

Supporting information:

The mechanism for N₂ activation in the E₄-state of nitrogenase.

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The starting E₄ structure with two hydrides in **Figure 1 and 2**. # means fixed atom
Energies: E= -7921.479734, solv = -0.202761, disp = -230.64 Z₀ = 894.84

| | | | |
|-----|----------------|----------------|----------------|
| Mo1 | 16.3411878090 | -5.8843224691 | 53.3532482045 |
| Fe2 | 9.8545237449 | -8.7066672616 | 55.8026803599 |
| Fe3 | 11.1270830736 | -6.1567857625 | 55.2253963209 |
| Fe4 | 11.2975412550 | -7.8791910044 | 53.1939275092 |
| Fe5 | 12.4004711229 | -8.7721346694 | 55.7826411927 |
| Fe6 | 14.5828727439 | -8.0468881788 | 54.3097782500 |
| Fe7 | 13.9710400141 | -5.7325498335 | 55.4475370195 |
| Fe8 | 13.2849575036 | -6.0681983570 | 52.9644078942 |
| C9 | 17.6826441859 | -2.2589053299 | 54.3195294106 |
| H10 | 17.8384919968 | -1.2545925665 | 53.9210344378 |
| H11 | 16.6046985230 | -2.3860228098 | 54.4827461332 |
| C12 | 18.1490916089 | -3.3294888351 | 53.3066023869 |
| C13 | 19.6205941297 | -3.0741902320 | 52.9009842022 |
| H14 | 20.2451659748 | -3.1818351138 | 53.7935819454 |
| H15 | 19.6926868002 | -2.0373160710 | 52.5549727621 |
| C16 | 20.1256658531 | -4.0148389529 | 51.7871779042 |
| H17 | 19.6151226762 | -3.8053958370 | 50.8451575598 |
| H18 | 19.9209928568 | -5.0510016584 | 52.0769603817 |
| C19 | 17.3109458328 | -3.4189019885 | 51.9976756549 |
| O20 | 16.8868131451 | -4.6179283585 | 51.7026256488 |
| O21 | 17.1890581818 | -2.4195844689 | 51.2905840319 |
| O22 | 18.0371388030 | -4.6068516786 | 53.9600244506 |
| C23 | 12.6703429290 | -7.2370369276 | 54.4920100332 |
| S24 | 12.3157255346 | -4.6567520170 | 56.8687276896 |
| S25 | 16.0758574362 | -6.7283949943 | 55.6923376397 |
| S26 | 9.4625045707 | -4.9381587745 | 53.9288238078 |
| S28 | 14.4626583560 | -10.1118021486 | 55.6799683710 |
| S29 | 14.4754472099 | -4.1580799740 | 53.6650878874 |
| S30 | 10.0380570449 | -9.7078565374 | 53.6279410778 |
| S31 | 15.0144651125 | -7.5224654096 | 52.0632631740 |
| S32 | 11.6130691052 | -6.5318388603 | 51.1209386392 |
| H33 | 13.6351742031# | -2.1902105282# | 49.0425559854# |
| C34 | 13.2979245689# | -2.0241172350# | 50.0550231810# |
| H35 | 13.9034573660 | -2.6598888494 | 50.7056694277 |
| H36 | 13.4458796854 | -0.9759837742 | 50.3384609648 |
| N37 | 11.8837648438 | -2.4084978367 | 50.1233956643 |
| H38 | 11.2953624729 | -2.0817310269 | 49.3700215198 |
| C39 | 11.2184954364 | -2.8361532489 | 51.2147486715 |
| N40 | 11.7993980766 | -3.0468706509 | 52.3782661061 |
| H41 | 11.2465556981 | -3.5295639622 | 53.1004721498 |
| H42 | 12.8174814132 | -3.1088642410 | 52.5167372597 |
| N43 | 9.8636686496 | -2.9870417022 | 51.1220582283 |
| H44 | 9.5059159338 | -3.2738784432 | 50.2198237743 |
| H45 | 9.4353741924 | -3.4837118621 | 51.9147680080 |
| H46 | 7.9311775757 | 0.3969127240 | 59.4142474362 |
| C47 | 8.3601754768 | -1.3536927130 | 60.6733970028 |
| H48 | 8.2198839164 | -1.5872878048 | 61.7357893086 |
| H49 | 7.5979341439 | -1.9169598563 | 60.1227019719 |
| C50 | 9.7342740982 | -1.8208202775 | 60.2990237029 |
| N51 | 10.7434350030 | -1.8645251239 | 61.2445204061 |

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|------|----------------|-----------------|----------------|
| C52 | 10.2173002769 | -2.2368975484 | 59.0790733622 |
| H53 | 9.7528195690 | -2.3761937290 | 58.1160708509 |
| C54 | 11.8067447778 | -2.3077230738 | 60.5997409865 |
| H55 | 12.7794232071 | -2.4938842201 | 61.0333020138 |
| N56 | 11.5445812744 | -2.5368910735 | 59.2853935335 |
| H57 | 19.2247459747 | -4.4001181294 | 57.4827423718 |
| H58 | 16.7207626868 | -8.8606035832 | 50.7823707470 |
| C59 | 18.3600442894 | -7.4209545971 | 50.6554863816 |
| H60 | 17.7203439277 | -6.5342444729 | 50.6265155384 |
| H61 | 19.1973292499 | -7.2324642976 | 49.9691587286 |
| C62 | 18.9076235659 | -7.5720035941 | 52.0408482857 |
| N63 | 18.1761048537 | -7.2359640103 | 53.1707608275 |
| C64 | 20.1357264525 | -8.0388899954 | 52.4430320023 |
| H65 | 20.9854226467 | -8.3939914895 | 51.8805623874 |
| C66 | 18.9398448911 | -7.4917565622 | 54.2223093263 |
| H67 | 18.6892631800 | -7.2983533025 | 55.2536852542 |
| N68 | 20.1310839156 | -7.9892042367 | 53.8265468999 |
| H69 | 20.8990905948 | -8.1757620497 | 54.4545171469 |
| H70 | 6.9632433529 | -10.5490125668 | 56.9226286093 |
| C71 | 6.1750521330# | -9.8249632781# | 56.6900008432# |
| H72 | 5.5309558047# | -10.2322288176# | 56.0424860987# |
| H73 | 5.6932327346# | -9.5371417035# | 57.6127207581# |
| S74 | 8.1208576459 | -7.9022504903 | 57.1032182752 |
| H75 | 12.1562091462 | -2.9523415094 | 58.5858874360 |
| H76 | 18.2516973875 | -4.4020611156 | 54.9525044855 |
| C78 | 18.3652903901 | -2.3659105397 | 55.7119717248 |
| O79 | 18.6559616188 | -3.5646337195 | 56.1110449935 |
| O80 | 18.5502542807 | -1.3253137664 | 56.3655395988 |
| C81 | 21.6036263071 | -3.8760164504 | 51.5491089153 |
| O82 | 22.1579211357 | -3.4773493276 | 50.5434515634 |
| O83 | 22.3208176811# | -4.2658020416# | 52.6398596358# |
| H84 | 15.7024656862# | -0.1996317006# | 61.4912312798# |
| C85 | 14.8549934097# | -0.0829911871# | 60.8320021209# |
| H86 | 13.9165015895# | -0.2867338793# | 61.3260937710# |
| H87 | 14.8279483830 | 0.9915817637 | 60.5848765406 |
| C88 | 15.0599857654# | -0.8751944034# | 59.5441990369# |
| H89 | 14.3835077641 | -0.4989717751 | 58.7665435195 |
| H90 | 14.7960412608 | -1.9266333706 | 59.7063201181 |
| C91 | 16.5031908365 | -0.8295814611 | 59.0342498621 |
| H92 | 16.9263363375 | 0.1792276503 | 59.1532367752 |
| H93 | 16.5564164622 | -1.0382358650 | 57.9599109557 |
| C94 | 17.4223544696 | -1.8256625768 | 59.7544369704 |
| O95 | 17.0868747364 | -2.4202248520 | 60.7847792022 |
| N96 | 18.6426525153 | -1.9792378187 | 59.1743279626 |
| H97 | 19.1605083577 | -2.7954550928 | 59.4787839270 |
| H98 | 18.7530174722 | -1.7209760024 | 58.1836447215 |
| C99 | 10.6519926369# | 0.0100033143# | 53.3460014096# |
| H100 | 11.1636988658# | 0.9592721141# | 53.2872696758# |
| H101 | 9.5863320405# | 0.1850132805# | 53.3579375021# |
| H102 | 10.9190941953 | -0.5834696714 | 52.4698598363 |
| C103 | 11.0702392862 | -0.6567050972 | 54.6716574163 |
| H104 | 10.7268855377 | -1.6990700515 | 54.6626107529 |
| C105 | 10.3874199892 | 0.0520433737 | 55.8508273284 |
| H106 | 9.2941105711 | -0.0085625901 | 55.7743167664 |
| H107 | 10.6617587762 | 1.1164166532 | 55.8783296763 |
| H108 | 10.6800093892 | -0.3902336710 | 56.8090000043 |
| C109 | 12.5945539536 | -0.6513049755 | 54.8507560345 |
| H110 | 13.1103480538 | -1.1313470011 | 54.0130682885 |
| H111 | 12.8894572896 | -1.1896090156 | 55.7581333620 |
| H112 | 12.9697410042 | 0.3790919023 | 54.9313980916 |
| H113 | 13.4550779485# | -12.2303887427# | 53.1883137695# |
| C114 | 13.9110016728# | -11.6210552681# | 52.4219872140# |
| H115 | 14.6576041196 | -10.9550734117 | 52.8624419645 |
| H116 | 14.3408188816 | -12.2308993538 | 51.6231944423 |
| N117 | 12.7296192230 | -10.8923147133 | 51.9338144653 |
| H118 | 11.9410187228 | -10.7991659610 | 52.5954798966 |
| C119 | 12.6212753307 | -10.1560446683 | 50.8405302031 |
| N120 | 13.7167480288 | -9.8445348858 | 50.1013882126 |
| H121 | 13.5281926408 | -9.2378159386 | 49.3113290911 |
| H122 | 14.5084804678 | -9.4951839573 | 50.6517771371 |
| N123 | 11.3879907874 | -9.7805114819 | 50.4131415055 |
| H124 | 10.6406278249 | -9.9925322111 | 51.0801011599 |
| H125 | 11.3275121517 | -8.7969058836 | 50.1340149323 |
| H126 | 19.2019475911 | -8.2163304887 | 61.7093235311 |
| C127 | 19.5978933129# | -7.2298795947# | 61.9900500755# |

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|------|----------------|----------------|----------------|
| H128 | 20.6406211045 | -7.3641195038 | 62.2959595225 |
| C129 | 18.8344260642 | -6.6814960099 | 63.1941988421 |
| O130 | 19.3879045594 | -6.1891041430 | 64.1746597346 |
| C131 | 19.4918720166# | -6.2717980482# | 60.7990634787# |
| H132 | 19.8694283581 | -5.2838229886 | 61.0857811629 |
| H133 | 18.4386122989 | -6.1229671825 | 60.5398528431 |
| C134 | 20.2371381416 | -6.7782439484 | 59.5494357355 |
| H135 | 20.0032393899 | -7.8335889829 | 59.3637796029 |
| H136 | 21.3241023671 | -6.7419869233 | 59.7148158998 |
| C137 | 19.9683223809 | -6.0624745740 | 58.2188044511 |
| O138 | 20.2354348347 | -6.5877909236 | 57.1480801485 |
| O139 | 19.4567873948 | -4.8433600258 | 58.3627774851 |
| N140 | 17.4797149232 | -6.7629628212 | 63.0492541790 |
| H141 | 17.1210565606 | -7.0987283314 | 62.1637624911 |
| C142 | 16.5368854076# | -6.0058843383# | 63.8530414920# |
| H143 | 15.8865455666 | -6.6972524048 | 64.4083744961 |
| H144 | 17.1205535772 | -5.4402388817 | 64.5836011345 |
| C145 | 15.6691451794 | -5.0681382096 | 62.9801187655 |
| H146 | 16.2844349341 | -4.2474953653 | 62.5958149885 |
| H147 | 14.8984296854 | -4.6249419249 | 63.6254221775 |
| C148 | 15.0285031061 | -5.8029697076 | 61.8160639212 |
| C149 | 13.9878756299 | -6.7249763181 | 62.0183930931 |
| H150 | 13.5859771134 | -6.8694631672 | 63.0200441311 |
| C151 | 15.5168434008 | -5.6198177031 | 60.5116791622 |
| H152 | 16.2911891507 | -4.8764291974 | 60.3369114161 |
| C153 | 13.4543795337 | -7.4489764885 | 60.9501748969 |
| H154 | 12.6401173417 | -8.1487283297 | 61.1207050466 |
| C155 | 14.9912354408 | -6.3498437026 | 59.4395958371 |
| H156 | 15.3801018175 | -6.1966463631 | 58.4367901867 |
| C157 | 13.9604063090 | -7.2683739588 | 59.6584325686 |
| H158 | 13.5459782377 | -7.8339105804 | 58.8275632984 |
| H159 | 9.0037560472# | 0.7050733335# | 60.7752693345# |
| C160 | 8.1269803484# | 0.1560803014# | 60.4649996132# |
| H161 | 7.2836720063# | 0.4592420217# | 61.0677700037# |
| H268 | 8.5766101054 | -4.5759831878 | 54.8844187042 |
| H269 | 18.2592781145# | -9.4987529070# | 50.1505401512# |
| C270 | 17.5839755707# | -8.6559201270# | 50.1520260987# |
| H271 | 17.2773626234# | -8.4419892695# | 49.1387987548# |
| H273 | 23.2543263111 | -4.1142159740 | 52.4015686380 |
| H274 | 10.4518484760 | -5.9043092316 | 51.4249389337 |
| H275 | 15.1465914384 | -9.5512893930 | 56.7013887979 |
| H277 | 12.2829812034 | -5.5530729437 | 57.8783241365 |
| H278 | 11.1931465340 | -9.7873804705 | 56.5321306707 |
| H279 | 10.9167755393 | -7.4658591505 | 56.4837484366 |
| C280 | 6.7703109854 | -8.5758097809 | 56.0541926573 |
| H281 | 5.9982599804 | -7.8042500554 | 55.9381843529 |
| H282 | 7.1567885251 | -8.7950033546 | 55.0517510584 |
| H283 | 7.1493941107# | -5.8354098952# | 59.8218942714# |
| C284 | 6.9590149674# | -4.8009333484# | 59.5000035989# |
| H285 | 5.9039260033# | -4.4903549879# | 59.5181449819# |
| H286 | 7.4684022920 | -4.1801929256 | 60.2526418680 |
| C287 | 7.5586458473 | -4.4488296119 | 58.1343715581 |
| H288 | 8.6201961954 | -4.7324350866 | 58.1076955378 |
| H289 | 7.5129755415 | -3.3587528818 | 58.0098877403 |
| O290 | 6.8623416785 | -4.9995052066 | 57.0275377134 |
| H291 | 7.2185473731 | -5.9102330485 | 56.9244449392 |

The TS structure for the allowed formation of H₂ from two hydrides in **Figure 3**
Energies: E = -7921.453280, solv = -0.200796, disp = -228.55 Z₀ = 892.69

| | | | |
|-----|---------------|---------------|---------------|
| Mo1 | 16.2546360000 | -5.9428990000 | 53.4426960000 |
| Fe2 | 9.9246470000 | -9.0193980000 | 55.6594990000 |
| Fe3 | 10.9700700000 | -6.3743250000 | 55.3626530000 |
| Fe4 | 11.2264280000 | -8.0938240000 | 53.3027000000 |
| Fe5 | 12.4302860000 | -8.9143300000 | 55.8245890000 |
| Fe6 | 14.5306870000 | -8.1439680000 | 54.3444850000 |
| Fe7 | 13.8489780000 | -5.8945150000 | 55.5760650000 |
| Fe8 | 13.1892260000 | -6.2034930000 | 53.0682590000 |
| C9 | 17.6187330000 | -2.2819720000 | 54.4201410000 |
| H10 | 17.7785540000 | -1.2869200000 | 54.0010270000 |
| H11 | 16.5414180000 | -2.4019410000 | 54.5945860000 |
| C12 | 18.0671190000 | -3.3751700000 | 53.4251770000 |

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| C13 | 19.5458920000 | -3.1512730000 | 53.0185920000 |
| H14 | 20.1665900000 | -3.2388200000 | 53.9163240000 |
| H15 | 19.6291710000 | -2.1256860000 | 52.6423760000 |
| C16 | 20.0478920000 | -4.1295990000 | 51.9362840000 |
| H17 | 19.4835040000 | -3.9976250000 | 51.0109260000 |
| H18 | 19.9087170000 | -5.1559610000 | 52.2894530000 |
| C19 | 17.2179390000 | -3.4464590000 | 52.1257900000 |
| O20 | 16.7845050000 | -4.6374090000 | 51.8197370000 |
| O21 | 17.0837100000 | -2.4364200000 | 51.4369280000 |
| O22 | 17.9238910000 | -4.6433930000 | 54.0909630000 |
| C23 | 12.5568470000 | -7.3610280000 | 54.6148270000 |
| S24 | 12.1184410000 | -4.9444710000 | 57.0656770000 |
| S25 | 15.9926560000 | -6.8398270000 | 55.7711680000 |
| S26 | 9.4890150000 | -4.9591520000 | 54.0160310000 |
| S27 | 14.4346750000 | -10.2815040000 | 55.6238240000 |
| S28 | 14.3509730000 | -4.2839300000 | 53.8078810000 |
| S29 | 10.0933540000 | -10.0592300000 | 53.5529560000 |
| S30 | 14.9629250000 | -7.5791040000 | 52.1091890000 |
| S31 | 11.5006660000 | -6.6774460000 | 51.2507800000 |
| H32 | 13.6351740000 | -2.1902110000 | 49.0425560000 |
| C33 | 13.2979250000 | -2.0241170000 | 50.0550230000 |
| H34 | 13.9448320000 | -2.6085750000 | 50.7143560000 |
| H35 | 13.3786100000 | -0.9629830000 | 50.3164660000 |
| N36 | 11.9082060000 | -2.4963750000 | 50.1220850000 |
| H37 | 11.3235870000 | -2.2617650000 | 49.3328630000 |
| C38 | 11.2422570000 | -2.9279450000 | 51.2123400000 |
| N39 | 11.8116070000 | -3.0803750000 | 52.3916110000 |
| H40 | 11.2607010000 | -3.5513070000 | 53.1214700000 |
| H41 | 12.8265240000 | -3.1508290000 | 52.5362720000 |
| N42 | 9.8984950000 | -3.1384410000 | 51.1061310000 |
| H43 | 9.5562710000 | -3.4297170000 | 50.1998980000 |
| H44 | 9.4841110000 | -3.6541280000 | 51.8927030000 |
| H45 | 7.9301440000 | 0.3900490000 | 59.4127660000 |
| C46 | 8.3658420000 | -1.3529500000 | 60.6890350000 |
| H47 | 8.1863800000 | -1.5756190000 | 61.7482210000 |
| H48 | 7.6267230000 | -1.9261770000 | 60.1173710000 |
| C49 | 9.7537350000 | -1.8298420000 | 60.3722500000 |
| N50 | 10.7445900000 | -1.8039140000 | 61.3381600000 |
| C51 | 10.2603050000 | -2.3410490000 | 59.1971620000 |
| H52 | 9.8161110000 | -2.5519920000 | 58.2375130000 |
| C53 | 11.8189920000 | -2.2996430000 | 60.7519100000 |
| H54 | 12.7820290000 | -2.4539790000 | 61.2184500000 |
| N55 | 11.5823620000 | -2.6294290000 | 59.4529580000 |
| H56 | 19.1759960000 | -4.3673970000 | 57.5432580000 |
| H57 | 16.7151170000 | -8.8851020000 | 50.7671670000 |
| C58 | 18.3271530000 | -7.4200270000 | 50.6984960000 |
| H59 | 17.6687970000 | -6.5463850000 | 50.6824620000 |
| H60 | 19.1720950000 | -7.1954040000 | 50.0328250000 |
| C61 | 18.8547290000 | -7.5935120000 | 52.0909550000 |
| N62 | 18.1175260000 | -7.2594460000 | 53.2194900000 |
| C63 | 20.0804000000 | -8.0630680000 | 52.4994980000 |
| H64 | 20.9352580000 | -8.4115510000 | 51.9402070000 |
| C65 | 18.8769150000 | -7.5176360000 | 54.2734940000 |
| H66 | 18.6182480000 | -7.3297820000 | 55.3038210000 |
| N67 | 20.0700260000 | -8.0146810000 | 53.8827620000 |
| H68 | 20.8350980000 | -8.2018430000 | 54.5140760000 |
| H69 | 6.9382230000 | -10.5742740000 | 56.9329810000 |
| C70 | 6.1750520000 | -9.8249630000 | 56.6900010000 |
| H71 | 5.5309560000 | -10.2322290000 | 56.0424860000 |
| H72 | 5.6932330000 | -9.5371420000 | 57.6127210000 |
| S73 | 8.3221570000 | -8.0312360000 | 57.0048590000 |
| H74 | 12.1982260000 | -3.1161630000 | 58.8046350000 |
| H75 | 18.1365470000 | -4.4418630000 | 55.0846070000 |
| C76 | 18.3165600000 | -2.3771210000 | 55.8010880000 |
| O77 | 18.5538250000 | -3.5786510000 | 56.2232520000 |
| O78 | 18.5637160000 | -1.3335960000 | 56.4260860000 |
| C79 | 21.5027540000 | -3.9304930000 | 51.6023930000 |
| O80 | 21.9621200000 | -3.5244760000 | 50.5532190000 |
| O81 | 22.3208180000 | -4.2658020000 | 52.6398600000 |
| H82 | 15.7024660000 | -0.1996320000 | 61.4912310000 |
| C83 | 14.8549930000 | -0.0829910000 | 60.8320020000 |
| H84 | 13.9165020000 | -0.2867340000 | 61.3260940000 |
| H85 | 14.8292240000 | 0.9919990000 | 60.5866230000 |
| C86 | 15.0599860000 | -0.8751940000 | 59.5441990000 |
| H87 | 14.3903070000 | -0.4915960000 | 58.7641340000 |

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|------|---------------|----------------|---------------|
| H88 | 14.7848230000 | -1.9240620000 | 59.7043780000 |
| C89 | 16.5039950000 | -0.8445980000 | 59.0406730000 |
| H90 | 16.9333220000 | 0.1636450000 | 59.1372130000 |
| H91 | 16.5599140000 | -1.0784780000 | 57.9716080000 |
| C92 | 17.4126730000 | -1.8324160000 | 59.7845780000 |
| O93 | 17.0464470000 | -2.4487280000 | 60.7892480000 |
| N94 | 18.6606860000 | -1.9503020000 | 59.2518620000 |
| H95 | 19.1735810000 | -2.7690300000 | 59.5581160000 |
| H96 | 18.7854390000 | -1.6942360000 | 58.2630570000 |
| C97 | 10.6519930000 | 0.0100030000 | 53.3460010000 |
| H98 | 11.1636990000 | 0.9592720000 | 53.2872700000 |
| H99 | 9.5863320000 | 0.1850130000 | 53.3579380000 |
| H100 | 10.9209050000 | -0.5856820000 | 52.4716090000 |
| C101 | 11.0636350000 | -0.6602470000 | 54.6741400000 |
| H102 | 10.7137300000 | -1.7010800000 | 54.6676570000 |
| C103 | 10.3822630000 | 0.0483470000 | 55.8559120000 |
| H104 | 9.2887000000 | 0.0116550000 | 55.7670450000 |
| H105 | 10.6783070000 | 1.1061750000 | 55.9028690000 |
| H106 | 10.6554110000 | -0.4146120000 | 56.8108110000 |
| C107 | 12.5874230000 | -0.6620220000 | 54.8579810000 |
| H108 | 13.1035800000 | -1.1547390000 | 54.0280210000 |
| H109 | 12.8755730000 | -1.1899620000 | 55.7735200000 |
| H110 | 12.9684640000 | 0.3668490000 | 54.9287980000 |
| H111 | 13.4550780000 | -12.2303890000 | 53.1883140000 |
| C112 | 13.9110020000 | -11.6210550000 | 52.4219870000 |
| H113 | 14.6243420000 | -10.9252910000 | 52.8712790000 |
| H114 | 14.3945330000 | -12.2374650000 | 51.6585340000 |
| N115 | 12.7353890000 | -10.9417710000 | 51.8657910000 |
| H116 | 11.9098980000 | -10.8677970000 | 52.4964350000 |
| C117 | 12.6550500000 | -10.2161000000 | 50.7670240000 |
| N118 | 13.7698260000 | -9.8741030000 | 50.0696930000 |
| H119 | 13.5889090000 | -9.2797070000 | 49.2683810000 |
| H120 | 14.5144660000 | -9.4800760000 | 50.6564060000 |
| N121 | 11.4279380000 | -9.8699880000 | 50.2882200000 |
| H122 | 10.6678900000 | -10.1065990000 | 50.9317060000 |
| H123 | 11.3561110000 | -8.8826650000 | 50.0299430000 |
| H124 | 19.2063060000 | -8.2182800000 | 61.7095210000 |
| C125 | 19.5978930000 | -7.2298800000 | 61.9900500000 |
| H126 | 20.6404980000 | -7.3596610000 | 62.2982760000 |
| C127 | 18.8300380000 | -6.6834150000 | 63.1900520000 |
| O128 | 19.3811760000 | -6.2012060000 | 64.1763030000 |
| C129 | 19.4918720000 | -6.2717980000 | 60.7990630000 |
| H130 | 19.8624660000 | -5.2827210000 | 61.0903830000 |
| H131 | 18.4390610000 | -6.1260220000 | 60.5359660000 |
| C132 | 20.2406280000 | -6.7682450000 | 59.5511940000 |
| H133 | 20.0062140000 | -7.8214300000 | 59.3532470000 |
| H134 | 21.3277190000 | -6.7327200000 | 59.7152650000 |
| C135 | 19.9610020000 | -6.0298780000 | 58.2370600000 |
| O136 | 20.2337040000 | -6.5271090000 | 57.1546900000 |
| O137 | 19.4265600000 | -4.8269550000 | 58.4128210000 |
| N138 | 17.4760700000 | -6.7471180000 | 63.0338490000 |
| H139 | 17.1141120000 | -7.0969440000 | 62.1555750000 |
| C140 | 16.5368850000 | -6.0058840000 | 63.8530410000 |
| H141 | 15.9246810000 | -6.7019540000 | 64.4451090000 |
| H142 | 17.1277010000 | -5.4076410000 | 64.5516160000 |
| C143 | 15.6123080000 | -5.1080000000 | 62.9962870000 |
| H144 | 16.1988020000 | -4.2991430000 | 62.5466290000 |
| H145 | 14.8781260000 | -4.6465480000 | 63.6705020000 |
| C146 | 14.9086450000 | -5.8972820000 | 61.9082610000 |
| C147 | 13.8659490000 | -6.7857780000 | 62.2167290000 |
| H148 | 13.5000200000 | -6.8469330000 | 63.2405430000 |
| C149 | 15.3481680000 | -5.8184030000 | 60.5772430000 |
| H150 | 16.1233790000 | -5.1000180000 | 60.3182560000 |
| C151 | 13.2905520000 | -7.5857230000 | 61.2288980000 |
| H152 | 12.4772140000 | -8.2614300000 | 61.4826720000 |
| C153 | 14.7822070000 | -6.6274280000 | 59.5852340000 |
| H154 | 15.1383540000 | -6.5557330000 | 58.5607930000 |
| C155 | 13.7554060000 | -7.5177190000 | 59.9113480000 |
| H156 | 13.3120870000 | -8.1473660000 | 59.1436330000 |
| H157 | 9.0037560000 | 0.7050730000 | 60.7752690000 |
| C158 | 8.1269800000 | 0.1560800000 | 60.4650000000 |
| H159 | 7.2836720000 | 0.4592420000 | 61.0677700000 |
| H160 | 8.6034780000 | -4.5234410000 | 54.9406010000 |
| H161 | 18.2592780000 | -9.4987530000 | 50.1505400000 |
| C162 | 17.5839760000 | -8.6559200000 | 50.1520260000 |

| | | | |
|------|---------------|---------------|---------------|
| H163 | 17.2773630000 | -8.4419890000 | 49.1387990000 |
| H164 | 23.2230980000 | -4.0703700000 | 52.3259990000 |
| H165 | 10.3487910000 | -6.0591740000 | 51.6053590000 |
| H166 | 15.1219200000 | -9.7653020000 | 56.6661930000 |
| H167 | 12.2017910000 | -5.8590930000 | 58.0567430000 |
| H168 | 11.5295660000 | -9.6155500000 | 57.0320710000 |
| H169 | 11.1215940000 | -8.5526970000 | 56.9328760000 |
| C170 | 6.8408750000 | -8.6038350000 | 56.0456110000 |
| H171 | 6.1260860000 | -7.7740640000 | 55.9794890000 |
| H172 | 7.1546590000 | -8.8424770000 | 55.0230530000 |
| H173 | 7.1493940000 | -5.8354100000 | 59.8218940000 |
| C174 | 6.9590150000 | -4.8009330000 | 59.5000040000 |
| H175 | 5.9039260000 | -4.4903550000 | 59.5181450000 |
| H176 | 7.4725740000 | -4.1744710000 | 60.2445120000 |
| C177 | 7.5697320000 | -4.4859510000 | 58.1304510000 |
| H178 | 8.6413700000 | -4.7282470000 | 58.1406440000 |
| H179 | 7.4841610000 | -3.4055760000 | 57.9508990000 |
| O180 | 6.9257160000 | -5.1253760000 | 57.0399090000 |
| H181 | 7.3634100000 | -6.0001420000 | 56.9444270000 |

The structure after the release of the two hydrides.

