

O₂

Gas phase Energy: -150.3166227 hartrees

Solvation Energy: 0.00000031291 hartrees

Zero Point Energy: 2.374 kcal/mol

Free Energy: -12.537 kcal/mol

angstroms

| atom | x | y | z |
|------|--------------|--------------|---------------|
| O1 | 0.0000000000 | 0.0000000000 | -0.0570704056 |
| O2 | 0.0000000000 | 0.0000000000 | 1.1570704056 |

1

Gas phase Energy: -1052.646614 hartrees

Solvation Energy: -0.01184732822 hartrees

Zero Point Energy: 290.181 kcal/mol

Free Energy: -31.007 kcal/mol

angstroms

| atom | x | y | z |
|------|---------------|---------------|---------------|
| Pd1 | 0.3155315840 | -0.5095382177 | -2.1796621847 |
| C2 | 1.1141360721 | -0.7460370358 | 1.2616487034 |
| C3 | -0.2224185427 | 1.2489675298 | 0.7518387277 |
| C4 | 0.8360197734 | 1.6826444901 | -0.2819844917 |
| N5 | 1.6570583930 | 0.5643493839 | -0.8447521025 |
| C6 | 2.2016467339 | -0.3104246467 | 0.2517499677 |
| C7 | 3.0268311286 | -1.4558904179 | -0.3475808479 |
| C8 | 4.2133060444 | -0.9061598177 | -1.1541795021 |
| C9 | 3.7291711512 | 0.1002624783 | -2.2074852533 |
| C10 | 2.8069791479 | 1.1579880748 | -1.5997144524 |
| C11 | 0.4963903818 | 0.5097158835 | 1.8905545047 |
| C12 | -0.0242996400 | -1.6396157596 | 0.7331509488 |
| N13 | -0.9129619505 | -0.9561122445 | -0.2368491704 |
| C14 | -1.3928457835 | 0.3937903517 | 0.2034397004 |
| C15 | -2.5699966004 | 0.3404912205 | 1.2072927491 |
| C16 | -3.1822083575 | -1.9418092437 | 0.3626757809 |
| C17 | -3.7167014670 | -0.5453315691 | 0.7015957383 |
| C18 | -2.0430912572 | -1.8321828703 | -0.6578293645 |
| H19 | 1.6380561984 | -1.3299670214 | 2.0292678272 |
| H20 | -0.6665019975 | 2.1793982463 | 1.1281178509 |
| H21 | 0.3756337192 | 2.2023423342 | -1.1267168175 |
| H22 | 1.5120108545 | 2.3956384969 | 0.2204753869 |
| H23 | 2.8984616771 | 0.3205251326 | 0.8349810511 |
| H24 | 3.3817400634 | -2.0962762178 | 0.4696004433 |
| H25 | 2.3871762003 | -2.0669350254 | -0.9954973064 |
| H26 | 4.9191731606 | -0.4170507181 | -0.4676827211 |
| H27 | 4.7594940867 | -1.7248331827 | -1.6353746474 |
| H28 | 4.5796454465 | 0.6136898381 | -2.6718325039 |
| H29 | 3.1877194728 | -0.4209148121 | -3.0030179991 |

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|-----|---------------|---------------|---------------|
| H30 | 2.3875423142 | 1.7969342217 | -2.3804130892 |
| H31 | 3.3773809769 | 1.7964962268 | -0.9027620478 |
| H32 | -0.1914887450 | 0.2436273271 | 2.6992564903 |
| H33 | 1.2728735868 | 1.1477729728 | 2.3301337636 |
| H34 | -0.5867313202 | -1.9988618956 | 1.6105456407 |
| H35 | 0.3746089034 | -2.5252368437 | 0.2287738913 |
| H36 | -1.7706845002 | 0.8720841226 | -0.7106725452 |
| H37 | -2.2323540912 | -0.0382594626 | 2.1799730593 |
| H38 | -2.9210145656 | 1.3660628796 | 1.3779726504 |
| H39 | -2.8466851106 | -2.4451443845 | 1.2798339573 |
| H40 | -3.9722741419 | -2.5703716449 | -0.0651919222 |
| H41 | -4.5144962638 | -0.5979793313 | 1.4514474908 |
| H42 | -4.1582932780 | -0.0978753243 | -0.1999755260 |
| H43 | -1.6199801087 | -2.8121411915 | -0.8966846968 |
| H44 | -2.4221992456 | -1.4356522687 | -1.6033091145 |
| C45 | -0.9047537223 | -1.4562100251 | -4.7014991943 |
| O46 | -1.0174273062 | -1.4462976836 | -3.3948218655 |
| O47 | -0.0217136017 | -0.9409667502 | -5.3771849837 |
| C48 | -2.0558631543 | -2.2199902232 | -5.3649523201 |
| H49 | -3.0109230847 | -1.7398534774 | -5.1269328469 |
| H50 | -1.9169985696 | -2.2388747038 | -6.4468216800 |
| H51 | -2.1025356133 | -3.2437136156 | -4.9801424513 |
| H52 | 1.0671829135 | -0.1542499397 | -3.4536287359 |

