Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Supplementary Information: A Computational Study on the Reduction of O_2 to H_2O_2 using Small Polycyclic Aromatic Molecules

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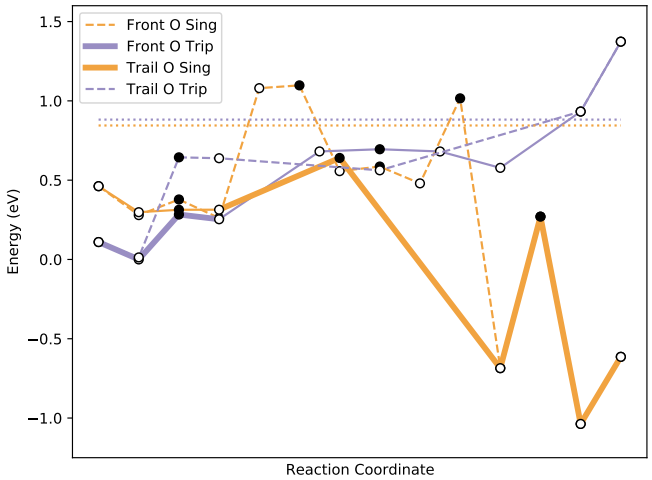

Figure 1: Reaction pathways calculated for the two types of transit across AHQ: with the front oxygen atom hydrogenated, and the training oxygen hydrogenated. This is a reproduction of the figure included in the main paper document with two extra pathways for completeness. The most favourable pathway is in bold.

Table 1: Summary of convergence test results.

		Monkhorst-Pack Grid		
		$1 \times 1 \times 1$	$2 \times 2 \times 1$	$3 \times 3 \times 1$
Grid Spacing	0.202	-0.245	-0.135	-0.165
	0.176	-0.238	**-0.154**	-0.191
	0.160	-0.239	-0.154	-0.185

Convergence Test

A convergence test was performed using $\vec{k}$-points and grid spacing on the adsorption energy of an oxygen molecule onto a functionalized graphene surface. The work presented in this manuscript is a part of a larger research program examining H_2O_2 synthesis on a variety of 1D and 2D carbon surfaces. To compare between systems, similar cells, grid spacings and $\vec{k}$-point meshes are used. The results of the convergence test are summarized in Table 1. We use a grid spacing of 0.176 and a Monkhorst-Pack grid of $2 \times 2 \times 1$ as a suitable compromise between accuracy and efficiency.

Molecular Positions for the AHQ Pathway

Trail O Sing Path: O2 Separated From AHQ Singlet (white point 1)
Absolute Energy: -187.47912176642373 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.83143082 7.42774826 9.69698669] 0.0
C [10.52513291 8.61609213 9.68260925] 0.0
C [9.82802662 9.84973101 9.62742606] 0.0
C [7.6656492 6.19491998 9.69457507] 0.0
C [8.40742362 7.39604665 9.65538414] 0.0
C [7.70399683 8.65514654 9.57679456] 0.0
C [8.4537582 9.86557091 9.57275959] 0.0
C [5.50388419 4.99874592 9.69253173] 0.0
C [6.25623751 6.20632375 9.6432606] 0.0
C [5.5538179 7.46373611 9.54090297] 0.0
C [6.29445078 8.66568781 9.51556172] 0.0
C [4.12987423 5.01416881 9.63591693] 0.0

C [3.43530443 6.24535728 9.52446382] 0.0
C [4.13083486 7.43209644 9.4787241] 0.0
O [1.66494123 12.79276933 11.34644863] 0.0
O [0.96472035 13.80262813 11.47110216] 0.0
O [8.26206056 4.9678303 9.78488057] 0.0
H [9.22353612 5.08786933 9.86211505] 0.0
O [5.69795888 9.89176523 9.43312284] 0.0
H [4.73244958 9.78254233 9.45581074] 0.0
H [7.91255481 10.80950662 9.52736197] 0.0
H [10.38716267 10.78596051 9.62955149] 0.0
H [11.61498457 8.61042491 9.71765228] 0.0
H [10.40751791 6.49862213 9.73765832] 0.0
H [3.55707089 8.3589311 9.38930975] 0.0
H [2.34596617 6.25172817 9.47470449] 0.0
H [3.57157631 4.07799525 9.67487312] 0.0
H [6.04275321 4.05591859 9.77625272] 0.0

Trail O Sing Path: O2 Hydrogen Bond On Top of AHQ Singlet (white point 2)
Absolute Energy: -187.64306213271695 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.90461906 7.4088747 9.72694113] 0.0
C [10.5311231 8.63415795 9.78923458] 0.0
C [9.76453028 9.82386376 9.82053878] 0.0
C [7.81002589 6.06187808 9.63872597] 0.0
C [8.48595412 7.30528117 9.69227514] 0.0
C [7.7113516 8.51994774 9.72085844] 0.0
C [8.38860245 9.76571219 9.78889371] 0.0
C [5.72180384 4.7441729 9.4579958] 0.0
C [6.40065997 5.9901444 9.55090713] 0.0
C [5.63387534 7.20630308 9.54107257] 0.0
C [6.29420235 8.45747669 9.6748326] 0.0
C [4.35108105 4.6990905 9.32824583] 0.0
C [3.59920566 5.89779823 9.27770846] 0.0
C [4.22595815 7.12066657 9.38494454] 0.0
O [4.51022272 9.38267464 12.06209375] 0.0
O [5.33083231 8.50768036 12.44299612] 0.0

O [8.47779871 4.87603504 9.65383024] 0.0
H [9.42775036 5.04639487 9.77698206] 0.0
O [5.59671391 9.61657909 9.67793143] 0.0
H [4.97812997 9.63307049 10.4713225] 0.0
H [7.78631866 10.67298887 9.80874487] 0.0
H [10.26997116 10.78907477 9.86947422] 0.0
H [11.61986901 8.68879731 9.81327675] 0.0
H [10.53497457 6.51506508 9.69263222] 0.0
H [3.64891152 8.04347869 9.33290719] 0.0
H [2.51734695 5.85201961 9.14637143] 0.0
H [3.8433635 3.73652519 9.25426124] 0.0
H [6.30658761 3.82585702 9.48494451] 0.0

Trail O Sing Path: Transition State for First Hydrogen Transfer Singlet (black point 1)
Absolute Energy: -187.62779484583442 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.87212416 7.44169851 9.7764098] 0.0
C [10.50584962 8.67096135 9.81488768] 0.0
C [9.75059333 9.85929179 9.8038711] 0.0
C [7.76868487 6.10133596 9.6847324] 0.0
C [8.45763695 7.34888141 9.72076019] 0.0
C [7.69977483 8.56091921 9.69870005] 0.0
C [8.36688763 9.79666545 9.74515055] 0.0
C [5.67924676 4.78011808 9.50166876] 0.0
C [6.35171576 6.02674495 9.5717445] 0.0
C [5.58759157 7.23171149 9.52217691] 0.0
C [6.24147845 8.53341406 9.62190883] 0.0
C [4.30277172 4.73397039 9.37744568] 0.0
C [3.55238825 5.92438361 9.31311273] 0.0
C [4.19059459 7.15274568 9.38502413] 0.0
O [4.52902626 9.75177464 11.86268298] 0.0
O [5.21533985 8.75938292 12.40221193] 0.0
O [8.43129194 4.91986203 9.74345649] 0.0
H [9.38310164 5.09042911 9.85829165] 0.0
O [5.57609349 9.61540887 9.60467169] 0.0
H [4.88744347 9.8050218 10.87002086] 0.0

H [7.75794968 10.70060525 9.73085949] 0.0
H [10.25673543 10.8242582 9.83812666] 0.0
H [11.59458925 8.71708729 9.85200031] 0.0
H [10.49952899 6.54504916 9.77794286] 0.0
H [3.62659781 8.08413028 9.33865456] 0.0
H [2.4678966 5.87776449 9.20725936] 0.0
H [3.79665441 3.76932103 9.32320407] 0.0
H [6.26098667 3.86050495 9.54504231] 0.0

