**Ab initio Investigation of the Structures and Energies of Spiropyran and Merocyanine Isomers**

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# Supplementary/Supporting Information

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | B97XD | -747.306489 | -747.306999 | -747.279174 | -747.277879 | -747.277162 | -747.276485 |
|  | MP2 | -745.253451 | -745.254087 | -745.220178 | -745.217577 | -745.216784 | -745.217246 |
| BIPS | B97XD | -865.220929 | -865.220570 | -865.192337 | -865.190721 | -865.188084 | -865.188276 |
|  | MP2 | -862.804215 | -862.804263 | -862.770916 | -862.767842 | -862.765579 | -862.767096 |
| nitroBIPS | B97XD | -1069.679261 | -1069.678858 | -1069.654761 | -1069.652962 | -1069.650160 | -1069.650872 |
|  | MP2 | -1066.832713 | -1066.832682 | -1066.801958 | -1066.798630 | -1066.796109 | -1066.798205 |
| dinitroBIPS | B97XD | -1274.123666 | --- | -1274.101777 | -1274.099355 | -1274.096757 | -1274.097795 |
|  | MP2 | -1270.85126 | -1270.850339 | -1270.821810 | -1270.817399 | -1270.814983 | -1270.817869 |

**S1: Gas phase electronic energies (in Eh), at B97XD and MP2 optimized geometries, with cc-pvdz basis. Note : for dinitroBIPS with B97XD only closed structure A exists.**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **Method** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | B97XD | -1.3 | 71.7 | 75.1 | 77.0 | 78.8 |
|  | MP2 | -1.7 | 87.4 | 94.2 | 96.3 | 95.1 |
| BIPS | B97XD | 0.9 | 75.1 | 79.3 | 86.2 | 85.7 |
|  | MP2 | -0.1 | 87.4 | 95.5 | 101.4 | 97.5 |
| nitroBIPS | B97XD | 1.1 | 64.3 | 69.0 | 76.4 | 74.5 |
|  | MP2 | 0.1 | 80.7 | 89.5 | 96.1 | 90.6 |
| dinitroBIPS | B97XD | --- | 57.5 | 63.8 | 70.6 | 67.9 |
|  | MP2 | 2.4 | 77.3 | 88.9 | 95.2 | 87.7 |

**S2: Electronic energies (kJ/mol) relative to the closed A form. For dinitroBIPS with B97XD closed form B does not exist**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Molecule | Method | Closed A | Closed B | TTC | TTT | CTT | CTC |
| SP0 | B97XD | -747.094030 | -747.094530 | -747.071639 | -747.070247 | -747.069814 | -747.069170 |
|  | MP2 | -745.043392 | -745.043981 | -745.015536 | -745.013613 | -745.013167 | -745.013529 |
| BIPS | B97XD | -864.928619 | -864.928626 | -864.904663 | -864.903583 | -864.901032 | -864.900959 |
|  | MP2 | -862.514077 | -862.513941 | -862.486752 | -862.484517 | -862.481225 | -862.482307 |
| nitroBIPS | B97XD | -1069.388163 | -1069.387804 | -1069.367802 | -1069.367066 | -1069.364150 | -1069.364139 |
|  | MP2 | -1066.544140 | -1066.543950 | -1066.518922 | -1066.516311 | -1066.514365 | -1066.512781 |
| dinitroBIPS | B97XD | -1273.833312 | -1273.833312 | -1273.816156 | -1273.814593 | -1273.811375 | -1273.812239 |
|  | MP2 | -1270.563575 | -1270.563284 | -1270.540025 | -1270.536430 | -1270.532815 | -1270.535193 |

**S3: Total energies (in Eh) including free energies in gas phase**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | B97XD | -1.3 | 58.8 | 62.4 | 63.6 | 65.3 |
|  | MP2 | -1.5 | 73.1 | 78.2 | 79.4 | 78.4 |
| BIPS | B97XD | 0.0 | 62.9 | 65.7 | 72.4 | 72.6 |
|  | MP2 | 0.4 | 71.7 | 77.6 | 86.3 | 83.4 |
| nitroBIPS | B97XD | 0.9 | 53.5 | 55.4 | 63.0 | 63.1 |
|  | MP2 | 0.5 | 66.2 | 73.1 | 78.2 | 82.3 |
| dinitroBIPS | B97XD | 0.0 | 45.0 | 49.1 | 57.6 | 55.3 |
|  | MP2 | 0.8 | 61.8 | 71.3 | 80.8 | 74.5 |