Energies: E= -7920.281890, solv = -0.199815, disp = -226.64 Z₀ = 885.74

| | | | |
|-----|----------------|----------------|----------------|
| Mo1 | 15.9786157245 | -6.0530086731 | 53.3713978187 |
| Fe2 | 9.3481601484 | -9.3112767567 | 54.7677527995 |
| Fe3 | 10.4484024847 | -6.3183215552 | 54.6777932723 |
| Fe4 | 11.0371418867 | -8.3110448022 | 52.7984635305 |
| Fe5 | 11.8750582339 | -8.9512876818 | 55.2395193576 |
| Fe6 | 14.1753459189 | -8.2044621520 | 54.2845004621 |
| Fe7 | 13.3130584704 | -5.9607140118 | 55.3169342185 |
| Fe8 | 12.9320505252 | -6.3144394860 | 52.7497163676 |
| C9 | 17.3409128478 | -2.4230577899 | 54.3334515170 |
| H10 | 17.4696046076 | -1.4293468647 | 53.9010739329 |
| H11 | 16.2674793448 | -2.5870129097 | 54.4939238054 |
| C12 | 17.8603230461 | -3.5130124806 | 53.3672349884 |
| C13 | 19.3525087131 | -3.2281604668 | 53.0498003317 |
| H14 | 19.9164319624 | -3.2531414760 | 53.9888520821 |
| H15 | 19.3985372337 | -2.2091550547 | 52.6514204633 |
| C16 | 20.0062314999 | -4.1851448074 | 52.0299372002 |
| H17 | 19.4580273945 | -4.1477890589 | 51.0849791395 |
| H18 | 19.9905421465 | -5.2077817201 | 52.4150178484 |
| C19 | 17.0810135048 | -3.6155257578 | 52.0228670069 |
| O20 | 16.6120866421 | -4.8004037530 | 51.7453430758 |
| O21 | 17.0223621639 | -2.6326649501 | 51.2848977890 |
| O22 | 17.7011339066 | -4.7786752419 | 54.0363101289 |
| C23 | 12.1090210134 | -7.3488425461 | 54.2488350680 |
| S24 | 11.3975683454 | -4.8792066444 | 56.5129317644 |
| S25 | 15.5030633764 | -6.8239706303 | 55.7172163983 |
| S26 | 8.8704325489 | -5.0212217650 | 53.3560497541 |
| S28 | 13.8183834085 | -10.3289260959 | 55.6324768613 |
| S29 | 14.0526012566 | -4.3821900167 | 53.5826582133 |
| S30 | 9.7536823092 | -10.2420036190 | 52.7478505053 |
| S31 | 14.7799879504 | -7.7434003317 | 52.0563435530 |
| S32 | 11.5096314719 | -6.8498419000 | 50.7487267080 |
| H33 | 13.6351741874# | -2.1902105239# | 49.0425559793# |
| C34 | 13.2979245834# | -2.0241172419# | 50.0550231893# |
| H35 | 13.8095081243 | -2.7386245892 | 50.7037974193 |
| H36 | 13.5309561625 | -1.0057462099 | 50.3818932338 |
| N37 | 11.8477786588 | -2.2710807758 | 50.0409465413 |
| H38 | 11.3316501330 | -1.8421047133 | 49.2859970744 |
| C39 | 11.0801045709 | -2.8428688119 | 50.9878552937 |
| N40 | 11.5280804082 | -3.2239682624 | 52.1649283872 |
| H41 | 10.8971217469 | -3.7955841766 | 52.7431115572 |
| H42 | 12.5253309750 | -3.2995102944 | 52.4204754038 |
| N43 | 9.7399303599 | -2.9572968783 | 50.7291274615 |
| H44 | 9.4937711072 | -3.1699391184 | 49.7703763675 |
| H45 | 9.2300211980 | -3.5262876770 | 51.4172883982 |
| H46 | 7.9293738348 | 0.3951682480 | 59.4142172039 |
| C47 | 8.3619532911 | -1.3516577072 | 60.6739789071 |
| H48 | 8.3098741090 | -1.5685112139 | 61.7479630540 |
| H49 | 7.5453221847 | -1.9098855595 | 60.2000677305 |
| C50 | 9.6889112278 | -1.8565657928 | 60.1891584334 |
| N51 | 10.7631114790 | -1.9685560916 | 61.0546134017 |

| | | | |
|------|----------------|-----------------|----------------|
| C52 | 10.0574503299 | -2.2745740059 | 58.9308869127 |
| H53 | 9.5192463894 | -2.3661646930 | 58.0015833218 |
| C54 | 11.7505677067 | -2.4560278841 | 60.3272397826 |
| H55 | 12.7417902856 | -2.6980666247 | 60.6846298134 |
| N56 | 11.3797498928 | -2.6456058144 | 59.0311240421 |
| H57 | 18.9712031863 | -4.4557002682 | 57.4989376967 |
| H58 | 16.7034709120 | -8.9057624170 | 50.7432482405 |
| C59 | 18.3010028148 | -7.4374359273 | 50.7658730771 |
| H60 | 17.6594379037 | -6.5532029719 | 50.7062569796 |
| H61 | 19.2051697401 | -7.2189671696 | 50.1810092638 |
| C62 | 18.6987472707 | -7.6387238915 | 52.2007387100 |
| N63 | 17.8310612322 | -7.4038675082 | 53.2612303596 |
| C64 | 19.9035872273 | -8.0530223244 | 52.7166619979 |
| H65 | 20.8298088417 | -8.3269028183 | 52.2352420819 |
| C66 | 18.4948272201 | -7.6699835405 | 54.3746509717 |
| H67 | 18.1165463332 | -7.5416520410 | 55.3768462707 |
| N68 | 19.7499852108 | -8.0788042974 | 54.0933340641 |
| H69 | 20.4652847312 | -8.1933886652 | 54.7977133857 |
| H70 | 6.9415877129 | -10.5715359783 | 56.9230207610 |
| C71 | 6.1750524117# | -9.8249631450# | 56.6900008555# |
| H72 | 5.5309557423# | -10.2322287496# | 56.0424861180# |
| H73 | 5.6932326974# | -9.5371417149# | 57.6127207422# |
| S74 | 8.5605755112 | -8.2249355125 | 56.6357703027 |
| H75 | 11.8946678789 | -3.1211309955 | 58.2943251553 |
| H76 | 17.8676219633 | -4.5690143844 | 55.0287956395 |
| C78 | 18.0443658910 | -2.4755346447 | 55.7151926069 |
| O79 | 18.2456184474 | -3.6616678054 | 56.1942826563 |
| O80 | 18.3480658505 | -1.4071658751 | 56.2755955659 |
| C81 | 21.4264385479 | -3.7662150746 | 51.7369087287 |
| O82 | 21.7959557446 | -3.0463662642 | 50.8303085915 |
| O83 | 22.3208176210# | -4.2658020399# | 52.6398596315# |
| H84 | 15.7024656850# | -0.1996317030# | 61.4912312810# |
| C85 | 14.8549934399# | -0.0829911764# | 60.8320021192# |
| H86 | 13.9165015895# | -0.2867338793# | 61.3260937710# |
| H87 | 14.8246388773 | 0.9910003317 | 60.5813923386 |
| C88 | 15.0599857376# | -0.8751944209# | 59.5441990260# |
| H89 | 14.3503943675 | -0.5339410595 | 58.7799009973 |
| H90 | 14.8465785620 | -1.9364152596 | 59.7180283902 |
| C91 | 16.4905712506 | -0.7594129173 | 59.0028932876 |
| H92 | 16.8494178538 | 0.2775265456 | 59.0911773174 |
| H93 | 16.5367946218 | -0.9903519139 | 57.9334568702 |
| C94 | 17.4863211555 | -1.6710596029 | 59.7337844497 |
| O95 | 17.2445973083 | -2.1811954328 | 60.8336377441 |
| N96 | 18.6666602869 | -1.8497522206 | 59.0821266586 |
| H97 | 19.2298461159 | -2.6177004535 | 59.4285530329 |
| H98 | 18.6980955794 | -1.6827261042 | 58.0655364936 |
| C99 | 10.6519927028# | 0.0100032806# | 53.3460013412# |
| H100 | 11.1636988270# | 0.9592721370# | 53.2872697081# |
| H101 | 9.5863320423# | 0.1850132898# | 53.3579375313# |
| H102 | 10.9138370918 | -0.5783366384 | 52.4631050014 |
| C103 | 11.0744714500 | -0.6822626396 | 54.6547942212 |
| H104 | 10.6745018523 | -1.7055751714 | 54.6532670951 |
| C105 | 10.4720824536 | 0.0583055153 | 55.8572988505 |
| H106 | 9.3755281623 | 0.0774871636 | 55.8062245453 |
| H107 | 10.8224111539 | 1.0998255879 | 55.8888380323 |
| H108 | 10.7541233548 | -0.4158757426 | 56.8030054641 |
| C109 | 12.6001872748 | -0.7675359909 | 54.7807156214 |
| H110 | 13.0516793834 | -1.3172200687 | 53.9488367276 |
| H111 | 12.8920958417 | -1.2875482990 | 55.6995241772 |
| H112 | 13.0438204125 | 0.2380405916 | 54.8060654728 |
| H113 | 13.4550779258# | -12.2303887227# | 53.1883137719# |
| C114 | 13.9110017164# | -11.6210552920# | 52.4219871994# |
| H115 | 14.4914353211 | -10.8182412803 | 52.8824322588 |
| H116 | 14.5434736779 | -12.2274588495 | 51.7666147599 |
| N117 | 12.7516933533 | -11.1101259655 | 51.6783283282 |
| H118 | 11.8514298911 | -11.0772643542 | 52.1882947232 |
| C119 | 12.7656353081 | -10.4327667166 | 50.5422219362 |
| N120 | 13.9409424427 | -10.0740172546 | 49.9635260879 |
| H121 | 13.8329159625 | -9.5098283382 | 49.1280094088 |
| H122 | 14.6023674405 | -9.6353259303 | 50.6155041318 |
| N123 | 11.5937771861 | -10.1599325165 | 49.9071117000 |
| H124 | 10.7666137136 | -10.3747040811 | 50.4749434969 |
| H125 | 11.5320608137 | -9.1942774503 | 49.5759191597 |
| H126 | 19.2066221331 | -8.2171667823 | 61.7042894412 |
| C127 | 19.5978933700# | -7.2298795547# | 61.9900501054# |

| | | | |
|------|----------------|----------------|----------------|
| H128 | 20.6387003595 | -7.3639540322 | 62.3015805516 |
| C129 | 18.8229541742 | -6.7058338706 | 63.1966162387 |
| O130 | 19.3647527421 | -6.2935793475 | 64.2195521528 |
| C131 | 19.4918719313# | -6.2717981033# | 60.7990634579# |
| H132 | 19.9303737561 | -5.3030017516 | 61.0644281609 |
| H133 | 18.4385131549 | -6.0651983152 | 60.5845954651 |
| C134 | 20.1431766187 | -6.8110369086 | 59.5117250601 |
| H135 | 19.8650324098 | -7.8605405629 | 59.3531071715 |
| H136 | 21.2392341413 | -6.8092212994 | 59.6004661223 |
| C137 | 19.8023901133 | -6.0976686763 | 58.1943696950 |
| O138 | 20.0362082643 | -6.6164697955 | 57.1119290485 |
| O139 | 19.2603830787 | -4.8966757361 | 58.3645397920 |
| N140 | 17.4702073773 | -6.7290688670 | 63.0122778754 |
| H141 | 17.1206266920 | -6.9904373431 | 62.0988223870 |
| C142 | 16.5368854072# | -6.0058843436# | 63.8530414923# |
| H143 | 15.8175069514 | -6.7107433356 | 64.2945306254 |
| H144 | 17.1182965252 | -5.5701815783 | 64.6693690301 |
| C145 | 15.7735392645 | -4.9132375542 | 63.0695536558 |
| H146 | 16.4656922558 | -4.1131864953 | 62.7855154551 |
| H147 | 15.0299268633 | -4.4735430044 | 63.7486332110 |
| C148 | 15.0952589771 | -5.4519492986 | 61.8225003837 |
| C149 | 13.9749998003 | -6.2948723709 | 61.9064765812 |
| H150 | 13.5525541991 | -6.5321815827 | 62.8818083274 |
| C151 | 15.6103937826 | -5.1454763819 | 60.5517346480 |
| H152 | 16.4521934546 | -4.4625567992 | 60.4728998107 |
| C153 | 13.3872625241 | -6.8213874179 | 60.7536799211 |
| H154 | 12.5155395741 | -7.4661106346 | 60.8362849468 |
| C155 | 15.0256429449 | -5.6735793279 | 59.3953154900 |
| H156 | 15.4328658091 | -5.4378667205 | 58.4163170951 |
| C157 | 13.9153953145 | -6.5161950117 | 59.4948871811 |
| H158 | 13.4707614628 | -6.9258042325 | 58.5925079605 |
| H159 | 9.0037560430# | 0.7050733583# | 60.7752693026# |
| C160 | 8.1269803503# | 0.1560802579# | 60.4649996038# |
| H161 | 7.2836720136# | 0.4592420062# | 61.0677700217# |
| H268 | 8.3383159255 | -4.2806392467 | 54.3537621415 |
| H269 | 18.2592781072# | -9.4987529129# | 50.1505401614# |
| C270 | 17.5839754677# | -8.6559201455# | 50.1520261458# |
| H271 | 17.2773626691# | -8.4419892550# | 49.1387987440# |
| H273 | 23.1792159666 | -3.8817894912 | 52.3804389159 |
| H274 | 10.2918247550 | -6.2863965306 | 50.9385173672 |
| H275 | 14.2617735917 | -9.6952414115 | 56.7414325622 |
| H277 | 11.2361738372 | -5.7767055266 | 57.5109280121 |
| C280 | 6.8163438753 | -8.5816081749 | 56.0395791124 |
| H281 | 6.2238188556 | -7.6871198559 | 56.2539216885 |
| H282 | 6.8266476921 | -8.6925198147 | 54.9493463237 |
| H283 | 7.1493941634# | -5.8354098671# | 59.8218943305# |
| C284 | 6.9590148206# | -4.8009335304# | 59.5000034994# |
| H285 | 5.9039260167# | -4.4903549437# | 59.5181450068# |
| H286 | 7.4895591738 | -4.1573429560 | 60.2140153829 |
| C287 | 7.5421121473 | -4.5546501985 | 58.1041174706 |
| H288 | 8.6254344880 | -4.7216605826 | 58.1153151084 |
| H289 | 7.3852302917 | -3.5003305799 | 57.8355062464 |
| O290 | 6.9312308768 | -5.3427432753 | 57.0884387413 |
| H291 | 7.5480927902 | -6.0682842102 | 56.8731524370 |

The structure for N₂ in **Figure 4**.

Energies: E= -8029.790879, solv = -0.199051, disp = -238.63 Z₀ = 891.62

| | | | |
|-----|---------------|---------------|---------------|
| Mo1 | 16.2787090531 | -5.7390151085 | 53.1488740126 |
| Fe2 | 8.9151540968 | -7.0742319777 | 54.3801411975 |
| Fe3 | 11.0951762065 | -5.4303080208 | 54.9076875636 |
| Fe4 | 10.9370048500 | -7.1514308352 | 52.8055192059 |
| Fe5 | 11.7761269255 | -8.2995030988 | 55.0799319009 |
| Fe6 | 14.2636701137 | -7.7490549556 | 53.9035596539 |
| Fe7 | 13.8029061876 | -5.3957659377 | 55.0373223719 |
| Fe8 | 13.1425715055 | -5.6762538257 | 52.3843423109 |
| C9 | 17.7129949285 | -2.1752995951 | 54.2173352797 |
| H10 | 17.9220055745 | -1.1776326596 | 53.8269276703 |
| H11 | 16.6249066517 | -2.2647265066 | 54.3301420575 |
| C12 | 18.1843797360 | -3.2613624674 | 53.2265217226 |
| C13 | 19.6796456008 | -3.0655505155 | 52.8763002692 |
| H14 | 20.2736507924 | -3.2497689548 | 53.7767957617 |
| H15 | 19.8167485214 | -2.0183348814 | 52.5845455383 |

| | | | |
|-----|----------------|-----------------|----------------|
| C16 | 20.1633335739 | -3.9736087636 | 51.7255581582 |
| H17 | 19.6788435829 | -3.7005541438 | 50.7868366435 |
| H18 | 19.9076861272 | -5.0128757497 | 51.9610904810 |
| C19 | 17.4190130621 | -3.3179981828 | 51.8699839624 |
| O20 | 17.0240959764 | -4.5120131959 | 51.5280543761 |
| O21 | 17.3513465865 | -2.3044155511 | 51.1756101305 |
| O22 | 17.9933509025 | -4.5379951123 | 53.8716664542 |
| C23 | 12.4184203319 | -6.5939536150 | 54.0222741024 |
| S24 | 12.3132184867 | -4.2226709993 | 56.6006261501 |
| S25 | 15.7829607921 | -6.6019947038 | 55.4390667239 |
| S26 | 9.0897003108 | -4.8802942298 | 53.7900627604 |
| S27 | 13.7595845690 | -9.7956738894 | 55.1842211219 |
| S28 | 14.5215135842 | -3.9089543981 | 53.2580973109 |
| S29 | 9.9367069311 | -9.1559797960 | 53.6068759101 |
| S30 | 14.9025030917 | -7.2503221595 | 51.7219295602 |
| S31 | 11.5558610512 | -6.3053465299 | 50.5324422170 |
| H32 | 13.6351741733# | -2.1902104694# | 49.0425559659# |
| C33 | 13.2979244972# | -2.0241174665# | 50.0550234519# |
| H34 | 13.8410050191 | -2.7109163971 | 50.7094158245 |
| H35 | 13.5087877948 | -0.9935587327 | 50.3606089158 |
| N36 | 11.8544810957 | -2.3068194144 | 50.0810717315 |
| H37 | 11.3159444354 | -1.9975504228 | 49.2848394380 |
| C38 | 11.1366960765 | -2.7707355628 | 51.1183754317 |
| N39 | 11.6608966125 | -2.9979694532 | 52.3078036718 |
| H40 | 11.0923798518 | -3.5182426578 | 52.9857691444 |
| H41 | 12.6746234852 | -2.9861082850 | 52.5036917810 |
| N42 | 9.7921998763 | -2.9493773743 | 50.9572117192 |
| H43 | 9.4829016702 | -3.2003236416 | 50.0266301223 |
| H44 | 9.3434072373 | -3.5016858758 | 51.7024317719 |
| H45 | 7.9321911951 | 0.3970560075 | 59.4141771699 |
| C46 | 8.3443096069 | -1.3565684796 | 60.6762940323 |
| H47 | 8.1925875410 | -1.5885545903 | 61.7373929435 |
| H48 | 7.5776265658 | -1.9091079773 | 60.1194414684 |
| C49 | 9.7159216052 | -1.8413151843 | 60.3163722924 |
| N50 | 10.6969972957 | -1.9461230133 | 61.2863414242 |
| C51 | 10.2285532644 | -2.1974111228 | 59.0892545298 |
| H52 | 9.7968411285 | -2.2665370869 | 58.1030566705 |
| C53 | 11.7742685894 | -2.3662829134 | 60.6493768943 |
| H54 | 12.7337389496 | -2.5834011839 | 61.0979564458 |
| N55 | 11.5460425687 | -2.5224831253 | 59.3186069422 |
| H56 | 19.0743504188 | -4.3583495018 | 57.4963669947 |
| H57 | 16.7212917553 | -8.8480422708 | 50.7848167964 |
| C58 | 18.3829715687 | -7.4278982611 | 50.6399547175 |
| H59 | 17.7786102507 | -6.5206480690 | 50.5501965848 |
| H60 | 19.2537750756 | -7.2975167894 | 49.9825171368 |
| C61 | 18.8575028611 | -7.5468366885 | 52.0538250907 |
| N62 | 18.0437113545 | -7.2016841066 | 53.1221555741 |
| C63 | 20.0609762962 | -7.9895053647 | 52.5480836290 |
| H64 | 20.9522123788 | -8.3438038132 | 52.0532914381 |
| C65 | 18.7355334623 | -7.4281606254 | 54.2277751975 |
| H66 | 18.4044117112 | -7.2202951192 | 55.2331317295 |
| N67 | 19.9584683708 | -7.9164474921 | 53.9280835694 |
| H68 | 20.6868170395 | -8.0536145730 | 54.6140654157 |
| H69 | 6.9567389594 | -10.5594889093 | 56.9115091512 |
| C70 | 6.1750542860# | -9.8249628600# | 56.6900012482# |
| H71 | 5.5309554283# | -10.2322280016# | 56.0424859602# |
| H72 | 5.6932325576# | -9.5371415300# | 57.6127206113# |
| S73 | 8.2949197606 | -7.9659834914 | 56.7600210824 |
| H74 | 12.1850824585 | -2.8712512506 | 58.6088235991 |
| H75 | 18.1659118294 | -4.3626890862 | 54.8726092913 |
| C76 | 18.3297461629 | -2.3005157643 | 55.6363590491 |
| O77 | 18.5246477542 | -3.5037912610 | 56.0712615684 |
| O78 | 18.5559882730 | -1.2516190876 | 56.2689471658 |
| C79 | 21.6476007397 | -3.8956863082 | 51.5163589193 |
| O80 | 22.2429152426 | -3.5635604229 | 50.5094530199 |
| O81 | 22.3208172403# | -4.2658019944# | 52.6398596086# |
| H82 | 15.7024655200# | -0.1996320045# | 61.4912314402# |
| C83 | 14.8549937829# | -0.0829907282# | 60.8320018979# |
| H84 | 13.9165015893# | -0.2867338795# | 61.3260937710# |
| H85 | 14.8211820303 | 0.9907508080 | 60.5802990204 |
| C86 | 15.0599854361# | -0.8751945415# | 59.5441990510# |
| H87 | 14.3237979751 | -0.5639882682 | 58.7922789032 |
| H88 | 14.8897537817 | -1.9432733073 | 59.7274025096 |
| C89 | 16.4741858402 | -0.7074075199 | 58.9688776476 |
| H90 | 16.767777978 | 0.3533033702 | 58.9848836807 |