Trail O Sing Path: HOO Hydrogen Bond On Top of AHQ Singlet (white point 3)
Absolute Energy: -187.6273186676664 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.85543226 7.46070543 9.78543143] 0.0
C [10.49430266 8.68751259 9.81415499] 0.0
C [9.74392668 9.8778774 9.78550516] 0.0
C [7.74924674 6.12542355 9.69843163] 0.0
C [8.44103212 7.37196226 9.72531114] 0.0
C [7.68655993 8.58637725 9.6910277] 0.0
C [8.36037206 9.81892262 9.72362202] 0.0
C [5.65481197 4.8085238 9.54347359] 0.0
C [6.33139962 6.05387572 9.59408307] 0.0
C [5.57048656 7.26099555 9.54157941] 0.0
C [6.22667435 8.56332787 9.6204432] 0.0
C [4.27689881 4.76587985 9.43310586] 0.0
C [3.52909712 5.95784559 9.36934405] 0.0
C [4.17214154 7.18437582 9.42186656] 0.0
O [4.47976805 9.9247911 11.8467437] 0.0
O [5.04472106 8.88742255 12.44231461] 0.0
O [8.40821079 4.94237097 9.75917956] 0.0
H [9.36202045 5.10950679 9.86057332] 0.0
O [5.56385884 9.64509034 9.5959048] 0.0
H [4.86476701 9.90794225 10.87047697] 0.0
H [7.75525701 10.72473489 9.69824185] 0.0
H [10.25297172 10.84139089 9.80998913] 0.0
H [11.58275558 8.7291107 9.8591421] 0.0
H [10.48034806 6.56206744 9.80492747] 0.0

H [3.61030468 8.11693281 9.37638104] 0.0
H [2.44344498 5.91465464 9.27790707] 0.0
H [3.76878538 3.8016617 9.39440078] 0.0
H [6.23443394 3.88758121 9.59253642] 0.0

Trail O Sing Path: Transition State for HOO Transfer Across AHQ Singlet (black point 2)
Absolute Energy: -187.30098385190635 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.88016436 7.53849917 9.79115876] 0.0
C [10.53351842 8.75581095 9.67504889] 0.0
C [9.79749593 9.94115495 9.51302769] 0.0
C [7.75556464 6.23010874 9.87063806] 0.0
C [8.46778514 7.46451288 9.74259206] 0.0
C [7.73052357 8.67274581 9.57363013] 0.0
C [8.40929412 9.89213818 9.46748311] 0.0
C [5.6765275 4.89652302 9.62201437] 0.0
C [6.34825583 6.14224084 9.64831066] 0.0
C [5.60059449 7.33807233 9.45415505] 0.0
C [6.25368661 8.65965271 9.54263835] 0.0
C [4.31303389 4.84475152 9.382025] 0.0
C [3.57923556 6.0268231 9.17480886] 0.0
C [4.2201784 7.259055 9.22302812] 0.0
O [5.60740145 7.8663809 12.72253057] 0.0
O [6.90043733 7.60197405 12.43638689] 0.0
O [8.39306841 5.06925708 10.13504872] 0.0
H [9.32474324 5.25535286 10.35144076] 0.0
O [5.58911858 9.70970508 9.60745707] 0.0
H [5.30723048 8.47256913 11.99978418] 0.0
H [7.81066343 10.79648156 9.352483] 0.0
H [10.31650522 10.89562818 9.4218753] 0.0
H [11.62283375 8.78958226 9.70622237] 0.0
H [10.49167094 6.63784177 9.89926297] 0.0
H [3.67479953 8.19300072 9.08116839] 0.0
H [2.50745063 5.97473176 8.97947299] 0.0
H [3.80818269 3.87829279 9.35148395] 0.0
H [6.24474495 3.98207904 9.78589645] 0.0

Trail O Sing Path: HOO Bound to Carbon 10 Anthracene Moiety Singlet (white point 4)
Absolute Energy: -188.62651577256742 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.81736693 7.68222538 9.90827777] 0.0
C [10.4870229 8.85570552 9.55919158] 0.0
C [9.76621826 10.01473108 9.25582099] 0.0
C [7.68859876 6.39034693 10.40698449] 0.0
C [8.42146483 7.64755463 9.9437327] 0.0
C [7.69649553 8.8095677 9.62023446] 0.0
C [8.37618418 9.98859517 9.28459964] 0.0
C [5.62060903 5.05839527 9.81727131] 0.0
C [6.26459698 6.29777146 9.89095968] 0.0
C [5.55023618 7.46677409 9.56676374] 0.0
C [6.20820646 8.80285339 9.56087442] 0.0
C [4.28298112 4.98278629 9.42643066] 0.0
C [3.56911669 6.14478854 9.11573504] 0.0
C [4.20266535 7.38095892 9.18685843] 0.0
O [7.00606757 5.55305185 12.55976164] 0.0
O [7.71695775 6.62514517 11.85142674] 0.0
O [8.34993982 5.18890173 10.09707695] 0.0
H [9.09450658 5.10538033 10.71929412] 0.0
O [5.56093857 9.8424303 9.44101174] 0.0
H [6.14560433 5.99011574 12.72293825] 0.0
H [7.78314712 10.87141936 9.0431239] 0.0
H [10.29382952 10.93145183 8.9896707] 0.0
H [11.57727439 8.86604224 9.52399565] 0.0
H [10.39497334 6.78663969 10.13839601] 0.0
H [3.68106084 8.30583191 8.93741903] 0.0
H [2.52412208 6.07927961 8.80831211] 0.0
H [3.794789 4.00912948 9.36314682] 0.0
H [6.17926488 4.15791758 10.06531556] 0.0

Trail O Sing Path: Transition State for Second Hydrogen Transfer Singlet (black point 3)
Absolute Energy: -187.6711711440464 eV

Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.89700067 7.28777862 9.81674465] 0.0
C [10.56907627 8.50418907 9.84246562] 0.0
C [9.85328693 9.70808444 9.89260303] 0.0
C [7.77782225 5.9795994 9.82322697] 0.0
C [8.49099963 7.24991908 9.84464745] 0.0
C [7.77011317 8.46911474 9.88749508] 0.0
C [8.46256139 9.68600527 9.91451276] 0.0
C [5.64309289 4.74574816 9.54595943] 0.0
C [6.32899221 5.96556778 9.69437237] 0.0
C [5.59593325 7.17619401 9.7339566] 0.0
C [6.28481386 8.48649923 9.87599479] 0.0
C [4.25779182 4.73261257 9.43466165] 0.0
C [3.53382563 5.93160253 9.48087389] 0.0
C [4.20111028 7.14415474 9.63352384] 0.0
O [9.18118811 6.06498348 12.77871226] 0.0
O [8.35340098 5.36989711 11.88405294] 0.0
O [8.42957602 4.83106804 9.65010842] 0.0
H [8.85721059 4.7728583 10.6177046] 0.0
O [5.64846864 9.53948939 9.96066176] 0.0
H [8.62297025 6.11318261 13.58221191] 0.0
H [7.87713416 10.60549826 9.94621441] 0.0
H [10.38583345 10.65969702 9.91199882] 0.0
H [11.65948094 8.51975807 9.82172402] 0.0
H [10.45237531 6.35170488 9.76797217] 0.0
H [3.66258609 8.09156356 9.67450755] 0.0
H [2.44635526 5.91392119 9.39750775] 0.0
H [3.73270904 3.78377167 9.31716294] 0.0
H [6.21844913 3.8214985 9.52079227] 0.0