**S4: Total energy differences (in kJ/mol) including free energy in gas phase. Open forms all lowered.**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Molecule | Method | Closed A | Closed B | TTC | TTT | CTT | CTC |
| SP0 | B97XD | -747.314578 | -747.315344 | -747.297226 | -747.296421 | -747.294064 | -747.294461 |
|  | MP2 | -745.2608878 | -745.261803 | -745.235102 | -745.233265 | -745.230632 | -745.230632 |
| BIPS | B97XD | -865.2280201 | -865.227552 | -865.207584 | -865.206647 | -865.203629 | -865.204256 |
|  | MP2 | -862.8106723 | -862.810667 | -862.783354 | -862.781309 | -862.778332 | -862.780239 |
| nitroBIPS | B97XD | -1069.689906 | -1069.689906 | -1069.675773 | -1069.674190 | -1069.671404 | -1069.672913 |
|  | MP2 | -1066.84147 | -1066.841328 | -1066.819218 | -1066.816371 | -1066.813545 | -1066.816500 |
| dinitroBIPS | B97XD | -1274.138565 | -1274.138565 | -1274.130812 | -1274.129355 | -1274.126845 | -1274.128409 |
|  | MP2 | -1270.862745 | -1270.861823 | -1270.845684 | -1270.842436 | -1270.840158 | -1270.843382 |

**S5: Electronic energies (in Eh) in water at B97XD and MP2 optimiaed geometries using cc-pvdz basis**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **SPA** | **SPB** | **TTC** | **TTT** | **CTT** | **CTC** |
| 0.0 | -2.0 | 45.6 | 47.7 | 53.9 | 52.8 |
| 0.0 | -2.4 | 67.7 | 72.5 | 79.4 | 79.4 |
| 0.0 | 1.2 | 53.7 | 56.1 | 64.0 | 62.4 |
| 0.0 | 0.0 | 71.7 | 77.1 | 84.9 | 79.9 |
| 0.0 | 0.0 | 37.1 | 41.3 | 48.6 | 44.6 |
| 0.0 | 0.4 | 58.4 | 65.9 | 73.3 | 65.6 |
| 0.0 | 0.0 | 20.4 | 24.2 | 30.8 | 26.7 |
| 0.0 | 2.4 | 44.8 | 53.3 | 59.3 | 50.8 |

**S6: Differences in the electronic energies (kJ/mol), in water, relative to closed form A**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | B97XD | -21.2 | -21.9 | -47.4 | -48.7 | -44.4 | -47.2 |
|  | MP2 | -19.5 | -20.3 | -39.2 | -41.2 | -36.4 | -35.1 |
| BIPS | B97XD | -18.6 | -18.3 | -40.0 | -41.8 | -40.8 | -41.9 |
|  | MP2 | -17.0 | -16.8 | -32.6 | -35.4 | -33.5 | -34.5 |
| nitroBIPS | B97XD | -27.9 | -29.0 | -55.2 | -55.7 | -55.8 | -57.9 |
|  | MP2 | -23.0 | -22.7 | -45.3 | -46.6 | -45.8 | -48.0 |
| dinitroBIPS | B97XD | -39.1 | -39.1 | -76.2 | -78.7 | -79.0 | -80.4 |
|  | MP2 | -30.1 | -30.1 | -62.7 | -65.7 | -66.1 | -67.0 |

**S7: Solvation energies (kJ/mol) in water**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | B97XD | -747.3119349 | -747.3126137 | -747.2912914 | -747.2903945 | -747.288645 | -747.2884034 |
|  | MP2 | -745.2584572 | -745.2592781 | -745.2300843 | -745.2280077 | -745.226107 | -745.2269498 |
| BIPS | B97XD | -865.2255763 | -865.2251396 | -865.2025287 | -865.2014595 | -865.1986148 | -865.1987075 |
|  | MP2 | -862.8084572 | -862.8084447 | -862.7791697 | -862.7767954 | -862.7741186 | -862.7756808 |
| nitroBIPS | B97XD | -1069.686652 | -1069.686181 | -1069.669277 | -1069.667631 | -1069.664908 | -1069.66593 |
|  | MP2 | -1066.838751 | -1066.838647 | -1066.813662 | -1066.810523 | -1066.807818 | -1066.810394 |
| dinitroBIPS | B97XD | -1274.133647 | -1274.133647 | -1274.12208 | -1274.120094 | -1274.117594 | -1274.118924 |
|  | MP2 | -1270.858941 | -1270.858111 | -1270.838317 | -1270.834401 | -1270.831971 | -1270.835203 |