2_{trip}

Gas phase Energy: -1202.969099 hartrees

Solvation Energy: -0.00911188548 hartrees

Zero Point Energy: 293.234 kcal/mol

Free Energy: -35.953 kcal/mol

angstroms

| atom | x | y | z |
|------|---------------|---------------|---------------|
| Pd1 | 0.6375233055 | -0.2634049769 | -2.2374790439 |
| C2 | 1.1748042003 | -0.6034079709 | 1.2417311204 |
| C3 | -0.2052294014 | 1.3448728519 | 0.6622175709 |
| C4 | 0.9170025519 | 1.8558878187 | -0.2623275821 |
| N5 | 1.8330983746 | 0.7866866824 | -0.7770055279 |
| C6 | 2.3213485265 | -0.0987874016 | 0.3381174600 |
| C7 | 3.2367681610 | -1.1955577594 | -0.2202443919 |
| C8 | 4.4651236072 | -0.5805826474 | -0.9076467473 |
| C9 | 4.0312925145 | 0.4400843393 | -1.9689527445 |
| C10 | 3.0208708512 | 1.4445344758 | -1.4124226013 |
| C11 | 0.4502484795 | 0.6090382510 | 1.8413742086 |
| C12 | 0.1316276617 | -1.5319212097 | 0.5934077043 |
| N13 | -0.6994263556 | -0.8633724077 | -0.4369085147 |
| C14 | -1.2846617000 | 0.4543005626 | -0.0057799673 |
| C15 | -2.5263629905 | 0.3145547736 | 0.9091387429 |

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|-----|---------------|---------------|---------------|
| C16 | -2.9411560766 | -1.9885469322 | 0.0035301087 |
| C17 | -3.5820916217 | -0.6326134784 | 0.3229347156 |
| C18 | -1.7606391479 | -1.7771124051 | -0.9524795857 |
| H19 | 1.6577016133 | -1.1833406158 | 2.0387967371 |
| H20 | -0.7229343176 | 2.2437631582 | 1.0201891334 |
| H21 | 0.5074136197 | 2.3763366362 | -1.1321557851 |
| H22 | 1.5167569169 | 2.5812805028 | 0.3130872819 |
| H23 | 2.9427215189 | 0.5425585534 | 0.9903383059 |
| H24 | 3.5457178827 | -1.8471443233 | 0.6065708102 |
| H25 | 2.6783080372 | -1.8100955534 | -0.9361177616 |
| H26 | 5.0930989347 | -0.0885356671 | -0.1514013792 |
| H27 | 5.0794681880 | -1.3642881479 | -1.3643623817 |
| H28 | 4.8966850110 | 0.9977601517 | -2.3469450948 |
| H29 | 3.5779570674 | -0.0783367291 | -2.8192501110 |
| H30 | 2.6462246990 | 2.0955743259 | -2.2053595624 |
| H31 | 3.5049105225 | 2.0771684335 | -0.6488030947 |
| H32 | -0.2882146084 | 0.2931741130 | 2.5844028937 |
| H33 | 1.1588010023 | 1.2683143496 | 2.3580482284 |
| H34 | -0.4906789770 | -1.9357954982 | 1.4075452574 |
| H35 | 0.6136616899 | -2.3872600620 | 0.1095316793 |
| H36 | -1.6137471571 | 0.9244706517 | -0.9407581296 |
| H37 | -2.2394364528 | -0.0495810859 | 1.9036613945 |
| H38 | -2.9495659044 | 1.3161715274 | 1.0560875694 |
| H39 | -2.6292934568 | -2.4890747658 | 0.9304519382 |
| H40 | -3.6621970894 | -2.6567103806 | -0.4824020640 |
| H41 | -4.4187636340 | -0.7442970644 | 1.0225192358 |
| H42 | -3.9903645275 | -0.2020591172 | -0.6009606999 |
| H43 | -1.2773200869 | -2.7198831491 | -1.2245786013 |
| H44 | -2.1380271772 | -1.3223229871 | -1.8681812845 |
| C45 | -1.5186926080 | -0.5842157916 | -4.0929854282 |
| O46 | -0.4335969752 | -1.1985786672 | -3.7240989531 |
| O47 | -2.0372513530 | 0.3808825232 | -3.5164158708 |
| C48 | -2.1514155656 | -1.1829542934 | -5.3482116992 |
| H49 | -2.2027256922 | -2.2730124256 | -5.2698693646 |
| H50 | -3.1487318921 | -0.7688720202 | -5.5049136844 |
| H51 | -1.5245002568 | -0.9510847078 | -6.2160084240 |
| H52 | 1.4926525032 | 0.2442893461 | -3.4001952398 |
| O53 | 1.9499012742 | -2.0696175041 | -5.2012243833 |
| O54 | 2.3582512004 | -2.6080891106 | -4.1938719824 |