| | | | |
|------|----------------|-----------------|----------------|
| H91 | 16.5154964950 | -1.0031074099 | 57.9147242792 |
| C92 | 17.5401890602 | -1.5049712088 | 59.7340474661 |
| O93 | 17.3508526731 | -1.9565489679 | 60.8704057325 |
| N94 | 18.7167905433 | -1.6519352022 | 59.0731005144 |
| H95 | 19.3451939319 | -2.3414400465 | 59.4673826977 |
| H96 | 18.7585690360 | -1.5111794123 | 58.0506256638 |
| C97 | 10.6519926840# | 0.0100029641# | 53.3460013939# |
| H98 | 11.1636988660# | 0.9592721207# | 53.2872697838# |
| H99 | 9.5863320625# | 0.1850134171# | 53.3579374284# |
| H100 | 10.9222937132 | -0.5856403503 | 52.4743277598 |
| C101 | 11.0733483059 | -0.6424336403 | 54.6776912847 |
| H102 | 10.7251619280 | -1.6836328403 | 54.6926355758 |
| C103 | 10.4003366027 | 0.0904813315 | 55.8484041866 |
| H104 | 9.3061118612 | 0.0284371533 | 55.7825248465 |
| H105 | 10.6747853594 | 1.1553234857 | 55.8525079866 |
| H106 | 10.7029662548 | -0.3321296005 | 56.8122916836 |
| C107 | 12.5983323710 | -0.6362355795 | 54.8479139168 |
| H108 | 13.1111800158 | -1.1461995370 | 54.0263228839 |
| H109 | 12.8950131274 | -1.1449579855 | 55.7713239932 |
| H110 | 12.9759876270 | 0.3956672053 | 54.8921816780 |
| H111 | 13.4550778651# | -12.2303885056# | 53.1883139083# |
| C112 | 13.9110017574# | -11.6210555686# | 52.4219869583# |
| H113 | 14.7543022690 | -11.0690948729 | 52.8414846854 |
| H114 | 14.2174783374 | -12.2246652584 | 51.5631706690 |
| N115 | 12.8009695536 | -10.7341988102 | 52.0334467314 |
| H116 | 12.0650736255 | -10.5731387883 | 52.7256145038 |
| C117 | 12.6697556216 | -10.0482291806 | 50.9037252372 |
| N118 | 13.7426364744 | -9.8773772485 | 50.0844604342 |
| H119 | 13.5441444083 | -9.2939570676 | 49.2782036883 |
| H120 | 14.5553563747 | -9.5044869105 | 50.5859592998 |
| N121 | 11.4541161290 | -9.5954061330 | 50.5388852582 |
| H122 | 10.7389408787 | -9.6503006099 | 51.2768375567 |
| H123 | 11.4382021504 | -8.6683037525 | 50.1024417285 |
| H124 | 19.1993744344 | -8.2158808291 | 61.7092991956 |
| C125 | 19.5978934917# | -7.2298793897# | 61.9900503598# |
| H126 | 20.6393268880 | -7.3696688239 | 62.2977239981 |
| C127 | 18.8306260408 | -6.6945012722 | 63.1974856055 |
| O128 | 19.3794524831 | -6.2544492185 | 64.2049048709 |
| C129 | 19.4918716546# | -6.2717983710# | 60.7990633514# |
| H130 | 19.9370678878 | -5.3066563419 | 61.0685636111 |
| H131 | 18.4378065707 | -6.0565634398 | 60.5956992663 |
| C132 | 20.1262568212 | -6.7900591243 | 59.4948377446 |
| H133 | 19.7919723516 | -7.8153749698 | 59.2900258768 |
| H134 | 21.2196097782 | -6.8547163296 | 59.5918310156 |
| C135 | 19.8519101895 | -6.0122446645 | 58.1925409724 |
| O136 | 20.1619247470 | -6.4791405201 | 57.1065150153 |
| O137 | 19.2815322571 | -4.8233216929 | 58.3705385875 |
| N138 | 17.4757748975 | -6.7456735893 | 63.0313655166 |
| H139 | 17.1266982378 | -7.0155679131 | 62.1201283690 |
| C140 | 16.5368852960# | -6.0058844230# | 63.8530408424# |
| H141 | 15.7947914006 | -6.7017561089 | 64.2692392790 |
| H142 | 17.1052771146 | -5.5865999962 | 64.6868355370 |
| C143 | 15.8103547253 | -4.8951365747 | 63.0567097998 |
| H144 | 16.5042671257 | -4.0712124230 | 62.8584746087 |
| H145 | 15.0081086293 | -4.4980209861 | 63.6942916785 |
| C146 | 15.2499478968 | -5.3989419453 | 61.7382416018 |
| C147 | 14.1846033907 | -6.3138658228 | 61.6948089502 |
| H148 | 13.7023659386 | -6.6238506731 | 62.6209839577 |
| C149 | 15.8431181951 | -5.0013739322 | 60.5282827744 |
| H150 | 16.6428744851 | -4.2658069807 | 60.5473574472 |
| C151 | 13.7284531447 | -6.8235906674 | 60.4758796597 |
| H152 | 12.8949111018 | -7.5199413933 | 60.4520648115 |
| C153 | 15.3917337647 | -5.5137251498 | 59.3068252797 |
| H154 | 15.8571470355 | -5.2044927829 | 58.3752138965 |
| C155 | 14.3368200302 | -6.4295517724 | 59.2792872959 |
| H156 | 13.9947108056 | -6.8249934857 | 58.3283215392 |
| H157 | 9.0037559556# | 0.7050735312# | 60.7752692435# |
| C158 | 8.1269806174# | 0.1560800139# | 60.4649996035# |
| H159 | 7.2836720101# | 0.4592419705# | 61.0677700345# |
| H160 | 9.0199327620 | -9.0794438062 | 56.5140259276 |
| H161 | 18.2592782786# | -9.4987527756# | 50.1505401247# |
| C162 | 17.5839752144# | -8.6559202400# | 50.1520266901# |
| H163 | 17.2773627064# | -8.4419891426# | 49.1387987566# |
| H164 | 23.2658115084 | -4.1702395143 | 52.4180336890 |
| H165 | 10.4819035633 | -5.4839794952 | 50.5175381505 |

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|------|---------------|----------------|----------------|
| H166 | 14.2773876925 | -9.3762007616 | 56.3578633031 |
| H167 | 12.1793403048 | -5.1935063458 | 57.5359657273 |
| C168 | 6.7544796403 | -8.5929356148 | 55.9992340428 |
| H169 | 6.9600246583 | -8.8114842881 | 54.9444186755 |
| H170 | 6.0590447882 | -7.7499093823 | 56.0439486895 |
| N171 | 11.4867123401 | -8.1282083507 | 56.9407824704 |
| N172 | 11.3945438184 | -8.0237255726 | 58.0630835425 |
| H173 | 7.1493940556# | -5.8354099323# | 59.8218941849# |
| C174 | 6.9590147445# | -4.8009338198# | 59.5000033373# |
| H175 | 5.9039260094# | -4.4903549685# | 59.5181450083# |
| H176 | 7.4898406305 | -4.1647375238 | 60.2186561376 |
| C177 | 7.5606092248 | -4.5337163643 | 58.1211815932 |
| H178 | 8.6116928500 | -4.8522227199 | 58.1092380238 |
| H179 | 7.5466714556 | -3.4494228265 | 57.9258554438 |
| O180 | 6.8167704633 | -5.2135049221 | 57.1076708528 |
| H181 | 7.2990280798 | -5.0864520340 | 56.2685638180 |

The structure for N₂H in **Figure 5**.

Energies: E= -8029.788545, solv = -0.205882, disp = -233.78 Z₀ = 893.47

| | | | |
|-----|----------------|----------------|----------------|
| Mo1 | 16.5287270579 | -5.6484418271 | 53.1775028577 |
| Fe2 | 9.5616540122 | -7.5278030441 | 55.2931174584 |
| Fe3 | 11.4928743107 | -5.4749166752 | 55.0532196874 |
| Fe4 | 11.2318718674 | -7.1617052489 | 52.9502880257 |
| Fe5 | 12.2396091015 | -8.4333147633 | 55.1298524344 |
| Fe6 | 14.6705057532 | -7.7189090451 | 53.9968525480 |
| Fe7 | 14.1548121311 | -5.4015944273 | 55.1108972558 |
| Fe8 | 13.4077543915 | -5.6844974744 | 52.4882815643 |
| C9 | 17.8390906338 | -2.0784182062 | 54.2749126344 |
| H10 | 18.0126062481 | -1.0598121272 | 53.9223438685 |
| H11 | 16.7560641780 | -2.2004108813 | 54.4022433293 |
| C12 | 18.3259304314 | -3.1114808685 | 53.2352905179 |
| C13 | 19.7992378270 | -2.8450305027 | 52.8518155647 |
| H14 | 20.4201088334 | -3.0489974960 | 53.7292361990 |
| H15 | 19.8981453734 | -1.7834966162 | 52.6005823227 |
| C16 | 20.2724410433 | -3.6927926288 | 51.6504941318 |
| H17 | 19.8507076154 | -3.3139394852 | 50.7181750944 |
| H18 | 19.9344932614 | -4.7253012998 | 51.7937325475 |
| C19 | 17.5310474786 | -3.1809097569 | 51.8968297239 |
| O20 | 17.1796613797 | -4.3888571026 | 51.5489461548 |
| O21 | 17.4045864876 | -2.1650591122 | 51.2153845817 |
| O22 | 18.2157310613 | -4.4105292953 | 53.8497570622 |
| C23 | 12.7729858756 | -6.6849713962 | 54.1508770717 |
| S24 | 12.7134032722 | -4.2383734062 | 56.7003539045 |
| S25 | 16.1717084705 | -6.5311060387 | 55.4799486481 |
| S26 | 9.5555453478 | -5.4678556135 | 53.8457720085 |
| S27 | 14.2420970834 | -9.7970686967 | 55.2772576266 |
| S28 | 14.7090135657 | -3.8668801580 | 53.3379023927 |
| S29 | 10.3685296675 | -9.2512286790 | 53.6190067001 |
| S30 | 15.1545907337 | -7.2009838487 | 51.7859814222 |
| S31 | 11.8146110614 | -6.2712231077 | 50.6500688156 |
| H32 | 13.6351743325# | -2.1902103580# | 49.0425560006# |
| C33 | 13.2979242146# | -2.0241176836# | 50.0550234375# |
| H34 | 13.8912285777 | -2.6708780459 | 50.7066454288 |
| H35 | 13.4679511747 | -0.9798820454 | 50.3397106473 |
| N36 | 11.8730837231 | -2.3755638735 | 50.1365415092 |
| H37 | 11.2861000143 | -2.0922311282 | 49.3650356119 |
| C38 | 11.2264911489 | -2.8575129642 | 51.2118723630 |
| N39 | 11.8141134931 | -3.0470880680 | 52.3781683276 |
| H40 | 11.3177121425 | -3.6150405400 | 53.0731312557 |
| H41 | 12.8334226013 | -2.9901103357 | 52.5278189355 |
| N42 | 9.8852281935 | -3.0991502131 | 51.1199607765 |
| H43 | 9.5346102455 | -3.3604457909 | 50.2071586835 |
| H44 | 9.4971473951 | -3.6683132883 | 51.8805299101 |
| H45 | 7.9313440546 | 0.3894970973 | 59.4127744268 |
| C46 | 8.3508434637 | -1.3530609035 | 60.6891908819 |
| H47 | 8.2269357958 | -1.5715541134 | 61.7566550806 |
| H48 | 7.5754633491 | -1.9178478455 | 60.1584186590 |
| C49 | 9.7157120432 | -1.8306904534 | 60.3003397838 |
| N50 | 10.7274949043 | -1.9071476543 | 61.2405850076 |
| C51 | 10.1936786315 | -2.2016266668 | 59.0642544436 |

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|------|----------------|-----------------|----------------|
| H52 | 9.7240050203 | -2.3034570105 | 58.0986444259 |
| C53 | 11.7905654806 | -2.3195847062 | 60.5759486485 |
| H54 | 12.7671895066 | -2.5137573410 | 60.9970896318 |
| N55 | 11.5233207811 | -2.5012845133 | 59.2552043920 |
| H56 | 19.2821986855 | -4.3587242780 | 57.4784193480 |
| H57 | 16.7363276145 | -8.8289920583 | 50.8069514287 |
| C58 | 18.4103026114 | -7.4216734859 | 50.5798349999 |
| H59 | 17.7983656552 | -6.5177271932 | 50.5193100997 |
| H60 | 19.2311125823 | -7.2982006217 | 49.8594042062 |
| C61 | 18.9914079975 | -7.5175561054 | 51.9526726475 |
| N62 | 18.3013531477 | -7.0757957593 | 53.0692499138 |
| C63 | 20.2012999746 | -8.0251055632 | 52.3599636298 |
| H64 | 21.0195771987 | -8.4599070886 | 51.8068550100 |
| C65 | 19.0697323541 | -7.3081674550 | 54.1223315960 |
| H66 | 18.8469276052 | -7.0490820893 | 55.1459004912 |
| N67 | 20.2259953669 | -7.8914076625 | 53.7377957908 |
| H68 | 20.9901010280 | -8.0954112016 | 54.3648576190 |
| H69 | 6.9877733464 | -10.5230526089 | 56.9143159107 |
| C70 | 6.1750555335# | -9.8249627841# | 56.6900008871# |
| H71 | 5.5309550371# | -10.2322275824# | 56.0424860856# |
| H72 | 5.6932327490# | -9.5371414456# | 57.6127206849# |
| S73 | 7.9158214490 | -7.6519666425 | 56.9487971446 |
| H74 | 12.1493431216 | -2.8479674866 | 58.5321164998 |
| H75 | 18.4115939115 | -4.2324712443 | 54.8557008013 |
| C76 | 18.4767136909 | -2.2382124885 | 55.6854872685 |
| O77 | 18.7828001392 | -3.4442718559 | 56.0475788199 |
| O78 | 18.6113491187 | -1.2205311312 | 56.3866843718 |
| C79 | 21.7656091049 | -3.7119911984 | 51.5285196761 |
| O80 | 22.4527102203 | -3.3144059018 | 50.6079376218 |
| O81 | 22.3208169155# | -4.2658020060# | 52.6398596224# |
| H82 | 15.7024655098# | -0.1996320228# | 61.4912314498# |
| C83 | 14.8549939453# | -0.0829906450# | 60.8320018725# |
| H84 | 13.9165015891# | -0.2867338797# | 61.3260937709# |
| H85 | 14.8278226096 | 0.9916027779 | 60.5848356021 |
| C86 | 15.0599852571# | -0.8751946462# | 59.5441990181# |
| H87 | 14.3755919610 | -0.5064509366 | 58.7697975306 |
| H88 | 14.8073367009 | -1.9288379679 | 59.7100665131 |
| C89 | 16.4992029584 | -0.8186545785 | 59.0243471492 |
| H90 | 16.9118717067 | 0.1962232114 | 59.1259632526 |
| H91 | 16.5461933853 | -1.0409686741 | 57.9522665680 |
| C92 | 17.4360319354 | -1.7964675218 | 59.7473969906 |
| O93 | 17.1052182624 | -2.4069227913 | 60.7699517027 |
| N94 | 18.6649646626 | -1.9163781282 | 59.1776778565 |
| H95 | 19.1967791008 | -2.7240168907 | 59.4806822801 |
| H96 | 18.7794311392 | -1.6436352363 | 58.1905390331 |
| C97 | 10.6519925417# | 0.0100028386# | 53.3460013070# |
| H98 | 11.1636989364# | 0.9592720911# | 53.2872699184# |
| H99 | 9.5863320785# | 0.1850135178# | 53.3579373837# |
| H100 | 10.9222558932 | -0.5842834476 | 52.4723195015 |
| C101 | 11.0707488778 | -0.6459710557 | 54.6780883974 |
| H102 | 10.7328756067 | -1.6911717834 | 54.6838110056 |
| C103 | 10.3803759901 | 0.0714461168 | 55.8481361129 |
| H104 | 9.2878783148 | -0.0057863768 | 55.7756512230 |
| H105 | 10.6408976272 | 1.1395557372 | 55.8584951433 |
| H106 | 10.6825429147 | -0.3514514952 | 56.8118693195 |
| C107 | 12.5943712798 | -0.6254814515 | 54.8614323580 |
| H108 | 13.1227544835 | -1.1125596484 | 54.0355160190 |
| H109 | 12.8904134121 | -1.1442629802 | 55.7794259337 |
| H110 | 12.9578725325 | 0.4100655791 | 54.9266925708 |
| H111 | 13.4550780674# | -12.2303883715# | 53.1883141353# |
| C112 | 13.9110014305# | -11.6210557313# | 52.4219866186# |
| H113 | 14.7424832138 | -11.0592995133 | 52.8567805745 |
| H114 | 14.2571928933 | -12.2406719187 | 51.5895294714 |
| N115 | 12.8206229136 | -10.7506118672 | 51.9781498012 |
| H116 | 12.0589521559 | -10.5490922884 | 52.6472032711 |
| C117 | 12.7870606776 | -10.0288445347 | 50.8675590289 |
| N118 | 13.9082399997 | -9.8655571382 | 50.1140185188 |
| H119 | 13.7861675257 | -9.2337623350 | 49.3297730453 |
| H120 | 14.7259024213 | -9.5899905004 | 50.6596643943 |
| N121 | 11.6066644412 | -9.5304580976 | 50.4399624843 |
| H122 | 10.8507451198 | -9.6124835282 | 51.1285043193 |
| H123 | 11.6379007610 | -8.5791602211 | 50.0594209019 |
| H124 | 19.2080261076 | -8.2185932809 | 61.7078491076 |
| C125 | 19.5978936982# | -7.2298790835# | 61.9900505377# |
| H126 | 20.6402193088 | -7.3597449474 | 62.2992713136 |

| | | | |
|------|----------------|----------------|----------------|
| C127 | 18.8295288464 | -6.6906911381 | 63.1951778805 |
| O128 | 19.3806860806 | -6.2164076689 | 64.1859022804 |
| C129 | 19.4918713400# | -6.2717987584# | 60.7990632464# |
| H130 | 19.8623472246 | -5.2823330694 | 61.0911799163 |
| H131 | 18.4386120428 | -6.1248172211 | 60.5371552951 |
| C132 | 20.2418245996 | -6.7604338782 | 59.5451229941 |
| H133 | 19.9930205840 | -7.8077436971 | 59.3338115720 |
| H134 | 21.3275624281 | -6.7471266586 | 59.7212251052 |
| C135 | 20.0080836094 | -6.0179649940 | 58.2196885385 |
| O136 | 20.3217297285 | -6.5204008498 | 57.1511750477 |
| O137 | 19.4734111497 | -4.8070460327 | 58.3612661103 |
| N138 | 17.4752524110 | -6.7622730971 | 63.0434178278 |
| H139 | 17.1171540207 | -7.0785878588 | 62.1503675657 |
| C140 | 16.5368852913# | -6.0058845463# | 63.8530408404# |
| H141 | 15.8694784246 | -6.6958729875 | 64.3893493575 |
| H142 | 17.1223406243 | -5.4617818822 | 64.5983237950 |
| C143 | 15.6977068546 | -5.0396793877 | 62.9846245095 |
| H144 | 16.3386503440 | -4.2366641824 | 62.6049664964 |
| H145 | 14.9419574133 | -4.5751867353 | 63.6329200853 |
| C146 | 15.0286378565 | -5.7419351327 | 61.8153691648 |
| C147 | 13.9501832951 | -6.6201430055 | 62.0160831789 |
| H148 | 13.5565100741 | -6.7648644754 | 63.0212477368 |
| C149 | 15.5068944290 | -5.5577056619 | 60.5070752599 |
| H150 | 16.3112737903 | -4.8464970542 | 60.3336895595 |
| C151 | 13.3653721136 | -7.2929494493 | 60.9420508338 |
| H152 | 12.5220441624 | -7.9582105528 | 61.1088164273 |
| C153 | 14.9268700360 | -6.2372773468 | 59.4280009811 |
| H154 | 15.3068162413 | -6.0804717800 | 58.4213754396 |
| C155 | 13.8537111716 | -7.1076725120 | 59.6436959770 |
| H156 | 13.3869577483 | -7.6346208601 | 58.8159536269 |
| H157 | 9.0037560032# | 0.7050734313# | 60.7752692852# |
| C158 | 8.1269804386# | 0.1560799233# | 60.4649995411# |
| H159 | 7.2836720402# | 0.4592420300# | 61.0677700469# |
| H160 | 10.0222851072 | -8.2637396059 | 58.1865790999 |
| H161 | 18.2592784915# | -9.4987526048# | 50.1505401100# |
| C162 | 17.5839749424# | -8.6559205544# | 50.1520269459# |
| H163 | 17.2773626996# | -8.4419890680# | 49.1387987744# |
| H164 | 23.2850270105 | -4.2252764080 | 52.4988655158 |
| H165 | 10.7034706627 | -5.5046520663 | 50.6696187393 |
| H166 | 14.7513433485 | -9.2632933097 | 56.4084043570 |
| H167 | 12.6139704060 | -5.2114472172 | 57.6376798672 |
| C168 | 6.6940454658 | -8.5901390288 | 55.9613496909 |
| H169 | 7.1463472818 | -8.8923818341 | 55.0104852204 |
| H170 | 5.8536235990 | -7.9255684944 | 55.7232165319 |
| N171 | 11.0545328664 | -8.2695002609 | 56.6282904743 |
| N172 | 10.9720907207 | -8.5320015847 | 57.8325950151 |
| H173 | 7.1493940742# | -5.8354099020# | 59.8218942709# |
| C174 | 6.9590146408# | -4.8009336895# | 59.5000032469# |
| H175 | 5.9039259809# | -4.4903550635# | 59.5181449779# |
| H176 | 7.4809284358 | -4.1808717403 | 60.2440379539 |
| C177 | 7.4747144364 | -4.4188821941 | 58.1063079740 |
| H178 | 8.4858513720 | -4.8138210881 | 57.9349953836 |
| H179 | 7.5486021313 | -3.3241373198 | 58.0612180234 |
| O180 | 6.5945562278 | -4.8005185573 | 57.0630231376 |
| H181 | 6.8789848426 | -5.7046140093 | 56.8083192255 |

The structure for the TS for formation of N₂H in **Figure 6**.

Energies: E= -8029.768229, solv = -0.200267, disp = -232.62 Z₀ = 889.78

| | | | |
|-----|---------------|---------------|---------------|
| Mo1 | 16.3767690000 | -5.7211350000 | 53.3011880000 |
| Fe2 | 9.0111330000 | -7.1475150000 | 54.6000130000 |
| Fe3 | 11.2500700000 | -5.4546410000 | 55.0915090000 |
| Fe4 | 10.9828520000 | -7.0676470000 | 52.9987510000 |
| Fe5 | 11.8935330000 | -8.4461870000 | 55.1844830000 |
| Fe6 | 14.4608350000 | -7.7888200000 | 54.1079520000 |
| Fe7 | 13.9304020000 | -5.4958830000 | 55.2504680000 |
| Fe8 | 13.2758780000 | -5.7499410000 | 52.6083780000 |
| C9 | 17.7985160000 | -2.1161220000 | 54.3864830000 |
| H10 | 18.0004020000 | -1.1175040000 | 53.9944880000 |
| H11 | 16.7139340000 | -2.1980260000 | 54.5347130000 |
| C12 | 18.2257310000 | -3.1991500000 | 53.3747660000 |
| C13 | 19.7083200000 | -3.0182970000 | 52.9708660000 |

| | | | |
|-----|---------------|----------------|---------------|
| H14 | 20.3311430000 | -3.2050440000 | 53.8511590000 |
| H15 | 19.8472430000 | -1.9745380000 | 52.6673860000 |
| C16 | 20.1341530000 | -3.9407360000 | 51.8100720000 |
| H17 | 19.6193210000 | -3.6681950000 | 50.8875310000 |
| H18 | 19.8695260000 | -4.9734150000 | 52.0624530000 |
| C19 | 17.4108330000 | -3.2429690000 | 52.0511090000 |
| O20 | 17.0449360000 | -4.4410670000 | 51.6908710000 |
| O21 | 17.2818930000 | -2.2152230000 | 51.3887070000 |
| O22 | 18.0512650000 | -4.4770400000 | 54.0166190000 |
| C23 | 12.5682570000 | -6.7060350000 | 54.2779930000 |
| S24 | 12.4531740000 | -4.2248690000 | 56.7630930000 |
| S25 | 15.9712780000 | -6.6294430000 | 55.6018660000 |
| S26 | 9.4112150000 | -5.0634540000 | 53.6702240000 |
| S27 | 13.9227450000 | -9.9057690000 | 55.2430020000 |
| S28 | 14.5532980000 | -3.9488790000 | 53.4633570000 |
| S29 | 10.0500400000 | -9.1591130000 | 53.7305550000 |
| S30 | 15.0207580000 | -7.2913310000 | 51.9065900000 |
| S31 | 11.7536250000 | -6.3277750000 | 50.6939620000 |
| H32 | 13.6351740000 | -2.1902100000 | 49.0425560000 |
| C33 | 13.2979240000 | -2.0241170000 | 50.0550230000 |
| H34 | 13.8314530000 | -2.7248930000 | 50.7022180000 |
| H35 | 13.5311280000 | -1.0007950000 | 50.3685490000 |
| N36 | 11.8550950000 | -2.2842040000 | 50.0832990000 |
| H37 | 11.3103650000 | -1.9517730000 | 49.3010770000 |
| C38 | 11.1553360000 | -2.8030410000 | 51.1062320000 |
| N39 | 11.6908400000 | -3.0524990000 | 52.2842830000 |
| H40 | 11.1495330000 | -3.6338510000 | 52.9382590000 |
| H41 | 12.6940780000 | -2.9766850000 | 52.4941010000 |
| N42 | 9.8168500000 | -3.0171660000 | 50.9397500000 |
| H43 | 9.5179630000 | -3.2589880000 | 50.0034880000 |
| H44 | 9.3877380000 | -3.6007480000 | 51.6690070000 |
| H45 | 7.9321000000 | 0.3862130000 | 59.4118500000 |
| C46 | 8.3532590000 | -1.3544900000 | 60.6997190000 |
| H47 | 8.1436700000 | -1.5768360000 | 61.7531140000 |
| H48 | 7.6291430000 | -1.9252720000 | 60.1069590000 |
| C49 | 9.7496670000 | -1.8257570000 | 60.4264930000 |
| N50 | 10.6894530000 | -1.8571310000 | 61.4415300000 |
| C51 | 10.3191740000 | -2.2467420000 | 59.2452640000 |
| H52 | 9.9290730000 | -2.3855220000 | 58.2487250000 |
| C53 | 11.7995440000 | -2.2944720000 | 60.8769910000 |
| H54 | 12.7420090000 | -2.4685080000 | 61.3774310000 |
| N55 | 11.6293820000 | -2.5369710000 | 59.5493200000 |
| H56 | 19.2590430000 | -4.3054360000 | 57.5452120000 |
| H57 | 16.7185260000 | -8.8589480000 | 50.7799000000 |
| C58 | 18.3617170000 | -7.4222870000 | 50.6600950000 |
| H59 | 17.7278550000 | -6.5324880000 | 50.6118620000 |
| H60 | 19.2095250000 | -7.2461430000 | 49.9833770000 |
| C61 | 18.8880160000 | -7.5565550000 | 52.0566550000 |
| N62 | 18.1642300000 | -7.1390050000 | 53.1643360000 |
| C63 | 20.0901470000 | -8.0627560000 | 52.4913270000 |
| H64 | 20.9287730000 | -8.4783990000 | 51.9534910000 |
| C65 | 18.9063420000 | -7.3831610000 | 54.2331030000 |
| H66 | 18.6497950000 | -7.1419930000 | 55.2528830000 |
| N67 | 20.0772010000 | -7.9521450000 | 53.8714140000 |
| H68 | 20.8301470000 | -8.1457770000 | 54.5150080000 |
| H69 | 6.9484610000 | -10.5626770000 | 56.9348880000 |
| C70 | 6.1750540000 | -9.8249630000 | 56.6900010000 |
| H71 | 5.5309550000 | -10.2322280000 | 56.0424860000 |
| H72 | 5.6932330000 | -9.5371420000 | 57.6127210000 |
| S73 | 7.9953690000 | -7.6315450000 | 56.8101780000 |
| H74 | 12.3063480000 | -2.9014490000 | 58.8869940000 |
| H75 | 18.2550220000 | -4.3023020000 | 55.0136070000 |
| C76 | 18.4613480000 | -2.2574090000 | 55.7830010000 |
| O77 | 18.6837660000 | -3.4671170000 | 56.1866000000 |
| O78 | 18.6946090000 | -1.2263390000 | 56.4368840000 |
| C79 | 21.6090770000 | -3.8947190000 | 51.5419510000 |
| O80 | 22.1667480000 | -3.5884080000 | 50.5062780000 |
| O81 | 22.3208170000 | -4.2658020000 | 52.6398600000 |
| H82 | 15.7024660000 | -0.1996320000 | 61.4912310000 |
| C83 | 14.8549940000 | -0.0829910000 | 60.8320020000 |
| H84 | 13.9165020000 | -0.2867340000 | 61.3260940000 |
| H85 | 14.8276510000 | 0.9919930000 | 60.5858380000 |
| C86 | 15.0599850000 | -0.8751950000 | 59.5441990000 |
| H87 | 14.3708280000 | -0.5118780000 | 58.7714090000 |
| H88 | 14.8138930000 | -1.9301980000 | 59.7144200000 |