**S8: Electronic energies (in Eh) in chloroform**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | B97XD | 0.0 | -1.8 | 54.2 | 56.5 | 61.1 | 61.8 |
|  | MP2 | 0.0 | -2.2 | 74.5 | 79.9 | 84.9 | 82.7 |
| BIPS | B97XD | 0.0 | 1.1 | 60.5 | 63.3 | 70.8 | 70.5 |
|  | MP2 | 0.0 | 0.0 | 76.9 | 83.1 | 90.1 | 86.0 |
| nitroBIPS | B97XD | 0.0 | 1.2 | 45.6 | 49.9 | 57.1 | 54.4 |
|  | MP2 | 0.0 | 0.3 | 65.9 | 74.1 | 81.2 | 74.4 |
| dinitroBIPS | B97XD | 0.0 | 0.0 | 30.4 | 35.6 | 42.1 | 38.6 |
|  | MP2 | 0.0 | 2.2 | 54.1 | 64.4 | 70.8 | 62.3 |

**S9: Electronic energies (kJ/mol), in chloroform, relative to closed form A**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | B97XD | -14.3 | -14.7 | -31.8 | -32.9 | -30.1 | -31.3 |
|  | MP2 | -13.1 | -13.6 | -26.0 | -27.4 | -24.5 | -25.5 |
| BIPS | B97XD | -12.2 | -12.0 | -26.8 | -28.2 | -27.6 | -27.4 |
|  | MP2 | -11.1 | -11.0 | -21.7 | -23.5 | -22.4 | -22.5 |
| nitroBIPS | B97XD | -19.4 | -19.2 | -38.1 | -38.5 | -38.7 | -39.5 |
|  | MP2 | -15.9 | -15.7 | -30.7 | -31.2 | -30.7 | -32.0 |
| dinitroBIPS | B97XD | -26.2 | -26.2 | -53.3 | -54.5 | -54.7 | -55.5 |
|  | MP2 | -20.2 | -20.4 | -43.3 | -44.6 | -44.6 | -45.5 |

**S10: Solvation energies (kJ/mol) in chloroform**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | B97XD | 0.0 | -2.0 | 34.9 | 36.5 | 41.6 | 40.3 |
|  | MP2 | 0.0 | -2.4 | 57.1 | 61.3 | 67.2 | 66.9 |
| BIPS | B97XD | 0.0 | 0.9 | 41.5 | 42.9 | 45.7 | 50.2 |
|  | MP2 | 0.0 | -0.3 | 59.6 | 63.9 | 66.6 | 67.7 |
| nitroBIPS | B97XD | 0.0 | 0.0 | 26.0 | 24.3 | 37.5 | 36.6 |
|  | MP2 | 0.0 | 0.4 | 47.3 | 49.0 | 62.2 | 57.6 |
| dinitroBIPS | B97XD | 0.0 | 0.0 | 6.3 | 9.5 | 17.9 | 17.5 |
|  | MP2 | 0.0 | 2.4 | 30.8 | 38.6 | 46.4 | 41.7 |

**S11: Free energies (kJ/mol), in water, relative to closed form A**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | B97XD | 0.0 | -1.8 | 43.6 | 44.8 | 49.1 | 49.3 |
|  | MP2 | 0.0 | -2.2 | 63.9 | 68.2 | 72.8 | 70.2 |
| BIPS | B97XD | 0.0 | 0.6 | 48.5 | 50.7 | 52.4 | 56.2 |
|  | MP2 | 0.0 | -0.5 | 64.9 | 70.5 | 71.8 | 71.7 |
| nitroBIPS | B97XD | 0.0 | 0.9 | 38.6 | 35.3 | 46.8 | 43.9 |
|  | MP2 | 0.0 | -0.1 | 58.9 | 59.4 | 70.9 | 64.0 |
| dinitroBIPS | B97XD | 0.0 | 0.0 | 19.7 | 22.5 | 29.1 | 28.7 |
|  | MP2 | 0.0 | 2.2 | 43.5 | 51.3 | 57.8 | 52.4 |

