433967 | -2.452623 | H | 5.570472 | -2.798991 | 4.025388 |
| O | 0.937605 | -0.345400 | -1.843851 | C | 5.632000 | -1.187566 | 2.584153 |
| C | -4.038180 | -2.612560 | 0.755639 | H | 6.669134 | -0.918037 | 2.764546 |
| H | -4.701825 | -1.949398 | 0.205710 | C | 4.902885 | -0.484600 | 1.637895 |
| N | -0.257315 | -1.413295 | 0.725707 | H | 5.350399 | 0.326254 | 1.070605 |
| C | -4.501683 | -3.782605 | 1.335429 | C | -1.869779 | 0.244629 | 3.120168 |
| H | -5.550226 | -4.050486 | 1.238449 | H | -0.996007 | -0.405273 | 3.102925 |
| N | 1.044067 | -1.087913 | 0.856440 | C | -2.299698 | 0.853349 | 4.293096 |
| C | -3.606093 | -4.593491 | 2.034365 | H | -1.759234 | 0.680222 | 5.220074 |
| H | -3.943463 | -5.515675 | 2.501373 | C | -3.433253 | 1.660847 | 4.257047 |
| N | 3.607128 | -0.758342 | 1.373420 | H | -3.802985 | 2.143241 | 5.158935 |
| C | -2.275533 | -4.208429 | 2.120150 | C | -4.101998 | 1.828184 | 3.048069 |
| H | -1.550897 | -4.823286 | 2.648509 | H | -5.000067 | 2.439280 | 3.001036 |
| N | -2.503679 | 0.409449 | 1.945934 | C | -3.628327 | 1.190123 | 1.904403 |
| C | -1.859488 | -3.023407 | 1.511141 | C | -4.296844 | 1.251379 | 0.601507 |
| N | -3.722401 | 0.466399 | -0.345812 | C | -5.433125 | 1.996021 | 0.290982 |
| C | -0.505581 | -2.526015 | 1.510424 | H | -5.940741 | 2.639225 | 1.006044 |
| N | -2.445202 | -1.220052 | -1.815549 | C | -5.931996 | 1.900415 | -0.999734 |
| C | 0.652863 | -2.901440 | 2.169808 | C | -5.356775 | 1.088651 | -1.964674 |
| H | 0.790917 | -3.723783 | 2.861046 | H | -5.805203 | 1.043533 | -2.954605 |
| N | 3.521519 | -1.223172 | -1.366129 | C | -4.225263 | 0.358056 | -1.602910 |
| C | 1.602225 | -1.967544 | 1.740315 | C | -3.517203 | -0.620663 | -2.428854 |
| N | 4.011884 | 1.254781 | -0.809162 | C | -3.932984 | -1.016790 | -3.695779 |
| C | 2.991846 | -1.769904 | 2.063797 | H | -4.781636 | -0.529953 | -4.170212 |
| N | 2.303527 | 1.882386 | 1.069269 | C | -3.276610 | -2.063938 | -4.338497 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|----------|-----------|
| H | -3.597621 | -2.387675 | -5.325792 | C | 3.241203 | 4.063678 | 1.438880 |
| C | -2.233363 | -2.708137 | -3.681507 | H | 3.966187 | 4.828456 | 1.172259 |
| H | -1.719854 | -3.554143 | -4.130080 | C | 2.352298 | 4.281098 | 2.486447 |
| C | -1.851363 | -2.262780 | -2.421042 | H | 2.380830 | 5.213922 | 3.044676 |
| H | -1.047692 | -2.737858 | -1.865989 | C | 1.439611 | 3.281628 | 2.814506 |
| C | 3.272455 | -2.534801 | -1.507864 | H | 0.736319 | 3.407938 | 3.633414 |
| H | 2.432489 | -2.921448 | -0.934195 | C | 1.448894 | 2.102581 | 2.082483 |
| C | 4.026397 | -3.357148 | -2.337182 | H | 0.758019 | 1.287474 | 2.290160 |
| H | 3.789956 | -4.415135 | -2.409838 | O | -1.093955 | 1.435927 | -0.467689 |