3_{trip}

Gas phase Energy: -1202.992695 hartrees

Solvation Energy: -0.00909690815 hartrees

Zero Point Energy: 294.912 kcal/mol

Free Energy: -34.301 kcal/mol

angstroms

| atom | x | y | z |
|------|---------------|---------------|---------------|
| Pd1 | 0.0569777250 | -0.3303562022 | -2.1412322966 |
| C2 | 1.2091512007 | -1.0165094285 | 1.1584400532 |
| C3 | 0.1218195435 | 1.1843567338 | 1.1021828019 |
| C4 | 1.1051588145 | 1.6344283020 | 0.0053852387 |
| N5 | 1.6990448011 | 0.5250252755 | -0.7863233447 |
| C6 | 2.2332099927 | -0.5670538176 | 0.0892512442 |
| C7 | 2.7986915733 | -1.7069789957 | -0.7688056632 |
| C8 | 3.9306491122 | -1.1958500540 | -1.6721111743 |
| C9 | 3.4528030396 | -0.0017686819 | -2.5090676778 |
| C10 | 2.7917255348 | 1.0700200291 | -1.6383137614 |
| C11 | 0.8494802914 | 0.1960689961 | 2.0262163455 |
| C12 | -0.0941776287 | -1.6755228197 | 0.6607039608 |
| N13 | -0.9817776395 | -0.7424296921 | -0.0798362957 |
| C14 | -1.2081851955 | 0.5746112618 | 0.5961300946 |
| C15 | -2.2598044997 | 0.5153718933 | 1.7325924358 |
| C16 | -3.2866136266 | -1.5154503297 | 0.6779290515 |
| C17 | -3.5731508154 | -0.1343791981 | 1.2775861956 |
| C18 | -2.2688001137 | -1.3919538870 | -0.4628876036 |
| H19 | 1.7241067933 | -1.7714975963 | 1.7662974595 |
| H20 | -0.1437145782 | 2.0930995701 | 1.6574361376 |
| H21 | 0.6185951521 | 2.3159447887 | -0.7001904732 |
| H22 | 1.9153617456 | 2.1994256023 | 0.5013310740 |
| H23 | 3.0808145712 | -0.1388187903 | 0.6604119536 |
| H24 | 3.1683741245 | -2.4948652614 | -0.1005953017 |
| H25 | 1.9988100002 | -2.1462360171 | -1.3788669733 |
| H26 | 4.7822217561 | -0.8910583568 | -1.0467154072 |
| H27 | 4.2910911307 | -1.9983647762 | -2.3251770589 |
| H28 | 4.2916497669 | 0.4592614401 | -3.0441198550 |
| H29 | 2.7368488892 | -0.3356286202 | -3.2670548842 |
| H30 | 2.3606470392 | 1.8554826567 | -2.2665001761 |
| H31 | 3.5486485891 | 1.5402197480 | -0.9838696041 |
| H32 | 0.2256200381 | -0.1002765117 | 2.8754177546 |
| H33 | 1.7531092940 | 0.6589671256 | 2.4418679065 |
| H34 | -0.6029845711 | -2.0885042715 | 1.5472780148 |
| H35 | 0.1063073175 | -2.5117003865 | -0.0149680933 |
| H36 | -1.6155112018 | 1.2309700492 | -0.1853717420 |
| H37 | -1.8672352862 | -0.0451781615 | 2.5896172009 |
| H38 | -2.4377036963 | 1.5387721127 | 2.0864145514 |
| H39 | -2.9191962346 | -2.1945296989 | 1.4589615930 |
| H40 | -4.2019596329 | -1.9687504099 | 0.2791370862 |
| H41 | -4.2726384230 | -0.2037340105 | 2.1188495712 |
| H42 | -4.0545089139 | 0.4980790350 | 0.5181048928 |
| H43 | -2.0169091710 | -2.3591747344 | -0.9019224078 |
| H44 | -2.7040502637 | -0.7855145406 | -1.2649406713 |
| C45 | -1.1119726820 | -2.7110524888 | -3.5427566747 |

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|-----|---------------|---------------|---------------|
| O46 | -1.2566684893 | -1.4114815637 | -3.6139937126 |
| O47 | -0.6151543930 | -3.2994551214 | -2.5786169637 |
| C48 | -1.6339575954 | -3.4781996441 | -4.7527061599 |
| H49 | -1.0975320218 | -3.1622158555 | -5.6543787170 |
| H50 | -1.5040180907 | -4.5517983058 | -4.6098802195 |
| H51 | -2.6927738281 | -3.2506582851 | -4.9129969632 |
| H52 | -0.7196500404 | -0.5064789099 | -4.6638409706 |
| O53 | 0.6182540610 | 0.6428150950 | -4.0617270687 |
| O54 | -0.1612856761 | 0.2607008555 | -5.0863970164 |

3_{sing}

Gas phase Energy: -1203.018442 hartrees

Solvation Energy: -0.00923847507 hartrees

Zero Point Energy: 297.131 kcal/mol

Free Energy: -31.917 kcal/mol

angstroms

| atom | x | y | z |
|------|---------------|---------------|---------------|
| Pd1 | 0.0676312813 | -0.3749440894 | -2.1007686939 |
| C2 | 1.2098810773 | -0.9588043193 | 1.1154344321 |
| C3 | 0.0603146106 | 1.2045653093 | 0.9151288866 |
| C4 | 1.0527255202 | 1.6237908602 | -0.1852353912 |
| N5 | 1.6639257336 | 0.4763336262 | -0.9200731679 |
| C6 | 2.2293395065 | -0.5449488081 | 0.0319441385 |
| C7 | 2.8567511123 | -1.7147131484 | -0.7367623616 |
| C8 | 4.0068063985 | -1.2160401838 | -1.6221198093 |
| C9 | 3.5082726200 | -0.1051124805 | -2.5533790413 |
| C10 | 2.7651833542 | 0.9989492531 | -1.7967188461 |
| C11 | 0.7974940800 | 0.2900076303 | 1.9060906059 |
| C12 | -0.0554910654 | -1.6873138323 | 0.6267984344 |
| N13 | -0.9522442263 | -0.8247250194 | -0.1943797482 |
| C14 | -1.2401540915 | 0.5252614906 | 0.4174995638 |
| C15 | -2.3070570859 | 0.4888267715 | 1.5380096129 |
| C16 | -3.2368108138 | -1.6379231299 | 0.6073837138 |
| C17 | -3.5887054854 | -0.2344481728 | 1.1088100791 |
| C18 | -2.2207684378 | -1.5492120129 | -0.5349233135 |
| H19 | 1.7379545416 | -1.6609074000 | 1.7728252226 |
| H20 | -0.2460113201 | 2.1330828696 | 1.4131509468 |
| H21 | 0.5768868280 | 2.2690773627 | -0.9294142451 |
| H22 | 1.8579847186 | 2.2062271378 | 0.2933094118 |
| H23 | 3.0464185753 | -0.0354460155 | 0.5753718137 |
| H24 | 3.2212699614 | -2.4483620280 | -0.0068059589 |
| H25 | 2.0957780533 | -2.2121659539 | -1.3505638813 |
| H26 | 4.8182190464 | -0.8384108603 | -0.9826065708 |
| H27 | 4.4247381378 | -2.0427753949 | -2.2068424572 |
| H28 | 4.3462588075 | 0.3631293907 | -3.0839337310 |
| H29 | 2.8426382218 | -0.5164714366 | -3.3165089501 |

