

Supplementary Information

Non-classical CH...O hydrogen-bond determining the regio- and stereoselectivity in the [3+2] cycloaddition reaction of (Z) C-phenyl-N-methylnitrone with dimethyl 2-benzylidenecyclopropane-1,1-dicarboxylate. A topological electron-density study

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- S5** MPWB1K/6-31G(d) gas phase computed total electronic energies and cartesian coordinates of the stationary points involved in the 32CA reactions of C-phenyl-N-methylnitrone **7** with BCP **10** and BCPC **8**.

Table S1. B3LYP/6-31G(d) gas phase total (E, in a.u.) and relative^a energies (ΔE , in kcal mol⁻¹) of the stationary points involved in the 32CA reaction of *C*-phenyl-*N*-methylnitronone **7** with BCP **10**.

	E	ΔE
7	-440.17942	
10	-387.02396	
TS-10-on	-827.17016	20.8
TS-10-ox	-827.16707	22.8
TS-10-mn	-827.17253	19.4
TS-10-mx	-827.17022	20.8
11-on	-827.23340	-18.8
11-ox	-827.23960	-22.7
11-mn	-827.23035	-16.9
11-mx	-827.23918	-22.5

^a Relative to nitronone **7** and BCP **10**.

Table S2. MPWB1K/6-31+G(d)//MPWB1K/6-31G(d) total (E, in a.u.) and relative (ΔE , in kcal mol⁻¹) gas phase energies of the stationary points involved in the 32CA reaction between *C*-phenyl-*N*-methylnitronone **7** with BCPC **8**.

	E	ΔE
7	-439.96353	
8	-842.39655	
MC-8-on	-1282.36942	-30.7
TS-8-on	-1282.33606	-9.8
TS-8-ox	-1282.32615	-3.5
TS-8-mn	-1282.33133	-6.8
TS-8-mx	-1282.33035	-6.2
9-on	-1282.41276	-57.9
9-ox	-1282.41835	-61.4
9-mn	-1282.41322	-58.2
9-mx	-1282.41879	-61.7

^a Relative to nitronone **7** and BCPC **8**.

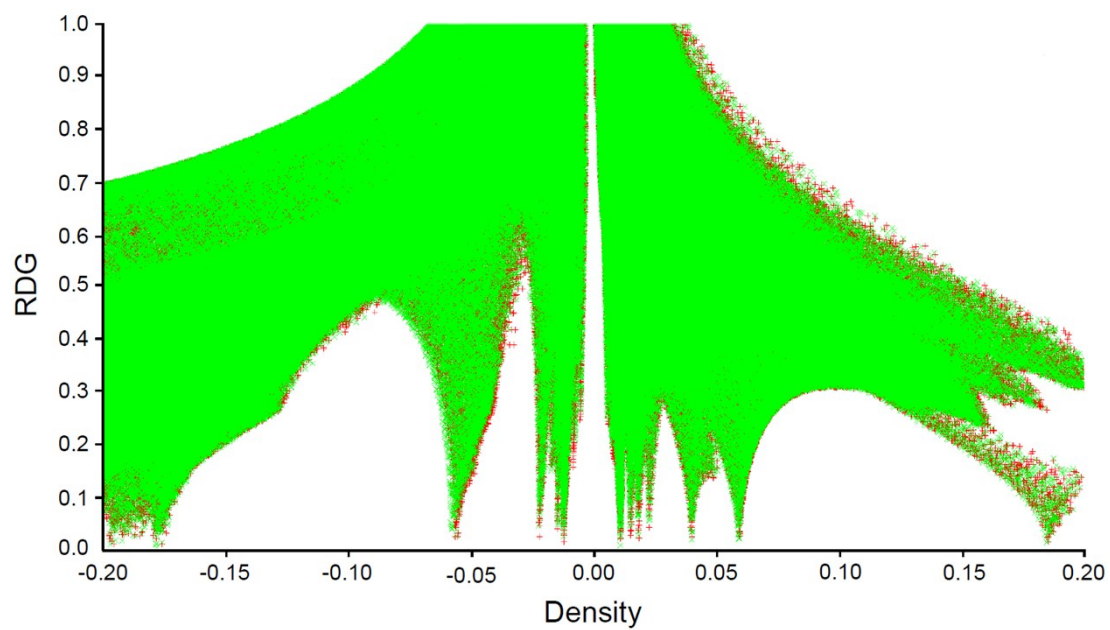


Figure S1. Overlaid plots of the RDG versus the electron-density multiplied by the sign of the second Hessian eigenvalue for the MPWB1K/6-31G(d) (in red) and MPWB1K/6-31+G(d) (in green) optimised geometry of **TS-8-on**. Both quantities are given in a.u.

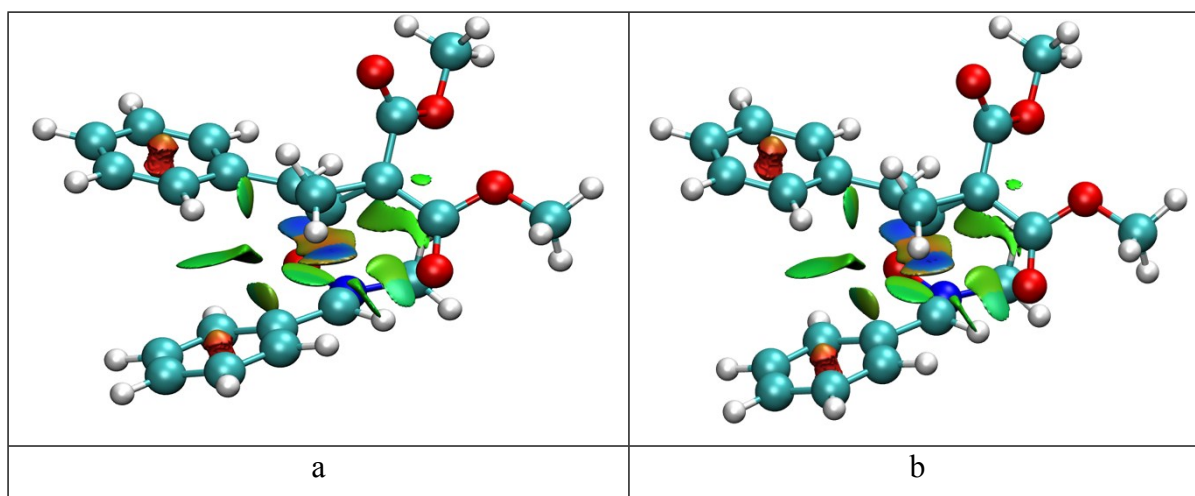


Figure S2. NCI gradient isosurfaces of the (a) MPWB1K/6-31G(d) and (b) MPWB1K/6-31+G(d) optimised geometry of **TS-8-on**. Blue indicates strong attractive interactions while red indicates strong non-bonded overlap.