Trail O Sing Path: H2O2 Hydrogen Bound to AQ Singlet (white point 5)
Absolute Energy: -188.97807439705798 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.66608052 7.56310641 9.8708669] 0.0
C [10.34761065 8.77332915 9.78841139] 0.0
C [9.65415393 9.95203848 9.48470727] 0.0

C [7.57058645 6.22390235 9.77643963] 0.0
C [8.28418285 7.51696697 9.64267231] 0.0
C [7.58725615 8.70259933 9.32958473] 0.0
C [8.28127139 9.91637649 9.25814598] 0.0
C [5.43889356 4.97197859 9.47000939] 0.0
C [6.1229174 6.19494828 9.44748619] 0.0
C [5.42662331 7.37791567 9.12524594] 0.0
C [6.11812532 8.69720621 9.09523692] 0.0
C [4.08050294 4.92298446 9.17089774] 0.0
C [3.38809882 6.09958734 8.8560204] 0.0
C [4.05794256 7.3198696 8.83659458] 0.0
O [7.70308713 6.85705236 12.77238294] 0.0
O [8.27187209 5.52447406 12.93967017] 0.0
O [8.156827 5.19689732 10.15002889] 0.0
H [8.34302535 5.2463753 11.99125537] 0.0
O [5.49641543 9.73884427 8.8870504] 0.0
H [6.80164093 6.70973699 13.12005998] 0.0
H [7.71826344 10.82130804 9.02783711] 0.0
H [10.18930537 10.90103219 9.42972651] 0.0
H [11.42213229 8.80828926 9.96987896] 0.0
H [10.1811898 6.63700113 10.12514303] 0.0
H [3.54301153 8.25067929 8.59713114] 0.0
H [2.323225 6.05899236 8.62383189] 0.0
H [3.55392172 3.96799967 9.18535452] 0.0
H [5.9981256 4.07123496 9.72351059] 0.0

Trail O Sing Path: H2O2 Separated from AQ Singlet (white point 6)
Absolute Energy: -188.5550938785082 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.85204021 7.41238186 9.83491535] 0.0
C [10.51677877 8.6354956 9.82515119] 0.0
C [9.7887239 9.8307582 9.74700245] 0.0
C [7.77052749 6.04367526 9.7651896] 0.0
C [8.45321193 7.36909223 9.76266186] 0.0
C [7.7205342 8.57184214 9.68606058] 0.0
C [8.39829395 9.79845975 9.68208556] 0.0
C [5.60812995 4.81166644 9.58600938] 0.0

C [6.28473991 6.03805476 9.63868233] 0.0
C [5.55318807 7.2420735 9.56328949] 0.0
C [6.23244953 8.56763556 9.60560369] 0.0
C [4.22237162 4.78098635 9.45584229] 0.0
C [3.49696463 5.97689892 9.38049444] 0.0
C [4.15886611 7.1997183 9.43631732] 0.0
O [13.36890571 -0.06560528 12.84436315] 0.0
O [12.17444118 0.45578 12.17856] 0.0
O [8.41095781 4.99705398 9.8573613] 0.0
H [12.37456441 0.21613671 11.25313378] 0.0
O [5.59144313 9.6179317 9.56519265] 0.0
H [12.9700177 -0.78204342 13.37610383] 0.0
H [7.80833761 10.71401616 9.62408462] 0.0
H [10.31165265 10.78858118 9.73683992] 0.0
H [11.60634864 8.66414607 9.87833384] 0.0
H [10.39414319 6.46825414 9.89682828] 0.0
H [3.61786279 8.14482982 9.38016085] 0.0
H [2.41141013 5.94873532 9.27637523] 0.0
H [3.69894815 3.82500487 9.41254521] 0.0
H [6.19447907 3.89471102 9.64975028] 0.0

Front O Trip Path: O2 Separated from AHQ Triplet (white point 1)
Absolute Energy: -187.83132749490233 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.8313581 7.42773251 9.69703866] 0.0
C [10.52498075 8.61560917 9.68300747] 0.0
C [9.8275356 9.84967488 9.62789904] 0.0
C [7.66563894 6.19470864 9.69435256] 0.0
C [8.40668087 7.39543506 9.65521771] 0.0
C [7.70297178 8.65510036 9.57676209] 0.0
C [8.45371986 9.86563798 9.57306936] 0.0
C [5.50433052 4.99846378 9.69232293] 0.0
C [6.25709547 6.20654626 9.64316381] 0.0
C [5.55427342 7.46438182 9.54105865] 0.0
C [6.2942981 8.66598977 9.51551853] 0.0
C [4.13079005 5.01306191 9.63522335] 0.0
C [3.43554665 6.24456671 9.52450961] 0.0

C [4.13055837 7.43117287 9.47967365] 0.0
O [1.6652279 12.79768297 11.34689178] 1.0
O [0.9648356 13.80007178 11.4720894] 1.0
O [8.26320559 4.96657889 9.78488273] 0.0
H [9.224381 5.08842091 9.86226569] 0.0
O [5.69610367 9.89331286 9.43331621] 0.0
H [4.73108221 9.78076869 9.45460444] 0.0
H [7.91265101 10.80968086 9.52762706] 0.0
H [10.38659819 10.7859773 9.62968257] 0.0
H [11.61492359 8.60982075 9.71794865] 0.0
H [10.40769287 6.49870999 9.73739673] 0.0
H [3.55578905 8.35755948 9.39140479] 0.0
H [2.34612206 6.25041273 9.47427859] 0.0
H [3.5728129 4.07662257 9.67356117] 0.0
H [6.04374682 4.05587949 9.77610585] 0.0

Front O Trip Path: O2 Hydrogen Bond in Front of AHQ Triplet (white point 2)
Absolute Energy: -187.94104371732396 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.87116943 7.46711751 9.72011493] 0.0
C [10.50627434 8.68823897 9.75540195] 0.0
C [9.74811732 9.88502675 9.77532578] 0.0
C [7.76778992 6.12967122 9.69535856] 0.0
C [8.45072353 7.36717884 9.69931749] 0.0
C [7.68514881 8.58962637 9.70190992] 0.0
C [8.37315975 9.83366891 9.74851668] 0.0
C [5.66915966 4.82803067 9.61269878] 0.0
C [6.35762663 6.07229721 9.64386102] 0.0
C [5.59312418 7.29574379 9.6137107] 0.0
C [6.27140745 8.53750168 9.67264379] 0.0
C [4.29535403 4.78154252 9.54109222] 0.0
C [3.54242114 5.9802309 9.48792974] 0.0
C [4.17595918 7.20238185 9.52001622] 0.0
O [3.27202451 10.10178968 11.23367921] 1.0
O [2.17105791 9.99565749 10.66213746] 1.0
O [8.42825051 4.9349992 9.74195773] 0.0

H [9.38417378 5.10338972 9.80089579] 0.0
O [5.61873199 9.72830734 9.6714005] 0.0
H [4.73217659 9.65828798 10.09128704] 0.0
H [7.78081072 10.74739146 9.76336802] 0.0
H [10.25885002 10.84753743 9.81095516] 0.0
H [11.59551056 8.73572979 9.77043262] 0.0
H [10.49438823 6.5683859 9.69979224] 0.0
H [3.57477613 8.10866313 9.45207281] 0.0
H [2.45559428 5.93637188 9.41039812] 0.0
H [3.78377051 3.81901352 9.51566228] 0.0
H [6.25337599 3.9095619 9.64278548] 0.0