| | | | |
|------|---------------|----------------|---------------|
| C89 | 16.4957180000 | -0.8132690000 | 59.0156630000 |
| H90 | 16.8877100000 | 0.2134720000 | 59.0612170000 |
| H91 | 16.5396030000 | -1.0907080000 | 57.9560910000 |
| C92 | 17.4561480000 | -1.7346090000 | 59.7803350000 |
| O93 | 17.1245230000 | -2.3376470000 | 60.8061940000 |
| N94 | 18.7049370000 | -1.8124170000 | 59.2459130000 |
| H95 | 19.2582330000 | -2.5917880000 | 59.5824850000 |
| H96 | 18.8306570000 | -1.5713550000 | 58.2514270000 |
| C97 | 10.6519930000 | 0.0100030000 | 53.3460010000 |
| H98 | 11.1636990000 | 0.9592720000 | 53.2872700000 |
| H99 | 9.5863320000 | 0.1850130000 | 53.3579370000 |
| H100 | 10.9229190000 | -0.5845370000 | 52.4722780000 |
| C101 | 11.0621770000 | -0.6585270000 | 54.6757900000 |
| H102 | 10.7143810000 | -1.7003590000 | 54.6698600000 |
| C103 | 10.3738270000 | 0.0527670000 | 55.8521110000 |
| H104 | 9.2806020000 | 0.0121600000 | 55.7599510000 |
| H105 | 10.6670770000 | 1.1117470000 | 55.8942600000 |
| H106 | 10.6459530000 | -0.4033040000 | 56.8105860000 |
| C107 | 12.5849740000 | -0.6548560000 | 54.8679710000 |
| H108 | 13.1105310000 | -1.1796960000 | 54.0638770000 |
| H109 | 12.8653160000 | -1.1509620000 | 55.8037260000 |
| H110 | 12.9665160000 | 0.3758160000 | 54.9041590000 |
| H111 | 13.4550780000 | -12.2303880000 | 53.1883140000 |
| C112 | 13.9110020000 | -11.6210560000 | 52.4219870000 |
| H113 | 14.7808020000 | -11.0997150000 | 52.8270900000 |
| H114 | 14.1783340000 | -12.2165810000 | 51.5443960000 |
| N115 | 12.8108690000 | -10.7049480000 | 52.0866240000 |
| H116 | 12.0869630000 | -10.5633820000 | 52.7950840000 |
| C117 | 12.6501250000 | -10.0016900000 | 50.9724010000 |
| N118 | 13.7024530000 | -9.8140290000 | 50.1290960000 |
| H119 | 13.4861610000 | -9.2100230000 | 49.3430310000 |
| H120 | 14.5382690000 | -9.4720630000 | 50.6122950000 |
| N121 | 11.4249790000 | -9.5479810000 | 50.6433250000 |
| H122 | 10.7310660000 | -9.6285320000 | 51.3982540000 |
| H123 | 11.4073400000 | -8.5979290000 | 50.2531140000 |
| H124 | 19.2165320000 | -8.2201710000 | 61.7010510000 |
| C125 | 19.5978940000 | -7.2298790000 | 61.9900500000 |
| H126 | 20.6387200000 | -7.3547750000 | 62.3059720000 |
| C127 | 18.8192700000 | -6.7069430000 | 63.1921690000 |
| O128 | 19.3635180000 | -6.2853090000 | 64.2096650000 |
| C129 | 19.4918720000 | -6.2717980000 | 60.7990630000 |
| H130 | 19.8227400000 | -5.2718940000 | 61.1021470000 |
| H131 | 18.4407260000 | -6.1558270000 | 60.5133050000 |
| C132 | 20.2795730000 | -6.7267750000 | 59.5591340000 |
| H133 | 20.0915330000 | -7.7860130000 | 59.3472340000 |
| H134 | 21.3612020000 | -6.6455790000 | 59.7431730000 |
| C135 | 19.9924110000 | -5.9874910000 | 58.2444060000 |
| O136 | 20.2339350000 | -6.5015120000 | 57.1631530000 |
| O137 | 19.4962380000 | -4.7662380000 | 58.4166610000 |
| N138 | 17.4661710000 | -6.7364700000 | 63.0137290000 |
| H139 | 17.1128670000 | -7.0098260000 | 62.1050600000 |
| C140 | 16.5368850000 | -6.0058840000 | 63.8530410000 |
| H141 | 15.8457460000 | -6.7099720000 | 64.3390230000 |
| H142 | 17.1296300000 | -5.5272590000 | 64.6366230000 |
| C143 | 15.7221360000 | -4.9623480000 | 63.0533220000 |
| H144 | 16.3865800000 | -4.1694340000 | 62.6926470000 |
| H145 | 15.0077830000 | -4.4998390000 | 63.7484830000 |
| C146 | 14.9870620000 | -5.5824470000 | 61.8789250000 |
| C147 | 13.8647970000 | -6.4025420000 | 62.0777230000 |
| H148 | 13.4762600000 | -6.5446810000 | 63.0853170000 |
| C149 | 15.4567020000 | -5.3970600000 | 60.5684550000 |
| H150 | 16.2939570000 | -4.7245360000 | 60.3975250000 |
| C151 | 13.2371380000 | -7.0307460000 | 61.0008640000 |
| H152 | 12.3633530000 | -7.6555950000 | 61.1702570000 |
| C153 | 14.8366320000 | -6.0334030000 | 59.4871460000 |
| H154 | 15.2131050000 | -5.8859710000 | 58.4779850000 |
| C155 | 13.7277690000 | -6.8562100000 | 59.7027830000 |
| H156 | 13.2462330000 | -7.3528650000 | 58.8641770000 |
| H157 | 9.0037560000 | 0.7050740000 | 60.7752690000 |
| C158 | 8.1269810000 | 0.1560800000 | 60.4650000000 |
| H159 | 7.2836720000 | 0.4592420000 | 61.0677700000 |
| H160 | 9.2352680000 | -8.5779870000 | 57.3855010000 |
| H161 | 18.2592780000 | -9.4987530000 | 50.1505400000 |
| C162 | 17.5839750000 | -8.6559200000 | 50.1520270000 |
| H163 | 17.2773630000 | -8.4419890000 | 49.1387990000 |

| | | | |
|------|---------------|---------------|---------------|
| H164 | 23.2571380000 | -4.1964410000 | 52.3758590000 |
| H165 | 10.6665590000 | -5.5264080000 | 50.6571820000 |
| H166 | 14.3358180000 | -9.5317790000 | 56.4722770000 |
| H167 | 12.2644430000 | -5.1643350000 | 57.7217050000 |
| C168 | 6.7744270000 | -8.6627600000 | 55.9141060000 |
| H169 | 7.2435140000 | -9.0616760000 | 55.0056180000 |
| H170 | 5.9766350000 | -7.9797430000 | 55.5977460000 |
| N171 | 11.2295400000 | -8.7240460000 | 56.9461410000 |
| N172 | 10.4273470000 | -8.8773510000 | 57.7833510000 |
| H173 | 7.1493940000 | -5.8354100000 | 59.8218940000 |
| C174 | 6.9590150000 | -4.8009340000 | 59.5000030000 |
| H175 | 5.9039260000 | -4.4903550000 | 59.5181450000 |
| H176 | 7.4863440000 | -4.1791150000 | 60.2375780000 |
| C177 | 7.4606410000 | -4.4291300000 | 58.1010290000 |
| H178 | 8.4593490000 | -4.8420920000 | 57.9060860000 |
| H179 | 7.5479880000 | -3.3370510000 | 58.0425290000 |
| O180 | 6.5458350000 | -4.8010610000 | 57.0779610000 |
| H181 | 6.7989330000 | -5.7068170000 | 56.8244260000 |

The structure of N₂H₂ in **Figure 7**.

Energies: E= -8029.807469, solv = -0.208632, disp = -238.61 Z₀ = 896.06

| | | | |
|-----|----------------|----------------|----------------|
| Mo1 | 16.5663093406 | -5.7480392576 | 53.2466704532 |
| Fe2 | 9.4148664771 | -6.9517217537 | 55.4254427764 |
| Fe3 | 11.6940324201 | -5.2991483036 | 55.6093294239 |
| Fe4 | 11.2070043822 | -6.7959480293 | 53.3136331463 |
| Fe5 | 12.2103536681 | -8.2685367550 | 55.3526792359 |
| Fe6 | 14.6804952081 | -7.8641118857 | 54.2864523601 |
| Fe7 | 14.3481253068 | -5.4120726513 | 55.2194799945 |
| Fe8 | 13.5236752013 | -5.7747065622 | 52.6363634529 |
| C9 | 17.8328289412 | -2.1394209024 | 54.2412700068 |
| H10 | 17.9935443457 | -1.1250056956 | 53.8707505645 |
| H11 | 16.7524661602 | -2.2695127877 | 54.3788543447 |
| C12 | 18.3244962226 | -3.1839931472 | 53.2133465517 |
| C13 | 19.7863586735 | -2.8910041940 | 52.8077660614 |
| H14 | 20.4202312950 | -3.0597775095 | 53.6831494981 |
| H15 | 19.8563336911 | -1.8333420214 | 52.5320352605 |
| C16 | 20.2710666846 | -3.7535518852 | 51.6223794732 |
| H17 | 19.8469798532 | -3.3972271862 | 50.6823075906 |
| H18 | 19.9450216733 | -4.7873112020 | 51.7833666692 |
| C19 | 17.5141892258 | -3.2986471006 | 51.8850717955 |
| O20 | 17.1824941688 | -4.5202526551 | 51.5673066994 |
| O21 | 17.3595239392 | -2.2997015432 | 51.1835558089 |
| O22 | 18.2528228909 | -4.4747828627 | 53.8506012481 |
| C23 | 12.8340475055 | -6.5945059115 | 54.4162474366 |
| S24 | 13.3139512312 | -3.9941395325 | 56.8640453848 |
| S25 | 16.3086700091 | -6.6061272258 | 55.5668191674 |
| S26 | 9.7788661941 | -4.9275225900 | 54.1698392965 |
| S27 | 13.8662250310 | -9.7641227742 | 55.3698010036 |
| S28 | 14.7719287447 | -3.9238865247 | 53.3822587967 |
| S29 | 10.2409575976 | -8.8399740697 | 54.0484892342 |
| S30 | 15.1439870397 | -7.4156850329 | 52.0154488575 |
| S31 | 11.7856634722 | -6.2432846531 | 50.8804021264 |
| H32 | 13.6351742119# | -2.1902104574# | 49.0425559768# |
| C33 | 13.2979244212# | -2.0241175138# | 50.0550234611# |
| H34 | 13.8983993023 | -2.6734435672 | 50.6975078804 |
| H35 | 13.4790006656 | -0.9813951574 | 50.3401329745 |
| N36 | 11.8780898138 | -2.3693106395 | 50.1610258741 |
| H37 | 11.2687264738 | -2.0422744109 | 49.4247739803 |
| C38 | 11.2617700373 | -2.8025695329 | 51.2765296484 |
| N39 | 11.8933083311 | -3.0074649764 | 52.4142868946 |
| H40 | 11.3905655715 | -3.5235687742 | 53.1485283969 |
| H41 | 12.9174677171 | -2.9911669929 | 52.5227380338 |
| N42 | 9.9073165784 | -2.9815964908 | 51.2457263999 |
| H43 | 9.5012541270 | -3.2440471030 | 50.3568397784 |
| H44 | 9.5240788009 | -3.4943219901 | 52.0475320327 |
| H45 | 7.9298855270 | 0.3931753930 | 59.4137431949 |
| C46 | 8.3356512060 | -1.3538025222 | 60.6818379100 |
| H47 | 8.2652927974 | -1.5706417679 | 61.7544694120 |
| H48 | 7.5218211845 | -1.9030603754 | 60.1931051735 |
| C49 | 9.6680955710 | -1.8482240169 | 60.2155046620 |
| N50 | 10.7218839534 | -1.9733485472 | 61.1009459186 |

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| C51 | 10.0802807376 | -2.1748488399 | 58.9432437541 |
| H52 | 9.5631273707 | -2.2210349218 | 57.9975261116 |
| C53 | 11.7456662811 | -2.3726498577 | 60.3689847491 |
| H54 | 12.7408818310 | -2.5862790643 | 60.7332115991 |
| N55 | 11.4117913114 | -2.5021181270 | 59.0572247816 |
| H56 | 19.2692877058 | -4.3602618586 | 57.4731429562 |
| H57 | 16.7332866612 | -8.8352930126 | 50.8018087748 |
| C58 | 18.4054588954 | -7.4211152873 | 50.5853829101 |
| H59 | 17.7864327608 | -6.5207291514 | 50.5535112074 |
| H60 | 19.2111949367 | -7.2756844826 | 49.8518534785 |
| C61 | 19.0202600148 | -7.5360718313 | 51.9431555500 |
| N62 | 18.3487201015 | -7.1437673588 | 53.0903230947 |
| C63 | 20.2545547334 | -8.0170802508 | 52.3061401394 |
| H64 | 21.0693130199 | -8.4144023517 | 51.7206698157 |
| C65 | 19.1518860944 | -7.3781074607 | 54.1169805192 |
| H66 | 18.9493383784 | -7.1462769626 | 55.1514297013 |
| N67 | 20.3131265950 | -7.9176381312 | 53.6862270551 |
| H68 | 21.1010649541 | -8.1151159174 | 54.2848524863 |
| H69 | 6.9596949203 | -10.5511952445 | 56.9300262444 |
| C70 | 6.1750544029# | -9.8249633580# | 56.6900008241# |
| H71 | 5.5309554274# | -10.2322282114# | 56.0424860931# |
| H72 | 5.6932325379# | -9.5371412374# | 57.6127205097# |
| S73 | 8.0421059581 | -7.8278656733 | 57.0800367612 |
| H74 | 12.0143761366 | -2.8207768562 | 58.2970206605 |
| H75 | 18.4635352425 | -4.2839770693 | 54.8505192107 |
| C76 | 18.4780827375 | -2.2676481850 | 55.6515091243 |
| O77 | 18.8035507653 | -3.4630134106 | 56.0305379939 |
| O78 | 18.5994915137 | -1.2374540633 | 56.3375759056 |
| C79 | 21.7647776218 | -3.7593628001 | 51.5062720356 |
| O80 | 22.4520286075 | -3.3883226188 | 50.5741950882 |
| O81 | 22.3208171359# | -4.2658019841# | 52.6398596058# |
| H82 | 15.7024655250# | -0.1996319952# | 61.4912314353# |
| C83 | 14.8549937912# | -0.0829907297# | 60.8320019002# |
| H84 | 13.9165015893# | -0.2867338795# | 61.3260937710# |
| H85 | 14.8268590480 | 0.9915611177 | 60.5842967544 |
| C86 | 15.0599854257# | -0.8751945445# | 59.5441990499# |
| H87 | 14.3642136115 | -0.5186014910 | 58.7744488877 |
| H88 | 14.8227584652 | -1.9319102071 | 59.7120087971 |
| C89 | 16.4939795088 | -0.8000533575 | 59.0109051634 |
| H90 | 16.8921756398 | 0.2214948080 | 59.1044552339 |
| H91 | 16.5337237116 | -1.0282580307 | 57.9397516811 |
| C92 | 17.4510289465 | -1.7594201881 | 59.7312719944 |
| O93 | 17.1437498078 | -2.3539325027 | 60.7713978166 |
| N94 | 18.6689788376 | -1.8835020798 | 59.1406152997 |
| H95 | 19.2126393136 | -2.6801703414 | 59.4519085762 |
| H96 | 18.7685572088 | -1.6285770871 | 58.1464800412 |
| C97 | 10.6519926765# | 0.0100029249# | 53.3460013947# |
| H98 | 11.1636988630# | 0.9592721235# | 53.2872698036# |
| H99 | 9.5863320648# | 0.1850134315# | 53.3579374282# |
| H100 | 10.9246007901 | -0.5873207308 | 52.4762778479 |
| C101 | 11.0735460556 | -0.6279509657 | 54.6856616703 |
| H102 | 10.7387292819 | -1.6737609484 | 54.7082248539 |
| C103 | 10.3810074750 | 0.1088649325 | 55.8425295594 |
| H104 | 9.2885980019 | 0.0289381030 | 55.7696762084 |
| H105 | 10.6394113981 | 1.1775448243 | 55.8341323449 |
| H106 | 10.6822320353 | -0.2956437878 | 56.8143731995 |
| C107 | 12.5971571469 | -0.5950836054 | 54.8674742948 |
| H108 | 13.1248354466 | -1.1018829939 | 54.0532766454 |
| H109 | 12.8984285348 | -1.0874168107 | 55.7980717723 |
| H110 | 12.9563783353 | 0.4435123740 | 54.9043265659 |
| H111 | 13.4550779241# | -12.2303883845# | 53.1883140395# |
| C112 | 13.9110016795# | -11.6210556879# | 52.4219867720# |
| H113 | 14.8128723926 | -11.1445665759 | 52.8128000622 |
| H114 | 14.1128643026 | -12.1917921808 | 51.5122560143 |
| N115 | 12.8352963455 | -10.6514625566 | 52.1755762552 |
| H116 | 12.2576366565 | -10.4209217688 | 52.9878017833 |
| C117 | 12.6126200778 | -9.9366002044 | 51.0838478283 |
| N118 | 13.6003867098 | -9.7805951298 | 50.1578733880 |
| H119 | 13.3386465184 | -9.1826927376 | 49.3812438711 |
| H120 | 14.4758187076 | -9.4579727859 | 50.5810556352 |
| N121 | 11.3804652988 | -9.4351103076 | 50.8569187276 |
| H122 | 10.7360760689 | -9.5137816005 | 51.6509198920 |
| H123 | 11.3536804313 | -8.4854632803 | 50.4691005731 |
| H124 | 19.1943342657 | -8.2146554450 | 61.7143140919 |
| C125 | 19.5978935100# | -7.2298793236# | 61.9900503808# |

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|------|----------------|----------------|----------------|
| H126 | 20.6412391703 | -7.3696898574 | 62.2916413635 |
| C127 | 18.8422164788 | -6.6705592332 | 63.1950979219 |
| O128 | 19.3989332221 | -6.1564886488 | 64.1622054430 |
| C129 | 19.4918715968# | -6.2717984572# | 60.7990633320# |
| H130 | 19.8804248345 | -5.2881390626 | 61.0875211311 |
| H131 | 18.4382699544 | -6.1113096983 | 60.5495133303 |
| C132 | 20.2202621713 | -6.7712605973 | 59.5372693015 |
| H133 | 19.9324641160 | -7.8068309382 | 59.3162177195 |
| H134 | 21.3062328349 | -6.8008622167 | 59.7087049521 |
| C135 | 20.0125120200 | -6.0087884264 | 58.2176466929 |
| O136 | 20.3740654594 | -6.4851007892 | 57.1528628334 |
| O137 | 19.4412255952 | -4.8141156971 | 58.3580581921 |
| N138 | 17.4868024003 | -6.7693607655 | 63.0635306644 |
| H139 | 17.1297969692 | -7.1217520922 | 62.1841314147 |
| C140 | 16.5368852110# | -6.0058844986# | 63.8530407246# |
| H141 | 15.8804542600 | -6.6951481673 | 64.4036926203 |
| H142 | 17.1121581311 | -5.4372794492 | 64.5879064701 |
| C143 | 15.6765562267 | -5.0686098721 | 62.9653282286 |
| H144 | 16.2793964220 | -4.2137938525 | 62.6408341171 |
| H145 | 14.8584409868 | -4.6755165385 | 63.5842012544 |
| C146 | 15.1301446471 | -5.7812615964 | 61.7393223069 |
| C147 | 14.1524986872 | -6.7847823538 | 61.8455668285 |
| H148 | 13.7097571696 | -7.0048946141 | 62.8159247874 |
| C149 | 15.6712785850 | -5.5063559289 | 60.4716421650 |
| H150 | 16.3998024986 | -4.7051074458 | 60.3713315626 |
| C151 | 13.7458726666 | -7.5096327761 | 60.7216177928 |
| H152 | 12.9950189895 | -8.2900491765 | 60.8281752497 |
| C153 | 15.2709680473 | -6.2351413818 | 59.3459015766 |
| H154 | 15.7084764026 | -6.0262792998 | 58.3731476410 |
| C155 | 14.3131709313 | -7.2470596468 | 59.4688763488 |
| H156 | 14.0271021448 | -7.8234804364 | 58.5928149492 |
| H157 | 9.0037559687# | 0.7050734955# | 60.7752692697# |
| C158 | 8.1269805825# | 0.1560800741# | 60.4649995132# |
| H159 | 7.2836720237# | 0.4592419581# | 61.0677700596# |
| H160 | 10.5718854507 | -6.1400231969 | 58.0398055671 |
| H161 | 18.2592784113# | -9.4987526692# | 50.1505401233# |
| C162 | 17.5839749970# | -8.6559203801# | 50.1520269010# |
| H163 | 17.2773627272# | -8.4419890734# | 49.1387987650# |
| H164 | 23.2852174382 | -4.2223160995 | 52.5009220222 |
| H165 | 10.7706798665 | -5.3547849358 | 50.8780869944 |
| H166 | 11.5866511697 | -8.0488253120 | 58.0731366646 |
| H167 | 13.3911078083 | -4.8422616132 | 57.9165260480 |
| C168 | 6.7769869643 | -8.6062452096 | 56.0110490767 |
| H169 | 7.2463530129 | -8.9039637702 | 55.0668543903 |
| H170 | 5.9877155160 | -7.8799535578 | 55.7765272331 |
| N171 | 11.5044296317 | -7.6450097503 | 57.1376027595 |
| N172 | 10.8820135627 | -6.4544072111 | 57.1163139114 |
| H173 | 7.1493940675# | -5.8354099124# | 59.8218942418# |
| C174 | 6.9590150104# | -4.8009332995# | 59.5000036690# |
| H175 | 5.9039259981# | -4.4903550046# | 59.5181449709# |
| H176 | 7.4950546431 | -4.1654202847 | 60.2191734539 |
| C177 | 7.4484201820 | -4.4724442203 | 58.0860669195 |
| H178 | 8.4932620819 | -4.7847458895 | 57.9446263934 |
| H179 | 7.4227813727 | -3.3834147458 | 57.9526544649 |
| O180 | 6.6174165546 | -5.0190598537 | 57.0786361976 |
| H181 | 6.9404942723 | -5.9415047205 | 56.9634578497 |

The structure of the reactant with two water.