MPWB1K/6-31G(d) gas phase computed total electronic energies (E, in a.u.) and cartesian coordinates of the stationary points involved in the 32CA reactions of *C*-phenyl-*N*-methylnitron **7** with BCP **10** and BCPC **8**.

7

E(RmPW+HF-B95) = -439.94778 a.u.

O	-2.08639700	1.31383100	0.00026000
C	-1.07026300	-0.72936400	-0.00019600
H	-1.29043100	-1.78298800	-0.00029200
N	-2.10429200	0.05709500	0.00002600
C	0.31132500	-0.31614500	-0.00010500
C	1.27541000	-1.32765600	0.00003800
C	0.73499500	1.01486400	-0.00017800
C	2.62003900	-1.02654600	0.00013900
H	0.95740000	-2.36097200	0.00005300
C	2.08604600	1.30559700	-0.00010100
H	-0.00225000	1.79747800	-0.00027900
C	3.03133300	0.29603900	0.00008000
H	3.34824300	-1.82337100	0.00027200
H	2.40274900	2.33768800	-0.00018600
H	4.08394100	0.53549300	0.00016900
C	-3.44706400	-0.50918500	-0.00000400
H	-3.95264600	-0.13357400	0.88241200
H	-3.95268500	-0.13337600	-0.88231400
H	-3.42402900	-1.59232100	-0.00013600

10

E(RmPW+HF-B95) = -386.81884 a.u.

C	0.98659400	-0.96744800	-0.00060000
H	1.05757400	-2.04818400	-0.00085600
C	2.10904900	-0.27476500	-0.00072100
C	2.78889100	1.01200400	0.00060100
C	3.56252900	-0.29314400	0.00045700
H	2.78944700	1.60126600	0.90830400
H	2.79131800	1.60187600	-0.90671800
H	4.08238400	-0.57112300	-0.90657700
H	4.08052600	-0.57241700	0.90816100
C	-0.36872000	-0.42363100	-0.00032200
C	-1.44923700	-1.29995900	0.00010100
C	-0.63078700	0.94520400	-0.00051100

C	-2.74931600	-0.83119700	0.00043900
H	-1.26208200	-2.36454500	0.00019000
C	-1.92807300	1.41412300	-0.00018300
H	0.19348700	1.64106600	-0.00095800
C	-2.99454300	0.52951800	0.00031200
H	-3.57173200	-1.53070400	0.00078800
H	-2.11090400	2.47838200	-0.00033800
H	-4.00834000	0.90014800	0.00056300

TS-10-on

E(RmPW+HF-B95) = -826.74045 a.u.

1 imaginary frequency = -475.9709 cm⁻¹

C	0.52364100	-1.67506100	0.28623300
O	-0.43215800	-1.35133800	-1.72915800
C	-1.94853100	-0.51639000	-0.32463300
H	-2.90893300	-0.71722900	0.13085200
N	-1.62808700	-1.36592800	-1.29728500
C	-0.58248100	-1.38948300	1.04588300
C	-0.83537500	-0.81259700	2.36923900
C	-1.39400900	-2.16782000	1.99893700
H	-1.52994600	0.01080200	2.47087100
H	-0.01161500	-0.77455800	3.06918800
H	-0.95233400	-3.04188100	2.45841600
H	-2.46595600	-2.24233600	1.86586900
C	-1.55718600	0.89340500	-0.32953300
C	-2.24148000	1.74536000	0.53628100
C	-0.58309100	1.43342600	-1.16655400
C	-1.95084700	3.09401000	0.58710000
H	-3.02419100	1.34433500	1.16569900
C	-0.30992400	2.78738200	-1.12432900
H	-0.04719400	0.78528500	-1.83605500
C	-0.98009300	3.62073700	-0.24676400
H	-2.49164000	3.73453100	1.26719700
H	0.44664800	3.19140300	-1.77974100
H	-0.75185400	4.67541800	-0.21547800
C	-2.27219000	-2.65672900	-1.35448300
H	-3.31515100	-2.57919400	-1.06678100
H	-2.19179700	-3.02372200	-2.37084400
H	-1.74596900	-3.33703100	-0.68337900
C	1.70294700	-0.82868900	0.19480300
C	2.83609100	-1.30727800	-0.46039700

C	1.76551100	0.43899200	0.77376700
C	3.99218500	-0.55569200	-0.52949600
H	2.79949800	-2.28315200	-0.92305900
C	2.92097700	1.19077600	0.70274300
H	0.89314600	0.84234200	1.26459400
C	4.04115600	0.69798700	0.05483500
H	4.85737400	-0.94884400	-1.04218200
H	2.94573200	2.17123500	1.15456700
H	4.94399800	1.28768000	0.00313200
H	0.64025100	-2.67689200	-0.10040300

TS-10-ox

E(RmPW+HF-B95) = -826.73645 a.u.

1 imaginary frequency = -481.6917 cm⁻¹

C	0.76199800	0.28083400	-0.69240300
O	0.18404600	0.81189600	1.37439300
C	-1.23915600	-0.83054100	0.89999000
H	-1.45942500	-1.86943100	1.10779100
N	-0.30349100	-0.31578800	1.69258700
C	0.01550500	-0.86480500	-0.82373100
C	0.27325100	-2.25415500	-1.24372900
C	-0.82332100	-1.43921900	-1.88489300
H	-0.02901000	-3.07210600	-0.60245100
H	1.15768000	-2.46575800	-1.83022700
H	-0.66475000	-1.09301600	-2.89645600
H	-1.84849300	-1.71288600	-1.67614600
C	-2.38015000	-0.05606900	0.40368600
C	-3.54045200	-0.76686600	0.10606400
C	-2.38103400	1.32580900	0.22519900
C	-4.67010200	-0.12716000	-0.36538300
H	-3.55757500	-1.83766900	0.25658700
C	-3.51826800	1.96230200	-0.23415800
H	-1.49549200	1.88749200	0.46389500
C	-4.66222600	1.24469600	-0.53764600
H	-5.55684300	-0.70013200	-0.59040200
H	-3.50740000	3.03451800	-0.36061800
H	-5.54201300	1.75199200	-0.90337100
C	0.59228600	-1.20266600	2.40256800
H	1.08517200	-0.61849100	3.16965400
H	0.03649700	-2.01925400	2.85095200
H	1.33676100	-1.58702600	1.70950300

H	0.30351500	1.20033600	-1.02802300
C	2.20230700	0.36852000	-0.46485200
C	2.81159900	1.62167500	-0.50739200
C	3.02102000	-0.74161400	-0.26007300
C	4.17468800	1.76402500	-0.34407700
H	2.19534400	2.49501300	-0.66517400
C	4.38418200	-0.60058800	-0.09411400
H	2.58546200	-1.72743400	-0.22678300
C	4.97175900	0.65221800	-0.13500600
H	4.61705800	2.74844700	-0.37934800
H	4.99422200	-1.47769300	0.06418300
H	6.03805600	0.76006100	-0.00711500

TS-10-mn

E(RmPW+HF-B95) = -826.74359 a.u.