Front O Trip Path: Transition State for First Hydrogen Transfer Triplet (black point 1)
Absolute Energy: -187.65764625091904 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.84961869 7.48828268 9.78682462] 0.0
C [10.48496523 8.71441845 9.81834664] 0.0
C [9.72732288 9.904474 9.82257635] 0.0
C [7.74990276 6.14915173 9.73570097] 0.0
C [8.4328281 7.39564382 9.75873376] 0.0
C [7.66908146 8.60933707 9.76000491] 0.0
C [8.34557739 9.84619925 9.79293331] 0.0
C [5.66004523 4.83121339 9.59081066] 0.0
C [6.33368583 6.0785624 9.65722406] 0.0
C [5.56561262 7.28918465 9.63607436] 0.0
C [6.22101911 8.57765661 9.71969159] 0.0
C [4.28332152 4.78112733 9.48720476] 0.0
C [3.53039632 5.97248383 9.44218349] 0.0
C [4.16221618 7.20164051 9.52109572] 0.0
O [3.73150178 10.18181402 11.23719133] 1.0
O [2.60742116 9.98639818 10.60302245] 1.0
O [8.41706896 4.96786193 9.7798596] 0.0
H [9.37178336 5.14166254 9.85741278] 0.0
O [5.56501146 9.68666407 9.72306948] 0.0
H [4.57374294 9.89239524 10.50903576] 0.0
H [7.74272031 10.75406515 9.79372863] 0.0

H [10.23570694 10.86857138 9.84877943] 0.0
H [11.57397619 8.76269963 9.84031908] 0.0
H [10.47562554 6.59082352 9.77374073] 0.0
H [3.57530345 8.12022621 9.48875042] 0.0
H [2.44527161 5.92756899 9.34381644] 0.0
H [3.77901147 3.81550349 9.43410649] 0.0
H [6.24652614 3.91394152 9.6166055] 0.0

Front O Trip Path: OOH Hydrogen Bond in Front of AHQ Triplet Triplet (white point 3)
Absolute Energy: -187.6876100180855 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.85506648 7.45905592 9.78135201] 0.0
C [10.50164385 8.68190864 9.7909444] 0.0
C [9.75519154 9.87553055 9.7508922] 0.0
C [7.74201449 6.13306653 9.71639943] 0.0
C [8.43969124 7.3761019 9.73038458] 0.0
C [7.68948741 8.59368684 9.70044393] 0.0
C [8.37072541 9.82370175 9.71179946] 0.0
C [5.64320406 4.82684355 9.57120492] 0.0
C [6.32279434 6.07001945 9.6281987] 0.0
C [5.56293761 7.28103548 9.59801695] 0.0
C [6.22725923 8.57967678 9.67325483] 0.0
C [4.26415727 4.78686157 9.4754811] 0.0
C [3.51896028 5.98106572 9.43298229] 0.0
C [4.16178068 7.20801308 9.49622896] 0.0
O [3.65294291 10.26573731 11.2678896] 1.0
O [2.52872245 9.92410992 10.6542813] 1.0
O [8.39422054 4.94601859 9.77923507] 0.0
H [9.35194586 5.1073642 9.85178285] 0.0
O [5.58166199 9.66820312 9.70707711] 0.0
H [4.41884775 9.98704805 10.61431769] 0.0
H [7.76890436 10.73226578 9.68761898] 0.0
H [10.26960147 10.83666626 9.75565475] 0.0
H [11.59069401 8.72138059 9.83153308] 0.0
H [10.47465953 6.55723047 9.80768348] 0.0
H [3.58623403 8.13500477 9.47313686] 0.0

H [2.43183153 5.94395369 9.35338069] 0.0
H [3.75282652 3.82423219 9.43091463] 0.0
H [6.22147148 3.90459681 9.60150175] 0.0

Front O Trip Path: OOH In First Intermediate Across AHQ Triplet (white point 4)
Absolute Energy: -187.25990775993336 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.89280791 7.50177151 9.93685839] 0.0
C [10.56034293 8.71388182 9.9001186] 0.0
C [9.85168864 9.90643233 9.66618918] 0.0
C [7.76907356 6.19947079 9.77017141] 0.0
C [8.48929154 7.43212854 9.73985673] 0.0
C [7.77911467 8.65014021 9.50556472] 0.0
C [8.47789389 9.86526148 9.47440152] 0.0
C [5.6473588 4.91994698 9.64760481] 0.0
C [6.35559042 6.14773929 9.60779145] 0.0
C [5.62635262 7.36018925 9.39878278] 0.0
C [6.31735447 8.66357073 9.30034712] 0.0
C [4.27260155 4.89923459 9.4888907] 0.0
C [3.55690138 6.0951021 9.2911182] 0.0
C [4.22991021 7.30767115 9.24550548] 0.0
O [5.24693775 8.49128297 12.41120521] 1.0
O [3.92752894 8.63877626 12.48723424] 1.0
O [8.3930981 5.01066076 9.96250055] 0.0
H [9.35025393 5.16196031 10.05699986] 0.0
O [5.69592488 9.71679424 9.07631831] 0.0
H [5.41489669 8.1546499 11.4868007] 0.0
H [7.89615624 10.7703546 9.29638524] 0.0
H [10.38359639 10.8573969 9.63881624] 0.0
H [11.63877403 8.74219541 10.05980855] 0.0
H [10.48524441 6.60250177 10.13156046] 0.0
H [3.70474189 8.24996108 9.08734751] 0.0
H [2.47397207 6.0673455 9.16867679] 0.0
H [3.74058196 3.94744951 9.51930222] 0.0
H [6.19902093 3.99398529 9.80270491] 0.0

Front O Trip Path: OOH In Transition State Moving Across AHQ Triplet (black point 2)
Absolute Energy: -187.24609960360485 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.84355559 7.53030579 9.92358015] 0.0
C [10.4928987 8.75168733 9.88028249] 0.0
C [9.77194384 9.92804946 9.60536145] 0.0
C [7.74700628 6.19148197 9.73434751] 0.0
C [8.44627439 7.43525077 9.69361261] 0.0
C [7.72273009 8.63688419 9.41752757] 0.0
C [8.40414527 9.86138181 9.37783123] 0.0
C [5.63985478 4.87659769 9.62550098] 0.0
C [6.33416059 6.11398603 9.54902503] 0.0
C [5.59315078 7.30844377 9.28277037] 0.0
C [6.26419041 8.62236858 9.17607395] 0.0
C [4.26800868 4.83351353 9.45094491] 0.0
C [3.54197678 6.01238783 9.19173693] 0.0
C [4.20243523 7.23051925 9.10846745] 0.0
O [5.93735266 7.39640907 12.62182102] 1.0
O [5.32879838 8.58361091 12.6465338] 1.0
O [8.38763619 5.01618109 9.96213162] 0.0
H [9.33793508 5.18796532 10.08651899] 0.0
O [5.63422698 9.65542737 8.90142288] 0.0
H [5.8140528 7.06095561 11.69421817] 0.0
H [7.81459084 10.75438044 9.16668701] 0.0
H [10.28993458 10.88723693 9.57493115] 0.0
H [11.56634282 8.79994748 10.06590383] 0.0
H [10.44323004 6.64336409 10.15046265] 0.0
H [3.67052193 8.1610891 8.90777691] 0.0
H [2.46114885 5.96634216 9.05588557] 0.0
H [3.74698777 3.87728429 9.51579103] 0.0
H [6.20063613 3.96529523 9.82797588] 0.0

Front O Trip Path: OOH In Second Intermediate Across AHQ Triplet (white point 5)
Absolute Energy: -187.26015044460348 eV
Cell: Cell([12.78, 14.75707288, 20.45])