| C | 5.076831 | -2.800204 | -3.058766 | H | -1.693807 | 2.074127 | -0.884405 |
| H | 5.683343 | -3.412630 | -3.721638 | H | -0.212444 | 1.571814 | -0.914864 |
| C | 5.353402 | -1.444476 | -2.907884 | H | 1.312712 | 1.831672 | -2.546648 |
| H | 6.181481 | -0.993664 | -3.449051 | O | 1.262938 | 2.115789 | -1.620875 |
| C | 4.576194 | -0.673767 | -2.047415 | H | 1.53014 | 3.076701 | -1.626871 |
| C | 4.840360 | 0.737011 | -1.749761 | H | 2.500632 | 5.020316 | -2.550662 |
| C | 5.854662 | 1.530005 | -2.287579 | O | 2.129348 | 4.711605 | -1.709995 |
| H | 6.528816 | 1.134762 | -3.042979 | H | 1.577472 | 5.451646 | -1.41584 |
| C | 6.001445 | 2.838584 | -1.834608 | H | 6.790557 | 3.466591 | -2.24101 |
| C | 5.153109 | 3.339243 | -0.847883 | O | -7.53266 | 2.578912 | -2.51117 |
| H | 5.279481 | 4.355552 | -0.484310 | O | -7.60618 | 3.39211 | -0.4713 |
| C | 4.150992 | 2.518456 | -0.334120 | N | -7.14179 | 2.700197 | -1.36222 |
| C | 3.212103 | 2.857307 | 0.743112 | | | | |

TS-3 A (4+ quartet)

E= -2977.536 04 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.007848 | -0.484763 | 0.106727 | C | 3.684091 | -2.434217 | 3.067855 |
| Ru | 2.544683 | 0.140741 | -0.115699 | H | 3.169295 | -3.222257 | 3.612220 |
| N | -2.767887 | -2.166633 | 0.992918 | C | 5.010560 | -2.133157 | 3.343087 |
| O | 0.747752 | -1.590895 | -2.260099 | H | 5.556611 | -2.685982 | 4.103426 |
| O | 0.984912 | -0.409193 | -1.936311 | C | 5.624891 | -1.105712 | 2.629117 |
| C | -4.068759 | -2.523844 | 0.983764 | H | 6.658834 | -0.826992 | 2.813809 |
| H | -4.742757 | -1.872096 | 0.432854 | C | 4.902351 | -0.429026 | 1.657416 |
| N | -0.265093 | -1.392899 | 0.759402 | H | 5.352896 | 0.369369 | 1.074987 |
| C | -4.529010 | -3.655494 | 1.637200 | C | -1.781470 | 0.443666 | 3.063740 |
| H | -5.586104 | -3.903986 | 1.599373 | H | -0.933921 | -0.240178 | 3.073038 |
| N | 1.042156 | -1.068611 | 0.857805 | C | -2.155471 | 1.153455 | 4.198157 |
| C | -3.619151 | -4.453835 | 2.332623 | H | -1.597552 | 1.025825 | 5.122238 |
| H | -3.953603 | -5.347023 | 2.854843 | C | -3.258351 | 2.000751 | 4.130119 |
| N | 3.614123 | -0.720358 | 1.380095 | H | -3.584707 | 2.562129 | 5.002579 |
| C | -2.279257 | -4.093436 | 2.344420 | C | -3.955313 | 2.103293 | 2.929861 |
| H | -1.544338 | -4.698738 | 2.869540 | H | -4.832647 | 2.741796 | 2.860748 |
| N | -2.440693 | 0.548455 | 1.896313 | C | -3.538448 | 1.364186 | 1.825660 |
| C | -1.867535 | -2.945406 | 1.665099 | C | -4.247706 | 1.343474 | 0.543801 |
| N | -3.734367 | 0.461370 | -0.351367 | C | -5.370270 | 2.098515 | 0.209949 |
| C | -0.508323 | -2.470150 | 1.596407 | H | -5.829747 | 2.817267 | 0.884478 |