**S12 Free energies (kJ/mol), in chloroform, relative to closed form A**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Basis** | **Closed A** | **Closed B** | **TTC** | **TTT** | **CTT** | **CTC** |
| SP0 | cc-pvdz | -745.253451 | -745.254087 | -745.220178 | -745.217577 | -745.216784 | -745.217246 |
| BIPS | cc-pvdz | -862.804215 | -862.804263 | -862.770916 | -862.767842 | -862.765579 | -862.767096 |
| nitroBIPS | cc-pvdz | -1066.832713 | -1066.832682 | -1066.801958 | -1066.798630 | -1066.796109 | -1066.798205 |
| dinitroBIPS | cc-pvdz | -1270.851260 | -1270.850339 | -1270.821810 | -1270.817399 | -1270.814983 | -1270.817869 |
| SP0 | cc-pvtz | -745.957711 | -745.958535 | -745.922265 | -745.919724 | -745.918966 | -745.919252 |
| BIPS | cc-pvtz | -863.631413 | -863.631594 | -863.596705 | BIPS | -863.591173 | -863.592684 |
| nitroBIPS | cc-pvtz | -1067.851427 | -1067.851507 | -1067.819744 | -1067.816393 | -1067.813595 | -1067.815826 |
| dinitroBIPS | cc-pvtz | -1272.059908 | -1272.059704 | -1272.030475 | -1272.025935 | -1272.023251 | -1272.026416 |
| SP0 | cc-pvqz | -746.190736 | -746.191645 | -746.156135 | -746.153548 | -746.152790 | -746.153081 |
| BIPS | cc-pvqz | -863.902309 | -863.902459 | -863.868688 | -863.865736 | -863.863032 | -863.864537 |
| nitroBIPS | cc-pvqz | -1068.187832 | -1068.187881 | -1068.157438 | -1068.154002 | -1068.151103 | -1068.153392 |
| dinitroBIPS | cc-pvqz | -1272.461139 | -1272.461043 | -1272.433413 | -1272.428762 | -1272.425989 | -1272.429254 |

**S13 Gas phase MP2 electronic energies (in Eh) with larger basis sets**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **CCC** | **CCT** | **TCC** | **TCT** |
| SP0 | B97XD | -747.306489 | -747.295691 | -747.271332 | -747.272205 | -747.268112 |
|  | MP2 | -745.253451 | -745.245956 | -745.212154 | -745.213551 | -745.209376 |
| BIPS | B97XD | -865.220929 | -865.186392 | -865.182042 |  | -865.175166 |
|  | MP2 | -862.804215 | -862.769385 | -862.760957 |  | -862.752318 |
| nitroBIPS | B97XD | -1069.679261 | -1069.650383 | -1069.644013 |  | -1069.636478 |
|  | MP2 | -1066.832713 | -1066.800999 | -1066.791627 |  | -1066.791627 |
| dinitroBIPS | B97XD | -1274.123666 | -1274.103691 | -1274.090632 |  | -1274.082679 |
|  | MP2 | -1270.851260 | -1270.827555 | -1270.811130 |  | -1270.802512 |

**S14 Electronic energies (in Eh) of the *cisoid* structures in gas phase**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **CCC** | **CCT** | **TCC** | **TCT** |
| SP0 | B97XD | -747.094030 | -747.087064 | -747.063368 | -747.06371 | -747.060613 |
|  | MP2 | -745.043392 | -745.0373291 | -745.0041898 | -745.0050557 | -745.001877 |
| BIPS | B97XD | -864.928619 | -864.89665 | -864.894285 |  | -864.888185 |
|  | MP2 | -862.514077 | -862.479643 | -862.4732 |  | -862.4653371 |
| nitroBIPS | B97XD | -1069.388163 | -1069.362215 | -1069.3572 |  | -1069.349788 |
|  | MP2 | -1066.544140 | -1066.512831 | -1066.504814 |  | -1066.504937 |
| dinitroBIPS | B97XD | -1273.833312 | -1273.815095 | -1273.80584 |  | -1273.796988 |
|  | MP2 | -1270.563575 | -1270.538958 | -1270.526337 |  | -1270.516821 |