Atom, Positions (Å), Magnetic Moment
C [9.80374305 7.55884662 9.91777586] 0.0
C [10.44317174 8.78550547 9.8682782] 0.0
C [9.7193115 9.9488775 9.55206893] 0.0
C [7.72096719 6.20295223 9.71707579] 0.0
C [8.41322554 7.44925228 9.65838272] 0.0
C [7.68537637 8.63809075 9.34261949] 0.0
C [8.35772731 9.86644308 9.29178601] 0.0
C [5.62234908 4.87013252 9.62819162] 0.0
C [6.30937911 6.11135459 9.52631542] 0.0
C [5.56626195 7.28991022 9.20688329] 0.0
C [6.22992989 8.60457353 9.08095382] 0.0
C [4.2545522 4.81088082 9.4229768] 0.0
C [3.52775838 5.97446427 9.10462465] 0.0
C [4.18278292 7.19462288 8.9981573] 0.0
O [6.24912793 6.97676786 12.73165177] 1.0
O [6.32788926 8.28568657 12.48787564] 1.0
O [8.36458019 5.0347682 9.9752072] 0.0
H [9.31727492 5.20881232 10.07372224] 0.0
O [5.59572228 9.62562308 8.77270122] 0.0
H [6.10002521 6.55693947 11.84209847] 0.0
H [7.76901998 10.75156461 9.0475717] 0.0
H [10.22825625 10.91231829 9.51649537] 0.0
H [11.50972624 8.84795036 10.08561117] 0.0
H [10.4017337 6.68368849 10.1902564] 0.0
H [3.64955926 8.11276468 8.74895734] 0.0
H [2.45141266 5.91389488 8.93895388] 0.0
H [3.73845382 3.85319915 9.50333494] 0.0
H [6.18671899 3.96837232 9.86311965] 0.0

Front O Trip Path: OOH Hydrogen Bond with Second OH-group Triplet (white point 6)
Absolute Energy: -187.36346864953077 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.70175207 7.47745764 10.08601208] 0.0
C [10.39461727 8.67284519 10.01732189] 0.0
C [9.71722274 9.87311119 9.73249851] 0.0

C [7.55887236 6.20953397 9.94000776] 0.0
C [8.29922095 7.43258301 9.87740324] 0.0
C [7.62372284 8.65257808 9.56404324] 0.0
C [8.34896903 9.85493554 9.50726202] 0.0
C [5.46817714 4.94440654 9.5226978] 0.0
C [6.18051007 6.16938272 9.56093129] 0.0
C [5.49399859 7.37439152 9.22930522] 0.0
C [6.18374478 8.66975846 9.27266482] 0.0
C [4.13596447 4.91787138 9.15124672] 0.0
C [3.4627119 6.1109742 8.82226614] 0.0
C [4.13650729 7.32197697 8.86932933] 0.0
O [9.99331217 4.06971889 12.84328571] 1.0
O [9.90662883 5.30808805 12.29642862] 1.0
O [8.11614997 5.04980115 10.3177254] 0.0
H [8.88379472 5.18132384 10.95477583] 0.0
O [5.57565414 9.74106789 9.05573544] 0.0
H [10.49656679 4.21674788 13.67767744] 0.0
H [7.80152006 10.76630359 9.26602508] 0.0
H [10.27068669 10.81122358 9.67680208] 0.0
H [11.47375565 8.68005866 10.17667363] 0.0
H [10.25120409 6.55767262 10.28364016] 0.0
H [3.63825162 8.26029961 8.62421888] 0.0
H [2.41306731 6.08060094 8.5269043] 0.0
H [3.60389404 3.96625031 9.11543724] 0.0
H [5.99358743 4.02635902 9.78255729] 0.0

Front O Trip Path: H2O2 Hydrogen Bond to AQ Triplet (white point 7)
Absolute Energy: -187.0083849334645 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.86230695 7.49145585 9.97902823] 0.0
C [10.51862621 8.70548089 9.8874661] 0.0
C [9.78431896 9.8978872 9.71753576] 0.0
C [7.78196053 6.14252961 9.99444532] 0.0
C [8.45225257 7.42280929 9.88889521] 0.0
C [7.71690461 8.62591124 9.70804302] 0.0
C [8.40325586 9.85713621 9.6351574] 0.0
C [5.67774838 4.85918503 9.72633495] 0.0

C [6.35303553 6.10187188 9.75999953] 0.0
C [5.60478455 7.29721539 9.57737241] 0.0
C [6.25934728 8.60301819 9.6130591] 0.0
C [4.3130074 4.80248367 9.50865392] 0.0
C [3.57349766 5.99081804 9.33182222] 0.0
C [4.21075139 7.2190265 9.37220371] 0.0
O [9.86759455 4.29662661 13.09278736] 1.0
O [8.62563503 4.90406145 12.7955154] 1.0
O [8.43534253 5.074973 10.3011701] 0.0
H [8.62035302 4.90089413 11.74636206] 0.0
O [5.59003438 9.6711378 9.56436683] 0.0
H [9.87343277 4.37859048 14.06832481] 0.0
H [7.81695667 10.76727828 9.50636213] 0.0
H [10.30284003 10.85507152 9.65023528] 0.0
H [11.6072643 8.73978412 9.94727368] 0.0
H [10.41317097 6.55953307 10.10888505] 0.0
H [3.65649173 8.14828164 9.23856844] 0.0
H [2.4966944 5.94417367 9.16246672] 0.0
H [3.80774882 3.83606265 9.47388597] 0.0
H [6.26902988 3.95329066 9.86363367] 0.0

Front O Trip Path: H2O2 Separated from AQ Triplet (white point 8)
Absolute Energy: -186.56762508633142 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.844749 7.41729533 9.83169018] 0.0
C [10.50418464 8.63297048 9.84031676] 0.0
C [9.77157585 9.83646506 9.77248307] 0.0
C [7.76633715 6.06728523 9.74636618] 0.0
C [8.43499076 7.36345314 9.75250221] 0.0
C [7.69868331 8.57377569 9.68303955] 0.0
C [8.39137251 9.80571119 9.69549388] 0.0
C [5.62652842 4.82946366 9.56575344] 0.0
C [6.31350103 6.06348296 9.61656364] 0.0
C [5.57673878 7.27393367 9.54824934] 0.0
C [6.2427268 8.57147774 9.59816005] 0.0
C [4.249345 4.79680232 9.44729151] 0.0
C [3.51565007 5.99961294 9.37967797] 0.0

C [4.1694565 7.21753573 9.43108493] 0.0
O [13.37151913 -0.09125693 12.79574331] 1.0
O [12.15292251 0.4243827 12.17877517] 1.0
O [8.4191469 4.98990472 9.8538811] 0.0
H [12.38460871 0.31021098 11.23650842] 0.0
O [5.58620635 9.65173446 9.56725893] 0.0
H [12.97813834 -0.72068713 13.43224057] 0.0
H [7.80511369 10.72328282 9.6387853] 0.0
H [10.29376806 10.79418283 9.77536651] 0.0
H [11.59293342 8.65971233 9.89948616] 0.0
H [10.39065715 6.47490781 9.88515624] 0.0
H [3.62134258 8.15905809 9.3800658] 0.0
H [2.42936758 5.97000485 9.28747409] 0.0
H [3.72962731 3.83864633 9.40965237] 0.0
H [6.2142148 3.91236084 9.62348051] 0.0

Front O Sing Path: O2 Hydrogen Bond in Front of AHQ Singlet (white point 2)
Absolute Energy: -187.6614518960024 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.8785773 7.47431925 9.73786313] 0.0
C [10.51630093 8.69534268 9.76967175] 0.0
C [9.76049814 9.89243997 9.79080227] 0.0
C [7.77324698 6.14200991 9.71299253] 0.0
C [8.45842976 7.3793498 9.72269932] 0.0
C [7.69459061 8.60151556 9.73317011] 0.0
C [8.38399246 9.84336439 9.77187865] 0.0
C [5.67715995 4.83963441 9.61344009] 0.0
C [6.36196475 6.08503614 9.66447124] 0.0
C [5.59766896 7.30803152 9.64910995] 0.0
C [6.27662166 8.55274258 9.71632355] 0.0
C [4.30285287 4.79251039 9.53312672] 0.0
C [3.55057595 5.99071922 9.49304865] 0.0
C [4.18200137 7.21463547 9.54894611] 0.0
O [3.32205229 10.10346348 11.19198191] 0.0
O [2.19808583 9.94520951 10.65442182] 0.0
O [8.43135352 4.94822927 9.74200893] 0.0