| N | -2.553882 | -1.371308 | -1.726283 | C | -5.920114 | 1.911522 | -1.049734 |
| C | 0.657612 | -2.827639 | 2.249420 | C | -5.407458 | 1.001399 | -1.960370 |
| H | 0.800675 | -3.619028 | 2.974855 | H | -5.893682 | 0.888093 | -2.926762 |
| N | 3.526281 | -1.284529 | -1.348131 | C | -4.286206 | 0.265845 | -1.576471 |
| C | 1.605841 | -1.918630 | 1.767634 | C | -3.634948 | -0.795663 | -2.344536 |
| N | 4.039281 | 1.208177 | -0.863161 | C | -4.109200 | -1.277696 | -3.560656 |
| C | 2.996363 | -1.715659 | 2.088462 | H | -4.964898 | -0.807948 | -4.039571 |
| N | 2.323420 | 1.918332 | 0.976389 | C | -3.501190 | -2.386450 | -4.143523 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|----------|-----------|
| H | -3.866391 | -2.777323 | -5.090380 | C | 3.271436 | 4.107325 | 1.269079 |
| C | -2.445724 | -3.002270 | -3.477756 | H | 4.003515 | 4.856445 | 0.978588 |
| H | -1.965515 | -3.890190 | -3.879795 | C | 2.375307 | 4.371917 | 2.299043 |
| C | -2.005340 | -2.471118 | -2.270985 | H | 2.404452 | 5.326229 | 2.819559 |
| H | -1.187473 | -2.918659 | -1.714081 | C | 1.455157 | 3.390520 | 2.659365 |
| C | 3.262690 | -2.595813 | -1.455731 | H | 0.746121 | 3.551455 | 3.467212 |
| H | 2.415686 | -2.956911 | -0.876073 | C | 1.464553 | 2.183352 | 1.974917 |
| C | 4.009521 | -3.448446 | -2.261267 | H | 0.773194 | 1.377964 | 2.216538 |
| H | 3.759369 | -4.504697 | -2.309034 | O | -1.116160 | 1.346089 | -0.678394 |
| C | 5.071389 | -2.923965 | -2.990285 | H | -1.681179 | 1.873719 | -1.264269 |
| H | 5.673382 | -3.560788 | -3.633943 | H | -0.191263 | 1.465779 | -1.031828 |
| C | 5.364800 | -1.568683 | -2.871629 | H | 1.373519 | 1.720218 | -2.632784 |
| H | 6.202080 | -1.142709 | -3.418708 | O | 1.301809 | 2.031208 | -1.716894 |
| C | 4.591159 | -0.766053 | -2.037229 | H | 1.565231 | 2.992275 | -1.745358 |
| C | 4.867751 | 0.650913 | -1.781554 | H | 2.538548 | 4.904275 | -2.735684 |
| C | 5.891252 | 1.416822 | -2.340996 | O | 2.163142 | 4.625255 | -1.886556 |
| H | 6.565773 | 0.990066 | -3.078662 | H | 1.608298 | 5.374088 | -1.6219 |
| C | 6.046292 | 2.739563 | -1.934503 | H | 6.842642 | 3.346224 | -2.35877 |
| C | 5.195128 | 3.282655 | -0.973112 | O | -7.5556 | 2.513075 | -2.55642 |
| H | 5.325866 | 4.311262 | -0.647648 | O | -7.52192 | 3.503555 | -0.59521 |
| C | 4.184264 | 2.488506 | -0.435644 | N | -7.1164 | 2.720151 | -1.43771 |
| C | 3.239994 | 2.874723 | 0.620500 | | | | |

TS-3 B (4+ doublet)

E= -2977.533 13 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.669593 | 0.045209 | -0.239330 | C | 2.107902 | -1.949815 | 4.181923 |
| Ru | 1.949791 | -0.300324 | 0.275051 | H | 1.347476 | -2.249686 | 4.898828 |
| N | -3.885803 | -0.542206 | 1.304874 | C | 3.455639 | -2.094778 | 4.476690 |