**S15 Free energies (in Eh) of the *cisoid* structures in gas phase**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **CCC** | **CCT** | **TCC** | **TCT** |
| SP0 | B97XD | -747.314578 | -747.305976 | -747.2855725 | -747.287771 | -747.2838295 |
|  | MP2 | -745.2608878 | -745.2554035 | -745.223511 | -745.227471 | -745.222257 |
| BIPS | B97XD | -865.2280201 | -865.1995179 | -865.1957606 |  | -865.1876354 |
|  | MP2 | -862.8106723 | -862.7800529 | -862.7720856 |  | -862.7631719 |
| nitroBIPS | B97XD | -1069.689906 | -1069.670093 | -1069.665506 |  | -1069.658729 |
|  | MP2 | -1066.84147 | -1066.817139 | -1066.810145 |  | -1066.803476 |
| dinitroBIPS | B97XD | -1274.138565 | -1274.1279 | -1274.123353 |  | -1274.11791 |
|  | MP2 | -1270.862745 | -1270.846642 | -1270.839453 |  | -1270.833442 |

**S16 Electronic energies (in Eh) of the *cisoid* structures in water**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **CCC** | **CCT** | **TCC** | **TCT** |
| SP0 | B97XD | -747.102462 | -747.097595 | -747.077813 | -747.079109 | -747.076237 |
|  | MP2 | -745.048772 | -745.0470225 | -745.0157515 | -745.018809 | -745.0146645 |
| BIPS | B97XD | -864.936082 | -864.910791 | -864.908412 |  | -864.900752 |
|  | MP2 | -862.518734 | -862.491326 | -862.484737 |  | -862.4762885 |
| nitroBIPS | B97XD | -1069.399618 | -1069.381814 | -1069.379253 |  | -1069.372664 |
|  | MP2 | -1066.551182 | -1066.528859 | -1066.523891 |  | -1066.517411 |
| dinitroBIPS | B97XD | -1273.848897 | -1273.840975 | -1273.836328 |  | -1273.833549 |
|  | MP2 | -1270.573077 | -1270.559717 | -1270.552428 |  | -1270.549081 |

**S17 Free energies (in Eh) of the *cisoid* structures in water**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **CCC** | **CCT** | **TCC** | **TCT** |
| SP0 | B97XD | -747.3119349 | -747.3026539 | -747.2808972 | -747.2825249 | -747.278652 |
|  | MP2 | -745.2584572 | -745.252392 | -745.219723 | -745.222711 | -745.219723 |
| BIPS | B97XD | -865.2255763 | -865.1947414 | -865.1911611 |  | -865.18347 |
|  | MP2 | -862.8084572 | -862.7761655 | -862.768316 |  | -862.7594241 |
| nitroBIPS | B97XD | -1069.686652 | -1069.663754 | -1069.658471 |  | -1069.650619 |
|  | MP2 | -1066.838751 | -1066.811755 | -1066.803388 |  | -1066.795744 |
| dinitroBIPS | B97XD | -1274.133647 | -1274.120074 | -1274.113211 |  | -1274.10609 |
|  | MP2 | -1270.858941 | -1270.840365 | -1270.82749 |  | -1270.822829 |

**S18 Electronic energies (in Eh) of the *cisoid* structures in chloroform**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **Method** | **Closed A** | **CCC** | **CCT** | **TCC** | **TCT** |
| SP0 | B97XD | -747.099700 | -747.094246 | -747.073146 | -747.073839 | -747.071108 |
|  | MP2 | -745.046222 | -745.0439841 | -745.0119718 | -745.0140251 | -745.012179 |
| BIPS | B97XD | -864.933507 | -864.905872 | -864.903851 |  | -864.896477 |
|  | MP2 | -862.516388 | -862.4872961 | -862.4810059 |  | -862.4724311 |
| nitroBIPS | B97XD | -1069.396093 | -1069.375755 | -1069.371002 |  | -1069.363503 |
|  | MP2 | -1066.548192 | -1066.523757 | -1066.515918 |  | -1066.508628 |
| dinitroBIPS | B97XD | -1273.843862 | -1273.832118 | -1273.827292 |  | -1273.821697 |
|  | MP2 | -1270.569157 | -1270.552409 | -1270.541571 |  | -1270.538436 |