H [9.388116 5.11375099 9.79967575] 0.0
O [5.63245953 9.74032366 9.72697233] 0.0
H [4.7314243 9.68368277 10.13598656] 0.0
H [7.7935571 10.75815271 9.7881584] 0.0
H [10.27356057 10.85416231 9.82338092] 0.0
H [11.60563894 8.74106571 9.78580693] 0.0
H [10.50061109 6.57420458 9.72006046] 0.0
H [3.57740491 8.11933175 9.49437148] 0.0
H [2.46385585 5.94799798 9.41143079] 0.0
H [3.79288026 3.82954456 9.49045961] 0.0
H [6.26293321 3.92179771 9.63510046] 0.0

Front O Sing Path: Transition State for First Hydrogen Transfer Singlet (black point 1)
Absolute Energy: -187.56281366413626 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.8457983 7.49413654 9.76134516] 0.0
C [10.48023408 8.7205992 9.78897739] 0.0
C [9.71911925 9.90866517 9.80735338] 0.0
C [7.7480296 6.14996509 9.73612749] 0.0
C [8.42882153 7.39700933 9.75031219] 0.0
C [7.66095401 8.60913261 9.75884319] 0.0
C [8.33769862 9.84786307 9.79019363] 0.0
C [5.66181528 4.82755827 9.61294291] 0.0
C [6.33187902 6.07696229 9.67158589] 0.0
C [5.5599927 7.2869019 9.65350344] 0.0
C [6.21753238 8.56895632 9.72738123] 0.0
C [4.28485727 4.77306436 9.52257218] 0.0
C [3.52749987 5.96211848 9.48196318] 0.0
C [4.15412532 7.19398767 9.54972108] 0.0
O [3.67451336 10.1021434 11.18424764] 0.0
O [2.58393942 9.96717108 10.4885833] 0.0
O [8.41689908 4.96964332 9.77702379] 0.0
H [9.37223843 5.14503971 9.84199481] 0.0
O [5.56118673 9.69001394 9.72448706] 0.0
H [4.61054269 9.82699767 10.4258147] 0.0
H [7.73473079 10.75546087 9.7993055] 0.0

H [10.22471404 10.87413327 9.83233028] 0.0
H [11.56943082 8.77081057 9.79706147] 0.0
H [10.47222817 6.59711814 9.73532601] 0.0
H [3.55956074 8.10724941 9.51406459] 0.0
H [2.44169774 5.91296066 9.39369499] 0.0
H [3.78278656 3.80588462 9.47516278] 0.0
H [6.2514404 3.91212316 9.63258994] 0.0

Front O Sing Path: HOO Hydrogen Bond in Front of AHQ Singlet (white point 3)
Absolute Energy: -187.6799767325234 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.86769656 7.46501329 9.78633764] 0.0
C [10.51279422 8.68937551 9.80722383] 0.0
C [9.76645009 9.88231767 9.77731714] 0.0
C [7.75526176 6.1385996 9.71661173] 0.0
C [8.45286974 7.38204627 9.73560018] 0.0
C [7.70317894 8.59854697 9.71102127] 0.0
C [8.38143043 9.82929536 9.73315562] 0.0
C [5.65919743 4.82880852 9.57627033] 0.0
C [6.33486189 6.07334636 9.6357771] 0.0
C [5.57252024 7.28238365 9.6127506] 0.0
C [6.23828109 8.58437714 9.68162622] 0.0
C [4.27897986 4.78476798 9.48631726] 0.0
C [3.53043325 5.97623814 9.45702265] 0.0
C [4.17089372 7.20576093 9.52153788] 0.0
O [3.60711917 10.35246329 11.21053359] 0.0
O [2.48552569 9.90878433 10.64674364] 0.0
O [8.4115937 4.95426599 9.76742227] 0.0
H [9.3678132 5.11959811 9.85000326] 0.0
O [5.59904415 9.67138009 9.70899196] 0.0
H [4.36819312 10.04309529 10.58624058] 0.0
H [7.77920825 10.73789346 9.71631403] 0.0
H [10.281316 10.84330206 9.79542615] 0.0
H [11.60179705 8.73016477 9.8506497] 0.0
H [10.48991894 6.56470162 9.80578495] 0.0
H [3.58855396 8.12926304 9.50954009] 0.0

H [2.44287418 5.93602854 9.38516087] 0.0
H [3.77175454 3.82028768 9.43856805] 0.0
H [6.2415469 3.90883498 9.59867658] 0.0

Front O Sing Path: HOO Physisorbed Moving Above AHQ Singlet (white point 4)
Absolute Energy: -186.86089319269692 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.8583004 7.48143859 9.78530904] 0.0
C [10.50980308 8.70274919 9.81140282] 0.0
C [9.77884538 9.89568981 9.66972867] 0.0
C [7.74983112 6.16454787 9.59249086] 0.0
C [8.45199406 7.40826174 9.61643108] 0.0
C [7.72046156 8.62511924 9.46284714] 0.0
C [8.40117879 9.84781187 9.49406897] 0.0
C [5.64816281 4.85663388 9.46461072] 0.0
C [6.33520845 6.09817826 9.4478561] 0.0
C [5.5887749 7.30384773 9.28352342] 0.0
C [6.25501209 8.6210174 9.23435261] 0.0
C [4.27035807 4.82196267 9.33712021] 0.0
C [3.53943248 6.01525234 9.19357511] 0.0
C [4.19591274 7.24014651 9.16528264] 0.0
O [5.42411197 8.4679822 12.18058681] 0.0
O [4.06936618 8.34632704 12.21168272] 0.0
O [8.39907027 4.9865954 9.7219163] 0.0
H [9.35469951 5.15260557 9.81791591] 0.0
O [5.63412733 9.66255717 8.98712949] 0.0
H [5.75492643 7.56851212 12.41059321] 0.0
H [7.80746816 10.75481935 9.37352234] 0.0
H [10.29643876 10.85495841 9.6963408] 0.0
H [11.59129683 8.73670787 9.9448829] 0.0
H [10.4683334 6.57997948 9.90035805] 0.0
H [3.65407776 8.17930803 9.05651701] 0.0
H [2.45366315 5.97746292 9.10129701] 0.0
H [3.75137265 3.86276752 9.34952956] 0.0
H [6.21639974 3.93477523 9.58119985] 0.0

Front O Sing Path: Transition State HOO Physisorbed Moving Above to Forming a Bond with and Interior Carbon of AHQ Singlet (black point 2)
Absolute Energy: -186.84327880407042 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.84106452 7.51859066 9.8252358] 0.0
C [10.48744252 8.74404562 9.83588123] 0.0
C [9.75894491 9.92818534 9.6317311] 0.0
C [7.74093578 6.18848649 9.60544962] 0.0
C [8.4430343 7.43447879 9.60924762] 0.0
C [7.71471127 8.64146665 9.39208823] 0.0
C [8.38802202 9.86780449 9.40899549] 0.0
C [5.64644738 4.86865784 9.45850876] 0.0
C [6.33034993 6.11028897 9.41452347] 0.0
C [5.58867461 7.30455457 9.18433253] 0.0
C [6.25389088 8.62423092 9.13959982] 0.0
C [4.27361733 4.82453671 9.28416324] 0.0
C [3.54653917 6.0066808 9.05816446] 0.0
C [4.20234049 7.23080839 9.01136147] 0.0
O [5.86108765 8.14800544 12.50774563] 0.0
O [4.55519771 8.10650822 12.10537451] 0.0
O [8.38828969 5.01547876 9.78829556] 0.0
H [9.33865151 5.18874315 9.91556809] 0.0
O [5.63092252 9.66507974 8.89771311] 0.0
H [5.95184342 7.37588045 13.11211178] 0.0
H [7.7937756 10.76717196 9.24362857] 0.0
H [10.27200053 10.89028826 9.64844977] 0.0
H [11.56305813 8.78724473 10.00868612] 0.0
H [10.44869795 6.62400743 9.99486422] 0.0
H [3.66378499 8.16524012 8.85486654] 0.0
H [2.46486416 5.96241994 8.92689354] 0.0
H [3.7543502 3.86604831 9.32684138] 0.0
H [6.21090791 3.95435574 9.63654448] 0.0