| O | -0.171238 | -1.923399 | -1.552712 | H | 3.770772 | -2.507846 | 5.431774 |
| O | 0.629840 | -0.966039 | -1.638606 | C | 4.396887 | -1.704287 | 3.523959 |
| C | -5.233162 | -0.472770 | 1.284942 | H | 5.463484 | -1.798980 | 3.709102 |
| H | -5.681675 | -0.069134 | 0.380663 | C | 3.960258 | -1.183765 | 2.316201 |
| N | -1.237377 | -0.621405 | 1.154975 | H | 4.662510 | -0.869103 | 1.549647 |
| C | -6.011397 | -0.887661 | 2.353500 | C | -2.356043 | 2.618496 | 1.442283 |
| H | -7.093409 | -0.811258 | 2.290270 | H | -1.735840 | 1.969843 | 2.057442 |
| N | 0.105501 | -0.734544 | 1.299669 | C | -2.566541 | 3.952691 | 1.760676 |
| C | -5.384014 | -1.396224 | 3.491633 | H | -2.108528 | 4.376132 | 2.650564 |
| H | -5.969999 | -1.730143 | 4.344532 | C | -3.392252 | 4.716825 | 0.940265 |
| N | 2.649853 | -1.034069 | 2.026439 | H | -3.589168 | 5.762032 | 1.167354 |
| C | -3.998834 | -1.469625 | 3.518439 | C | -3.991809 | 4.115912 | -0.162070 |
| H | -3.480237 | -1.861727 | 4.389848 | H | -4.663561 | 4.688281 | -0.796843 |
| N | -2.916539 | 2.036703 | 0.368079 | C | -3.754127 | 2.770349 | -0.429712 |
| C | -3.263471 | -1.037314 | 2.413000 | C | -4.410371 | 2.015728 | -1.501053 |
| N | -4.107375 | 0.696118 | -1.497544 | C | -5.310507 | 2.517485 | -2.439994 |
| C | -1.825015 | -1.066089 | 2.328140 | H | -5.574426 | 3.571718 | -2.451477 |
| N | -3.268711 | -1.726691 | -1.208250 | C | -5.878193 | 1.645665 | -3.367230 |
| C | -0.852786 | -1.459919 | 3.229228 | C | -5.551843 | 0.292337 | -3.344556 |
| H | -0.989352 | -1.850488 | 4.229970 | H | -5.998921 | -0.389951 | -4.062837 |
| N | 2.623756 | -2.169335 | -0.513991 | C | -4.647302 | -0.169990 | -2.387551 |
| C | 0.345389 | -1.234861 | 2.550263 | C | -4.206386 | -1.553385 | -2.193722 |
| N | 3.693758 | 0.182704 | -0.539010 | C | -4.714522 | -2.642809 | -2.896126 |
| C | 1.717344 | -1.419015 | 2.950464 | H | -5.456083 | -2.491881 | -3.676606 |
| N | 2.209893 | 1.641728 | 1.046626 | C | -4.286127 | -3.927787 | -2.577555 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|----------|-----------|
| H | -4.683770 | -4.786342 | -3.113622 | C | 3.733636 | 3.504430 | 1.039172 |
| C | -3.357830 | -4.095026 | -1.553371 | H | 4.643750 | 3.968327 | 0.666220 |
| H | -3.010796 | -5.082785 | -1.262881 | C | 2.974448 | 4.144958 | 2.014833 |
| C | -2.875149 | -2.973761 | -0.892272 | H | 3.284469 | 5.113048 | 2.402075 |
| H | -2.139721 | -3.050032 | -0.094501 | C | 1.836080 | 3.509716 | 2.506226 |
| C | 2.068673 | -3.376056 | -0.335825 | H | 1.235235 | 3.960367 | 3.292060 |
| H | 1.152592 | -3.392884 | 0.251697 | C | 1.491639 | 2.264012 | 1.996000 |
| C | 2.614373 | -4.536683 | -0.874613 | H | 0.621690 | 1.716278 | 2.354364 |