**S19 Free energies (in Eh) of the *cisoid* structures in chloroform**

GeomAB2.tif

**Figure 5A: Structure A of the closed form of spiropyran**

GeomAB1.tif

**Figure 5B: Structure B of the closed form of spiropyran**

**Geometries - SP0**

**SP0 B97XD/cc-pvdz optimized geometry - form A**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50601458

C 1.03136365 0.00000000 2.42965283

C 0.72211256 0.02911492 3.79581747

C -0.60797719 0.06028379 4.21118426

C -1.65715266 0.06345122 3.28559951

C -1.33327155 0.03155102 1.93453105

N -2.19525585 0.06959523 0.82792203

C -1.46519455 -0.38101606 -0.33446820

C -1.97820953 0.21905360 -1.61626770

C -1.93803762 -0.47196176 -2.75997882

C -1.47267858 -1.85704588 -2.76067797

C -1.22594316 -2.59601140 -3.92175878

C -0.83015399 -3.92818095 -3.84911848

C -0.69025128 -4.53740109 -2.60053882

C -0.93199681 -3.82028507 -1.43140793

C -1.31402246 -2.48256963 -1.51282714

O -1.58444377 -1.82408013 -0.35584611

H -3.10719918 -0.36333559 0.93586034

H 0.69706791 -0.70971036 -0.46548424

H 0.21976768 1.00516026 -0.39536001

H -0.63663859 -4.49320162 -4.76177604

H 2.07183771 -0.02905433 2.09888581

H 1.52374733 0.02416197 4.53576361

H -0.84005266 0.07864666 5.27783923

H -2.69684017 0.08587179 3.61692700

H -2.32059502 1.25346279 -1.56439802

H -2.26168240 -0.02375081 -3.70211094

H -1.35266783 -2.11147341 -4.89287459

H -0.38306654 -5.58269016 -2.53413682

H -0.82788557 -4.27644851 -0.44641862

**SP0 B97XD/cc-pvdz optimized geometry - form B**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50773433

C 1.03358637 0.00000000 2.42783539

C 0.72813236 0.02396700 3.79547031

C -0.60061575 0.04931217 4.21463612

C -1.65314281 0.05113750 3.29235059

C -1.33311105 0.02671217 1.94002255

N -2.18538472 0.06799464 0.83209249

C -1.45604204 -0.37896717 -0.34005061

C -2.03400665 0.23536103 -1.58651012

C -2.93168783 -0.43006821 -2.32201462

C -3.30079235 -1.79642544 -1.96497795

C -4.35852011 -2.49884014 -2.55359831

C -4.63587474 -3.81067603 -2.18465442

C -3.84304007 -4.43817356 -1.22015359

C -2.78662134 -3.75838604 -0.62111671

C -2.51936099 -2.44090665 -0.99165313

O -1.45189568 -1.82194654 -0.42764808

H -3.13547975 -0.27374426 0.92646669

H 0.69007902 -0.71946579 -0.45715985

H 0.22691634 1.00404102 -0.39204509

H -5.46414590 -4.34720183 -2.64918900

H 2.07329977 -0.02501311 2.09426033

H 1.53201599 0.01914464 4.53292295

H -0.82954346 0.06358074 5.28206094

H -2.69185047 0.06745460 3.62706197

H -1.74608140 1.26275741 -1.81331660

H -3.40033422 0.03165673 -3.19413159

H -4.96548770 -2.00000638 -3.31299538

H -4.05254218 -5.46859846 -0.92738495

H -2.15456179 -4.22862017 0.13285070

**SP0 open form TTC B97XD/cc-pvdz optimized geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50858566

C 1.03295167 0.00000000 2.43039265

C 0.72183439 -0.00000000 3.79623579

C -0.60726709 -0.00000000 4.21760300

C -1.66041807 -0.00000000 3.29704650

C -1.32873513 -0.00000000 1.94908586

N -2.16946056 -0.00000000 0.83396673

C -1.47930269 -0.00001229 -0.34645081

C -2.07461912 -0.00002731 -1.57783587

C -1.31493313 -0.00003966 -2.77383570

C -1.77572111 -0.00002736 -4.07584669

C -0.80762878 -0.00003261 -5.15015349

C -1.17650999 -0.00001474 -6.45537487

C -2.57703545 0.00002962 -6.79543876

C -3.54146595 0.00003578 -5.84224695

C -3.22365150 0.00000423 -4.41133844

O -4.12178777 0.00000100 -3.56371024

H 2.07342743 0.00000000 2.09977229

H 1.52416420 -0.00000000 4.53514008

H -0.83531107 -0.00000000 5.28463063