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|-----|---------------|---------------|---------------|
| H30 | 2.3091507160 | 1.6856917608 | -2.5110403459 |
| H31 | 3.4626757578 | 1.5550137800 | -1.1481253584 |
| H32 | 0.1670494468 | 0.0238350067 | 2.7601147592 |
| H33 | 1.6793890349 | 0.8015745932 | 2.3102288770 |
| H34 | -0.5874577377 | -2.0567740761 | 1.5158745879 |
| H35 | 0.1879213797 | -2.5521230815 | 0.0043756866 |
| H36 | -1.6538983100 | 1.1214634061 | -0.4063759185 |
| H37 | -1.9082630207 | -0.0018529353 | 2.4336162721 |
| H38 | -2.5240914416 | 1.5256797740 | 1.8232687776 |
| H39 | -2.8532421749 | -2.2482404327 | 1.4358965281 |
| H40 | -4.1256548830 | -2.1561399390 | 0.2286967513 |
| H41 | -4.2969641553 | -0.2756907570 | 1.9441747043 |
| H42 | -4.0807843783 | 0.3275554091 | 0.3026759714 |
| H43 | -1.9239377270 | -2.5319390742 | -0.9043628121 |
| H44 | -2.6673605375 | -1.0171891481 | -1.3790375959 |
| C45 | -1.1429047559 | -2.5964989497 | -3.4623825754 |
| O46 | -1.3181165943 | -1.3035292377 | -3.3862382690 |
| O47 | -0.4865720597 | -3.2723022623 | -2.6622479409 |
| C48 | -1.8376451620 | -3.2437104183 | -4.6561154590 |
| H49 | -1.3058601168 | -2.9693465852 | -5.5739468125 |
| H50 | -1.8311386769 | -4.3298133993 | -4.5527709653 |
| H51 | -2.8641910373 | -2.8788677937 | -4.7536035036 |
| H52 | -0.7945788130 | 0.1163593599 | -4.6403226531 |
| O53 | 0.8708754418 | 0.2594223107 | -3.7977616938 |
| O54 | -0.2169839120 | 0.8927636560 | -4.4958279846 |

4

Gas phase Energy: -1052.639169 hartrees

Solvation Energy: -0.00440728495 hartrees

Zero Point Energy: 290.335 kcal/mol

Free Energy: -31.974 kcal/mol

| | angstroms | | |
|------|---------------|---------------|---------------|
| atom | x | y | z |
| Pd1 | 0.3393109360 | -0.5829105468 | -2.2949476951 |
| C2 | 1.1411814000 | -0.6819127445 | 1.3605218238 |
| C3 | -0.2247649018 | 1.2823774285 | 0.8208237923 |
| C4 | 0.7859774272 | 1.6794629351 | -0.2742218428 |
| N5 | 1.6089794155 | 0.5607334178 | -0.8212356628 |
| C6 | 2.1766726605 | -0.2858112508 | 0.2809906214 |
| C7 | 2.9566463564 | -1.4587353472 | -0.3242816672 |
| C8 | 4.1254672107 | -0.9457453601 | -1.1801236314 |
| C9 | 3.6296893541 | 0.0671263116 | -2.2225899772 |
| C10 | 2.7448298655 | 1.1436000493 | -1.5905610494 |
| C11 | 0.5439223227 | 0.5970768797 | 1.9597729921 |
| C12 | -0.0164152118 | -1.6056194282 | 0.9366891478 |
| N13 | -0.9438431680 | -0.9642046718 | 0.0014906664 |