| H | 2.134362 | -5.494560 | -0.693677 | O | -1.453330 | 0.789791 | -1.890565 |
| C | 3.775005 | -4.444440 | -1.636516 | H | -1.437116 | 0.169776 | -2.638517 |
| H | 4.224400 | -5.331457 | -2.076395 | H | -0.493455 | 0.995177 | -1.716117 |
| C | 4.365007 | -3.196989 | -1.815974 | H | 1.559628 | 1.508885 | -2.447020 |
| H | 5.282391 | -3.103794 | -2.392222 | O | 1.143583 | 1.522522 | -1.570003 |
| C | 3.781552 | -2.072633 | -1.236319 | H | 1.040873 | 2.481891 | -1.326129 |
| C | 4.369894 | -0.732984 | -1.281607 | H | 0.906204 | 4.681472 | -0.380610 |
| C | 5.538238 | -0.361500 | -1.946995 | O | 0.404544 | 4.046162 | -0.911671 |
| H | 6.114640 | -1.046707 | -2.564247 | H | 0.11619 | 4.562934 | -1.67996 |
| C | 5.973621 | 0.945666 | -1.802116 | H | -6.58216 | 2.021851 | -4.1056 |
| C | 5.308260 | 1.870047 | -1.007978 | O | 7.539373 | 2.541169 | -2.35559 |
| H | 5.717272 | 2.873334 | -0.915980 | O | 7.767824 | 0.51889 | -3.18215 |
| C | 4.146378 | 1.454182 | -0.364775 | N | 7.212994 | 1.375304 | -2.51396 |
| C | 3.346982 | 2.248257 | 0.575446 | | | | |

TS-3 B (4+ quartet)

E= -2977.532 85 a.u.

| | | | | | | | |
|----|-----------|-----------|-----------|---|-----------|-----------|-----------|
| Ru | -2.670169 | 0.040632 | -0.238197 | C | 2.108685 | -1.828163 | 4.233445 |
| Ru | 1.958480 | -0.278839 | 0.285718 | H | 1.346821 | -2.130223 | 4.947907 |
| N | -3.886227 | -0.576282 | 1.294549 | C | 3.455968 | -1.929339 | 4.549950 |
| O | -0.100764 | -2.020378 | -1.559763 | H | 3.768470 | -2.312678 | 5.518190 |
| O | 0.597052 | -0.984802 | -1.625002 | C | 4.399151 | -1.532515 | 3.602553 |
| C | -5.234458 | -0.528762 | 1.266892 | H | 5.465278 | -1.594429 | 3.803580 |
| H | -5.684269 | -0.127291 | 0.362273 | C | 3.965111 | -1.051876 | 2.376850 |
| N | -1.234871 | -0.620401 | 1.155057 | H | 4.669282 | -0.736998 | 1.612100 |
| C | -6.011765 | -0.962070 | 2.328656 | C | -2.407455 | 2.597979 | 1.474337 |
| H | -7.094515 | -0.903017 | 2.259769 | H | -1.784931 | 1.950231 | 2.088319 |
| N | 0.110195 | -0.701291 | 1.312822 | C | -2.636154 | 3.926433 | 1.804295 |
| C | -5.382354 | -1.466374 | 3.467701 | H | -2.191271 | 4.345849 | 2.702801 |
| H | -5.967574 | -1.814313 | 4.315512 | C | -3.463946 | 4.689180 | 0.984523 |
| N | 2.655884 | -0.949668 | 2.064383 | H | -3.674979 | 5.729654 | 1.220594 |
| C | -3.996397 | -1.517592 | 3.502069 | C | -4.047741 | 4.092601 | -0.128664 |
| H | -3.476467 | -1.906309 | 4.374194 | H | -4.721335 | 4.663451 | -0.762879 |
| N | -2.951692 | 2.021450 | 0.389016 | C | -3.791746 | 2.752809 | -0.407905 |
| C | -3.261772 | -1.067541 | 2.403137 | C | -4.430488 | 2.000452 | -1.491426 |
| N | -4.109323 | 0.685125 | -1.498922 | C | -5.331803 | 2.498851 | -2.431011 |