1 imaginary frequency = -468.7789 cm⁻¹

O	-2.43725000	0.81103700	0.54565000
C	-1.00160300	-1.22269800	-0.51881800
C	-1.00171700	1.12678500	-1.13778900
H	-1.38652800	-1.53019100	-1.48449000
H	-0.93172500	1.15113800	-2.21526900
N	-2.23679000	1.18113200	-0.67252900
C	-1.92056300	-1.03507700	0.48991600
C	-2.08563200	-1.41002600	1.89258500
C	-3.19237700	-1.65436300	0.89326200
H	-2.24049800	-0.61970500	2.61277600
H	-1.52292500	-2.25741800	2.25899300
H	-3.37676500	-2.67296600	0.58097500
H	-4.07156700	-1.03361100	0.97584600
C	0.41611300	-1.46850000	-0.31415200
C	1.19088000	-1.93228900	-1.37773200
C	1.05941400	-1.24233900	0.90398200
C	2.54514200	-2.16092800	-1.23592600
H	0.71383200	-2.11567300	-2.33116500
C	2.41310400	-1.47323100	1.04568500
H	0.49183700	-0.86112500	1.73773300
C	3.16744500	-1.93144000	-0.02119200
H	3.11728500	-2.52225500	-2.07804500
H	2.88590900	-1.28268200	1.99796000
H	4.22607300	-2.10892200	0.09327900
C	0.18664400	1.52807100	-0.41446200

C	1.39014500	1.50636100	-1.11798200
C	0.19201600	1.94364100	0.91588000
C	2.56992000	1.89120600	-0.51656800
H	1.39489100	1.17367500	-2.14586000
C	1.37416800	2.34525500	1.50653300
H	-0.73059200	1.94601200	1.47031300
C	2.56463200	2.31509700	0.80060400
H	3.49298200	1.85654400	-1.07433500
H	1.36609300	2.67731900	2.53392800
H	3.48474700	2.61980700	1.27589800
C	-3.34674200	0.91944700	-1.55631900
H	-3.47974900	-0.15916500	-1.64983700
H	-4.23567800	1.35073100	-1.11131400
H	-3.16801200	1.36243600	-2.52992300

TS-10-mx

E(RmPW+HF-B95) = -826.74219 a.u.

1 imaginary frequency = -496.9429 cm⁻¹

O	0.61826600	2.03274200	0.80176600
C	-0.49011800	0.15227200	-0.78894900
C	0.67587000	-0.16166500	1.17860100
H	0.21191300	-0.49894500	-1.28875200
N	0.35606800	1.05251400	1.59223200
C	-0.23461600	1.50501600	-0.84995100
C	-0.91987200	2.74805900	-1.22733600
C	0.45462100	2.41892900	-1.76012200
H	-0.98766500	3.54378600	-0.50104700
H	-1.76181000	2.67340800	-1.90240900
H	0.54972100	2.13194500	-2.79729600
H	1.28102200	2.99372100	-1.36750900
C	-1.79837800	-0.44458900	-0.52393000
C	-1.94546700	-1.82875900	-0.63040200
C	-2.93173800	0.29586200	-0.18541700
C	-3.15908500	-2.44585400	-0.40203500
H	-1.08457100	-2.42409900	-0.90412200
C	-4.14626600	-0.32140900	0.04450100
H	-2.86043400	1.37025900	-0.11153500
C	-4.27100100	-1.69583700	-0.05927900
H	-3.23828800	-3.51902700	-0.49569000
H	-5.00635200	0.27968600	0.30135900
H	-5.22170700	-2.17474800	0.11849100

H	0.18006400	-0.95834000	1.71327400
C	1.94100600	-0.51917000	0.54678500
C	2.22140900	-1.87905600	0.42605300
C	2.87963000	0.40234500	0.08736100
C	3.40037600	-2.31318800	-0.14505100
H	1.50141400	-2.60104800	0.78600000
C	4.06468800	-0.03928600	-0.46841400
H	2.67127800	1.45419300	0.17447500
C	4.32994200	-1.39199800	-0.59424900
H	3.59672800	-3.37108700	-0.23169400
H	4.78778500	0.68461500	-0.81304300
H	5.25524400	-1.72603900	-1.03836300
C	-0.76805600	1.26999900	2.47261300
H	-0.94674100	0.38835700	3.07753700
H	-0.53444000	2.11301600	3.11414900
H	-1.64944800	1.50078400	1.88176200

11-on

E(RmPW+HF-B95) = -826.82673 a.u.

C	1.08678200	-1.17542600	0.44349100
O	0.25642100	-0.81866000	1.51460400
C	-1.26229100	-1.31631200	-0.08841500
H	1.49291000	-2.17406700	0.62576100
N	-0.88534500	-1.63554900	1.29652800
C	2.20353300	-0.18960700	0.31789300
C	3.31542300	-0.50677100	-0.45087500
C	2.15190400	1.04341200	0.94973900
C	4.34668100	0.40029500	-0.60514600
H	3.37862500	-1.47709000	-0.92466200
C	3.18943200	1.94722000	0.80407000
H	1.30220800	1.27625100	1.57177300
C	4.28596700	1.63232700	0.02270800
H	5.20403900	0.14032600	-1.20760400
H	3.14178700	2.90070400	1.30838800
H	5.09463000	2.33840500	-0.08985400
C	0.11230500	-1.26219400	-0.73828600
C	0.44348500	-2.06343800	-1.94787400
C	0.33132200	-0.57984800	-2.04250000
H	-0.33515000	-2.66926700	-2.38758700
H	1.42929500	-2.50447700	-2.00227800
H	1.23706900	-0.00534100	-2.16674300

H	-0.53622900	-0.16344600	-2.53238500
C	-1.83048100	-1.28228600	2.31825400
H	-2.74919200	-1.83268400	2.13206900
H	-1.42623300	-1.58863200	3.27804500
H	-2.05370400	-0.21405400	2.34039600
C	-2.08500400	-0.06714300	-0.24975000
C	-1.51664900	1.19792100	-0.15722800
C	-3.45392300	-0.16783000	-0.44693900
C	-2.30396000	2.32992600	-0.25200700
H	-0.44883400	1.28955600	-0.02652600
C	-4.24476200	0.96335500	-0.54819000
H	-3.90653400	-1.14716600	-0.52625100
C	-3.67013000	2.21657400	-0.44787000
H	-1.84805500	3.30614000	-0.18067800
H	-5.30791900	0.86480400	-0.70839300
H	-4.28166800	3.10252200	-0.52894300
H	-1.83879500	-2.16540100	-0.45349500

11-ox

E(RmPW+HF-B95) = -826.83063 a.u.