H -2.69942331 -0.00000000 3.62943036

H -3.16073790 -0.00001955 -1.66577200

H -0.22272778 -0.00005472 -2.66289438

H 0.25255359 -0.00006242 -4.87985088

H -2.86058852 0.00004363 -7.85128268

H -3.17893193 -0.00001555 0.87682116

H 0.49943049 -0.88654638 -0.42021075

H 0.49939609 0.88657162 -0.42020186

H -4.60307935 0.00005660 -6.09457956

H -0.42760340 -0.00002978 -7.24825428

**SP0 open form TTT B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50823888

C 1.03302448 0.00000000 2.42997879

C 0.72231759 0.00000000 3.79601659

C -0.60631126 0.00000000 4.21834128

C -1.65972409 0.00000000 3.29794023

C -1.32784389 0.00000000 1.95017031

N -2.17103589 0.00000836 0.83553644

C -1.47888955 -0.00002311 -0.34586108

C -2.05259147 -0.00006623 -1.58555395

C -1.26499642 -0.00009700 -2.76808473

C -1.68075991 -0.00012510 -4.07700201

C -3.06544785 -0.00012815 -4.48916886

C -3.41138327 -0.00015040 -5.79990075

C -2.38498081 -0.00017170 -6.81789944

C -1.06681780 -0.00017023 -6.50612240

C -0.60682596 -0.00015493 -5.11224580

O 0.58945582 -0.00016441 -4.82449861

H 2.07327729 0.00000000 2.09903530

H 1.52539190 0.00000000 4.53395038

H -0.83349702 0.00000000 5.28566762

H -2.69880872 0.00000000 3.63043196

H -3.14337296 -0.00007669 -1.64933633

H -0.17458084 -0.00009648 -2.65701473

H -3.84601405 -0.00010701 -3.72499524

H -2.69284744 -0.00018942 -7.86692470

H -3.17945257 -0.00007564 0.88680597

H 0.49950574 -0.88459194 -0.42349140

H 0.49946762 0.88461806 -0.42348164

H -0.29050749 -0.00018628 -7.27299232

H -4.46018561 -0.00015249 -6.09961840

**SP0 open form CTT B97XD/ccpvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50743251

C 1.02964950 0.00000000 2.43312646

C 0.71342294 -0.00000000 3.79766911

C -0.61728100 -0.00000000 4.21404191

C -1.66703362 -0.00000000 3.28973384

C -1.33003913 -0.00000000 1.94310843

N -2.17249154 0.00000531 0.82775175

C -1.47653478 -0.00001395 -0.35024973

C -1.99657636 -0.00003887 -1.61535168

C -3.39143511 -0.00005539 -1.88491683

C -4.03683023 -0.00006841 -3.09671575

C -3.36552976 -0.00006744 -4.37581395

C -4.06443425 -0.00008079 -5.53726500

C -5.50985515 -0.00009639 -5.51132154

C -6.20639095 -0.00009822 -4.34945515

C -5.52785299 -0.00008440 -3.04875496

O -6.15420238 -0.00008597 -1.98907325

H 2.07156654 0.00000000 2.10704519

H 1.51318593 -0.00000000 4.53922567

H -0.84906151 -0.00000000 5.28038121

H -2.70761340 -0.00000000 3.61712056

H -1.27767196 -0.00005150 -2.43565970

H -4.09047294 -0.00006081 -1.03939260

H -2.27360622 -0.00005568 -4.40124201

H -6.04691316 -0.00010695 -6.46354859

H -3.18086241 -0.00003139 0.88365136

H 0.49580866 -0.88617282 -0.42565736

H 0.49578909 0.88618718 -0.42565143

H -7.29735621 -0.00010999 -4.32827907

H -3.54833933 -0.00007993 -6.49821205

**SP0 open form CTC B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50673169

C 1.02796487 0.00000000 2.43451799

C 0.70990187 -0.00000000 3.79874229

C -0.62104054 -0.00000000 4.21410956

C -1.66936105 -0.00000000 3.28810374

C -1.33020390 -0.00000000 1.94207949

N -2.17144975 -0.00000000 0.82497150

C -1.47499070 -0.00000778 -0.35355050

C -1.97538534 -0.00002064 -1.62810933

C -3.36078810 -0.00002817 -1.93037435

C -3.96722129 -0.00005211 -3.17053062

C -5.41232554 -0.00005528 -3.23415083

C -6.08377164 -0.00007815 -4.41218213

C -5.34457827 -0.00010019 -5.65026669

C -3.98913423 -0.00009868 -5.66970363

C -3.19131482 -0.00007467 -4.43947982

O -1.95830577 -0.00007383 -4.48517559

H 2.07017574 0.00000000 2.10966606