| C | -1.822649 | -1.071526 | 2.326663 | H | -5.610528 | 3.549350 | -2.433717 |
| N | -3.243525 | -1.729120 | -1.223249 | C | -5.881974 | 1.628186 | -3.369961 |
| C | -0.849691 | -1.436907 | 3.238008 | C | -5.537792 | 0.279110 | -3.357906 |
| H | -0.985843 | -1.822791 | 4.240631 | H | -5.972033 | -0.402431 | -4.084750 |
| N | 2.619081 | -2.168998 | -0.446694 | C | -4.632810 | -0.180128 | -2.399752 |
| C | 0.349370 | -1.188041 | 2.567838 | C | -4.176255 | -1.559608 | -2.214204 |
| N | 3.703072 | 0.175670 | -0.539657 | C | -4.666005 | -2.650126 | -2.927676 |
| C | 1.721506 | -1.336289 | 2.985247 | H | -5.403865 | -2.503055 | -3.712402 |
| N | 2.216930 | 1.692252 | 0.986837 | C | -4.224080 | -3.932029 | -2.614515 |

| | | | | | | | |
|---|-----------|-----------|-----------|---|-----------|----------|-----------|
| H | -4.607357 | -4.791626 | -3.159325 | C | 3.746725 | 3.549234 | 0.923248 |
| C | -3.301960 | -4.095453 | -1.584179 | H | 4.661314 | 3.996319 | 0.540939 |
| H | -2.945574 | -5.081042 | -1.297713 | C | 2.980116 | 4.228986 | 1.865690 |
| C | -2.838146 | -2.973132 | -0.911312 | H | 3.289551 | 5.210277 | 2.218544 |
| H | -2.107725 | -3.045887 | -0.108589 | C | 1.833621 | 3.617316 | 2.367844 |
| C | 2.059508 | -3.368300 | -0.233410 | H | 1.225168 | 4.100286 | 3.128275 |
| H | 1.143794 | -3.364872 | 0.354592 | C | 1.490423 | 2.353678 | 1.902368 |
| C | 2.601138 | -4.547001 | -0.736067 | H | 0.613854 | 1.823496 | 2.270561 |
| H | 2.117507 | -5.497039 | -0.525847 | O | -1.450434 | 0.800865 | -1.876937 |
| C | 3.762438 | -4.482644 | -1.499206 | H | -1.454164 | 0.200246 | -2.640814 |
| H | 4.208760 | -5.384261 | -1.911689 | H | -0.483572 | 0.986460 | -1.715007 |
| C | 4.358124 | -3.243377 | -1.714622 | H | 1.561978 | 1.475690 | -2.502926 |
| H | 5.276733 | -3.171207 | -2.291903 | O | 1.156366 | 1.498295 | -1.621358 |
| C | 3.779426 | -2.099999 | -1.169294 | H | 1.034852 | 2.458227 | -1.393329 |
| C | 4.375142 | -0.765410 | -1.253633 | H | 0.737254 | 4.663536 | -0.456989 |
| C | 5.545627 | -0.419862 | -1.928884 | O | 0.296166 | 3.990685 | -0.995477 |
| H | 6.119608 | -1.125965 | -2.524479 | H | 0.000177 | 4.47957 | -1.77901 |
| C | 5.987038 | 0.889173 | -1.823782 | H | -6.58676 | 2.001806 | -4.10887 |
| C | 5.324710 | 1.840962 | -1.060270 | O | 7.559403 | 2.45996 | -2.42669 |
| H | 5.737253 | 2.845218 | -1.000322 | O | 7.781515 | 0.410997 | -3.18638 |
| C | 4.160277 | 1.450274 | -0.405901 | N | 7.228791 | 1.29075 | -2.54728 |
| C | 3.359471 | 2.278091 | 0.503212 | | | | |

- [1] F. Bozoglian, S. Romain, M. Z. Ertem, T. K. Todorova, C. Sens, J. Mola, M. Rodriguez, I. Romero, J. Benet-Buchholz, X. Fontrodona, C. J. Cramer, L. Gagliardi, A. Llobet, *J. Am. Chem. Soc.* **2009**, *131*, 15176-15187.