C	-1.12441200	0.33819900	-0.73840200
O	-0.75872300	1.65782000	-0.42512900
C	0.98435400	0.50985400	0.39277500
H	-0.99883400	0.17835300	-1.81232000
H	0.81467900	0.80560300	1.43661800
N	0.66078700	1.61739000	-0.49365200
C	-2.54451600	0.09257000	-0.34995000
C	-3.32419800	-0.77048600	-1.10282000
C	-3.08105500	0.66805400	0.79307900
C	-4.62041700	-1.06522200	-0.71763100
H	-2.91543500	-1.20997900	-2.00220200
C	-4.37906300	0.38438500	1.17145700
H	-2.47239300	1.34723800	1.36951600
C	-5.15096600	-0.48672100	0.42019200
H	-5.21791500	-1.73937800	-1.31257600
H	-4.79152400	0.84382900	2.05724500
H	-6.16424000	-0.70844100	0.71929500
C	-0.08388700	-0.50276400	0.00386400
C	0.20519500	-1.89852500	-0.41577900
C	-0.42141000	-1.63038100	0.91136200
H	1.23452700	-2.22303100	-0.44727500

H	-0.42402100	-2.31593200	-1.19007900
H	-1.46263100	-1.87858100	1.05361000
H	0.19830700	-1.75337100	1.78878400
C	2.40158700	0.06113800	0.22863200
C	3.15098200	-0.31217900	1.33265700
C	2.97337800	-0.02146800	-1.03483500
C	4.45089100	-0.76505500	1.18243600
H	2.71421100	-0.24208500	2.31926400
C	4.27348000	-0.46382300	-1.18513000
H	2.38582600	0.27735100	-1.88948500
C	5.01534600	-0.83923500	-0.07697500
H	5.02345700	-1.05242300	2.05142200
H	4.71088400	-0.51808300	-2.17082000
H	6.03059900	-1.18617600	-0.19647700
C	1.11644400	2.89152700	-0.01588100
H	2.20266000	2.87635600	-0.00843400
H	0.77784000	3.66689000	-0.69543900
H	0.74789300	3.10836000	0.99164800

11-mn

$E(\text{RmPW+HF-B95}) = -826.82399 \text{ a.u.}$

O	-2.39733200	0.30821400	0.65849800
C	-0.76863400	-0.89459500	-0.56037200
C	-0.95895100	0.57926900	-1.03318200
H	-1.16212500	-1.52436900	-1.35779200
H	-0.91494500	0.61616500	-2.11991400
N	-2.31551400	0.89098400	-0.61749600
C	-1.75395400	-0.94258700	0.59616400
C	-1.56525800	-1.61526000	1.89688900
C	-2.56594400	-2.14911500	0.91412100
H	-1.94598000	-1.09543500	2.76297700
H	-0.65335600	-2.16953500	2.05692300
H	-2.33350700	-3.07172600	0.40172500
H	-3.61137400	-1.99298300	1.13165600
C	0.62678000	-1.36090500	-0.28523800
C	1.22695600	-2.26150000	-1.15341900
C	1.35230100	-0.92059800	0.81699100
C	2.51743500	-2.71181500	-0.93828600
H	0.67200100	-2.61790100	-2.01041800
C	2.63912100	-1.37176900	1.03804100
H	0.90261100	-0.21370700	1.49872900

C	3.22701600	-2.26848700	0.16145400
H	2.96363300	-3.41384400	-1.62654300
H	3.18727700	-1.01814700	1.89821200
H	4.23228000	-2.62010000	0.33808800
C	0.02685000	1.57243500	-0.48175600
C	1.29196700	1.66266000	-1.04534100
C	-0.29845400	2.40711600	0.57635500
C	2.21885000	2.56633800	-0.56105400
H	1.55674800	1.00922200	-1.86523700
C	0.63034800	3.31025200	1.06311400
H	-1.28245500	2.34532500	1.01119900
C	1.89004100	3.39300500	0.49858800
H	3.19801200	2.62394400	-1.01219000
H	0.36434800	3.95675700	1.88614500
H	2.61143600	4.10074100	0.87872100
C	-3.33274700	0.31131200	-1.46394200
H	-3.23566900	-0.77019500	-1.59654900
H	-4.30058300	0.52188500	-1.02106300
H	-3.28343600	0.79675300	-2.43495400

11-mx

E(RmPW+HF-B95) = -826.82559 a.u.

O	-0.09015200	2.71387800	-0.57533300
C	-0.51797700	0.47500900	-0.53601100
C	0.64560900	0.74878900	0.42754100
H	-0.09445400	0.34158700	-1.53159700
N	0.94129800	2.16958100	0.24233900
C	-1.16414600	1.83325200	-0.51907500
C	-2.37640200	2.21755400	0.26145700
C	-2.38143900	2.23537600	-1.24201300
H	-2.33864000	3.17262200	0.76190200
H	-2.95711200	1.45584200	0.75820700
H	-2.93678800	1.46382100	-1.75449200
H	-2.36342800	3.19399500	-1.73660500
C	-1.36993600	-0.71122100	-0.21126600
C	-1.66820000	-1.63064900	-1.20711300
C	-1.88845700	-0.92915400	1.06127000
C	-2.46303400	-2.73291800	-0.94777800
H	-1.26389300	-1.48114600	-2.19785700
C	-2.68260200	-2.02927700	1.32513200
H	-1.67153300	-0.23127200	1.85689500

C	-2.97355600	-2.93572300	0.32044100
H	-2.67862200	-3.43593100	-1.73810000
H	-3.07434600	-2.17964300	2.31988600
H	-3.59134100	-3.79625300	0.52751300
H	0.28375000	0.58123200	1.44656400
C	1.83976000	-0.13161200	0.19268400
C	1.85021600	-1.41786600	0.71431200
C	2.91224500	0.29635600	-0.57325600
C	2.91312600	-2.26665500	0.46802400
H	1.01669000	-1.75590200	1.31466800
C	3.97827900	-0.55213600	-0.81543200
H	2.89993800	1.30330600	-0.96004000
C	3.98173600	-1.83495500	-0.29820000
H	2.90927700	-3.26481300	0.87964000
H	4.81176900	-0.20703700	-1.40904600
H	4.81554700	-2.49449100	-0.48638000
C	0.94391000	2.89654000	1.48558200
H	1.74549600	2.49890500	2.10372000
H	1.14771800	3.94336700	1.28478900
H	-0.00269600	2.80947600	2.02882300

8

E(RmPW+HF-B95) = -842.37274 a.u.