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|-----|---------------|---------------|---------------|
| C14 | -1.4037457073 | 0.3952134706 | 0.3542710268 |
| C15 | -2.5689182051 | 0.4033984918 | 1.3779057420 |
| C16 | -3.2036916315 | -1.9161721746 | 0.6117648943 |
| C17 | -3.7229243620 | -0.5054431226 | 0.9248083280 |
| C18 | -2.0565524076 | -1.8329559521 | -0.4105076868 |
| H19 | 1.7102450959 | -1.2226461613 | 2.1285058289 |
| H20 | -0.6597352805 | 2.2259110094 | 1.1763222930 |
| H21 | 0.2807935083 | 2.1528899487 | -1.1204018590 |
| H22 | 1.4615920133 | 2.4316327743 | 0.1747925656 |
| H23 | 2.9105030271 | 0.3468570556 | 0.8197117670 |
| H24 | 3.3275089864 | -2.0987410830 | 0.4866853238 |
| H25 | 2.2743277296 | -2.0548780779 | -0.9436560264 |
| H26 | 4.8688300407 | -0.4690411035 | -0.5251822523 |
| H27 | 4.6340842464 | -1.7812487711 | -1.6749912486 |
| H28 | 4.4754177857 | 0.5549869055 | -2.7235289339 |
| H29 | 3.0370084397 | -0.4499657793 | -2.9870209482 |
| H30 | 2.3212615019 | 1.7922403401 | -2.3620510922 |
| H31 | 3.3503509940 | 1.7747331847 | -0.9120768853 |
| H32 | -0.1110862219 | 0.3614438909 | 2.8055056168 |
| H33 | 1.3338319908 | 1.2570155521 | 2.3408170116 |
| H34 | -0.5062539417 | -1.9475203430 | 1.8698961209 |
| H35 | 0.3698445325 | -2.5050162352 | 0.4429719138 |
| H36 | -1.7952065093 | 0.8209344649 | -0.5829839429 |
| H37 | -2.2153355201 | 0.0668967927 | 2.3612075257 |
| H38 | -2.9242575293 | 1.4339720105 | 1.5097894566 |
| H39 | -2.8576597916 | -2.3988089686 | 1.5362855445 |
| H40 | -4.0070805906 | -2.5470055173 | 0.2108689819 |
| H41 | -4.5076893167 | -0.5359132645 | 1.6904159232 |
| H42 | -4.1838609076 | -0.0839084393 | 0.0195710471 |
| H43 | -1.6477570060 | -2.8251041988 | -0.6302990151 |
| H44 | -2.4476048414 | -1.4401621641 | -1.3583098490 |
| C45 | -0.5880294261 | -1.2759812423 | -4.9537202970 |
| O46 | -0.9011711136 | -1.5731463656 | -3.7936393247 |
| O47 | 0.4055691058 | -0.4526792141 | -5.2191839409 |
| C48 | -1.3113834003 | -1.8203988530 | -6.1543901062 |
| H49 | -1.7600954522 | -0.9969874400 | -6.7186834923 |
| H50 | -0.6031095427 | -2.3235131891 | -6.8191325614 |
| H51 | -2.0871063264 | -2.5176424844 | -5.8381695406 |
| H52 | 0.7635501404 | -0.1957854874 | -4.2744533283 |

ζ_{trip}

Gas phase Energy: -1202.99324 hartrees

Solvation Energy: -0.01172931785 hartrees

Zero Point Energy: 294.834 kcal/mol

Free Energy: -34.806 kcal/mol

angstroms

| atom | x | y | z |
|------|---------------|---------------|---------------|
| Pd1 | 0.1234439256 | -0.6955385574 | -2.0245579469 |
| C2 | 1.2758892709 | -0.6083120201 | 1.4203061809 |
| C3 | -0.0838240805 | 1.3544960339 | 0.8529899031 |
| C4 | 0.8986560442 | 1.6913086976 | -0.2860519220 |
| N5 | 1.6740148224 | 0.5313802973 | -0.7944580793 |
| C6 | 2.2904088326 | -0.2635230884 | 0.3056736687 |
| C7 | 3.0352479363 | -1.4747345427 | -0.2704927504 |
| C8 | 4.1424701842 | -1.0245982304 | -1.2341358858 |
| C9 | 3.5582827406 | -0.1144616559 | -2.3213272042 |
| C10 | 2.7245227576 | 1.0231408838 | -1.7278506117 |
| C11 | 0.7121389841 | 0.6987418259 | 1.9914920392 |
| C12 | 0.0999008966 | -1.5292286320 | 1.0401841259 |
| N13 | -0.8638975718 | -0.9174318650 | 0.0902813564 |
| C14 | -1.2962385555 | 0.4720170990 | 0.4618954260 |
| C15 | -2.3879182663 | 0.5111207527 | 1.5604813098 |
| C16 | -3.0768300401 | -1.8276155178 | 0.9735629872 |
| C17 | -3.5770654710 | -0.4026849739 | 1.2364048418 |
| C18 | -2.0329904597 | -1.8096108027 | -0.1504263050 |
| H19 | 1.8448493568 | -1.1403555574 | 2.1938894536 |
| H20 | -0.4973346786 | 2.3144999756 | 1.1877737681 |
| H21 | 0.3770775158 | 2.1330932082 | -1.1410002728 |
| H22 | 1.5975449686 | 2.4556816749 | 0.1013904964 |
| H23 | 3.0500611289 | 0.3792785791 | 0.7949031532 |
| H24 | 3.4552019714 | -2.0586210443 | 0.5585456276 |
| H25 | 2.3229576202 | -2.1181141917 | -0.8032026052 |
| H26 | 4.9139538002 | -0.4830931284 | -0.6677131392 |
| H27 | 4.6353042595 | -1.8942985645 | -1.6837462099 |
| H28 | 4.3561244151 | 0.3263680070 | -2.9306840670 |
| H29 | 2.9230301953 | -0.6929506873 | -2.9991136941 |
| H30 | 2.2194786157 | 1.5576903340 | -2.5369429733 |
| H31 | 3.3790114833 | 1.7270979590 | -1.1805691517 |
| H32 | 0.0873861285 | 0.5072129005 | 2.8699580144 |
| H33 | 1.5242580872 | 1.3603550864 | 2.3168636449 |
| H34 | -0.3985731872 | -1.8185608235 | 1.9801235598 |
| H35 | 0.4597096746 | -2.4525077395 | 0.5757996859 |
| H36 | -1.7431591098 | 0.8840127857 | -0.4530037655 |
| H37 | -1.9697171140 | 0.2144771008 | 2.5300439923 |
| H38 | -2.7202589071 | 1.5508546366 | 1.6715379571 |
| H39 | -2.6590710432 | -2.2540065718 | 1.8954172882 |
| H40 | -3.9011206887 | -2.4851980093 | 0.6721702239 |
| H41 | -4.3052759183 | -0.3830954843 | 2.0555133804 |
| H42 | -4.0970549812 | -0.0306763538 | 0.3420982031 |
| H43 | -1.6410183457 | -2.8103225531 | -0.3538227697 |
| H44 | -2.5082457190 | -1.4762444468 | -1.0768741808 |
| C45 | -1.7060185069 | -2.1555518040 | -4.3955857727 |