Energies: E=-8182.639843, solv = -0.209678, disp= 242.53, Z₀ = 925.12

| | | | |
|-----|---------------|---------------|---------------|
| Mo1 | 16.6578216559 | -5.2711516497 | 53.0753841506 |
| Fe2 | 9.5809669492 | -7.2319310951 | 55.2157569591 |
| Fe3 | 11.6848824330 | -5.3824372312 | 55.4019727481 |
| Fe4 | 11.3716466974 | -6.8545789614 | 52.9771309216 |
| Fe5 | 12.5741047766 | -8.2195608510 | 55.0300157298 |
| Fe6 | 14.8987677638 | -7.3536100981 | 53.9140479083 |
| Fe7 | 14.3991619257 | -5.1060569928 | 55.1041121525 |
| Fe8 | 13.6759957209 | -5.4214493104 | 52.6360398515 |
| C9 | 18.0053451383 | -1.7844065024 | 54.3437632205 |
| H10 | 18.2038365917 | -0.7507386590 | 54.0539860221 |
| H11 | 16.9188940542 | -1.8905807796 | 54.4571595144 |
| C12 | 18.4797353598 | -2.7673517343 | 53.2493285524 |
| C13 | 19.9611202972 | -2.5105485169 | 52.8898141460 |

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|-----|----------------|-----------------|----------------|
| H14 | 20.5665243722 | -2.7769990200 | 53.7617385619 |
| H15 | 20.0889248606 | -1.4402650414 | 52.6976169285 |
| C16 | 20.4249551408 | -3.3068386668 | 51.6475378149 |
| H17 | 20.0989543130 | -2.8125171028 | 50.7310335341 |
| H18 | 19.9785093195 | -4.3062222351 | 51.6850992600 |
| C19 | 17.6850817036 | -2.7623020321 | 51.9069290896 |
| O20 | 17.2917805957 | -3.9452724048 | 51.5131861913 |
| O21 | 17.5914601929 | -1.7207206508 | 51.2620861748 |
| O22 | 18.3490578989 | -4.0920789209 | 53.7980555444 |
| C23 | 12.9610022354 | -6.4029757127 | 54.2178844459 |
| S24 | 13.1125053984 | -3.9612429092 | 56.8226627618 |
| S25 | 16.4114675756 | -6.2162466905 | 55.3650700267 |
| S26 | 9.7382244798 | -5.1627313260 | 54.0131909796 |
| S27 | 14.5898878358 | -9.5849708733 | 54.9425153378 |
| S28 | 14.8312605967 | -3.4876603921 | 53.3630788213 |
| S29 | 10.4764390145 | -8.9498899793 | 53.7219461464 |
| S30 | 15.3268471545 | -6.8209075118 | 51.6609288834 |
| S31 | 11.9848275078 | -6.0688838127 | 50.7012002500 |
| H32 | 13.6351742682# | -2.1902104965# | 49.0425560021# |
| C33 | 13.2979242878# | -2.0241175178# | 50.0550234980# |
| H34 | 13.8574800589 | -2.7058474867 | 50.7001319986 |
| H35 | 13.5213616771 | -0.9942046727 | 50.3551805211 |
| N36 | 11.8607563835 | -2.3057501143 | 50.1369835284 |
| H37 | 11.2782640774 | -1.9771842050 | 49.3801379296 |
| C38 | 11.2079209034 | -2.7751672022 | 51.2138576453 |
| N39 | 11.7882496509 | -2.9765384477 | 52.3786875268 |
| H40 | 11.2878063809 | -3.5567576296 | 53.0640942601 |
| H41 | 12.8044755521 | -2.8996752981 | 52.5321003685 |
| N42 | 9.8581580305 | -2.9873500425 | 51.1141354245 |
| H43 | 9.5246693830 | -3.3000639054 | 50.2107841697 |
| H44 | 9.4569953695 | -3.5161830008 | 51.8935499579 |
| H45 | 7.9325520585 | 0.3810724355 | 59.4110396270 |
| C46 | 8.3275019849 | -1.3523154916 | 60.7097562809 |
| H47 | 8.2155205306 | -1.5517403439 | 61.7822940323 |
| H48 | 7.5309362758 | -1.9079414889 | 60.2000968654 |
| C49 | 9.6745464777 | -1.8592644117 | 60.3059059774 |
| N50 | 10.6905065379 | -1.9794078491 | 61.2354476986 |
| C51 | 10.1344365178 | -2.2068828764 | 59.0564406934 |
| H52 | 9.6549993432 | -2.2652882150 | 58.0915499210 |
| C53 | 11.7396390142 | -2.3973354389 | 60.5507550439 |
| H54 | 12.7164168434 | -2.6200142155 | 60.9578067192 |
| N55 | 11.4566366480 | -2.5423431227 | 59.2294943191 |
| H56 | 19.3585225335 | -4.2983398779 | 57.4918990267 |
| H57 | 16.7461156054 | -8.8008624944 | 50.8265453052 |
| C58 | 18.4240586471 | -7.4046785106 | 50.5171686968 |
| H59 | 17.8132296727 | -6.5058748163 | 50.4055781010 |
| H60 | 19.2345812223 | -7.3313375164 | 49.7778769780 |
| C61 | 19.0254427091 | -7.4028605153 | 51.8845732467 |
| N62 | 18.4561332171 | -6.7151998265 | 52.9448045539 |
| C63 | 20.1719963996 | -8.0180871318 | 52.3257372153 |
| H64 | 20.8971160673 | -8.6335357556 | 51.8160249694 |
| C65 | 19.2382504091 | -6.9095800247 | 53.9973138618 |
| H66 | 19.0980748172 | -6.5142915475 | 54.9907455291 |
| N67 | 20.2832130676 | -7.6969211517 | 53.6668057671 |
| H68 | 21.0182725716 | -7.9555452365 | 54.3080607226 |
| H69 | 6.9357268503 | -10.5751531843 | 56.9374999191 |
| C70 | 6.1750550015# | -9.8249632122# | 56.6900010349# |
| H71 | 5.5309554297# | -10.2322280462# | 56.0424859867# |
| H72 | 5.6932323806# | -9.5371412703# | 57.6127204378# |
| S73 | 8.2809464172 | -8.0253814216 | 56.9685978529 |
| H74 | 12.0804659411 | -2.8613669007 | 58.4883315170 |
| H75 | 18.5476371626 | -3.9710929924 | 54.8200123384 |
| C76 | 18.6278419037 | -2.0408928244 | 55.7490513592 |
| O77 | 18.9026716248 | -3.2740951029 | 56.0438161840 |
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| H82 | 15.7024655411# | -0.1996319657# | 61.4912314196# |
| C83 | 14.8549938557# | -0.0829907525# | 60.8320019245# |
| H84 | 13.9165015893# | -0.2867338795# | 61.3260937710# |
| H85 | 14.8290324677 | 0.9920186360 | 60.5864443157 |
| C86 | 15.0599853666# | -0.8751945622# | 59.5441989904# |
| H87 | 14.3890209674 | -0.4954939783 | 58.7637611062 |
| H88 | 14.7890309355 | -1.9249254552 | 59.7037552199 |

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|------|----------------|-----------------|----------------|
| C89 | 16.5031024529 | -0.8419998846 | 59.0363043277 |
| H90 | 16.9277863544 | 0.1693742574 | 59.1184816641 |
| H91 | 16.5520329162 | -1.0864436886 | 57.9689672367 |
| C92 | 17.4261451748 | -1.8189996238 | 59.7777249138 |
| O93 | 17.0620269549 | -2.4674287423 | 60.7647873215 |
| N94 | 18.6840038895 | -1.8967589074 | 59.2649052818 |
| H95 | 19.2140071902 | -2.7074063332 | 59.5624669335 |
| H96 | 18.8441358290 | -1.5833077284 | 58.2965418839 |
| C97 | 10.6519927169# | 0.0100028348# | 53.3460013160# |
| H98 | 11.1636988471# | 0.9592721347# | 53.2872698475# |
| H99 | 9.5863320724# | 0.1850134768# | 53.3579374361# |
| H100 | 10.9256149468 | -0.5853263175 | 52.4757690214 |
| C101 | 11.0723839906 | -0.6324646982 | 54.6840160596 |
| H102 | 10.7709425023 | -1.6886797121 | 54.6858647733 |
| C103 | 10.3410757795 | 0.0616075163 | 55.8435082004 |
| H104 | 9.2528349817 | -0.0536620906 | 55.7560239915 |
| H105 | 10.5634666265 | 1.1383109133 | 55.8558526242 |
| H106 | 10.6450167756 | -0.3490795195 | 56.8121820058 |
| C107 | 12.5913314901 | -0.5547421462 | 54.8865171208 |
| H108 | 13.1472972375 | -1.0244230331 | 54.0689340577 |
| H109 | 12.8975109052 | -1.0588459458 | 55.8090147120 |
| H110 | 12.9137421568 | 0.4945516587 | 54.9516550429 |
| H111 | 13.4550781473# | -12.2303882858# | 53.1883142507# |
| C112 | 13.9110013104# | -11.6210558142# | 52.4219864809# |
| H113 | 14.7773029320 | -11.1099126361 | 52.8475560378 |
| H114 | 14.2029400053 | -12.2458209422 | 51.5710970185 |
| N115 | 12.8497220429 | -10.6998463699 | 52.0153253701 |
| H116 | 12.1003423773 | -10.4977861486 | 52.6895864147 |
| C117 | 12.8808665077 | -9.8903404298 | 50.9610754706 |
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| H119 | 14.0032590797 | -8.9756919818 | 49.5735867384 |
| H120 | 14.8699161991 | -9.7011848091 | 50.7989598009 |
| N121 | 11.7436825331 | -9.2957744420 | 50.5517822423 |
| H122 | 10.9745217815 | -9.3605506389 | 51.2258405584 |
| H123 | 11.8320297115 | -8.3291244463 | 50.2104488412 |
| H124 | 19.2328863548 | -8.2255187848 | 61.6978416670 |
| C125 | 19.5978935435# | -7.2298792579# | 61.9900504987# |
| H126 | 20.6379535540 | -7.3428617584 | 62.3131780086 |
| C127 | 18.8084444927 | -6.7273458057 | 63.1944295967 |
| O128 | 19.3417158675 | -6.3731872403 | 64.2442896406 |
| C129 | 19.4918715082# | -6.2717985410# | 60.7990633049# |
| H130 | 19.8190764921 | -5.2709280911 | 61.1039555699 |
| H131 | 18.4420771454 | -6.1567961026 | 60.5084562594 |
| C132 | 20.2857727663 | -6.7207264834 | 59.5558538026 |
| H133 | 20.0864910305 | -7.7756640659 | 59.3327195115 |
| H134 | 21.3660636347 | -6.6601803753 | 59.7552501307 |
| C135 | 20.0475348852 | -5.9786240905 | 58.2285391798 |
| O136 | 20.3470002301 | -6.4872032058 | 57.1593743634 |
| O137 | 19.5332838027 | -4.7570597625 | 58.3700446042 |
| N138 | 17.4631813750 | -6.6969917700 | 62.9809898103 |
| H139 | 17.1125013410 | -6.9364553170 | 62.0616932640 |
| C140 | 16.5368851203# | -6.0058846251# | 63.8530404166# |
| H141 | 15.8676293828 | -6.7306852604 | 64.3397920124 |
| H142 | 17.1339506328 | -5.5304390267 | 64.6356297064 |
| C143 | 15.6884460522 | -4.9638435770 | 63.0882706430 |
| H144 | 16.3368632275 | -4.1731239316 | 62.6955211733 |
| H145 | 15.0001765657 | -4.5005815516 | 63.8079139346 |
| C146 | 14.9155251195 | -5.6043344210 | 61.9532903855 |
| C147 | 13.7580330138 | -6.3579599073 | 62.2037798490 |
| H148 | 13.3637584461 | -6.4130031962 | 63.2173327232 |
| C149 | 15.3992059139 | -5.5296823092 | 60.6360884080 |
| H150 | 16.2583245934 | -4.8979605066 | 60.4228386507 |
| C151 | 13.1057722267 | -7.0307802477 | 61.1692910336 |
| H152 | 12.2067698312 | -7.6058577450 | 61.3776825667 |
| C153 | 14.7625753482 | -6.2246298910 | 59.6023488572 |
| H154 | 15.1688713662 | -6.1919141298 | 58.5954194183 |
| C155 | 13.6147438558 | -6.9771650729 | 59.8683622268 |
| H156 | 13.1318977983 | -7.5262261142 | 59.0670112182 |
| H157 | 9.0037559686# | 0.7050735180# | 60.7752692304# |
| C158 | 8.1269805500# | 0.1560800299# | 60.4649995645# |
| H159 | 7.2836720285# | 0.4592419800# | 61.0677700553# |
| H160 | 10.9056528716 | -6.6219726077 | 57.9579776464 |
| H161 | 18.2592785842# | -9.4987525305# | 50.1505400606# |
| C162 | 17.5839749693# | -8.6559204856# | 50.1520272309# |
| H163 | 17.2773626316# | -8.4419890790# | 49.1387987928# |

| | | | |
|------|---------------|----------------|----------------|
| H164 | 23.2935001408 | -4.2989887519 | 52.5768836499 |
| H165 | 10.8038707898 | -5.4137028256 | 50.6202590143 |
| H166 | 15.0687726129 | -9.3154631097 | 56.1965327973 |
| H167 | 13.3271723435 | -4.8557524449 | 57.8145899618 |
| C168 | 6.8367036026 | -8.6346013207 | 56.0063928062 |
| H169 | 7.1849024801 | -8.9368563530 | 55.0122801031 |
| H170 | 6.1112200181 | -7.8231007536 | 55.8697469074 |
| N171 | 11.8393540257 | -7.8751741576 | 56.8156456930 |
| N172 | 11.2194374819 | -6.7928351595 | 56.9823508174 |
| H173 | 7.1493939976# | -5.8354099045# | 59.8218943085# |
| C174 | 6.9590150824# | -4.8009333946# | 59.5000036940# |
| H175 | 5.9039260003# | -4.4903549913# | 59.5181448624# |
| H176 | 7.5027250719 | -4.1569425719 | 60.2042722989 |
| C177 | 7.4716104327 | -4.5422575696 | 58.0799013537 |
| H178 | 8.5365382030 | -4.8039967418 | 57.9993895515 |
| H179 | 7.3901247479 | -3.4691054557 | 57.8592291284 |
| O180 | 6.7114117285 | -5.2248944607 | 57.0979848420 |
| H181 | 7.1588033677 | -6.0907711693 | 56.9796842785 |
| O182 | 12.7305260266 | -10.3036864961 | 57.9711376085 |
| H183 | 12.2854552855 | -9.4347425973 | 57.7963616027 |
| H184 | 12.8427803510 | -10.6522009050 | 57.0698056347 |
| O185 | 15.3052821647 | -9.2985835707 | 58.0991454074 |
| H186 | 14.4098943659 | -9.7021351540 | 58.2155298278 |
| H187 | 15.9301816639 | -9.9845522749 | 58.3766847954 |

The structure of the TS with two water molecules in **Figure 8**.

Energies: E = -8182.627859, solv = -0.212304, disp = -243.34, Z₀ = 922.22

| | | | |
|-----|---------------|---------------|---------------|
| Mo1 | 16.5222710000 | -5.7099350000 | 53.3117920000 |
| Fe2 | 9.3558970000 | -7.0541860000 | 55.2066470000 |
| Fe3 | 11.5971170000 | -5.3305210000 | 55.5228220000 |
| Fe4 | 11.2195220000 | -6.8823150000 | 53.1265090000 |
| Fe5 | 12.1256710000 | -8.3090750000 | 55.3237040000 |
| Fe6 | 14.6480060000 | -7.8560300000 | 54.3947850000 |
| Fe7 | 14.3370680000 | -5.4038490000 | 55.3196640000 |
| Fe8 | 13.6434740000 | -5.7907070000 | 52.8533880000 |
| C9 | 17.8609020000 | -2.0818600000 | 54.3254530000 |
| H10 | 18.0543500000 | -1.0792960000 | 53.9387440000 |
| H11 | 16.7780080000 | -2.1728860000 | 54.4737370000 |
| C12 | 18.3046330000 | -3.1575270000 | 53.3105450000 |
| C13 | 19.7727010000 | -2.9258620000 | 52.8842620000 |
| H14 | 20.4109380000 | -3.1052700000 | 53.7544660000 |
| H15 | 19.8795830000 | -1.8756880000 | 52.5910250000 |
| C16 | 20.2076480000 | -3.8243660000 | 51.7073420000 |
| H17 | 19.7423980000 | -3.4988640000 | 50.7755530000 |
| H18 | 19.8909470000 | -4.8529690000 | 51.9129450000 |
| C19 | 17.4802420000 | -3.2542280000 | 51.9936420000 |
| O20 | 17.1467170000 | -4.4739200000 | 51.6612200000 |
| O21 | 17.3202400000 | -2.2505770000 | 51.3033830000 |
| O22 | 18.1909970000 | -4.4354190000 | 53.9642300000 |
| C23 | 12.7794650000 | -6.5727160000 | 54.4600220000 |
| S24 | 13.1548160000 | -3.9853070000 | 56.9183260000 |
| S25 | 16.2871660000 | -6.6199110000 | 55.6458530000 |
| S26 | 9.6918460000 | -5.0015580000 | 54.0697920000 |
| S27 | 13.8128260000 | -9.9352810000 | 55.3448200000 |
| S28 | 14.7849180000 | -3.8603660000 | 53.5183130000 |
| S29 | 10.0833970000 | -8.8568730000 | 53.7973710000 |
| S30 | 15.1920560000 | -7.4598760000 | 52.1374780000 |
| S31 | 12.0513910000 | -6.2206540000 | 50.8845510000 |
| H32 | 13.6351740000 | -2.1902110000 | 49.0425560000 |
| C33 | 13.2979240000 | -2.0241180000 | 50.0550230000 |
| H34 | 13.8879970000 | -2.6819610000 | 50.6983810000 |
| H35 | 13.4854980000 | -0.9844220000 | 50.3463880000 |
| N36 | 11.8751940000 | -2.3615490000 | 50.1449050000 |
| H37 | 11.2728080000 | -2.0111400000 | 49.4138740000 |
| C38 | 11.2471620000 | -2.8275320000 | 51.2418750000 |
| N39 | 11.8627020000 | -3.0459280000 | 52.3847870000 |
| H40 | 11.3597680000 | -3.6072240000 | 53.0840940000 |
| H41 | 12.8847500000 | -3.0511720000 | 52.5012090000 |
| N42 | 9.8952960000 | -3.0221510000 | 51.1828480000 |
| H43 | 9.5162290000 | -3.2857860000 | 50.2825570000 |
| H44 | 9.5078830000 | -3.5601300000 | 51.9660300000 |

| | | | |
|------|---------------|----------------|---------------|
| H45 | 7.9319230000 | 0.3854060000 | 59.4118020000 |
| C46 | 8.3427320000 | -1.3540230000 | 60.7005570000 |
| H47 | 8.1771970000 | -1.5695910000 | 61.7630410000 |
| H48 | 7.5879990000 | -1.9187380000 | 60.1408840000 |
| C49 | 9.7219670000 | -1.8265840000 | 60.3636530000 |
| N50 | 10.7057320000 | -1.8738840000 | 61.3336420000 |
| C51 | 10.2433670000 | -2.1990950000 | 59.1449400000 |
| H52 | 9.8048460000 | -2.3103380000 | 58.1650210000 |
| C53 | 11.7966010000 | -2.2710770000 | 60.7039090000 |
| H54 | 12.7643390000 | -2.4403510000 | 61.1549920000 |
| N55 | 11.5707720000 | -2.4739000000 | 59.3784690000 |
| H56 | 19.3112280000 | -4.3022310000 | 57.5267780000 |
| H57 | 16.7277080000 | -8.8408830000 | 50.7951690000 |
| C58 | 18.3819140000 | -7.4157810000 | 50.6146590000 |
| H59 | 17.7461300000 | -6.5269600000 | 50.5893880000 |
| H60 | 19.1918920000 | -7.2454080000 | 49.8913640000 |
| C61 | 18.9863180000 | -7.5304250000 | 51.9797690000 |
| N62 | 18.3429140000 | -7.0687460000 | 53.1181360000 |
| C63 | 20.1991210000 | -8.0585950000 | 52.3530670000 |
| H64 | 20.9921140000 | -8.5096770000 | 51.7761610000 |
| C65 | 19.1415820000 | -7.3061940000 | 54.1471280000 |
| H66 | 18.9569730000 | -7.0369980000 | 55.1758430000 |
| N67 | 20.2731010000 | -7.9144640000 | 53.7278060000 |
| H68 | 21.0511840000 | -8.1375880000 | 54.3301070000 |
| H69 | 6.9549920000 | -10.5579030000 | 56.9279050000 |
| C70 | 6.1750550000 | -9.8249630000 | 56.6900010000 |
| H71 | 5.5309550000 | -10.2322280000 | 56.0424860000 |
| H72 | 5.6932320000 | -9.5371410000 | 57.6127200000 |
| S73 | 8.1353510000 | -7.8783310000 | 57.0106010000 |
| H74 | 12.2324230000 | -2.7848440000 | 58.6681270000 |
| H75 | 18.4033900000 | -4.2414980000 | 54.9643940000 |
| C76 | 18.5154520000 | -2.2153500000 | 55.7289580000 |
| O77 | 18.7950470000 | -3.4181640000 | 56.1208560000 |
| O78 | 18.6853670000 | -1.1843600000 | 56.4010760000 |
| C79 | 21.6933910000 | -3.8327750000 | 51.5140750000 |
| O80 | 22.3220090000 | -3.5190270000 | 50.5222520000 |
| O81 | 22.3208170000 | -4.2658020000 | 52.6398600000 |
| H82 | 15.7024660000 | -0.1996320000 | 61.4912310000 |
| C83 | 14.8549940000 | -0.0829910000 | 60.8320020000 |
| H84 | 13.9165020000 | -0.2867340000 | 61.3260940000 |
| H85 | 14.8271150000 | 0.9920590000 | 60.5860880000 |
| C86 | 15.0599850000 | -0.8751950000 | 59.5441990000 |
| H87 | 14.3670420000 | -0.5164880000 | 58.7729950000 |
| H88 | 14.8188130000 | -1.9310930000 | 59.7127620000 |
| C89 | 16.4934860000 | -0.8059800000 | 59.0105870000 |
| H90 | 16.8865380000 | 0.2197400000 | 59.0710680000 |
| H91 | 16.5330830000 | -1.0677560000 | 57.9468920000 |
| C92 | 17.4568020000 | -1.7383830000 | 59.7571320000 |
| O93 | 17.1336230000 | -2.3509530000 | 60.7802000000 |
| N94 | 18.7004130000 | -1.8150680000 | 59.2101500000 |
| H95 | 19.2544200000 | -2.5998180000 | 59.5328210000 |
| H96 | 18.8204220000 | -1.5595400000 | 58.2189950000 |
| C97 | 10.6519930000 | 0.0100030000 | 53.3460010000 |
| H98 | 11.1636990000 | 0.9592720000 | 53.2872700000 |
| H99 | 9.5863320000 | 0.1850130000 | 53.3579370000 |
| H100 | 10.9227350000 | -0.5850400000 | 52.4729710000 |
| C101 | 11.0744150000 | -0.6455010000 | 54.6775680000 |
| H102 | 10.7485140000 | -1.6944470000 | 54.6780190000 |
| C103 | 10.3751330000 | 0.0593570000 | 55.8509430000 |
| H104 | 9.2830650000 | -0.0230260000 | 55.7744580000 |
| H105 | 10.6294190000 | 1.1289360000 | 55.8722400000 |
| H106 | 10.6777090000 | -0.3703110000 | 56.8121850000 |
| C107 | 12.5977090000 | -0.6054250000 | 54.8620780000 |
| H108 | 13.1290860000 | -1.0957510000 | 54.0401610000 |
| H109 | 12.9004170000 | -1.1109980000 | 55.7851080000 |
| H110 | 12.9499980000 | 0.4349130000 | 54.9158350000 |
| H111 | 13.4550780000 | -12.2303880000 | 53.1883140000 |
| C112 | 13.9110010000 | -11.6210560000 | 52.4219860000 |
| H113 | 14.8007580000 | -11.1317190000 | 52.8249170000 |
| H114 | 14.1416860000 | -12.2047940000 | 51.5262260000 |
| N115 | 12.8367060000 | -10.6665110000 | 52.1251520000 |
| H116 | 12.2080540000 | -10.4404730000 | 52.8987900000 |
| C117 | 12.6931280000 | -9.9409640000 | 51.0253570000 |
| N118 | 13.7285280000 | -9.8258910000 | 50.1479630000 |
| H119 | 13.5459580000 | -9.1868700000 | 49.3817280000 |

| | | | |
|------|--------------|---------------|---------------|
| H120 | 14.613200000 | -9.598617000 | 50.604448000 |
| N121 | 11.496514000 | -9.396239000 | 50.727465000 |
| H122 | 10.802907000 | -9.449228000 | 51.482389000 |
| H123 | 11.537862000 | -8.440646000 | 50.351667000 |
| H124 | 19.219229000 | -8.221627000 | 61.702834000 |
| C125 | 19.597894000 | -7.229879000 | 61.990051000 |
| H126 | 20.640012000 | -7.352305000 | 62.303571000 |
| C127 | 18.823870000 | -6.709755000 | 63.197136000 |
| O128 | 19.368973000 | -6.310510000 | 64.223663000 |
| C129 | 19.491871000 | -6.271799000 | 60.799063000 |
| H130 | 19.822926000 | -5.272056000 | 61.103051000 |
| H131 | 18.441945000 | -6.156001000 | 60.510517000 |
| C132 | 20.283497000 | -6.726169000 | 59.561007000 |
| H133 | 20.081759000 | -7.780767000 | 59.338423000 |
| H134 | 21.364486000 | -6.664638000 | 59.756604000 |
| C135 | 20.029408000 | -5.977626000 | 58.244031000 |
| O136 | 20.311817000 | -6.480660000 | 57.167986000 |
| O137 | 19.516682000 | -4.759784000 | 58.403818000 |
| N138 | 17.474950000 | -6.713119000 | 63.006104000 |
| H139 | 17.124478000 | -6.984666000 | 62.096122000 |
| C140 | 16.536885000 | -6.005885000 | 63.853040000 |
| H141 | 15.885596000 | -6.726367000 | 64.369771000 |
| H142 | 17.122424000 | -5.483608000 | 64.614173000 |
| C143 | 15.662889000 | -5.016754000 | 63.041912000 |
| H144 | 16.275169000 | -4.171481000 | 62.709300000 |
| H145 | 14.890878000 | -4.621783000 | 63.716035000 |
| C146 | 15.033183000 | -5.687212000 | 61.835658000 |
| C147 | 13.972817000 | -6.597098000 | 61.974725000 |
| H148 | 13.527254000 | -6.754905000 | 62.955949000 |
| C149 | 15.580359000 | -5.483429000 | 60.558585000 |
| H150 | 16.368497000 | -4.744704000 | 60.432511000 |
| C151 | 13.486880000 | -7.304298000 | 60.872959000 |
| H152 | 12.665479000 | -8.007199000 | 60.988258000 |
| C153 | 15.106988000 | -6.200697000 | 59.454781000 |
| H154 | 15.548476000 | -6.046518000 | 58.473588000 |
| C155 | 14.065514000 | -7.118528000 | 59.613168000 |
| H156 | 13.709180000 | -7.683439000 | 58.757812000 |
| H157 | 9.003756000 | 0.705074000 | 60.775269000 |
| C158 | 8.126981000 | 0.156080000 | 60.465000000 |
| H159 | 7.283672000 | 0.459242000 | 61.067770000 |
| H160 | 10.765030000 | -6.261355000 | 58.159956000 |
| H161 | 18.259279000 | -9.498753000 | 50.150540000 |
| C162 | 17.583975000 | -8.655921000 | 50.152027000 |
| H163 | 17.277363000 | -8.441989000 | 49.138799000 |
| H164 | 23.274010000 | -4.230630000 | 52.437074000 |
| H165 | 11.038939000 | -5.340393000 | 50.720926000 |
| H166 | 13.713135000 | -10.193031000 | 57.014647000 |
| H167 | 13.229166000 | -4.852797000 | 57.954939000 |
| C168 | 6.782746000 | -8.609687000 | 56.007146000 |
| H169 | 7.191699000 | -8.904190000 | 55.034999000 |
| H170 | 6.005904000 | -7.855214000 | 55.827915000 |
| N171 | 11.384284000 | -7.732399000 | 57.072322000 |
| N172 | 11.049512000 | -6.523834000 | 57.197644000 |
| H173 | 7.149394000 | -5.835410000 | 59.821894000 |
| C174 | 6.959015000 | -4.800933000 | 59.500004000 |
| H175 | 5.903926000 | -4.490355000 | 59.518145000 |
| H176 | 7.494932000 | -4.166018000 | 60.219778000 |
| C177 | 7.461893000 | -4.489176000 | 58.087521000 |
| H178 | 8.510008000 | -4.797936000 | 57.964303000 |
| H179 | 7.429402000 | -3.402454000 | 57.933617000 |
| O180 | 6.646277000 | -5.065116000 | 57.082275000 |
| H181 | 7.004995000 | -5.970310000 | 56.955248000 |
| O182 | 11.354717000 | -9.562435000 | 58.815340000 |
| H183 | 11.332425000 | -8.681873000 | 58.132793000 |
| H184 | 10.566754000 | -10.058286000 | 58.535177000 |
| O185 | 13.511277000 | -10.546653000 | 58.132723000 |
| H186 | 12.516050000 | -10.157271000 | 58.440708000 |
| H187 | 13.436839000 | -11.512670000 | 58.0499730000 |

Optimized TS for the reaction between a proton on S2B and a hydride in **Figure 10**.