C	-1.12266100	0.11009100	-0.58946800
C	-0.17560400	-0.12521300	0.29543000
C	0.30327600	-0.45173000	1.61066500
C	1.28510500	-0.14237700	0.48245100
H	0.27368500	-1.48625900	1.92538500
H	0.26303700	0.29508200	2.39264100
C	-2.55993900	0.03666200	-0.35265100
C	-3.42980800	0.32351800	-1.39903200
C	-3.09839200	-0.31325100	0.88339200
C	-4.79881200	0.26341000	-1.22157300
H	-3.02322300	0.59513300	-2.36276600
C	-4.46470700	-0.37363400	1.06090700
H	-2.43579600	-0.54059200	1.70416700
C	-5.32107600	-0.08591900	0.00985500
H	-5.45772900	0.48897800	-2.04629600
H	-4.86689100	-0.64778000	2.02451200
H	-6.38982100	-0.13506100	0.15264200
H	-0.81766000	0.37764400	-1.59258000

C	1.93264900	1.20210100	0.53200700
O	1.94451200	1.91579600	1.49511700
O	2.43024800	1.54630200	-0.64667800
C	2.03270500	-1.31927400	-0.03528000
O	1.54779800	-2.40743600	-0.17256900
O	3.30851500	-1.04626900	-0.26902900
C	3.04192000	2.82135400	-0.68468700
H	3.86343800	2.86955600	0.02343200
H	3.40547000	2.94530800	-1.69682400
H	2.32139400	3.59585400	-0.44004600
C	4.07491200	-2.14451800	-0.72754600
H	5.07465600	-1.76140900	-0.88696600
H	4.08203000	-2.93743800	0.01386800
H	3.66142400	-2.53347800	-1.65272100

MC-8-on

$E(\text{RmPW+HF-B95}) = -1282.33217 \text{ a.u.}$

C	0.07730800	1.08044200	0.37947800
O	0.88855000	-1.09629300	2.66268600
C	0.67021800	-2.17191800	0.65693700
H	-0.04505400	-2.70436400	0.05715900
N	0.25118300	-1.79681600	1.82302100
C	-0.78805400	0.85997400	-0.59103700
C	-1.24178300	0.94879100	-1.95117400
C	-2.19999900	0.51395700	-0.84105100
H	-0.96097500	0.16719200	-2.64473800
H	-1.45327200	1.91918200	-2.38094800
C	1.94465500	-1.84445800	0.06648400
C	2.05220200	-2.02753300	-1.31311000
C	3.04890900	-1.37047700	0.77357900
C	3.22573200	-1.73535500	-1.97481900
H	1.19255300	-2.38518400	-1.86216200
C	4.22466800	-1.09279600	0.10427000
H	2.96352900	-1.21276300	1.83334700
C	4.31899300	-1.26774200	-1.26500400
H	3.28990500	-1.87386300	-3.04361900
H	5.07154500	-0.71727700	0.65847100
H	5.24016200	-1.03705900	-1.77872600
C	-1.10537300	-2.12409600	2.23457200
H	-1.58350200	-2.78318800	1.51988500
H	-1.04436300	-2.58510600	3.21372300

H	-1.65675400	-1.19106200	2.31693400
C	1.43343400	1.59139800	0.23060100
C	2.17055700	1.85467300	1.38039500
C	2.01317900	1.83594800	-1.01061300
C	3.44320400	2.38439200	1.29392800
H	1.74011200	1.61684800	2.34197700
C	3.28409700	2.36577200	-1.09586500
H	1.45648200	1.61574400	-1.90872200
C	4.00159700	2.64667100	0.05562300
H	4.00179900	2.58886700	2.19491400
H	3.72111900	2.55586200	-2.06462600
H	4.99523400	3.06330800	-0.01433700
H	-0.23198700	0.87692500	1.39549200
C	-3.17918200	1.53770600	-0.37100000
O	-3.47972300	2.52799400	-0.97458700
O	-3.62148900	1.25220100	0.84710800
C	-2.60895200	-0.91058000	-0.88369300
O	-1.87453400	-1.82374200	-1.15643500
O	-3.90328300	-1.06698100	-0.64787500
C	-4.53207100	2.19445700	1.38200300
H	-5.41358500	2.26839300	0.75254000
H	-4.79633600	1.82719500	2.36544400
H	-4.06673600	3.17282100	1.45096300
C	-4.37675000	-2.39808000	-0.72534000
H	-5.44305000	-2.34292000	-0.54850400
H	-4.17092800	-2.81891200	-1.70432100
H	-3.89987900	-3.01522200	0.03053700

TS-8-on

E(RmPW+HF-B95) = -1282.30146 a.u.

1 imaginary frequency = -417.7525 cm⁻¹

C	0.27125300	1.16294100	0.43842600
O	0.95431600	0.20558300	2.20470100
C	0.14387800	-1.59477400	1.15604800
H	-0.70301800	-2.25597400	1.10826000
N	0.14317700	-0.77912600	2.19586700
C	-0.34170900	0.11276500	-0.20349900
C	-0.52463900	-0.26840900	-1.59066100
C	-1.74081900	0.04145700	-0.73210800
H	-0.41579800	-1.30855200	-1.86821300
H	-0.31143400	0.45229100	-2.36923900

C	1.33850100	-2.05918800	0.45934100
C	1.14837500	-3.05875300	-0.49463800
C	2.62910300	-1.60418200	0.71522200
C	2.22026200	-3.58618600	-1.18630000
H	0.14532400	-3.41551900	-0.68409700
C	3.69825700	-2.15027900	0.03046000
H	2.78120300	-0.82462500	1.44056400
C	3.50192500	-3.13405900	-0.92299900
H	2.05596100	-4.35700400	-1.92404100
H	4.69561600	-1.79429200	0.24025500
H	4.34364600	-3.54786500	-1.45757000
C	-1.09709600	-0.54039900	2.89877900
H	-1.67710000	-1.45408800	2.96713700
H	-0.85381800	-0.17525200	3.88925300
H	-1.66281500	0.22292800	2.35983100
C	1.54030300	1.76748100	0.05388000
C	1.92992300	2.94115100	0.69292400
C	2.37029800	1.24225800	-0.93280500
C	3.10685100	3.57835500	0.35803200
H	1.29792900	3.34815800	1.46900100
C	3.54969900	1.87986100	-1.26707700
H	2.09540100	0.32195500	-1.42457200
C	3.92260100	3.04941000	-0.62695500
H	3.38988700	4.48758100	0.86680900
H	4.18298500	1.45851500	-2.03340100
H	4.84436600	3.54396000	-0.89366400
H	-0.34265700	1.77248400	1.08643900
C	-2.37290100	1.37956500	-0.92142100
O	-2.36170700	2.02098600	-1.93253500
O	-2.90123600	1.81815800	0.22066200
C	-2.64716500	-1.09998500	-0.46844500
O	-2.30767600	-2.25265800	-0.38143400
O	-3.91619900	-0.72112000	-0.39588000
C	-3.51769600	3.08885700	0.13763900
H	-4.32397100	3.07178900	-0.58919100
H	-3.90369200	3.29806400	1.12740100
H	-2.79504400	3.84331000	-0.15788600
C	-4.84916700	-1.76990500	-0.21620600
H	-5.82307700	-1.29823400	-0.19473500
H	-4.78464200	-2.47903100	-1.03541700
H	-4.65770400	-2.29221100	0.71606800

TS-8-ox

E(RmPW+HF-B95) = -1282.29169 a.u.