Front O Sing Path: HOO Bound to Interior Carbon of AHQ Singlet (white point 5)
Absolute Energy: -187.38417269709382 eV
Cell: Cell([12.78, 14.75707288, 20.45])

Atom, Positions (Å), Magnetic Moment
C [9.8392057 7.47978748 9.81579999] 0.0
C [10.51544172 8.69800716 9.75020881] 0.0
C [9.80771088 9.88976681 9.57611793] 0.0
C [7.71180435 6.15438586 9.68827311] 0.0
C [8.43938724 7.42309096 9.70936416] 0.0
C [7.73028161 8.64023621 9.56197494] 0.0
C [8.41732172 9.85265055 9.48180286] 0.0
C [5.6325612 4.8306303 9.55613661] 0.0
C [6.33790494 6.07555274 9.6809841] 0.0
C [5.54053877 7.32651417 9.88375726] 0.0
C [6.24776853 8.63667215 9.49873048] 0.0
C [4.28705532 4.81455151 9.32820395] 0.0
C [3.56669972 6.05001721 9.13894053] 0.0
C [4.15559192 7.25158452 9.33828795] 0.0
O [6.44306217 7.46899991 12.18760554] 0.0
O [5.2317503 7.50602898 11.37505141] 0.0
O [8.42273816 4.99393184 9.63539602] 0.0
H [9.36496881 5.20286935 9.51182974] 0.0
O [5.60452312 9.63762511 9.2135342] 0.0
H [6.44958002 6.52950505 12.45806701] 0.0
H [7.82854508 10.76224168 9.35715854] 0.0
H [10.33827444 10.84057933 9.525319] 0.0
H [11.60183872 8.71351748 9.84104582] 0.0
H [10.43583451 6.57781585 9.98026253] 0.0
H [3.64709372 8.19884525 9.16924502] 0.0
H [2.53331142 6.00697045 8.78881569] 0.0
H [3.76185444 3.86605547 9.21268675] 0.0
H [6.20086311 3.90127445 9.59299763] 0.0

Front O Sing Path: Transition State for OOH to Leave Bond with Interior Carbon to be Physisorbed Above Center of AHQ Singlet (black point 3)
Absolute Energy: -187.35515668304248 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.8315001 7.50560279 9.86428544] 0.0
C [10.50477555 8.72377801 9.81943966] 0.0
C [9.79509912 9.91332461 9.62562325] 0.0

C [7.70211538 6.18278885 9.7263721] 0.0
C [8.43170343 7.44595135 9.72666479] 0.0
C [7.7236589 8.65831292 9.53471841] 0.0
C [8.41133033 9.87178298 9.47294217] 0.0
C [5.6219304 4.86246556 9.53063772] 0.0
C [6.32092297 6.1110666 9.60846227] 0.0
C [5.55090025 7.35244973 9.66425625] 0.0
C [6.24637023 8.65268777 9.3566669] 0.0
C [4.2661368 4.83334361 9.34933251] 0.0
C [3.53307302 6.05620285 9.1948172] 0.0
C [4.14658054 7.26663732 9.30676975] 0.0
O [6.5197901 7.28800033 12.16001694] 0.0
O [5.44399554 7.79648878 11.40097982] 0.0
O [8.38903559 5.01522981 9.7933247] 0.0
H [9.34199444 5.20543756 9.84706172] 0.0
O [5.63189296 9.6530362 8.99774481] 0.0
H [6.21097648 6.38564845 12.38703651] 0.0
H [7.82560409 10.77797288 9.31409912] 0.0
H [10.32259308 10.86718753 9.59984575] 0.0
H [11.58822753 8.74523085 9.94010407] 0.0
H [10.43383213 6.6048714 10.01918987] 0.0
H [3.61581529 8.20535378 9.15398238] 0.0
H [2.46919944 6.00791508 8.95509588] 0.0
H [3.74503932 3.87859437 9.27158511] 0.0
H [6.19586739 3.93782443 9.58224935] 0.0

Front O Sing Path: HOO Physisorbed Above Center of AHQ Singlet (white point 6)
Absolute Energy: -187.46131256163193 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.7594024 7.53337375 9.98703583] 0.0
C [10.40671529 8.75248607 9.94369025] 0.0
C [9.66960089 9.93345818 9.71619097] 0.0
C [7.64125374 6.22082549 9.91361909] 0.0
C [8.35504822 7.45288993 9.80954016] 0.0
C [7.61730289 8.65039201 9.59459497] 0.0
C [8.29965383 9.87834221 9.53610659] 0.0

C [5.57224081 4.86356222 9.62875481] 0.0
C [6.23713207 6.11426243 9.62053935] 0.0
C [5.49879656 7.29974968 9.36292995] 0.0
C [6.15486969 8.63069932 9.33618151] 0.0
C [4.20894659 4.80082493 9.39206597] 0.0
C [3.48031311 5.97780909 9.13787382] 0.0
C [4.12196875 7.20840891 9.11786435] 0.0
O [6.86618191 7.17450299 12.13673319] 0.0
O [6.32708574 8.3734475 11.74664814] 0.0
O [8.27334753 5.06324097 10.17464443] 0.0
H [9.20550734 5.24963787 10.39338125] 0.0
O [5.53844664 9.65646504 9.03288946] 0.0
H [6.10690817 6.54669645 12.10914633] 0.0
H [7.70514744 10.77267892 9.34933283] 0.0
H [10.1885491 10.89200461 9.67670625] 0.0
H [11.48722771 8.80075811 10.07971226] 0.0
H [10.36725571 6.63660259 10.14833561] 0.0
H [3.58456398 8.13688392 8.9229796] 0.0
H [2.40684675 5.9202593 8.95358662] 0.0
H [3.70316924 3.83414599 9.40056493] 0.0
H [6.14195597 3.95517569 9.82137602] 0.0

Front O Sing Path: Transition State for HOO Physisorbed Above Center of AHQ to Bind to Carbon 10 Singlet (black point 4)
Absolute Energy: -186.92516348621805 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.84250564 7.52204242 9.71027743] 0.0
C [10.5079507 8.73736505 9.6841364] 0.0
C [9.78283878 9.93397717 9.56073308] 0.0
C [7.71225125 6.22720658 9.65819904] 0.0
C [8.43089977 7.46292016 9.61720446] 0.0
C [7.7052641 8.68224096 9.48850617] 0.0
C [8.39645791 9.89783519 9.4629536] 0.0
C [5.60941108 4.92667346 9.5097537] 0.0
C [6.29580718 6.16488541 9.50745734] 0.0
C [5.55485957 7.37241224 9.3695552] 0.0
C [6.22763148 8.68975455 9.3830628] 0.0

C [4.23201067 4.89292592 9.36654071] 0.0
C [3.50387457 6.08722357 9.22555575] 0.0
C [4.16384012 7.31143225 9.23214793] 0.0
O [7.34910499 6.33698379 12.96460428] 0.0
O [6.68719559 7.4725666 12.56917844] 0.0
O [8.34458116 5.05104326 9.8288916] 0.0
H [9.28705546 5.21427218 10.0153535] 0.0
O [5.59107808 9.74876426 9.29488891] 0.0
H [6.94228456 6.1171912 13.83230813] 0.0
H [7.80684349 10.81022422 9.36776318] 0.0
H [10.30924653 10.88877126 9.54088938] 0.0
H [11.59542288 8.76097669 9.75850426] 0.0
H [10.44594101 6.61339881 9.79726228] 0.0
H [3.62314201 8.25367635 9.13778962] 0.0
H [2.41933994 6.05190398 9.11541879] 0.0
H [3.71230728 3.9340086 9.36575729] 0.0
H [6.17569643 4.00385235 9.6264038] 0.0