| | | | |
|-----|---------------|---------------|---------------|
| O46 | -1.5047665223 | -2.0375747914 | -3.1795826003 |
| O47 | -1.0068481873 | -1.5701067622 | -5.3336857646 |
| C48 | -2.8243925993 | -3.0219124937 | -4.9316362918 |
| H49 | -3.5147406167 | -2.4069511788 | -5.5174052939 |
| H50 | -2.4125454143 | -3.7777059991 | -5.6071826245 |
| H51 | -3.3582937205 | -3.5038759293 | -4.1128375350 |
| H52 | -0.2646838998 | -0.9714202213 | -4.9148882407 |
| O53 | 0.6831145510 | -0.2323382574 | -4.0663875888 |
| O54 | 1.0282276179 | 1.0075581193 | -4.3817422276 |

ϕ_{sing}

Gas phase Energy: -1202.993871 hartrees

Solvation Energy: -0.0142512133 hartrees

Zero Point Energy: 296.388 kcal/mol

Free Energy: -32.374 kcal/mol

angstroms

| atom | x | y | z |
|------|---------------|---------------|---------------|
| Pd1 | 0.1032343452 | -0.7194734063 | -2.0194448527 |
| C2 | 1.2603239819 | -0.6406168084 | 1.3144882112 |
| C3 | -0.0849844905 | 1.3196605167 | 0.6855101537 |
| C4 | 0.8940905015 | 1.6240400557 | -0.4636467671 |
| N5 | 1.6553330380 | 0.4312162119 | -0.9348445092 |
| C6 | 2.2720791232 | -0.3407374308 | 0.1891146747 |
| C7 | 3.0163784179 | -1.5687199661 | -0.3512204647 |
| C8 | 4.1341288896 | -1.1468941802 | -1.3161651532 |
| C9 | 3.5648210861 | -0.2575941905 | -2.4288850844 |
| C10 | 2.7313185989 | 0.8968405291 | -1.8723753813 |
| C11 | 0.7048904551 | 0.6886731423 | 1.8434585688 |
| C12 | 0.0874380951 | -1.5670170908 | 0.9494382405 |
| N13 | -0.8634146996 | -0.9770165552 | -0.0343662098 |
| C14 | -1.3001997909 | 0.4304993775 | 0.3148728273 |
| C15 | -2.3850760685 | 0.4854887095 | 1.4174417520 |
| C16 | -3.0696692468 | -1.8645095437 | 0.8979308089 |
| C17 | -3.5745100277 | -0.4362107527 | 1.1245045506 |
| C18 | -2.0429243156 | -1.8780774624 | -0.2384829292 |
| H19 | 1.8236807691 | -1.1539554987 | 2.1042211888 |
| H20 | -0.4986901399 | 2.2876986873 | 0.9942297338 |
| H21 | 0.3931320953 | 2.0265351077 | -1.3518262316 |
| H22 | 1.6088003810 | 2.3821766191 | -0.1019265965 |
| H23 | 3.0301282700 | 0.3217317326 | 0.6465251162 |
| H24 | 3.4267379337 | -2.1316112548 | 0.4967748978 |
| H25 | 2.3083389586 | -2.2261409712 | -0.8718674940 |
| H26 | 4.9044053363 | -0.5982622881 | -0.7552673675 |
| H27 | 4.6241796843 | -2.0303978563 | -1.7408468654 |
| H28 | 4.3725850947 | 0.1687977494 | -3.0354622510 |
| H29 | 2.9395291140 | -0.8462525928 | -3.1057681396 |