1 imaginary frequency = -413.7801 cm⁻¹

C	1.39619300	-0.09877700	0.53598800
O	1.31531000	-2.23907900	0.42913300
C	-0.40675300	-1.77153400	-0.89849200
H	-0.72486900	-1.73075200	-1.93084700
N	0.76577500	-2.35785900	-0.70837100
C	0.48769000	0.20509600	-0.45110500
C	0.54717200	1.13786600	-1.57162700
C	-0.55181600	1.25959600	-0.52414200
H	0.18202800	0.85005400	-2.54796100
H	1.31329000	1.90333800	-1.56704700
C	-1.49568000	-1.87379600	0.08034400
C	-2.77599400	-2.06143600	-0.43804400
C	-1.33238500	-1.86727000	1.46286800
C	-3.86166200	-2.24652700	0.39441800
H	-2.91389100	-2.05882100	-1.50917000
C	-2.42415900	-2.04560400	2.29223100
H	-0.35044300	-1.74352800	1.88063400
C	-3.68944500	-2.23590600	1.76694000
H	-4.84206800	-2.40359600	-0.03047500
H	-2.28044700	-2.03721700	3.36204300
H	-4.53518300	-2.37692800	2.42284600
C	1.63100300	-2.62431300	-1.84287800
H	2.61095500	-2.84529300	-1.44184500
H	1.25312000	-3.47113600	-2.40851800
H	1.68677300	-1.75242000	-2.49090800
H	1.04305500	-0.09294200	1.55447900
C	2.84747700	-0.02986200	0.38539600
C	3.64233600	-0.05826100	1.52968100
C	3.48681400	0.09323600	-0.84685400
C	5.01751900	0.02675400	1.44835500
H	3.16507600	-0.14758500	2.49451000
C	4.86301100	0.17383900	-0.92948500
H	2.90582800	0.12217900	-1.75434200
C	5.63780000	0.14124100	0.21653100
H	5.60820900	0.00324300	2.35189500
H	5.33374400	0.26630000	-1.89712500
H	6.71316600	0.20647600	0.15043100
C	-1.91251500	0.95385500	-1.04955200

O	-2.12757800	0.41447400	-2.10305300
O	-2.86400500	1.35036500	-0.22165300
C	-0.45985400	2.41971600	0.41361600
O	0.13135300	2.43600900	1.45536300
O	-1.09062600	3.47999000	-0.08402200
C	-4.18731800	1.20880000	-0.70065100
H	-4.82848300	1.56350500	0.09615300
H	-4.32621100	1.80719100	-1.59630500
H	-4.39998700	0.17034900	-0.92553200
C	-1.07146200	4.62508100	0.74429300
H	-1.63078600	5.38553600	0.21387000
H	-1.53580000	4.40871800	1.70175100
H	-0.05095800	4.95351000	0.91691800

TS-8-mn

E(RmPW+HF-B95) = -1282.29716 a.u.

1 imaginary frequency = -435.6845 cm⁻¹

O	-0.65696300	-1.84317100	-0.20116900
C	0.11051500	0.63117000	0.58974400
C	0.91263700	-1.52621400	1.35712500
H	-0.32381100	0.85975900	1.55616300
H	1.06492700	-1.41642000	2.42023800
N	-0.27780900	-1.98224500	1.02266900
C	-0.71864700	0.06642100	-0.35294500
C	-1.11208300	0.39322900	-1.71297700
C	-2.16701400	0.30300400	-0.63925300
H	-1.17920700	-0.40420300	-2.43885000
H	-0.85033400	1.37082300	-2.09138300
C	1.35126600	1.31631900	0.26672100
C	1.95802200	2.12798600	1.22524600
C	1.98755300	1.18297000	-0.96841600
C	3.14518300	2.78301600	0.96301100
H	1.48288800	2.24466800	2.18978900
C	3.17492300	1.83759500	-1.22860500
H	1.56214300	0.53590500	-1.71944600
C	3.76276100	2.64216800	-0.26742100
H	3.58951400	3.40793400	1.72381400
H	3.65057300	1.70943200	-2.18973000
H	4.69163700	3.15164300	-0.47422800
C	2.10778700	-1.60508500	0.54359300
C	3.29616300	-1.16846500	1.12819800

C	2.14049200	-2.10059700	-0.75902200
C	4.48678200	-1.21716700	0.43408900
H	3.27827800	-0.77740100	2.13518700
C	3.33969700	-2.16339900	-1.44126400
H	1.22822300	-2.43246800	-1.22299200
C	4.51180500	-1.71685500	-0.85603800
H	5.39368900	-0.86298400	0.89919200
H	3.35577300	-2.55922600	-2.44556200
H	5.44157300	-1.75937800	-1.40284400
C	-1.35413200	-1.96721100	1.98656100
H	-1.86151700	-1.00181400	1.94676000
H	-2.05848600	-2.74451300	1.71404000
H	-0.96518900	-2.15425200	2.98121300
C	-3.10377500	-0.85295200	-0.78973000
O	-3.14412900	-1.55976100	-1.75587400
O	-3.90502800	-1.00552100	0.25650200
C	-2.66384200	1.52081700	0.06023800
O	-3.09502100	1.52552700	1.18041000
O	-2.51437200	2.61874000	-0.67056700
C	-4.82811000	-2.06969200	0.13469000
H	-5.41436400	-2.05878200	1.04492600
H	-5.46522000	-1.92257600	-0.73205500
H	-4.30579100	-3.01534700	0.02276400
C	-2.84840600	3.82258100	-0.00681200
H	-2.68071700	4.61413200	-0.72598900
H	-3.88652600	3.80555200	0.30999600
H	-2.21675400	3.96089000	0.86550400

TS-8-mx

E(RmPW+HF-B95) = -1282.29604 a.u.