Energies: E= -7921.449548, solv = -0.201939, disp = -229.81 Z₀ = 892.83

| | | | |
|-----|---------------|----------------|---------------|
| Mo1 | 16.3679620000 | -5.6352600000 | 53.2479690000 |
| Fe2 | 10.0227010000 | -8.3632910000 | 56.0110220000 |
| Fe3 | 11.1856240000 | -5.7755490000 | 54.9548510000 |
| Fe4 | 11.2990670000 | -7.6702080000 | 53.1473690000 |
| Fe5 | 12.6065660000 | -8.6713440000 | 55.5416660000 |
| Fe6 | 14.6863490000 | -7.7230190000 | 54.1244620000 |
| Fe7 | 13.9249480000 | -5.3952190000 | 55.3789900000 |
| Fe8 | 13.3091590000 | -5.8724810000 | 52.8453580000 |
| C9 | 17.7966750000 | -2.0592940000 | 54.3383230000 |
| H10 | 18.0062930000 | -1.0548190000 | 53.9658930000 |
| H11 | 16.7110610000 | -2.1376950000 | 54.4823370000 |
| C12 | 18.2263790000 | -3.1288060000 | 53.3123250000 |
| C13 | 19.7114420000 | -2.9455630000 | 52.9195250000 |
| H14 | 20.3258410000 | -3.1217930000 | 53.8079600000 |
| H15 | 19.8487600000 | -1.9043440000 | 52.6075120000 |
| C16 | 20.1530230000 | -3.8796290000 | 51.7735360000 |
| H17 | 19.6635890000 | -3.6019680000 | 50.8383770000 |
| H18 | 19.8703170000 | -4.9078690000 | 52.0243100000 |
| C19 | 17.4084930000 | -3.1582390000 | 51.9913400000 |
| O20 | 16.9857470000 | -4.3435690000 | 51.6439390000 |
| O21 | 17.3105860000 | -2.1341670000 | 51.3194630000 |
| O22 | 18.0491660000 | -4.4096700000 | 53.9428130000 |
| C23 | 12.6985680000 | -7.0080770000 | 54.3861950000 |
| S24 | 12.2638640000 | -4.3890760000 | 56.6696130000 |
| S25 | 16.0493470000 | -6.4200350000 | 55.5905560000 |
| S26 | 9.2983250000 | -4.9741080000 | 53.6893860000 |
| S27 | 14.6572480000 | -9.9064420000 | 55.3821430000 |
| S28 | 14.4874760000 | -3.9392360000 | 53.4770070000 |
| S29 | 10.3116260000 | -9.5666670000 | 53.9523530000 |
| S30 | 15.0515800000 | -7.2255370000 | 51.8627760000 |
| S31 | 11.5971920000 | -6.4729240000 | 50.9933500000 |
| H32 | 13.6351740000 | -2.1902110000 | 49.0425560000 |
| C33 | 13.2979250000 | -2.0241170000 | 50.0550230000 |
| H34 | 13.8490640000 | -2.7060870000 | 50.7079260000 |
| H35 | 13.4963980000 | -0.9914250000 | 50.3616370000 |
| N36 | 11.8622850000 | -2.3323840000 | 50.0737020000 |
| H37 | 11.3168800000 | -1.9889680000 | 49.2963640000 |
| C38 | 11.1457400000 | -2.7758190000 | 51.1228050000 |
| N39 | 11.6730080000 | -3.0057320000 | 52.3058560000 |
| H40 | 11.0887600000 | -3.4754150000 | 53.0070620000 |
| H41 | 12.6844540000 | -3.0261500000 | 52.4980120000 |
| N42 | 9.7958620000 | -2.9249090000 | 50.9635690000 |
| H43 | 9.4852400000 | -3.2041440000 | 50.0419200000 |
| H44 | 9.3368000000 | -3.4372820000 | 51.7254090000 |
| H45 | 7.9327580000 | 0.3836580000 | 59.4111830000 |
| C46 | 8.3565360000 | -1.3521590000 | 60.7050850000 |
| H47 | 8.1964790000 | -1.5586850000 | 61.7706680000 |
| H48 | 7.5957720000 | -1.9219990000 | 60.1581510000 |
| C49 | 9.7292810000 | -1.8564890000 | 60.3701340000 |
| N50 | 10.7159550000 | -1.9134300000 | 61.3388350000 |
| C51 | 10.2208830000 | -2.3321800000 | 59.1743760000 |
| H52 | 9.7773680000 | -2.4733490000 | 58.2013550000 |
| C53 | 11.7721670000 | -2.4255120000 | 60.7308330000 |
| H54 | 12.7266640000 | -2.6406030000 | 61.1913870000 |
| N55 | 11.5263270000 | -2.6858880000 | 59.4194240000 |
| H56 | 19.2300670000 | -4.3354010000 | 57.5135530000 |
| H57 | 16.7220740000 | -8.8577410000 | 50.7840610000 |
| C58 | 18.3625060000 | -7.4131770000 | 50.6405710000 |
| H59 | 17.7283050000 | -6.5248590000 | 50.5706810000 |
| H60 | 19.2105470000 | -7.2526850000 | 49.9604730000 |
| C61 | 18.8873560000 | -7.5127440000 | 52.0400370000 |
| N62 | 18.1709310000 | -7.0520680000 | 53.1357200000 |
| C63 | 20.0814430000 | -8.0259510000 | 52.4883490000 |
| H64 | 20.9120180000 | -8.4711010000 | 51.9620000000 |
| C65 | 18.9109440000 | -7.2790540000 | 54.2107210000 |
| H66 | 18.6645010000 | -7.0074670000 | 55.2251390000 |
| N67 | 20.0710690000 | -7.8760320000 | 53.8643380000 |
| H68 | 20.8158400000 | -8.0726040000 | 54.5168250000 |
| H69 | 6.9200170000 | -10.5883850000 | 56.9481570000 |
| C70 | 6.1750520000 | -9.8249630000 | 56.6900010000 |
| H71 | 5.5309560000 | -10.2322290000 | 56.0424860000 |
| H72 | 5.6932330000 | -9.5371420000 | 57.6127210000 |
| S73 | 8.1485600000 | -8.0037510000 | 57.2974810000 |
| H74 | 12.1225940000 | -3.1563080000 | 58.7387340000 |

| | | | |
|------|---------------|----------------|---------------|
| H75 | 18.2638790000 | -4.2388340000 | 54.9491110000 |
| C76 | 18.4545130000 | -2.2288290000 | 55.7362150000 |
| O77 | 18.6873090000 | -3.4467710000 | 56.1136690000 |
| O78 | 18.6768030000 | -1.2114240000 | 56.4119390000 |
| C79 | 21.6361410000 | -3.8498460000 | 51.5397230000 |
| O80 | 22.2187060000 | -3.5171120000 | 50.5265080000 |
| O81 | 22.3208180000 | -4.2658020000 | 52.6398600000 |
| H82 | 15.7024660000 | -0.1996320000 | 61.4912310000 |
| C83 | 14.8549930000 | -0.0829910000 | 60.8320020000 |
| H84 | 13.9165020000 | -0.2867340000 | 61.3260940000 |
| H85 | 14.8276830000 | 0.9921970000 | 60.5857630000 |
| C86 | 15.0599860000 | -0.8751940000 | 59.5441990000 |
| H87 | 14.3700440000 | -0.5139630000 | 58.7715580000 |
| H88 | 14.8126430000 | -1.9293790000 | 59.7140460000 |
| C89 | 16.4964890000 | -0.8066100000 | 59.0170120000 |
| H90 | 16.8888280000 | 0.2192500000 | 59.0824350000 |
| H91 | 16.5430160000 | -1.0643190000 | 57.9525850000 |
| C92 | 17.4572240000 | -1.7370530000 | 59.7694000000 |
| O93 | 17.1352480000 | -2.3371290000 | 60.7995930000 |
| N94 | 18.7004360000 | -1.8258470000 | 59.2214350000 |
| H95 | 19.2512190000 | -2.6086140000 | 59.5536480000 |
| H96 | 18.8210880000 | -1.5807470000 | 58.2285100000 |
| C97 | 10.6519930000 | 0.0100030000 | 53.3460010000 |
| H98 | 11.1636990000 | 0.9592720000 | 53.2872700000 |
| H99 | 9.5863320000 | 0.1850130000 | 53.3579380000 |
| H100 | 10.9223770000 | -0.5771990000 | 52.4675930000 |
| C101 | 11.0739480000 | -0.6668030000 | 54.6672420000 |
| H102 | 10.7424680000 | -1.7133980000 | 54.6564470000 |
| C103 | 10.3861360000 | 0.0196100000 | 55.8578650000 |
| H104 | 9.2923800000 | -0.0348250000 | 55.7750210000 |
| H105 | 10.6641840000 | 1.0821450000 | 55.9129320000 |
| H106 | 10.6744540000 | -0.4492920000 | 56.8048240000 |
| C107 | 12.5976620000 | -0.6527700000 | 54.8503680000 |
| H108 | 13.1219510000 | -1.1075470000 | 54.0034180000 |
| H109 | 12.8889140000 | -1.2189220000 | 55.7412110000 |
| H110 | 12.9635140000 | 0.3788780000 | 54.9579110000 |
| H111 | 13.4550780000 | -12.2303890000 | 53.1883140000 |
| C112 | 13.9110020000 | -11.6210550000 | 52.4219870000 |
| H113 | 14.7084060000 | -11.0094140000 | 52.8509010000 |
| H114 | 14.2826070000 | -12.2314000000 | 51.5947750000 |
| N115 | 12.7562210000 | -10.8227900000 | 51.9868100000 |
| H116 | 12.0051220000 | -10.6942110000 | 52.6815980000 |
| C117 | 12.6392830000 | -10.0872260000 | 50.8925200000 |
| N118 | 13.7265280000 | -9.7777060000 | 50.1444710000 |
| H119 | 13.5296980000 | -9.1850810000 | 49.3455020000 |
| H120 | 14.5135290000 | -9.4069510000 | 50.6868000000 |
| N121 | 11.4046710000 | -9.7105080000 | 50.4741300000 |
| H122 | 10.6566050000 | -9.9449850000 | 51.1267560000 |
| H123 | 11.3365450000 | -8.7261320000 | 50.1908400000 |
| H124 | 19.2259210000 | -8.2228850000 | 61.6971090000 |
| C125 | 19.5978930000 | -7.2298800000 | 61.9900500000 |
| H126 | 20.6371450000 | -7.3480590000 | 62.3126770000 |
| C127 | 18.8071620000 | -6.7226090000 | 63.1898330000 |
| O128 | 19.3410050000 | -6.3573130000 | 64.2348310000 |
| C129 | 19.4918720000 | -6.2717980000 | 60.7990630000 |
| H130 | 19.8631280000 | -5.2823720000 | 61.0898350000 |
| H131 | 18.4384930000 | -6.1188710000 | 60.5390590000 |
| C132 | 20.2299140000 | -6.7559510000 | 59.5387750000 |
| H133 | 19.9948350000 | -7.8076820000 | 59.3351570000 |
| H134 | 21.3183630000 | -6.7205120000 | 59.6947330000 |
| C135 | 19.9464730000 | -6.0157070000 | 58.2230160000 |
| O136 | 20.1848450000 | -6.5352020000 | 57.1430870000 |
| O137 | 19.4583640000 | -4.7896170000 | 58.3865570000 |
| N138 | 17.4599510000 | -6.7015540000 | 62.9805490000 |
| H139 | 17.1084680000 | -6.9340940000 | 62.0600630000 |
| C140 | 16.5368850000 | -6.0058840000 | 63.8530420000 |
| H141 | 15.8691670000 | -6.7294600000 | 64.3435990000 |
| H142 | 17.1393320000 | -5.5338120000 | 64.6334690000 |
| C143 | 15.6934720000 | -4.9598840000 | 63.0961340000 |
| H144 | 16.3455360000 | -4.1696130000 | 62.7080540000 |
| H145 | 15.0164490000 | -4.4936090000 | 63.8258200000 |
| C146 | 14.8940820000 | -5.5671970000 | 61.9577500000 |
| C147 | 13.8413840000 | -6.4607380000 | 62.2128480000 |
| H148 | 13.5687860000 | -6.6895220000 | 63.2423550000 |
| C149 | 15.2161200000 | -5.2732770000 | 60.6234920000 |

| | | | |
|------|---------------|---------------|---------------|
| H150 | 16.0065190000 | -4.5550940000 | 60.4164320000 |
| C151 | 13.1300200000 | -7.0465640000 | 61.1650300000 |
| H152 | 12.3085170000 | -7.7261980000 | 61.3796690000 |
| C153 | 14.5024390000 | -5.8582350000 | 59.5714640000 |
| H154 | 14.7466020000 | -5.6091210000 | 58.5430590000 |
| C155 | 13.4591810000 | -6.7474240000 | 59.8394550000 |
| H156 | 12.8945070000 | -7.1859270000 | 59.0213550000 |
| H157 | 9.0037560000 | 0.7050730000 | 60.7752690000 |
| C158 | 8.1269800000 | 0.1560800000 | 60.4650000000 |
| H159 | 7.2836720000 | 0.4592420000 | 61.0677700000 |
| H160 | 8.5127620000 | -4.5675980000 | 54.7138740000 |
| H161 | 18.2592780000 | -9.4987530000 | 50.1505400000 |
| C162 | 17.5839750000 | -8.6559200000 | 50.1520260000 |
| H163 | 17.2773630000 | -8.4419890000 | 49.1387990000 |
| H164 | 23.2631710000 | -4.1959410000 | 52.3987660000 |
| H165 | 10.4172040000 | -5.8442570000 | 51.2104630000 |
| H166 | 15.2532550000 | -9.3716210000 | 56.4711060000 |
| H167 | 11.2469110000 | -5.9074260000 | 56.8699990000 |
| H168 | 11.4999640000 | -9.0384330000 | 56.8387980000 |
| H169 | 10.7361900000 | -6.6333400000 | 56.6471480000 |
| C170 | 6.8818380000 | -8.6156770000 | 56.0980160000 |
| H171 | 6.1706860000 | -7.8043620000 | 55.9018420000 |
| H172 | 7.3626130000 | -8.8692420000 | 55.1470940000 |
| H173 | 7.1493940000 | -5.8354100000 | 59.8218940000 |
| C174 | 6.9590150000 | -4.8009330000 | 59.5000040000 |
| H175 | 5.9039260000 | -4.4903550000 | 59.5181450000 |
| H176 | 7.4690370000 | -4.1778720000 | 60.2495290000 |
| C177 | 7.5685650000 | -4.4606140000 | 58.1359730000 |
| H178 | 8.6376910000 | -4.7133350000 | 58.1355930000 |
| H179 | 7.4943510000 | -3.3764680000 | 57.9809440000 |
| O180 | 6.9105860000 | -5.0627310000 | 57.0290400000 |
| H181 | 7.2781800000 | -5.9716060000 | 56.9791910000 |

Optimized TS for the reaction between a proton on S1A and a hydride in **Figure 11**.

Energies: E= -7921.427857, solv = -0.203768, disp = -227.86 Z₀ = 891.42

| | | | |
|-----|---------------|----------------|---------------|
| Mo1 | 16.1147450000 | -6.0168710000 | 53.4621550000 |
| Fe2 | 9.5001490000 | -9.5249710000 | 54.3030630000 |
| Fe3 | 10.6819880000 | -7.0498320000 | 55.4919440000 |
| Fe4 | 10.6380670000 | -7.4440280000 | 52.6752040000 |
| Fe5 | 12.0510460000 | -9.3420940000 | 54.6191390000 |
| Fe6 | 14.4752770000 | -8.2310520000 | 54.4988160000 |
| Fe7 | 13.4141960000 | -6.0220600000 | 55.3334660000 |
| Fe8 | 13.1759890000 | -6.4111160000 | 52.7729190000 |
| C9 | 17.5025640000 | -2.3402050000 | 54.4082110000 |
| H10 | 17.6503380000 | -1.3519190000 | 53.9688510000 |
| H11 | 16.4269800000 | -2.4703380000 | 54.5878770000 |
| C12 | 17.9637200000 | -3.4493710000 | 53.4370060000 |
| C13 | 19.4509400000 | -3.2206910000 | 53.0565180000 |
| H14 | 20.0527240000 | -3.2602890000 | 53.9705780000 |
| H15 | 19.5210470000 | -2.2083050000 | 52.6434560000 |
| C16 | 20.0080670000 | -4.2241460000 | 52.0243920000 |
| H17 | 19.4272310000 | -4.1762050000 | 51.1007380000 |
| H18 | 19.9428380000 | -5.2372680000 | 52.4311110000 |
| C19 | 17.1366210000 | -3.5449990000 | 52.1239420000 |
| O20 | 16.7102840000 | -4.7422910000 | 51.8326340000 |
| O21 | 17.0103850000 | -2.5465490000 | 51.4166680000 |
| O22 | 17.7985160000 | -4.7023620000 | 54.1204480000 |
| C23 | 12.1711820000 | -7.4445430000 | 54.1281010000 |
| S24 | 11.6443160000 | -5.3400590000 | 56.9439240000 |
| S25 | 15.6749610000 | -6.6983360000 | 55.8180880000 |
| S26 | 9.4742560000 | -5.3925240000 | 53.7139300000 |
| S27 | 13.9493380000 | -10.1473450000 | 55.8141600000 |
| S28 | 14.1700940000 | -4.4067190000 | 53.6620540000 |
| S29 | 8.9486860000 | -9.0391210000 | 52.1758640000 |
| S30 | 15.0252840000 | -7.8585560000 | 52.2583130000 |
| S31 | 11.8997450000 | -6.5882040000 | 50.6464650000 |
| H32 | 13.6351740000 | -2.1902110000 | 49.0425560000 |
| C33 | 13.2979250000 | -2.0241170000 | 50.0550230000 |
| H34 | 13.9411030000 | -2.6024650000 | 50.7230230000 |

| | | | |
|------|---------------|----------------|---------------|
| H35 | 13.3571650000 | -0.9616380000 | 50.3125410000 |
| N36 | 11.9052490000 | -2.5075680000 | 50.0836940000 |
| H37 | 11.4144350000 | -2.5036300000 | 49.2024180000 |
| C38 | 11.2123700000 | -2.9735680000 | 51.1374190000 |
| N39 | 11.7509610000 | -3.0774040000 | 52.3421900000 |
| H40 | 11.1761900000 | -3.5241260000 | 53.0544540000 |
| H41 | 12.7588890000 | -3.2740100000 | 52.4914540000 |
| N42 | 9.8928220000 | -3.2664660000 | 50.9967150000 |
| H43 | 9.5143150000 | -3.3649630000 | 50.0651230000 |
| H44 | 9.5100000000 | -3.9143530000 | 51.6995560000 |
| H45 | 7.9292940000 | 0.3927200000 | 59.4135250000 |
| C46 | 8.3650070000 | -1.3508760000 | 60.6815600000 |
| H47 | 8.2889660000 | -1.5636420000 | 61.7551090000 |
| H48 | 7.5609930000 | -1.9136950000 | 60.1917640000 |
| C49 | 9.7045110000 | -1.8564130000 | 60.2311490000 |
| N50 | 10.7700020000 | -1.9195730000 | 61.1118490000 |
| C51 | 10.0881690000 | -2.3357070000 | 58.9986830000 |
| H52 | 9.5564210000 | -2.4717320000 | 58.0700420000 |
| C53 | 11.7673930000 | -2.4386910000 | 60.4203890000 |
| H54 | 12.7559680000 | -2.6598680000 | 60.7992400000 |
| N55 | 11.4109040000 | -2.6952130000 | 59.1312510000 |
| H56 | 19.1638870000 | -4.3669290000 | 57.5372060000 |
| H57 | 16.7059160000 | -8.9143700000 | 50.7405970000 |
| C58 | 18.2969820000 | -7.4385910000 | 50.7721230000 |
| H59 | 17.6397510000 | -6.5647730000 | 50.7512810000 |
| H60 | 19.1752960000 | -7.1907360000 | 50.1596690000 |
| C61 | 18.7570760000 | -7.6514190000 | 52.1890850000 |
| N62 | 17.9903290000 | -7.3075020000 | 53.2962300000 |
| C63 | 19.9540800000 | -8.1556580000 | 52.6415830000 |
| H64 | 20.8206080000 | -8.5217810000 | 52.1121050000 |
| C65 | 18.7020720000 | -7.5896840000 | 54.3744270000 |
| H66 | 18.4117080000 | -7.3963070000 | 55.3954840000 |
| N67 | 19.8958910000 | -8.1164180000 | 54.0242770000 |
| H68 | 20.6352070000 | -8.3158440000 | 54.6819830000 |
| H69 | 6.9102560000 | -10.5978290000 | 56.9440400000 |
| C70 | 6.1750520000 | -9.8249630000 | 56.6900010000 |
| H71 | 5.5309560000 | -10.2322290000 | 56.0424860000 |
| H72 | 5.6932330000 | -9.5371420000 | 57.6127210000 |
| S73 | 8.7260090000 | -8.6407230000 | 56.3916810000 |
| H74 | 11.9350630000 | -3.2155950000 | 58.4332530000 |
| H75 | 18.0128330000 | -4.4919070000 | 55.1050030000 |
| C76 | 18.2184050000 | -2.4027650000 | 55.7838860000 |
| O77 | 18.4631310000 | -3.5913740000 | 56.2335540000 |
| O78 | 18.4820250000 | -1.3415480000 | 56.3740110000 |
| C79 | 21.4391740000 | -3.9230390000 | 51.6569420000 |
| O80 | 21.8298840000 | -3.4223260000 | 50.6209610000 |
| O81 | 22.3208180000 | -4.2658020000 | 52.6398600000 |
| H82 | 15.7024660000 | -0.1996320000 | 61.4912310000 |
| C83 | 14.8549930000 | -0.0829910000 | 60.8320020000 |
| H84 | 13.9165020000 | -0.2867340000 | 61.3260940000 |
| H85 | 14.8296490000 | 0.9921210000 | 60.5860860000 |
| C86 | 15.0599860000 | -0.8751940000 | 59.5441990000 |
| H87 | 14.3721610000 | -0.5090310000 | 58.7712630000 |
| H88 | 14.8086360000 | -1.9284490000 | 59.7163050000 |
| C89 | 16.4981910000 | -0.8186800000 | 59.0251830000 |
| H90 | 16.9112560000 | 0.1959420000 | 59.1274600000 |
| H91 | 16.5499090000 | -1.0424350000 | 57.9538890000 |
| C92 | 17.4306460000 | -1.7948210000 | 59.7556100000 |
| O93 | 17.0901880000 | -2.4078740000 | 60.7717260000 |
| N94 | 18.6696430000 | -1.9027510000 | 59.2002230000 |
| H95 | 19.1975840000 | -2.7117480000 | 59.5074080000 |
| H96 | 18.7678230000 | -1.6634690000 | 58.2034310000 |
| C97 | 10.6519930000 | 0.0100030000 | 53.3460010000 |
| H98 | 11.1636990000 | 0.9592720000 | 53.2872700000 |
| H99 | 9.5863320000 | 0.1850130000 | 53.3579380000 |
| H100 | 10.9210340000 | -0.5871780000 | 52.4722920000 |
| C101 | 11.0684110000 | -0.6617740000 | 54.6707250000 |
| H102 | 10.6834210000 | -1.6912390000 | 54.6769300000 |
| C103 | 10.4344950000 | 0.0794830000 | 55.8587030000 |
| H104 | 9.3387420000 | 0.0850660000 | 55.7890770000 |
| H105 | 10.7717090000 | 1.1253450000 | 55.8906980000 |
| H106 | 10.7064590000 | -0.3851880000 | 56.8129070000 |
| C107 | 12.5948380000 | -0.7150120000 | 54.8207270000 |
| H108 | 13.0699270000 | -1.2499900000 | 53.9930980000 |
| H109 | 12.8866960000 | -1.2272450000 | 55.7441670000 |