| | | | |
|-----|---------------|---------------|---------------|
| H30 | 2.2216234962 | 1.4460329643 | -2.6693136378 |
| H31 | 3.3775849667 | 1.5894026687 | -1.3060991771 |
| H32 | 0.0808298124 | 0.5287539765 | 2.7284736839 |
| H33 | 1.5229291458 | 1.3518739388 | 2.1487265301 |
| H34 | -0.4383416471 | -1.8181015357 | 1.8822031171 |
| H35 | 0.4434802580 | -2.5071019590 | 0.5184345094 |
| H36 | -1.7503896601 | 0.8187538615 | -0.6068993577 |
| H37 | -1.9609295174 | 0.2150148895 | 2.3916065957 |
| H38 | -2.7154398866 | 1.5277817581 | 1.5025668841 |
| H39 | -2.6464620249 | -2.2665353514 | 1.8280474193 |
| H40 | -3.8916612090 | -2.5335041116 | 0.6173446049 |
| H41 | -4.2955254416 | -0.3971022087 | 1.9488107246 |
| H42 | -4.1014587415 | -0.0895474927 | 0.2247696639 |
| H43 | -1.6502495830 | -2.8808532973 | -0.4240894234 |
| H44 | -2.5229225125 | -1.5670406919 | -1.1677365035 |
| C45 | -1.4763741984 | -2.0107616364 | -4.2571730749 |
| O46 | -1.2849547912 | -2.0000819304 | -2.9854600646 |
| O47 | -0.8756410413 | -1.3048293941 | -5.0974789404 |
| C48 | -2.5522313430 | -2.9631640088 | -4.7578118839 |
| H49 | -3.4255389203 | -2.3778613097 | -5.0652562196 |
| H50 | -2.1870695656 | -3.4916271157 | -5.6420681291 |
| H51 | -2.8506929216 | -3.6752449488 | -3.9871917257 |
| H52 | 0.0896103426 | -0.4258892423 | -4.4302871155 |
| O53 | 0.7757717912 | 0.0259374541 | -3.7848617738 |
| O54 | 0.3666327090 | 1.3819799555 | -3.6663727302 |

TS2-3

Gas phase Energy: -1202.949641 hartrees

Solvation Energy: -0.01103253135 hartrees

Zero Point Energy: 287.96 kcal/mol

Free Energy: -31.088 kcal/mol

| | angstroms | | |
|------|---------------|---------------|---------------|
| atom | x | y | z |
| Pd1 | 0.1140286634 | -0.3763248382 | -2.2916097402 |
| C2 | 1.1970066546 | -0.9922016941 | 0.9870392726 |
| C3 | -0.0293284939 | 1.1323147375 | 0.8380079297 |
| C4 | 0.9425241645 | 1.6109655725 | -0.2583614183 |
| N5 | 1.6159099732 | 0.5125279231 | -1.0170251970 |
| C6 | 2.2016737969 | -0.5207596479 | -0.0889858729 |
| C7 | 2.8581531733 | -1.6469662291 | -0.8990313028 |
| C8 | 3.9967160778 | -1.0917738540 | -1.7678484540 |
| C9 | 3.4857034850 | 0.0541397706 | -2.6500386956 |
| C10 | 2.7200516274 | 1.1036666952 | -1.8399022248 |
| C11 | 0.7464981657 | 0.2253117571 | 1.8052726368 |
| C12 | -0.0517325689 | -1.7524931665 | 0.4996545591 |
| N13 | -0.9823180593 | -0.9038574248 | -0.2814999899 |

| | | | |
|-----|---------------|---------------|---------------|
| C14 | -1.3093100920 | 0.4186867151 | 0.3360557772 |
| C15 | -2.3826049408 | 0.3296533273 | 1.4480265823 |
| C16 | -3.2502481046 | -1.7964389722 | 0.4297923047 |
| C17 | -3.6378427585 | -0.4166670097 | 0.9746123136 |
| C18 | -2.2079170820 | -1.6464563325 | -0.6847915722 |
| H19 | 1.7548804810 | -1.6871690678 | 1.6273183052 |
| H20 | -0.3611003264 | 2.0410646512 | 1.3561710829 |
| H21 | 0.4337927350 | 2.2455068539 | -0.9903614871 |
| H22 | 1.7169579926 | 2.2256948633 | 0.2307004474 |
| H23 | 3.0062091864 | -0.0079076156 | 0.4701323216 |
| H24 | 3.2434635007 | -2.3980222219 | -0.1983734093 |
| H25 | 2.1087653376 | -2.1417580460 | -1.5296500706 |
| H26 | 4.8049957265 | -0.7278255340 | -1.1174582017 |
| H27 | 4.4250219587 | -1.8855858063 | -2.3893409642 |
| H28 | 4.3153997203 | 0.5580312564 | -3.1591968621 |
| H29 | 2.8317481179 | -0.3462691170 | -3.4306429827 |
| H30 | 2.2789588376 | 1.8463779677 | -2.5094909059 |
| H31 | 3.4111433222 | 1.6251650538 | -1.1557653118 |
| H32 | 0.1284866170 | -0.0818737083 | 2.6547069005 |
| H33 | 1.6113968121 | 0.7595728643 | 2.2173821908 |
| H34 | -0.5451379218 | -2.1712414910 | 1.3920972518 |
| H35 | 0.2184214736 | -2.5932350660 | -0.1457539589 |
| H36 | -1.7410901109 | 1.0159649993 | -0.4792289830 |
| H37 | -1.9793622269 | -0.1782643748 | 2.3326805172 |
| H38 | -2.6360421535 | 1.3499515485 | 1.7624848824 |
| H39 | -2.8665832812 | -2.4265367649 | 1.2435663192 |
| H40 | -4.1245282875 | -2.3163939552 | 0.0204226815 |
| H41 | -4.3590163518 | -0.5032978053 | 1.7954136709 |
| H42 | -4.1312701568 | 0.1605474287 | 0.1797607569 |
| H43 | -1.8799032128 | -2.6119226184 | -1.0764242286 |
| H44 | -2.6482877490 | -1.1025446555 | -1.5266235553 |
| C45 | -1.0900136458 | -2.4655436749 | -3.7219292832 |
| O46 | -1.2577100056 | -1.1794652214 | -3.6140199088 |
| O47 | -0.3131545087 | -3.1384591456 | -3.0283574602 |
| C48 | -1.9506172426 | -3.1155568154 | -4.8002053555 |
| H49 | -1.6234434928 | -2.7703996136 | -5.7867857043 |
| H50 | -1.8627801156 | -4.2018175831 | -4.7502105540 |
| H51 | -2.9968828808 | -2.8166211976 | -4.6864877937 |
| H52 | 0.7017068791 | 0.2898484771 | -3.6771848775 |
| O53 | 0.9218601330 | 0.8225583320 | -4.8805620575 |
| O54 | 1.6850299162 | 1.8318350220 | -4.8348138084 |