1 imaginary frequency = -491.3184 cm⁻¹

O	-0.49637800	0.22921200	1.88370700
C	0.99473700	-0.28769600	-0.31364100
C	1.17629400	1.48433000	1.09316600
H	0.75438800	0.36993600	-1.13485100
N	0.63397900	0.80229900	2.09245600
C	-0.06618100	-0.88750600	0.32246600
C	-0.49977200	-2.21964500	0.69980700
C	-1.43571200	-1.30364300	-0.07814000
H	-0.79585900	-2.41672500	1.71829500
H	-0.09092800	-3.05164800	0.14161300

C	2.36517300	-0.80584800	-0.32391000
C	3.30887200	-0.17248400	-1.13334100
C	2.78943000	-1.90449900	0.42177600
C	4.61758000	-0.60783400	-1.18895200
H	2.99676700	0.67368500	-1.73020400
C	4.10001700	-2.33957300	0.36746500
H	2.08586900	-2.43538700	1.04428000
C	5.02454100	-1.69452500	-0.43428800
H	5.32295700	-0.09823500	-1.82855600
H	4.39891700	-3.19639900	0.95324900
H	6.04661600	-2.03849800	-0.47644200
H	2.23438600	1.66372500	1.21736100
C	0.48557700	2.45475600	0.25203900
C	1.29132800	3.32480900	-0.48068800
C	-0.89755200	2.56122100	0.14332100
C	0.73305700	4.27979600	-1.30575200
H	2.36680700	3.24862400	-0.39716400
C	-1.44930800	3.52563000	-0.67760600
H	-1.53373400	1.88727200	0.68729300
C	-0.64329800	4.38429000	-1.40522600
H	1.37209400	4.94547400	-1.86582700
H	-2.52357300	3.59276800	-0.75555800
H	-1.08524700	5.12935100	-2.04927700
C	1.47512100	0.10744700	3.03940200
H	2.41035300	0.63797800	3.17577200
H	0.94183700	0.05037000	3.98175300
H	1.66602500	-0.89696400	2.67039700
C	-1.62276400	-1.67052500	-1.50913300
O	-0.73601400	-2.03176200	-2.23197500
O	-2.89369600	-1.61499500	-1.88076600
C	-2.60181700	-0.68070100	0.62051900
O	-3.19756300	0.27661300	0.21372900
O	-2.89736000	-1.29573500	1.75761800
C	-3.13642800	-1.98189100	-3.22461100
H	-2.82682400	-3.00767300	-3.40053000
H	-4.20325800	-1.87306000	-3.37235600
H	-2.58934700	-1.33071300	-3.89919200
C	-3.88321700	-0.64838400	2.53592000
H	-4.03481800	-1.27461200	3.40617200
H	-3.53213600	0.33588900	2.83160900
H	-4.80512700	-0.54305700	1.97290800

9-on

$E(\text{RmPW+HF-B95}) = -1282.37986 \text{ a.u.}$

C	-0.19610600	-1.41393900	0.38141400
O	-0.19591700	-1.20700200	1.76881400
C	-0.22229900	0.91853800	0.90582200
H	0.60731800	1.45563200	1.36574800
N	-0.87649600	0.03749100	1.87980900
C	0.33350800	-0.08126500	-0.11428600
C	0.65229200	0.22459800	-1.51287900
C	1.79738100	-0.03701900	-0.57515600
H	0.52248400	1.24856200	-1.83302300
H	0.50869600	-0.53822800	-2.26327200
C	-1.21050500	1.91453300	0.35293200
C	-0.75856000	3.11671600	-0.17732900
C	-2.57430300	1.65393200	0.36002800
C	-1.65137700	4.03057400	-0.70772900
H	0.29836500	3.33092000	-0.16863200
C	-3.46521000	2.57234900	-0.16649500
H	-2.92583300	0.73021700	0.78973000
C	-3.00819400	3.76096900	-0.70604900
H	-1.28426300	4.96046100	-1.11609100
H	-4.52306000	2.35570500	-0.15191000
H	-3.70571700	4.47629700	-1.11568600
C	-0.70945500	0.47301400	3.23601300
H	-1.19415900	1.44052200	3.33469200
H	-1.19875700	-0.23342400	3.89910400
H	0.34421300	0.56442800	3.51665100
C	-1.56390200	-1.82053800	-0.11725700
C	-2.20546100	-2.85059000	0.55937900
C	-2.18910000	-1.25500200	-1.21533600
C	-3.43840600	-3.31027500	0.14258600
H	-1.73006100	-3.27739600	1.43020500
C	-3.42697600	-1.71401600	-1.63510400
H	-1.73137400	-0.43313600	-1.74034400
C	-4.05292400	-2.74439200	-0.96263700
H	-3.92269300	-4.11093300	0.68138500
H	-3.90209900	-1.25612100	-2.48953700
H	-5.01637400	-3.10362800	-1.29158900
H	0.49666800	-2.23237900	0.20569600
C	2.45527600	-1.36947600	-0.71360900
O	2.28958700	-2.11500400	-1.63953200

O	3.17458600	-1.67666700	0.35405600
C	2.66639100	1.12392300	-0.27894100
O	2.27562300	2.23629200	-0.03919900
O	3.95255800	0.82744900	-0.39217300
C	3.82252700	-2.93326300	0.29759100
H	4.51444400	-2.96428800	-0.53851900
H	4.35333800	-3.03473000	1.23533500
H	3.09555300	-3.73120000	0.18115300
C	4.83855200	1.91407700	-0.19598400
H	5.83292900	1.51258600	-0.34216800
H	4.63402600	2.70319000	-0.91274000
H	4.73144500	2.31326200	0.80757800

9-ox

E(RmPW+HF-B95) = -1282.38565 a.u.

C	-1.26699300	-0.72147300	-0.68560200
O	-0.79952700	-2.02740800	-0.92926000
C	0.57006600	-1.39164900	0.73924200
H	0.75365000	-1.50402800	1.80442100
N	-0.30640900	-2.48724300	0.32621100
C	-0.36859100	-0.22940500	0.46618900
C	-0.89848400	0.61368700	1.55643300
C	0.09819700	1.20077100	0.60041500
H	-0.52292800	0.45462700	2.55607600
H	-1.92169700	0.94904100	1.47710400
C	1.88909700	-1.32282000	0.01408800
C	3.01613700	-1.86816300	0.61413100
C	2.01263300	-0.75875500	-1.24917800
C	4.23702400	-1.87082200	-0.03391400
H	2.93337700	-2.28821500	1.60691100
C	3.23468200	-0.75567000	-1.89903100
H	1.15730700	-0.29574600	-1.71897000
C	4.34781200	-1.31557500	-1.29734400
H	5.10213200	-2.30023800	0.44870500
H	3.31547100	-0.31165900	-2.87971600
H	5.29917600	-1.31357300	-1.80780100
C	0.33148800	-3.74613500	0.05557500
H	-0.43253200	-4.46026300	-0.23543100
H	1.08281200	-3.67740600	-0.73253600
H	0.80239000	-4.08947200	0.97329100
H	-1.07714400	-0.15706200	-1.59213100