Trail O Trip Path: O2 Hydrogen Bond On Top of AHQ Triplet (white point 2)
Absolute Energy: -187.92814945445525 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.88019567 7.48893465 9.80824526] 0.0
C [10.51676955 8.70866295 9.83538392] 0.0
C [9.76106514 9.90749486 9.79399152] 0.0
C [7.77829474 6.1540037 9.71858689] 0.0
C [8.46135824 7.3914654 9.72802219] 0.0
C [7.69813629 8.61543211 9.66827043] 0.0
C [8.38840462 9.85917917 9.71459346] 0.0
C [5.68485114 4.84869324 9.53988656] 0.0
C [6.37448066 6.092645 9.5887343] 0.0
C [5.61866924 7.31569388 9.48682781] 0.0
C [6.28979576 8.5584602 9.56871474] 0.0
C [4.31962479 4.80516219 9.37408335] 0.0
C [3.57720276 6.00539979 9.2424554] 0.0
C [4.21155464 7.22570764 9.29712576] 0.0
O [4.14930536 9.41353943 11.92014095] 1.0

O [5.01885647 8.69609263 12.43651327] 1.0
O [8.43335318 4.96036526 9.82321973] 0.0
H [9.38161454 5.12992128 9.95490889] 0.0
O [5.61225375 9.74167883 9.50280691] 0.0
H [4.80412051 9.67951316 10.05765965] 0.0
H [7.79912662 10.77473303 9.6848538] 0.0
H [10.27366172 10.86966235 9.82671675] 0.0
H [11.60481799 8.7535051 9.8919425] 0.0
H [10.49997683 6.58775972 9.83639791] 0.0
H [3.63057711 8.13978824 9.17139483] 0.0
H [2.49877341 5.96159997 9.08499793] 0.0
H [3.80723095 3.84342409 9.33154356] 0.0
H [6.26232943 3.9291884 9.6251036] 0.0

Trail O Trip Path: Transition State for First Hydrogen Transfer Triplet (black point 1)
Absolute Energy: -187.29713215709745 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.92117061 7.47999411 9.90673941] 0.0
C [10.59311145 8.68992609 9.88264578] 0.0
C [9.88891732 9.88860281 9.66610992] 0.0
C [7.79150272 6.19084288 9.74993148] 0.0
C [8.51650719 7.41963585 9.71926218] 0.0
C [7.80968322 8.64314958 9.50618331] 0.0
C [8.51381447 9.85608647 9.48257584] 0.0
C [5.66636534 4.91861365 9.61329469] 0.0
C [6.37828294 6.14326859 9.57690766] 0.0
C [5.6562496 7.35652424 9.36870715] 0.0
C [6.34460085 8.66290629 9.34255398] 0.0
C [4.29259673 4.90088688 9.44486169] 0.0
C [3.58281202 6.09708959 9.2298338] 0.0
C [4.26225993 7.30778327 9.19268711] 0.0
O [5.07130652 8.41291064 12.44521783] 1.0
O [6.16621617 7.73028197 12.7796951] 1.0
O [8.40968681 5.00080742 9.94750408] 0.0
H [9.36080287 5.15192303 10.09017608] 0.0
O [5.7095208 9.72786985 9.22234819] 0.0

H [4.97309189 8.28196561 11.46409065] 0.0
H [7.93730821 10.7677494 9.32159573] 0.0
H [10.42465144 10.83793207 9.64727593] 0.0
H [11.67276659 8.71111521 10.03509683] 0.0
H [10.50979501 6.57433049 10.08281812] 0.0
H [3.74218129 8.25073711 9.01445057] 0.0
H [2.50210231 6.07202863 9.08629882] 0.0
H [3.75768701 3.95090903 9.47905263] 0.0
H [6.21310187 3.99239703 9.78284872] 0.0

Trail O Trip Path: HOO Hydrogen Bond On Top of AHQ Triplet (white point 3)
Absolute Energy: -187.30279285215883 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.91003148 7.48680193 9.93297752] 0.0
C [10.58753002 8.69353094 9.89607915] 0.0
C [9.89050935 9.89235354 9.65837955] 0.0
C [7.77624531 6.20323888 9.77256891] 0.0
C [8.50659266 7.42880825 9.73584463] 0.0
C [7.80804703 8.65196262 9.49549612] 0.0
C [8.51740063 9.86127717 9.46154041] 0.0
C [5.64502355 4.94053642 9.6507835] 0.0
C [6.36320186 6.16158221 9.59764145] 0.0
C [5.64844311 7.3759786 9.36244975] 0.0
C [6.34761202 8.67695061 9.28924818] 0.0
C [4.27368232 4.92455334 9.46757395] 0.0
C [3.5705609 6.12078263 9.22858569] 0.0
C [4.25471482 7.32807438 9.1799091] 0.0
O [5.22053442 8.31710463 12.44708958] 1.0
O [6.31659645 7.62897121 12.76558151] 1.0
O [8.39029552 5.01093157 9.97037755] 0.0
H [9.34237755 5.15859137 10.10989562] 0.0
O [5.73154818 9.73867834 9.08255847] 0.0
H [5.07563608 8.13803048 11.47815126] 0.0
H [7.94519704 10.77146877 9.27950783] 0.0
H [10.42933367 10.83997575 9.63374684] 0.0
H [11.66610241 8.71216733 10.0568712] 0.0

H [10.49452444 6.58196652 10.1272118] 0.0
H [3.73860148 8.26946146 8.98549542] 0.0
H [2.49101241 6.09818037 9.07667447] 0.0
H [3.73492367 3.97691062 9.51081965] 0.0
H [6.18667812 4.01518426 9.84026668] 0.0

Trail O Trip Path: HOO Hydrogen Bound to Other OH Triplet (white point 4)
Absolute Energy: -187.379024944124 eV
Cell: Cell([12.78, 14.75707288, 20.45])
Atom, Positions (Å), Magnetic Moment
C [9.70507392 7.49162487 10.0038934] 0.0
C [10.38799359 8.69390018 9.95440507] 0.0
C [9.69708271 9.89740585 9.71722163] 0.0
C [7.56211986 6.21758856 9.90963571] 0.0
C [8.29862365 7.44244802 9.82568213] 0.0
C [7.6133933 8.66228037 9.53455649] 0.0
C [8.32775059 9.87225548 9.50086655] 0.0
C [5.47055267 4.94396434 9.51166757] 0.0
C [6.182038 6.1701525 9.53684349] 0.0
C [5.48956136 7.37249877 9.20536938] 0.0
C [6.1715648 8.67296857 9.25339802] 0.0
C [4.13456584 4.91362013 9.1531066] 0.0
C [3.45545773 6.10388046 8.82636405] 0.0
C [4.12862612 7.31592064 8.85980398] 0.0
O [9.32354279 6.12304192 13.15675834] 1.0
O [9.97119072 5.32728868 12.27007804] 1.0
O [8.12044985 5.0672142 10.31801841] 0.0
H [8.88103516 5.21561992 10.95981453] 0.0
O [5.55713791 9.74369123 9.05434667] 0.0
H [9.97673912 6.25073315 13.88336786] 0.0
H [7.76993797 10.78479914 9.28896558] 0.0
H [10.24171708 10.84155714 9.68056002] 0.0
H [11.47104033 8.70349877 10.08507736] 0.0
H [10.26109819 6.56846573 10.16575035] 0.0
H [3.62616465 8.25367475 8.62067676] 0.0
H [2.40080315 6.07152742 8.54931069] 0.0
H [3.60278423 3.96129587 9.12778463] 0.0

H [5.99753774 4.02709891 9.77305868] 0.0