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|------|--------------|---------------|--------------|
| H110 | 13.014690000 | 0.300402000 | 54.854446000 |
| H111 | 13.455078000 | -12.230389000 | 53.188314000 |
| C112 | 13.911002000 | -11.621055000 | 52.421987000 |
| H113 | 14.590436000 | -10.899213000 | 52.880777000 |
| H114 | 14.422636000 | -12.232770000 | 51.673018000 |
| N115 | 12.727376000 | -10.972901000 | 51.825883000 |
| H116 | 11.890527000 | -10.974995000 | 52.411503000 |
| C117 | 12.676992000 | -10.222797000 | 50.729130000 |
| N118 | 13.827018000 | -9.911506000 | 50.074187000 |
| H119 | 13.694733000 | -9.255160000 | 49.312004000 |
| H120 | 14.568344000 | -9.576294000 | 50.699833000 |
| N121 | 11.488726000 | -9.853029000 | 50.212459000 |
| H122 | 10.657487000 | -9.959785000 | 50.816634000 |
| H123 | 11.482594000 | -8.917325000 | 49.801001000 |
| H124 | 19.218515000 | -8.221261000 | 61.703048000 |
| C125 | 19.597893000 | -7.229880000 | 61.990050000 |
| H126 | 20.638946000 | -7.351292000 | 62.306509000 |
| C127 | 18.818228000 | -6.701936000 | 63.189189000 |
| O128 | 19.360883000 | -6.278427000 | 64.207180000 |
| C129 | 19.491872000 | -6.271798000 | 60.799063000 |
| H130 | 19.847890000 | -5.278210000 | 61.093238000 |
| H131 | 18.438833000 | -6.135740000 | 60.529382000 |
| C132 | 20.253117000 | -6.752178000 | 59.551267000 |
| H133 | 20.070691000 | -7.817749000 | 59.369910000 |
| H134 | 21.338001000 | -6.653335000 | 59.705276000 |
| C135 | 19.914657000 | -6.045232000 | 58.233888000 |
| O136 | 20.071070000 | -6.595758000 | 57.154262000 |
| O137 | 19.470453000 | -4.804071000 | 58.400329000 |
| N138 | 17.467530000 | -6.719581000 | 63.003250000 |
| H139 | 17.108443000 | -7.023237000 | 62.106833000 |
| C140 | 16.536885000 | -6.005884000 | 63.853042000 |
| H141 | 15.914599000 | -6.720246000 | 64.412248000 |
| H142 | 17.136494000 | -5.451032000 | 64.579555000 |
| C143 | 15.619614000 | -5.058807000 | 63.046170000 |
| H144 | 16.211407000 | -4.239519000 | 62.622856000 |
| H145 | 14.898874000 | -4.617229000 | 63.747907000 |
| C146 | 14.894988000 | -5.799493000 | 61.939521000 |
| C147 | 13.875450000 | -6.718439000 | 62.237452000 |
| H148 | 13.540196000 | -6.830837000 | 63.267683000 |
| C149 | 15.296746000 | -5.655740000 | 60.602697000 |
| H150 | 16.058167000 | -4.918503000 | 60.355037000 |
| C151 | 13.292563000 | -7.492557000 | 61.233994000 |
| H152 | 12.506165000 | -8.201299000 | 61.483005000 |
| C153 | 14.719819000 | -6.436469000 | 59.594418000 |
| H154 | 15.050174000 | -6.325477000 | 58.565721000 |
| C155 | 13.724999000 | -7.365825000 | 59.909980000 |
| H156 | 13.295813000 | -7.990781000 | 59.130394000 |
| H157 | 9.003756000 | 0.705073000 | 60.775269000 |
| C158 | 8.126980000 | 0.156080000 | 60.465000000 |
| H159 | 7.283672000 | 0.459242000 | 61.067770000 |
| H160 | 8.196007000 | -5.825504000 | 53.673798000 |
| H161 | 18.259278000 | -9.498753000 | 50.150540000 |
| C162 | 17.583975000 | -8.655920000 | 50.152026000 |
| H163 | 17.277363000 | -8.441989000 | 49.138799000 |
| H164 | 23.192766000 | -3.986710000 | 52.303681000 |
| H165 | 10.989007000 | -5.596800000 | 50.536603000 |
| H166 | 12.662054000 | -9.422905000 | 56.481400000 |
| H167 | 12.141116000 | -6.100216000 | 57.945797000 |
| H168 | 10.931390000 | -10.664050000 | 54.196140000 |
| H169 | 11.639250000 | -8.879311000 | 56.454103000 |
| C170 | 6.888661000 | -8.615364000 | 56.033296000 |
| H171 | 6.476395000 | -7.673819000 | 56.402237000 |
| H172 | 6.753377000 | -8.631619000 | 54.947021000 |
| H173 | 7.149394000 | -5.835410000 | 59.821894000 |
| C174 | 6.959015000 | -4.800933000 | 59.500004000 |
| H175 | 5.903926000 | -4.490355000 | 59.518145000 |
| H176 | 7.485562000 | -4.154837000 | 60.214593000 |
| C177 | 7.572267000 | -4.585351000 | 58.115218000 |
| H178 | 8.660773000 | -4.691591000 | 58.175948000 |
| H179 | 7.365125000 | -3.559743000 | 57.776536000 |
| O180 | 7.044680000 | -5.485775000 | 57.140634000 |
| H181 | 7.768775000 | -6.066840000 | 56.857126000 |

Optimized TS for the reaction between a proton on S2A and a hydride in **Figure 12**.

Energies: E= -7921.455527, solv = -0.202302, disp = -230.02 Z₀ = 892.88

| | | | |
|-----|---------------|---------------|---------------|
| Mo1 | 16.4618420000 | -5.4542580000 | 53.2002070000 |
| Fe2 | 9.9176320000 | -8.2084630000 | 56.0041510000 |
| Fe3 | 11.2935110000 | -5.6742600000 | 55.1076770000 |
| Fe4 | 11.1335510000 | -7.1654420000 | 53.0031990000 |
| Fe5 | 12.5037000000 | -8.3533010000 | 55.3383580000 |
| Fe6 | 14.6924080000 | -7.5527310000 | 54.0066300000 |
| Fe7 | 14.0603620000 | -5.3059750000 | 55.1647750000 |
| Fe8 | 13.4870940000 | -5.6746810000 | 52.6360010000 |
| C9 | 17.8749050000 | -1.9093620000 | 54.3931070000 |
| H10 | 18.0903990000 | -0.8958410000 | 54.0498060000 |
| H11 | 16.7879500000 | -1.9880580000 | 54.5249180000 |
| C12 | 18.3106120000 | -2.9523670000 | 53.3427920000 |
| C13 | 19.7967650000 | -2.7592910000 | 52.9597150000 |
| H14 | 20.4090220000 | -2.9908820000 | 53.8369890000 |
| H15 | 19.9462070000 | -1.7044490000 | 52.7049830000 |
| C16 | 20.2273250000 | -3.6326440000 | 51.7607020000 |
| H17 | 19.7810010000 | -3.2611960000 | 50.8367390000 |
| H18 | 19.8863440000 | -4.6595840000 | 51.9298720000 |
| C19 | 17.5059510000 | -2.9583440000 | 52.0122770000 |
| O20 | 17.1038750000 | -4.1424060000 | 51.6339180000 |
| O21 | 17.4108700000 | -1.9228130000 | 51.3593650000 |
| O22 | 18.1325690000 | -4.2484760000 | 53.9421740000 |
| C23 | 12.7510840000 | -6.7017670000 | 54.2228500000 |
| S24 | 12.3906880000 | -4.2284730000 | 56.6857720000 |
| S25 | 16.1197980000 | -6.3333090000 | 55.5171710000 |
| S26 | 9.5174000000 | -5.3165120000 | 53.2104190000 |
| S27 | 14.5008920000 | -9.7315620000 | 55.2342990000 |
| S28 | 14.5940300000 | -3.7202510000 | 53.4280720000 |
| S29 | 10.4318150000 | -9.2480280000 | 53.9009300000 |
| S30 | 15.2304430000 | -7.0668480000 | 51.7912680000 |
| S31 | 12.0084130000 | -6.2650690000 | 50.6526060000 |
| H32 | 13.6351740000 | -2.1902100000 | 49.0425560000 |
| C33 | 13.2979250000 | -2.0241170000 | 50.0550230000 |
| H34 | 13.7879460000 | -2.7615030000 | 50.6946300000 |
| H35 | 13.5805960000 | -1.0199640000 | 50.3886940000 |
| N36 | 11.8458440000 | -2.2141030000 | 50.0652480000 |
| H37 | 11.3202140000 | -1.8328250000 | 49.2921830000 |
| C38 | 11.1191020000 | -2.7637930000 | 51.0533490000 |
| N39 | 11.6210190000 | -3.0598760000 | 52.2353200000 |
| H40 | 11.0677480000 | -3.7124520000 | 52.8213380000 |
| H41 | 12.6209860000 | -2.9960450000 | 52.4538550000 |
| N42 | 9.7825440000 | -2.9595010000 | 50.8448060000 |
| H43 | 9.5227000000 | -3.2171530000 | 49.9003620000 |
| H44 | 9.3477470000 | -3.5611830000 | 51.5609080000 |
| H45 | 7.9329470000 | 0.3863160000 | 59.4118810000 |
| C46 | 8.3550300000 | -1.3536390000 | 60.6987060000 |
| H47 | 8.1663480000 | -1.5747480000 | 61.7562770000 |
| H48 | 7.6197470000 | -1.9254540000 | 60.1210930000 |
| C49 | 9.7466310000 | -1.8215850000 | 60.3977450000 |
| N50 | 10.7077250000 | -1.8512870000 | 61.3930060000 |
| C51 | 10.2932690000 | -2.2346750000 | 59.2039130000 |
| H52 | 9.8786950000 | -2.3752770000 | 58.2179630000 |
| C53 | 11.8080290000 | -2.2805070000 | 60.8042210000 |
| H54 | 12.7614400000 | -2.4509130000 | 61.2845670000 |
| N55 | 11.6120650000 | -2.5176050000 | 59.4789130000 |
| H56 | 19.2684080000 | -4.2838050000 | 57.5427100000 |
| H57 | 16.7290110000 | -8.8432410000 | 50.7951180000 |
| C58 | 18.3755620000 | -7.4051210000 | 50.6053180000 |
| H59 | 17.7456120000 | -6.5167960000 | 50.5129850000 |
| H60 | 19.2163600000 | -7.2719300000 | 49.9099520000 |
| C61 | 18.9172200000 | -7.4572850000 | 52.0006870000 |
| N62 | 18.2693050000 | -6.8688510000 | 53.0783740000 |
| C63 | 20.0792630000 | -8.0337100000 | 52.4561840000 |
| H64 | 20.8587860000 | -8.5751680000 | 51.9421050000 |
| C65 | 19.0188200000 | -7.0844810000 | 54.1493410000 |
| H66 | 18.8204880000 | -6.7424100000 | 55.1524630000 |
| N67 | 20.1189740000 | -7.7927830000 | 53.8180950000 |
| H68 | 20.8536390000 | -8.0263980000 | 54.4696080000 |

| | | | |
|------|--------------|---------------|--------------|
| H69 | 6.896000000 | -10.608768000 | 56.957107000 |
| C70 | 6.175052000 | -9.824963000 | 56.690001000 |
| H71 | 5.530956000 | -10.232229000 | 56.042486000 |
| H72 | 5.693233000 | -9.537142000 | 57.612721000 |
| S73 | 8.179444000 | -8.176718000 | 57.490734000 |
| H74 | 12.277361000 | -2.876336000 | 58.802509000 |
| H75 | 18.334791000 | -4.101118000 | 54.954013000 |
| C76 | 18.517528000 | -2.116202000 | 55.793668000 |
| O77 | 18.742418000 | -3.343238000 | 56.146334000 |
| O78 | 18.732840000 | -1.115875000 | 56.497444000 |
| C79 | 21.716894000 | -3.654819000 | 51.584710000 |
| O80 | 22.365561000 | -3.207896000 | 50.659616000 |
| O81 | 22.320818000 | -4.265802000 | 52.639860000 |
| H82 | 15.702466000 | -0.199632000 | 61.491231000 |
| C83 | 14.854993000 | -0.082991000 | 60.832002000 |
| H84 | 13.916502000 | -0.286734000 | 61.326094000 |
| H85 | 14.827649000 | 0.991756000 | 60.585847000 |
| C86 | 15.059986000 | -0.875194000 | 59.544199000 |
| H87 | 14.377444000 | -0.507040000 | 58.768043000 |
| H88 | 14.807716000 | -1.928883000 | 59.712984000 |
| C89 | 16.499541000 | -0.819433000 | 59.026844000 |
| H90 | 16.900331000 | 0.202891000 | 59.088124000 |
| H91 | 16.550937000 | -1.083303000 | 57.964269000 |
| C92 | 17.445124000 | -1.758114000 | 59.788517000 |
| O93 | 17.092715000 | -2.388637000 | 60.790729000 |
| N94 | 18.705151000 | -1.821153000 | 59.279554000 |
| H95 | 19.251900000 | -2.609525000 | 59.605208000 |
| H96 | 18.852960000 | -1.543926000 | 58.298252000 |
| C97 | 10.651993000 | 0.010003000 | 53.346001000 |
| H98 | 11.163699000 | 0.959272000 | 53.287270000 |
| H99 | 9.586332000 | 0.185013000 | 53.357938000 |
| H100 | 10.919680000 | -0.580278000 | 52.468847000 |
| C101 | 11.076064000 | -0.663493000 | 54.667345000 |
| H102 | 10.751491000 | -1.712510000 | 54.648413000 |
| C103 | 10.380954000 | 0.020817000 | 55.854934000 |
| H104 | 9.288552000 | -0.056366000 | 55.778281000 |
| H105 | 10.638429000 | 1.089100000 | 55.895444000 |
| H106 | 10.682870000 | -0.427127000 | 56.808197000 |
| C107 | 12.600003000 | -0.630019000 | 54.847578000 |
| H108 | 13.128442000 | -1.101420000 | 54.013000000 |
| H109 | 12.904804000 | -1.161192000 | 55.756050000 |
| H110 | 12.954451000 | 0.407956000 | 54.927273000 |
| H111 | 13.455078000 | -12.230389000 | 53.188314000 |
| C112 | 13.911002000 | -11.621055000 | 52.421987000 |
| H113 | 14.757089000 | -11.072562000 | 52.844232000 |
| H114 | 14.223879000 | -12.232856000 | 51.570694000 |
| N115 | 12.802247000 | -10.743618000 | 52.032250000 |
| H116 | 12.065248000 | -10.576825000 | 52.732400000 |
| C117 | 12.733353000 | -9.965702000 | 50.960025000 |
| N118 | 13.833994000 | -9.735108000 | 50.199774000 |
| H119 | 13.696446000 | -9.047896000 | 49.465879000 |
| H120 | 14.674369000 | -9.521741000 | 50.735481000 |
| N121 | 11.538801000 | -9.471487000 | 50.570116000 |
| H122 | 10.780056000 | -9.638527000 | 51.232327000 |
| H123 | 11.558733000 | -8.484507000 | 50.267308000 |
| H124 | 19.212577000 | -8.219966000 | 61.705892000 |
| C125 | 19.597893000 | -7.229880000 | 61.990050000 |
| H126 | 20.639305000 | -7.356108000 | 62.303455000 |
| C127 | 18.823347000 | -6.694924000 | 63.190407000 |
| O128 | 19.371507000 | -6.240837000 | 64.191423000 |
| C129 | 19.491872000 | -6.271798000 | 60.799063000 |
| H130 | 19.853450000 | -5.280789000 | 61.096856000 |
| H131 | 18.437834000 | -6.128781000 | 60.536455000 |
| C132 | 20.241197000 | -6.739612000 | 59.539842000 |
| H133 | 20.001845000 | -7.785750000 | 59.313530000 |
| H134 | 21.327860000 | -6.714718000 | 59.709195000 |
| C135 | 19.981562000 | -5.972334000 | 58.233904000 |
| O136 | 20.254433000 | -6.462776000 | 57.149089000 |
| O137 | 19.472281000 | -4.755582000 | 58.411098000 |
| N138 | 17.469437000 | -6.745984000 | 63.024612000 |
| H139 | 17.112484000 | -7.046250000 | 62.126021000 |
| C140 | 16.536885000 | -6.005884000 | 63.853042000 |
| H141 | 15.865323000 | -6.705972000 | 64.370813000 |
| H142 | 17.129512000 | -5.490293000 | 64.612836000 |
| C143 | 15.699758000 | -5.001363000 | 63.026797000 |

| | | | |
|------|---------------|---------------|---------------|
| H144 | 16.3470830000 | -4.1990850000 | 62.6562610000 |
| H145 | 14.9683100000 | -4.5426280000 | 63.7064980000 |
| C146 | 14.9888240000 | -5.6561970000 | 61.8554110000 |
| C147 | 13.9149700000 | -6.5384150000 | 62.0580780000 |
| H148 | 13.5503930000 | -6.7166080000 | 63.0687200000 |
| C149 | 15.4276290000 | -5.4278950000 | 60.5412780000 |
| H150 | 16.2294200000 | -4.7137560000 | 60.3687620000 |
| C151 | 13.3008300000 | -7.1793660000 | 60.9811220000 |
| H152 | 12.4630370000 | -7.8504280000 | 61.1545210000 |
| C153 | 14.8193960000 | -6.0755730000 | 59.4593650000 |
| H154 | 15.1734460000 | -5.8884920000 | 58.4484740000 |
| C155 | 13.7552730000 | -6.9554450000 | 59.6769050000 |
| H156 | 13.2767030000 | -7.4574860000 | 58.8391540000 |
| H157 | 9.0037560000 | 0.7050730000 | 60.7752690000 |
| C158 | 8.1269800000 | 0.1560800000 | 60.4650000000 |
| H159 | 7.2836720000 | 0.4592420000 | 61.0677700000 |
| H160 | 9.3526530000 | -5.8834640000 | 54.8382570000 |
| H161 | 18.2592780000 | -9.4987530000 | 50.1505400000 |
| C162 | 17.5839750000 | -8.6559200000 | 50.1520260000 |
| H163 | 17.2773630000 | -8.4419890000 | 49.1387990000 |
| H164 | 23.2775150000 | -4.2119100000 | 52.4584870000 |
| H165 | 10.8241320000 | -5.6167760000 | 50.7162270000 |
| H166 | 15.1287660000 | -9.2242390000 | 56.3171260000 |
| H167 | 12.3946920000 | -5.2103580000 | 57.6191670000 |
| H168 | 11.5237490000 | -8.4044670000 | 56.8009180000 |
| H169 | 9.5768840000 | -6.3081640000 | 55.6580330000 |
| C170 | 6.9378430000 | -8.6187130000 | 56.1786840000 |
| H171 | 6.2736770000 | -7.7639700000 | 56.0098780000 |
| H172 | 7.4439960000 | -8.8363400000 | 55.2309580000 |
| H173 | 7.1493940000 | -5.8354100000 | 59.8218940000 |
| C174 | 6.9590150000 | -4.8009330000 | 59.5000040000 |
| H175 | 5.9039260000 | -4.4903550000 | 59.5181450000 |
| H176 | 7.4831910000 | -4.1659550000 | 60.2288350000 |
| C177 | 7.5291900000 | -4.5174930000 | 58.1084030000 |
| H178 | 8.6103410000 | -4.7186400000 | 58.0965100000 |
| H179 | 7.3975030000 | -3.4529680000 | 57.8730520000 |
| O180 | 6.8708160000 | -5.2423230000 | 57.0832200000 |
| H181 | 7.2871120000 | -6.1286290000 | 57.0970370000 |

Optimized position for a water molecule in the Fe2, Fe6, Val70 region
in **Figure 13**.

Energies: E= -7997.906419, solv = -0.204742, disp = -241.15 Z₀ = 911.62

| | | | |
|-----|---------------|----------------|---------------|
| Mo1 | 16.3773842157 | -6.2201207089 | 53.6474057688 |
| Fe2 | 10.0021115268 | -9.5121256834 | 55.8780721718 |
| Fe3 | 11.2166256958 | -6.9810213039 | 55.8038580223 |
| Fe4 | 11.2468952393 | -8.2380549797 | 53.4862448904 |
| Fe5 | 12.5645161938 | -9.5097942105 | 55.8843894581 |
| Fe6 | 14.7052867869 | -8.5487598585 | 54.5255511070 |
| Fe7 | 14.0546160447 | -6.4428888370 | 55.9316277417 |
| Fe8 | 13.3312772622 | -6.5012158796 | 53.4010277233 |
| C9 | 17.5210584587 | -2.4521832477 | 54.4797326076 |
| H10 | 17.6043389762 | -1.4562099689 | 54.0411031966 |
| H11 | 16.4608522611 | -2.6354656044 | 54.6952148731 |
| C12 | 18.0059403564 | -3.5283828502 | 53.4768672485 |
| C13 | 19.4432430596 | -3.1850292045 | 53.0081256304 |
| H14 | 20.0886256530 | -3.1532830126 | 53.8929435277 |
| H15 | 19.4151988128 | -2.1815597793 | 52.5696225248 |
| C16 | 20.0276372874 | -4.1763373827 | 51.9800747246 |
| H17 | 19.4616293395 | -4.1315980433 | 51.0462865318 |
| H18 | 19.9629077411 | -5.1894964300 | 52.3853053098 |
| C19 | 17.0761780407 | -3.6639392596 | 52.2367207563 |
| O20 | 16.6624665283 | -4.8705394579 | 51.9863324722 |
| O21 | 16.8337330827 | -2.6661967278 | 51.5518144030 |
| O22 | 18.0042402693 | -4.8029865256 | 54.1497690693 |
| C23 | 12.7568244156 | -7.8369207535 | 54.7917931763 |
| S24 | 12.3968347627 | -5.7239092096 | 57.5951299408 |
| S25 | 16.2493343995 | -7.2973359360 | 55.9241434812 |
| S26 | 9.7217832456 | -5.5706433588 | 54.4020703103 |
| S28 | 14.6903476626 | -10.7163068213 | 55.7514127672 |
| S29 | 14.4842013984 | -4.6540635300 | 54.2964525749 |

| | | | |
|------|----------------|-----------------|----------------|
| S30 | 9.9458982094 | -10.0966951957 | 53.5702927346 |
| S31 | 15.0768167396 | -7.8363453775 | 52.3334969995 |
| S32 | 11.6928694549 | -6.7547840164 | 51.5107951137 |
| H33 | 13.6351741281# | -2.1902107774# | 49.0425560013# |
| C34 | 13.2979245943# | -2.0241170144# | 50.0550233218# |
| H35 | 14.1359585917 | -2.3250165164 | 50.6902535814 |
| H36 | 13.1087999689 | -0.9538177343 | 50.2034971020 |
| N37 | 12.0998930518 | -2.8146239454 | 50.3514994437 |
| H38 | 11.4618837277 | -3.0009648129 | 49.5919400546 |
| C39 | 11.6428197161 | -3.0623752503 | 51.6001411740 |
| N40 | 12.4393896182 | -2.9180445221 | 52.6515368081 |
| H41 | 12.0922041096 | -3.1473501368 | 53.5908380197 |
| H42 | 13.4381620281 | -3.1082782482 | 52.5714497761 |
| N43 | 10.3425618437 | -3.3691960135 | 51.7958918394 |
| H44 | 9.7521132126 | -3.5260404061 | 50.9915715923 |
| H45 | 10.0877875570 | -3.9161951278 | 52.6318008717 |
| H46 | 7.9178694891 | 0.4395073261 | 59.4259050264 |
| C47 | 8.3735220212 | -1.3544951836 | 60.5727334882 |
| H48 | 8.5012702887 | -1.6314588044 | 61.6260837225 |
| H49 | 7.4850857680 | -1.8869998595 | 60.2099004194 |
| C50 | 9.5972841869 | -1.8110531719 | 59.8334568705 |
| N51 | 10.7898637231 | -2.0274290618 | 60.4969756057 |
| C52 | 9.7618589505 | -2.0586992670 | 58.4887390428 |
| H53 | 9.0820240150 | -2.0161707049 | 57.6526691112 |
| C54 | 11.6423709473 | -2.4149673257 | 59.5659018555 |
| H55 | 12.6701185573 | -2.6977700008 | 59.7399402997 |
| N56 | 11.0768445696 | -2.4349698271 | 58.3284459875 |
| H57 | 19.0905762860 | -4.4381567114 | 57.5468643487 |
| H58 | 16.7171758104 | -8.8904254477 | 50.7660039878 |
| C59 | 18.3326901889 | -7.4273728372 | 50.7034026644 |
| H60 | 17.6584000188 | -6.5680917422 | 50.7642710069 |
| H61 | 19.1351904036 | -7.1585841308 | 50.0022760790 |
| C62 | 18.9457280578 | -7.6576059465 | 52.0512932266 |
| N63 | 18.2714493615 | -7.4155559766 | 53.2400429949 |
| C64 | 20.2033768280 | -8.1188396693 | 52.3550002750 |
| H65 | 21.0280405465 | -8.4144262021 | 51.7248946612 |
| C66 | 19.0984162345 | -7.7155527832 | 54.2306106346 |
| H67 | 18.9033856544 | -7.5890014452 | 55.2850365529 |
| N68 | 20.2761957645 | -8.1568236131 | 53.7367944167 |
| H69 | 21.0823278981 | -8.3764592381 | 54.3024325260 |
| H70 | 6.8930128508 | -10.6129674494 | 56.9523300316 |
| C71 | 6.1750524232# | -9.8249631940# | 56.6900007489# |
| H72 | 5.5309557341# | -10.2322287736# | 56.0424861413# |
| H73 | 5.6932327210# | -9.5371417037# | 57.6127207510# |
| S74 | 8.4325682323 | -8.2768850626 | 57.1045185452 |
| H75 | 11.4741770610 | -2.8161293847 | 57.4660649040 |
| H76 | 18.2340249235 | -4.5685309864 | 55.1347972672 |
| C78 | 18.2645562658 | -2.4882360678 | 55.8348942000 |
| O79 | 18.5754507746 | -3.6759324043 | 56.2500818677 |
| O80 | 18.4808479689 | -1.4327167526 | 56.4496390961 |
| C81 | 21.4672545989 | -3.8704539216 | 51.6504941501 |
| O82 | 21.8864386700 | -3.3314593505 | 50.6449474241 |
| O83 | 22.3208176291# | -4.2658020463# | 52.6398596376# |
| H84 | 15.7024656764# | -0.1996317185# | 61.4912312893# |
| C85 | 14.8549934557# | -0.0829911608# | 60.8320021121# |
| H86 | 13.9165015895# | -0.2867338793# | 61.3260937710# |
| H87 | 14.8316706074 | 0.9919586761 | 60.5856276345 |
| C88 | 15.0599857050# | -0.8751944201# | 59.5441990054# |
| H89 | 14.4191750147 | -0.4676256614 | 58.7521311649 |
| H90 | 14.7537014123 | -1.9171737751 | 59.6871036995 |
| C91 | 16.5152343257 | -0.8864137962 | 59.0747735861 |
| H92 | 16.9836820958 | 0.0984378788 | 59.2216362751 |
| H93 | 16.5902818124 | -1.0805976723 | 57.9992822792 |
| C94 | 17.3647488299 | -1.9380277712 | 59.8012463344 |
| O95 | 16.9592585112 | -2.5699659698 | 60.7797120932 |
| N96 | 18.6173007855 | -2.0912830170 | 59.2829191982 |
| H97 | 19.0860843785 | -2.9452612157 | 59.5637869053 |
| H98 | 18.7574536666 | -1.8168626221 | 58.3028758741 |
| C99 | 10.6519926687# | 0.0100032631# | 53.3460013693# |
| H100 | 11.1636988274# | 0.9592721372# | 53.2872697144# |
| H101 | 9.5863320466# | 0.1850133191# | 53.3579374811# |
| H102 | 10.9514479228 | -0.6441049895 | 52.5280118340 |
| C103 | 11.0409037046 | -0.4873435781 | 54.7544143792 |
| H104 | 10.7639315313 | -1.5364136960 | 54.8709483742 |
| C105 | 10.2766353642 | 0.3362872317 | 55.8030743243 |