TS1-4

Gas phase Energy: -1052.635561 hartrees

Solvation Energy: -0.00617678318 hartrees

Zero Point Energy: 290.803 kcal/mol

Free Energy: -34.921 kcal/mol

| | angstroms | | |
|------|---------------|---------------|---------------|
| atom | x | y | z |
| Pd1 | 0.2678281273 | -0.5733206202 | -2.2427294652 |
| C2 | 1.1646353079 | -0.6883394408 | 1.3066817586 |
| C3 | -0.2024744799 | 1.2827718336 | 0.7917647527 |
| C4 | 0.8022714680 | 1.6845533607 | -0.3073487286 |
| N5 | 1.6086035255 | 0.5608334868 | -0.8717689333 |
| C6 | 2.1937696273 | -0.2864114070 | 0.2219475820 |
| C7 | 2.9771747921 | -1.4541850187 | -0.3895835807 |
| C8 | 4.1297543588 | -0.9354229252 | -1.2638157098 |
| C9 | 3.6104833931 | 0.0625774949 | -2.3088986154 |
| C10 | 2.7285762832 | 1.1386255027 | -1.6725296683 |
| C11 | 0.5733866520 | 0.5872891430 | 1.9196888533 |
| C12 | 0.0008401388 | -1.6069500992 | 0.8860024887 |
| N13 | -0.9349192578 | -0.9593482830 | -0.0435528525 |
| C14 | -1.3896198942 | 0.4030907065 | 0.3281054675 |
| C15 | -2.5446889447 | 0.4033849382 | 1.3606048551 |
| C16 | -3.1949390293 | -1.9078395006 | 0.5881132560 |
| C17 | -3.7056837776 | -0.4956262616 | 0.9067771369 |
| C18 | -2.0589804319 | -1.8287912418 | -0.4443179553 |
| H19 | 1.7374868385 | -1.2362855099 | 2.0663563301 |
| H20 | -0.6323080826 | 2.2247965139 | 1.1566999887 |
| H21 | 0.2952971428 | 2.1721223774 | -1.1444932555 |
| H22 | 1.4906642525 | 2.4241657717 | 0.1413372241 |
| H23 | 2.9271678488 | 0.3506755417 | 0.7545909227 |
| H24 | 3.3648258773 | -2.0848717902 | 0.4205685187 |
| H25 | 2.2955934426 | -2.0644401131 | -0.9951013286 |
| H26 | 4.8753258268 | -0.4449273669 | -0.6217592367 |
| H27 | 4.6414291880 | -1.7695358543 | -1.7572450959 |
| H28 | 4.4453436903 | 0.5553957591 | -2.8223863969 |
| H29 | 3.0211447280 | -0.4649852191 | -3.0665832704 |
| H30 | 2.2865392307 | 1.7766316173 | -2.4422319327 |
| H31 | 3.3408646300 | 1.7792209291 | -1.0106100781 |
| H32 | -0.0754215772 | 0.3464629513 | 2.7685052949 |
| H33 | 1.3669418665 | 1.2432978795 | 2.2992834499 |
| H34 | -0.4892661892 | -1.9465304950 | 1.8178769241 |
| H35 | 0.3787733399 | -2.5065750985 | 0.3872781523 |
| H36 | -1.7890955354 | 0.8372242971 | -0.6011497500 |
| H37 | -2.1852736696 | 0.0564646661 | 2.3379938259 |
| H38 | -2.8932041105 | 1.4345301235 | 1.5036172118 |
| H39 | -2.8453251694 | -2.3945101208 | 1.5089873645 |
| H40 | -4.0026527403 | -2.5340701870 | 0.1895599601 |
| H41 | -4.4882409040 | -0.5239149285 | 1.6742806147 |
| H42 | -4.1657673844 | -0.0680218204 | 0.0041188972 |
| H43 | -1.6519664424 | -2.8202788867 | -0.6683857660 |

| | | | |
|-----|---------------|---------------|---------------|
| H44 | -2.4566435627 | -1.4364091955 | -1.3883700789 |
| C45 | -0.5019050002 | -1.2590420411 | -4.8765188136 |
| O46 | -0.9684785797 | -1.5283773752 | -3.7373307795 |
| O47 | 0.5422075710 | -0.5331327901 | -5.0500114855 |
| C48 | -1.1847791199 | -1.7922969143 | -6.1154554325 |
| H49 | -1.5812668955 | -0.9543790916 | -6.6976728190 |
| H50 | -0.4547508240 | -2.3071188311 | -6.7460413502 |
| H51 | -1.9966306478 | -2.4706315938 | -5.8518366802 |
| H52 | 0.8265463263 | -0.2738384629 | -3.8101833035 |