C	-2.73549700	-0.67489800	-0.37102200
C	-3.51495500	0.36252400	-0.85847200
C	-3.32392600	-1.65186100	0.42096300
C	-4.86436300	0.43072600	-0.55135100
H	-3.06406300	1.11529200	-1.48929000
C	-4.67093900	-1.58678700	0.71912300
H	-2.71104700	-2.45432200	0.80062100
C	-5.44526900	-0.54371600	0.23773700
H	-5.46221200	1.24181200	-0.93955900
H	-5.12115900	-2.35364400	1.33184400
H	-6.49760500	-0.49482300	0.47408100
C	1.47048000	1.37974600	1.15117800
O	1.85608600	0.88459700	2.17423500
O	2.23131500	2.09905200	0.34194400
C	-0.32665500	2.24424400	-0.37520100
O	-0.62666100	2.06495900	-1.52465000
O	-0.33780400	3.43806000	0.19918500
C	3.59961500	2.15688600	0.70394600
H	4.07480700	2.78691200	-0.03681900
H	3.71192100	2.57931700	1.69721700
H	4.02543100	1.15763700	0.68603300
C	-0.66660200	4.51406900	-0.65908200
H	-0.61036100	5.40680600	-0.04966600
H	0.03801700	4.56827900	-1.48317100
H	-1.66789600	4.38779600	-1.05925000

9-mn

E(RmPW+HF-B95) = -1282.38122 a.u.

O	-0.41413900	-1.85913200	-0.39786400
C	0.26585100	0.14529200	0.63681300
C	0.99245200	-1.12043400	1.17639800
H	-0.38655200	0.47963400	1.44118100
H	1.10335300	-1.03523500	2.25530200
N	0.04222700	-2.18409700	0.89801000
C	-0.60733300	-0.48541000	-0.43558100
C	-1.01061400	0.09873100	-1.71573500
C	-2.04148500	0.03824500	-0.62845600
H	-1.17768600	-0.59846800	-2.52321100
H	-0.63458500	1.07574400	-1.97614000
C	1.08162500	1.32511700	0.21297600
C	1.04541300	2.48189600	0.97866700

C	1.87121400	1.30749200	-0.93110600
C	1.78996200	3.59378200	0.62458600
H	0.42376800	2.50666500	1.86382700
C	2.61116400	2.41733100	-1.28991300
H	1.90929200	0.41316500	-1.53590400
C	2.57546500	3.56276800	-0.51213700
H	1.75269200	4.48327100	1.23541800
H	3.22239200	2.38629600	-2.17910300
H	3.15666900	4.42758600	-0.79439900
C	2.33937500	-1.40273800	0.57267200
C	3.43741700	-0.66800800	0.99807300
C	2.51672500	-2.37950500	-0.39494100
C	4.69077600	-0.89748000	0.46380700
H	3.30681600	0.09754800	1.75035700
C	3.77212500	-2.60851700	-0.93117900
H	1.66798700	-2.95940900	-0.71848200
C	4.86096200	-1.86913500	-0.50666500
H	5.53470300	-0.31824500	0.80690100
H	3.89847000	-3.37365400	-1.68254000
H	5.83898300	-2.05222700	-0.92573000
C	-1.09956800	-2.20465500	1.79013100
H	-1.65686300	-1.26324400	1.83049200
H	-1.76776300	-2.99232000	1.45529500
H	-0.74294200	-2.45594300	2.78501900
C	-3.08108800	-1.00814000	-0.77457000
O	-3.05594500	-1.85964800	-1.61812800
O	-4.02706600	-0.91685900	0.15090000
C	-2.36731600	1.25659200	0.15997700
O	-2.66119700	1.25484900	1.32488700
O	-2.23929500	2.36508500	-0.55749800
C	-5.02975300	-1.91120200	0.07019500
H	-5.73047900	-1.68896600	0.86475800
H	-5.52191600	-1.87791200	-0.89699400
H	-4.59578000	-2.89727800	0.20674600
C	-2.47034500	3.56818800	0.14993300
H	-2.35326400	4.36422200	-0.57407300
H	-3.47121800	3.57345400	0.56987000
H	-1.74868400	3.67837800	0.95330200

9-mx

E(RmPW+HF-B95) = -1282.38681 a.u.

O	-0.06052600	-1.30041200	-1.47249300
C	-1.03621600	0.02117500	0.14446100
C	-0.75560700	0.85576000	-1.12611800
H	-0.73302100	0.56575300	1.02896200
N	0.20420900	0.04584900	-1.88021300
C	-0.13860600	-1.16766100	-0.10682700
C	0.02128000	-2.36115900	0.70563800
C	1.18481600	-1.39576600	0.65980200
H	0.16542100	-3.29962000	0.19684300
H	-0.51280300	-2.38288400	1.64326100
C	-2.46612800	-0.40884600	0.30795300
C	-3.09153200	-0.26176100	1.53700100
C	-3.16898800	-0.99987600	-0.73502500
C	-4.39774100	-0.68127400	1.71849200
H	-2.54375100	0.17941000	2.35735100
C	-4.47210600	-1.42150900	-0.55460000
H	-2.68390400	-1.14332700	-1.69009900
C	-5.09261100	-1.25976000	0.67256400
H	-4.87207500	-0.55516500	2.68013400
H	-5.00545500	-1.87932200	-1.37422800
H	-6.11232000	-1.58542700	0.81205900
H	-1.68832800	0.98018900	-1.68423300
C	-0.16184400	2.19935800	-0.82070600
C	-0.93393400	3.34657200	-0.89707600
C	1.15932100	2.29206500	-0.39900000
C	-0.40150400	4.57571600	-0.54783300
H	-1.96057300	3.27745400	-1.22870500
C	1.68897300	3.52017000	-0.05091900
H	1.76957100	1.39980500	-0.37075200
C	0.91061300	4.66431200	-0.12218100
H	-1.01219000	5.46369600	-0.61252700
H	2.71817300	3.58534700	0.26945200
H	1.32889300	5.62241000	0.14752500
C	0.00792300	0.08925200	-3.29975000
H	0.17755800	1.11319300	-3.62050000
H	0.73765800	-0.55263800	-3.78278700
H	-1.00030800	-0.21999500	-3.59419600
C	1.38425400	-0.59237200	1.88595000
O	0.50759900	-0.40964900	2.69414800
O	2.59989400	-0.09455500	2.01399400
C	2.34133200	-1.67678500	-0.23615200
O	3.18186700	-0.88145300	-0.54451300

O	2.31888200	-2.92404100	-0.69735000
C	2.79141500	0.72659500	3.15008900
H	2.54459600	0.18678100	4.05871700
H	3.83804600	1.00227800	3.13859000
H	2.16379700	1.61022900	3.08074300
C	3.32157400	-3.21647500	-1.64939000
H	3.15402900	-4.24243900	-1.95216700
H	3.23981500	-2.54778300	-2.50084200
H	4.30786400	-3.10439500	-1.20966100