| | | | |
|------|----------------|-----------------|----------------|
| H106 | 9.1903562109 | 0.2115194054 | 55.6984654883 |
| H107 | 10.4984253443 | 1.4084154334 | 55.6943049794 |
| H108 | 10.5493356513 | 0.0394305603 | 56.8201001557 |
| C109 | 12.5511551277 | -0.3622684244 | 54.9938692121 |
| H110 | 13.1316494193 | -0.9059214384 | 54.2418894511 |
| H111 | 12.8286228243 | -0.7566631135 | 55.9764853267 |
| H112 | 12.8599191367 | 0.6928349522 | 54.9550720600 |
| H113 | 13.4550780847# | -12.2303887257# | 53.1883138641# |
| C114 | 13.9110014278# | -11.6210552988# | 52.4219871242# |
| H115 | 14.6099268803 | -10.9059066635 | 52.8616892510 |
| H116 | 14.3990756578 | -12.2340558602 | 51.6594437413 |
| N117 | 12.7104603946 | -10.9672165738 | 51.8717090384 |
| H118 | 11.8814508046 | -10.9524065345 | 52.4922359813 |
| C119 | 12.6087346440 | -10.1946731779 | 50.8044846749 |
| N120 | 13.7106813016 | -9.7996334830 | 50.1208417789 |
| H121 | 13.5190229982 | -9.1634420472 | 49.3553705897 |
| H122 | 14.4671577019 | -9.4448123002 | 50.7198901148 |
| N123 | 11.3724298490 | -9.8521174447 | 50.3451944659 |
| H124 | 10.6211018301 | -10.1203661858 | 50.9862747804 |
| H125 | 11.2956496889 | -8.8521136879 | 50.1414554368 |
| H126 | 19.1649531103 | -8.2046407000 | 61.7255501856 |
| C127 | 19.5978932924# | -7.2298795333# | 61.9900501767# |
| H128 | 20.6425970791 | -7.3919678445 | 62.2751186909 |
| C129 | 18.8636769750 | -6.6300364800 | 63.1926976657 |
| O130 | 19.4295588396 | -6.0044780889 | 64.0856707634 |
| C131 | 19.4918719702# | -6.2717980970# | 60.7990634052# |
| H132 | 19.9843618893 | -5.3246166398 | 61.0436112828 |
| H133 | 18.4423128549 | -6.0284900833 | 60.6136958201 |
| C134 | 20.0963278592 | -6.8770340899 | 59.5214193551 |
| H135 | 19.7177530832 | -7.8952299568 | 59.3648707023 |
| H136 | 21.1867639152 | -6.9805187798 | 59.6185847235 |
| C137 | 19.8305233652 | -6.1281361404 | 58.2158681899 |
| O138 | 20.0861334254 | -6.6180187491 | 57.1248644854 |
| O139 | 19.3171045824 | -4.9217994557 | 58.4127484181 |
| N140 | 17.5106594801 | -6.8094347499 | 63.1278127998 |
| H141 | 17.1490053424 | -7.2724177776 | 62.3028548767 |
| C142 | 16.5368854453# | -6.0058843768# | 63.8530414353# |
| H143 | 15.9828725082 | -6.6415891000 | 64.5589750187 |
| H144 | 17.0938856471 | -5.2677980330 | 64.4360935171 |
| C145 | 15.5431386222 | -5.3229843948 | 62.8793260282 |
| H146 | 16.0511817435 | -4.5129525125 | 62.3442791963 |
| H147 | 14.7406320366 | -4.8688809440 | 63.4750294919 |
| C148 | 14.9746561330 | -6.3186137224 | 61.8855598199 |
| C149 | 14.0216069362 | -7.2749761443 | 62.2726614081 |
| H150 | 13.6095489718 | -7.2428512661 | 63.2798661651 |
| C151 | 15.4769065297 | -6.3710250053 | 60.5748530347 |
| H152 | 16.1755632312 | -5.6061287423 | 60.2439705223 |
| C153 | 13.5934605708 | -8.2610872526 | 61.3818624681 |
| H154 | 12.8442942538 | -8.9845482520 | 61.6936895003 |
| C155 | 15.0631244588 | -7.3660199938 | 59.6833297655 |
| H156 | 15.4622192259 | -7.3800838616 | 58.6727394579 |
| C157 | 14.1220709975 | -8.3172099884 | 60.0877421956 |
| H158 | 13.7870136483 | -9.0844652800 | 59.3941303646 |
| H159 | 9.0037560460# | 0.7050733324# | 60.7752693400# |
| C160 | 8.1269803486# | 0.1560802985# | 60.4649995486# |
| H161 | 7.2836720179# | 0.4592420071# | 61.0677700273# |
| H268 | 8.6306183113 | -5.4598366652 | 55.1948900265 |
| H269 | 18.2592781541# | -9.4987528752# | 50.1505401201# |
| C270 | 17.5839755870# | -8.6559201244# | 50.1520261842# |
| H271 | 17.2773625962# | -8.4419892869# | 49.1387987594# |
| H273 | 23.2042271274 | -3.9798789799 | 52.3412840500 |
| H274 | 10.5611113384 | -6.0997811266 | 51.8525720396 |
| H275 | 15.3187669771 | -10.1634682011 | 56.8124318575 |
| H277 | 12.5533259559 | -6.7437724931 | 58.4630775105 |
| H278 | 11.3467457687 | -10.7274407363 | 56.2919533440 |
| H279 | 11.1950880210 | -8.5371357179 | 56.8387620328 |
| C280 | 6.9383949387 | -8.6554879299 | 56.0791138990 |
| H281 | 6.3097724277 | -7.7593173679 | 56.0275085240 |
| H282 | 7.2605190468 | -8.8906734545 | 55.0589784375 |
| H283 | 7.1493941354# | -5.8354098835# | 59.8218942939# |
| C284 | 6.9590149597# | -4.8009334214# | 59.5000035190# |
| H285 | 5.9039260052# | -4.4903549822# | 59.5181449940# |
| H286 | 7.4947047716 | -4.1546393089 | 60.2071924483 |
| C287 | 7.5324089474 | -4.5705797736 | 58.0970944140 |
| H288 | 8.6238221857 | -4.6880950801 | 58.1161160584 |

| | | | |
|------|---------------|---------------|---------------|
| H289 | 7.3236987217 | -3.5403568452 | 57.7857873726 |
| O290 | 6.9561257098 | -5.4110938534 | 57.1042462352 |
| H291 | 7.4468141575 | -6.2590214156 | 57.1514306919 |
| O292 | 11.7867711517 | -3.3674876907 | 55.5746999925 |
| H293 | 12.6693334330 | -3.7951719711 | 55.5828297792 |
| H294 | 11.1489866929 | -4.1081108886 | 55.4313715520 |

Optimized TS for the reaction between a proton on S2A and a hydride after an addition of a water molecule in **Figure 14**.

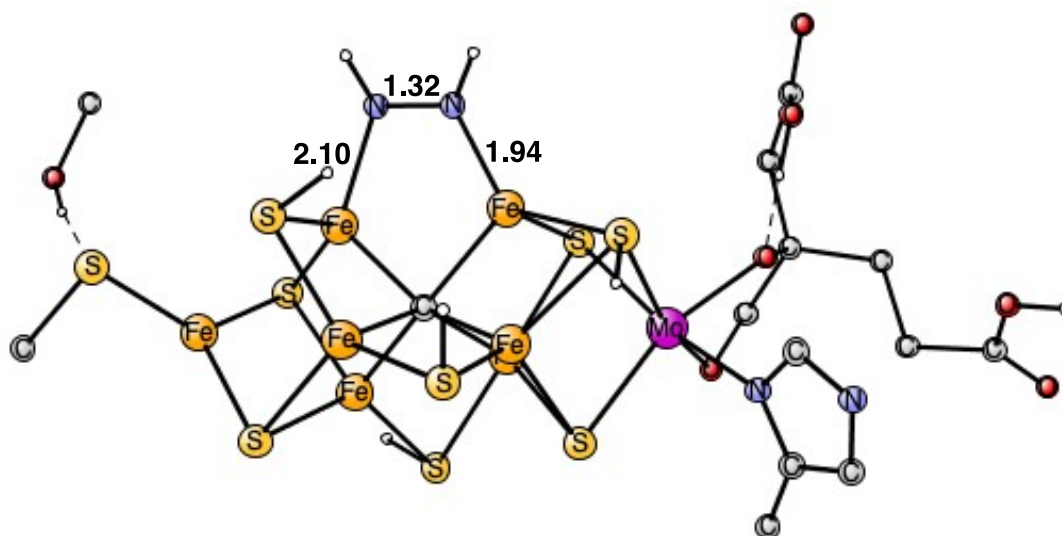
Energies: E= -7997.871643, solv = -0.206917, disp = -237.69 Z₀ = 908.99

| | | | |
|-----|---------------|----------------|---------------|
| Mo1 | 16.7137430000 | -6.0433800000 | 53.7395300000 |
| Fe2 | 10.1118000000 | -8.7224260000 | 56.5280670000 |
| Fe3 | 12.0025490000 | -6.4928810000 | 56.3085980000 |
| Fe4 | 11.3736400000 | -7.5335460000 | 53.9021490000 |
| Fe5 | 12.7012470000 | -9.2290190000 | 55.9420980000 |
| Fe6 | 14.9949360000 | -8.3696160000 | 54.7297070000 |
| Fe7 | 14.7369150000 | -6.1736670000 | 56.0616580000 |
| Fe8 | 13.8193070000 | -6.3217220000 | 53.5388240000 |
| C9 | 17.8017690000 | -2.2475960000 | 54.5340630000 |
| H10 | 17.8806650000 | -1.2535800000 | 54.0895710000 |
| H11 | 16.7458330000 | -2.4142630000 | 54.7787970000 |
| C12 | 18.2434130000 | -3.3283940000 | 53.5227700000 |
| C13 | 19.6486410000 | -2.9979340000 | 52.9682540000 |
| H14 | 20.3531040000 | -3.0302530000 | 53.8056870000 |
| H15 | 19.6286590000 | -1.9754410000 | 52.5757100000 |
| C16 | 20.1062970000 | -3.9650390000 | 51.8565400000 |
| H17 | 19.5683490000 | -3.7688140000 | 50.9266900000 |
| H18 | 19.8948840000 | -4.9901520000 | 52.1753810000 |
| C19 | 17.2729270000 | -3.4977570000 | 52.3209200000 |
| O20 | 16.9433790000 | -4.7297980000 | 52.0567370000 |
| O21 | 16.9483920000 | -2.5119360000 | 51.6582650000 |
| O22 | 18.2994600000 | -4.5955180000 | 54.2121420000 |
| C23 | 13.1440980000 | -7.4632160000 | 55.0687090000 |
| S24 | 13.3357930000 | -5.2611390000 | 57.8692990000 |
| S25 | 16.7800130000 | -7.2532610000 | 55.9745560000 |
| S26 | 9.9451920000 | -5.6456630000 | 54.1765720000 |
| S27 | 14.6747350000 | -10.6315150000 | 55.7545170000 |
| S28 | 14.8845520000 | -4.4215030000 | 54.3994360000 |
| S29 | 10.5862530000 | -9.7039380000 | 54.4083810000 |
| S30 | 15.4444820000 | -7.7866810000 | 52.5370420000 |
| S31 | 12.3755840000 | -6.4710360000 | 51.5298830000 |
| H32 | 13.6351740000 | -2.1902110000 | 49.0425560000 |
| C33 | 13.2979250000 | -2.0241170000 | 50.0550240000 |
| H34 | 14.1423170000 | -2.3103010000 | 50.6885670000 |
| H35 | 13.1089820000 | -0.9521500000 | 50.1946490000 |
| N36 | 12.1081860000 | -2.8071600000 | 50.3607370000 |
| H37 | 11.5312260000 | -3.1353150000 | 49.6020280000 |
| C38 | 11.6851560000 | -3.0680240000 | 51.6170060000 |
| N39 | 12.5086550000 | -2.9147220000 | 52.6489680000 |
| H40 | 12.1546200000 | -3.0482500000 | 53.6060220000 |
| H41 | 13.5039740000 | -3.1086690000 | 52.5575840000 |
| N42 | 10.4032330000 | -3.4033610000 | 51.8406750000 |
| H43 | 9.7543230000 | -3.4200520000 | 51.0670010000 |
| H44 | 10.1744670000 | -4.0223350000 | 52.6503270000 |
| H45 | 7.9170920000 | 0.4387320000 | 59.4257030000 |
| C46 | 8.3816330000 | -1.3551250000 | 60.5725440000 |
| H47 | 8.5367680000 | -1.6255290000 | 61.6239090000 |
| H48 | 7.4846370000 | -1.8906070000 | 60.2358830000 |
| C49 | 9.5861260000 | -1.8203040000 | 59.8023700000 |
| N50 | 10.7922740000 | -2.0635740000 | 60.4316940000 |
| C51 | 9.7088180000 | -2.0681420000 | 58.4519790000 |
| H52 | 9.0056290000 | -2.0114620000 | 57.6359570000 |
| C53 | 11.6133600000 | -2.4634510000 | 59.4767610000 |
| H54 | 12.6414020000 | -2.7646800000 | 59.6104090000 |
| N55 | 11.0098040000 | -2.4760400000 | 58.2555630000 |
| H56 | 19.4404230000 | -4.2384330000 | 57.6199880000 |
| H57 | 16.7252930000 | -8.8807610000 | 50.7776560000 |
| C58 | 18.3415840000 | -7.4096040000 | 50.6612590000 |
| H59 | 17.6526450000 | -6.5680730000 | 50.7714140000 |

| | | | |
|------|---------------|----------------|---------------|
| H60 | 19.0725530000 | -7.1202180000 | 49.8928680000 |
| C61 | 19.0871170000 | -7.5925050000 | 51.9514760000 |
| N62 | 18.5934080000 | -7.1940470000 | 53.1871600000 |
| C63 | 20.3448280000 | -8.1125600000 | 52.1420510000 |
| H64 | 21.0636370000 | -8.5181230000 | 51.4464170000 |
| C65 | 19.5239910000 | -7.4577980000 | 54.0927170000 |
| H66 | 19.4715200000 | -7.2371040000 | 55.1497470000 |
| N67 | 20.5986730000 | -8.0244230000 | 53.4992830000 |
| H68 | 21.4498130000 | -8.2768340000 | 53.9780540000 |
| H69 | 6.8609790000 | -10.6361900000 | 56.9742480000 |
| C70 | 6.1750530000 | -9.8249630000 | 56.6900010000 |
| H71 | 5.5309560000 | -10.2322290000 | 56.0424860000 |
| H72 | 5.6932330000 | -9.5371420000 | 57.6127210000 |
| S73 | 8.1573570000 | -8.2562980000 | 57.6251910000 |
| H74 | 11.3943420000 | -2.8242310000 | 57.3744540000 |
| H75 | 18.5863530000 | -4.3392880000 | 55.1844850000 |
| C76 | 18.5720670000 | -2.2725570000 | 55.8748590000 |
| O77 | 18.9822360000 | -3.4405310000 | 56.2600930000 |
| O78 | 18.7086390000 | -1.2179160000 | 56.5115540000 |
| C79 | 21.5784350000 | -3.8580420000 | 51.5730950000 |
| O80 | 22.1080670000 | -3.4689830000 | 50.5509400000 |
| O81 | 22.3208170000 | -4.2658020000 | 52.6398600000 |
| H82 | 15.7024660000 | -0.1996320000 | 61.4912310000 |
| C83 | 14.8549930000 | -0.0829910000 | 60.8320020000 |
| H84 | 13.9165020000 | -0.2867340000 | 61.3260940000 |
| H85 | 14.8298390000 | 0.9926610000 | 60.5867240000 |
| C86 | 15.0599860000 | -0.8751940000 | 59.5441990000 |
| H87 | 14.3905910000 | -0.4955700000 | 58.7619410000 |
| H88 | 14.7891700000 | -1.9238130000 | 59.7089340000 |
| C89 | 16.5056110000 | -0.8439150000 | 59.0445920000 |
| H90 | 16.9239240000 | 0.1717130000 | 59.1067080000 |
| H91 | 16.5677940000 | -1.1143820000 | 57.9841940000 |
| C92 | 17.4237960000 | -1.7950320000 | 59.8254120000 |
| O93 | 17.0451570000 | -2.4288920000 | 60.8117590000 |
| N94 | 18.7019060000 | -1.8555420000 | 59.3494690000 |
| H95 | 19.2306220000 | -2.6572460000 | 59.6732920000 |
| H96 | 18.8652880000 | -1.5836320000 | 58.3723630000 |
| C97 | 10.6519930000 | 0.0100030000 | 53.3460010000 |
| H98 | 11.1636990000 | 0.9592720000 | 53.2872700000 |
| H99 | 9.5863320000 | 0.1850130000 | 53.3579370000 |
| H100 | 10.9539030000 | -0.6494080000 | 52.5331600000 |
| C101 | 11.0338150000 | -0.4749860000 | 54.7633930000 |
| H102 | 10.7357500000 | -1.5174380000 | 54.8973950000 |
| C103 | 10.2769840000 | 0.3746660000 | 55.7985590000 |
| H104 | 9.1898260000 | 0.2581920000 | 55.6948310000 |
| H105 | 10.5094360000 | 1.4425820000 | 55.6727940000 |
| H106 | 10.5451210000 | 0.0922730000 | 56.8214620000 |
| C107 | 12.5455520000 | -0.3639500000 | 55.0029580000 |
| H108 | 13.1218070000 | -0.9009000000 | 54.2436550000 |
| H109 | 12.8234270000 | -0.7697630000 | 55.9810730000 |
| H110 | 12.8611990000 | 0.6893680000 | 54.9744610000 |
| H111 | 13.4550780000 | -12.2303890000 | 53.1883140000 |
| C112 | 13.9110010000 | -11.6210550000 | 52.4219870000 |
| H113 | 14.7319290000 | -11.0296770000 | 52.8362180000 |
| H114 | 14.2385740000 | -12.2206210000 | 51.5686660000 |
| N115 | 12.7439110000 | -10.7972590000 | 52.0654720000 |
| H116 | 12.0170670000 | -10.7285640000 | 52.7913600000 |
| C117 | 12.6167790000 | -9.9147220000 | 51.0870200000 |
| N118 | 13.6796190000 | -9.5460260000 | 50.3339840000 |
| H119 | 13.4784900000 | -8.7878420000 | 49.6900410000 |
| H120 | 14.5220120000 | -9.3395310000 | 50.8806420000 |
| N121 | 11.3859590000 | -9.4224810000 | 50.7910770000 |
| H122 | 10.6658290000 | -9.7019060000 | 51.4561640000 |
| H123 | 11.4077610000 | -8.3939630000 | 50.6974520000 |
| H124 | 19.1816310000 | -8.2119690000 | 61.7238990000 |
| C125 | 19.5978930000 | -7.2298790000 | 61.9900500000 |
| H126 | 20.6424600000 | -7.3738440000 | 62.2846470000 |
| C127 | 18.8501860000 | -6.6264800000 | 63.1793260000 |
| O128 | 19.4077670000 | -5.9582480000 | 64.0448740000 |
| C129 | 19.4918720000 | -6.2717980000 | 60.7990630000 |
| H130 | 19.9133830000 | -5.3008830000 | 61.0804100000 |
| H131 | 18.4394990000 | -6.0826430000 | 60.5630710000 |
| C132 | 20.1952620000 | -6.8063740000 | 59.5431500000 |
| H133 | 19.7966730000 | -7.7919740000 | 59.2706000000 |
| H134 | 21.2657340000 | -6.9647790000 | 59.7391200000 |

| | | | |
|------|---------------|----------------|---------------|
| C135 | 20.0986450000 | -5.9575960000 | 58.2727850000 |
| O136 | 20.4794510000 | -6.3824700000 | 57.1929180000 |
| O137 | 19.5894640000 | -4.7490950000 | 58.4821810000 |
| N138 | 17.4983830000 | -6.8333260000 | 63.1386820000 |
| H139 | 17.1283170000 | -7.3540140000 | 62.3531470000 |
| C140 | 16.5368850000 | -6.0058840000 | 63.8530410000 |
| H141 | 16.0299790000 | -6.5970800000 | 64.6296930000 |
| H142 | 17.1053730000 | -5.2164370000 | 64.3515730000 |
| C143 | 15.4848900000 | -5.4057940000 | 62.8912930000 |
| H144 | 15.9808530000 | -4.7135760000 | 62.2004710000 |
| H145 | 14.7811710000 | -4.8129580000 | 63.4887530000 |
| C146 | 14.7378420000 | -6.4843740000 | 62.1321430000 |
| C147 | 13.6306610000 | -7.1330020000 | 62.7014140000 |
| H148 | 13.2637990000 | -6.8057530000 | 63.6725990000 |
| C149 | 15.1777500000 | -6.9143460000 | 60.8705300000 |
| H150 | 15.9997910000 | -6.3938340000 | 60.3842190000 |
| C151 | 12.9835450000 | -8.1736650000 | 62.0341420000 |
| H152 | 12.1139550000 | -8.6464250000 | 62.4842760000 |
| C153 | 14.5438060000 | -7.9703050000 | 60.2059500000 |
| H154 | 14.9013340000 | -8.2761060000 | 59.2258170000 |
| C155 | 13.4407640000 | -8.6020140000 | 60.7842430000 |
| H156 | 12.9275530000 | -9.3991430000 | 60.2532850000 |
| H157 | 9.0037560000 | 0.7050730000 | 60.7752690000 |
| C158 | 8.1269800000 | 0.1560800000 | 60.4649990000 |
| H159 | 7.2836720000 | 0.4592420000 | 61.0677700000 |
| H160 | 10.0307710000 | -6.1244260000 | 55.8856500000 |
| H161 | 18.2592780000 | -9.4987530000 | 50.1505400000 |
| C162 | 17.5839750000 | -8.6559200000 | 50.1520260000 |
| H163 | 17.2773630000 | -8.4419890000 | 49.1387990000 |
| H164 | 23.2496410000 | -4.1335680000 | 52.3740710000 |
| H165 | 11.2553060000 | -5.7659110000 | 51.7855800000 |
| H166 | 15.2620870000 | -10.2751980000 | 56.9195160000 |
| H167 | 13.4559860000 | -6.2640050000 | 58.7677770000 |
| H168 | 11.6092530000 | -9.3243980000 | 57.3552270000 |
| H169 | 10.2240460000 | -6.5231470000 | 56.7021880000 |
| C170 | 7.0144180000 | -8.6588320000 | 56.2146480000 |
| H171 | 6.4055810000 | -7.7769020000 | 55.9895120000 |
| H172 | 7.5924400000 | -8.9025630000 | 55.3179790000 |
| H173 | 7.1493940000 | -5.8354100000 | 59.8218940000 |
| C174 | 6.9590150000 | -4.8009340000 | 59.5000030000 |
| H175 | 5.9039260000 | -4.4903550000 | 59.5181450000 |
| H176 | 7.5058450000 | -4.1511090000 | 60.1955970000 |
| C177 | 7.4683700000 | -4.5663220000 | 58.0758460000 |
| H178 | 8.5521280000 | -4.7352410000 | 58.0205270000 |
| H179 | 7.2908940000 | -3.5214290000 | 57.7949760000 |
| O180 | 6.7818400000 | -5.3587240000 | 57.1188960000 |
| H181 | 7.2219970000 | -6.2302040000 | 57.1563830000 |
| O182 | 11.8370210000 | -3.4326790000 | 55.4438300000 |
| H183 | 12.7272930000 | -3.8411380000 | 55.4606550000 |
| H184 | 11.2251990000 | -4.1571260000 | 55.1386660000 |

A structure obtained for N_2H_2 after the addition of two protons to E_4 . **Figure S1.**



| | | | |
|-----|----------------|----------------|----------------|
| Mo1 | 16.9176041605 | -5.7874763238 | 53.6672310367 |
| Fe2 | 9.4823507382 | -7.5137492816 | 55.3683287822 |
| Fe3 | 11.8868105016 | -6.1045156819 | 56.3929799229 |
| Fe4 | 11.8383078709 | -7.3505634718 | 53.8654590789 |
| Fe5 | 12.5170268338 | -8.8734614724 | 55.9458908744 |
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