H 1.50893325 -0.00000000 4.54113574

H -0.85388173 -0.00000000 5.28022501

H -2.71025360 -0.00000000 3.61499160

H -1.27451886 -0.00003116 -2.46029305

H -4.06032684 -0.00001528 -1.08269209

H -5.96420722 -0.00003844 -2.28922690

H -5.89943821 -0.00011849 -6.59217486

H -3.17867185 -0.00000426 0.88536563

H 0.49499162 -0.88491150 -0.42896826

H 0.49497441 0.88492451 -0.42896441

H -3.42420222 -0.00011529 -6.60334555

H -7.17411754 -0.00008007 -4.43470629

**SP0 open form CCC B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.49936714

C 1.01253409 0.00000000 2.44742755

C 0.65573689 0.00232643 3.80004321

C -0.68727205 0.00594774 4.18852595

C -1.71061782 0.00650114 3.23925502

C -1.34403093 0.00226810 1.89857676

N -2.21159502 -0.00055125 0.78597004

C -1.48782872 -0.00603139 -0.29021696

C -1.99837257 -0.04552265 -1.64827997

C -3.20991442 -0.42285319 -2.11909868

C -4.47897148 -0.86259992 -1.51754975

C -5.14191080 -1.90125333 -2.20783837

C -6.38862869 -2.36793511 -1.83007060

C -7.04109731 -1.75865911 -0.75266361

C -6.42870858 -0.72201551 -0.06939279

C -5.14842088 -0.26051018 -0.42356777

O -4.66625032 0.78371992 0.26370943

H 2.06380964 -0.00083645 2.15304798

H 1.43626919 0.00264862 4.56267777

H -0.93815766 0.00746290 5.25065559

H -2.76276608 0.00908615 3.52576679

H -1.24140465 0.17008243 -2.40770464

H -3.24517108 -0.47854601 -3.21366311

H -4.64147950 -2.35026907 -3.06981337

H -8.03458320 -2.09563571 -0.45003410

H -3.72270505 0.57452635 0.51373938

H 0.49064929 -0.88267157 -0.44135851

H 0.47924408 0.89040675 -0.43932157

H -6.91950251 -0.22532537 0.76860849

H -6.86030737 -3.18398946 -2.37874598

**SP0 open form CCT B97XD/cc-pvtz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50748269

C 1.02911616 0.00000000 2.43388066

C 0.71223226 0.00075466 3.79837100

C -0.61877327 0.00260399 4.21404528

C -1.66779231 0.00515598 3.28899252

C -1.33032007 0.00364759 1.94229115

N -2.17391704 0.01423413 0.82900545

C -1.47878671 -0.03438081 -0.35011286

C -1.97983236 -0.17212383 -1.61476853

C -3.35211922 -0.31104849 -1.99906378

C -4.48715488 0.25348788 -1.46614441

C -4.48868828 1.38134564 -0.55690383

C -5.64419854 1.90403858 -0.07802344

C -6.91676674 1.34062440 -0.47517897

C -6.99635288 0.32089666 -1.36109963

C -5.79368740 -0.29046302 -1.94694173

O -5.86932728 -1.20720774 -2.75962188

H -0.85099177 0.00173887 5.28034573

H 1.51168684 -0.00110590 4.54031391

H 2.07127814 -0.00341484 2.10847765

H -2.70893315 0.00712173 3.61451274

H -1.23419812 -0.36139154 -2.39005291

H -3.54905724 -0.98045423 -2.84498609

H -7.95325002 -0.09067310 -1.68638349

H -3.53608483 1.85231023 -0.30562647

H -7.83103742 1.77393138 -0.06142449

H -5.62881270 2.77670247 0.57667004

H -3.18160527 -0.06424270 0.87720167

H 0.52435013 -0.86668065 -0.42963585

H 0.46785882 0.90484362 -0.41938163

**SP0 open form TCT B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50776776

C 1.03431680 0.00000000 2.42825239

C 0.72647498 0.02992863 3.79458033

C -0.60142695 0.06654814 4.21803690

C -1.65566827 0.07461372 3.29874406

C -1.32710440 0.04033664 1.94994062

N -2.17132055 0.04795580 0.83796378

C -1.47777610 -0.07732430 -0.34560451

C -2.07726453 -0.36890499 -1.53692462

C -1.40634194 -0.61649038 -2.78050990

C -0.32621483 0.02895479 -3.32407562

C 0.14681660 1.32056462 -2.87445257

C 1.22384072 1.91596542 -3.43941773

C 1.93122889 1.26061098 -4.52052608

C 1.51137261 0.08203724 -5.03565702

C 0.33022925 -0.61489070 -4.50365951

O -0.06561508 -1.67274395 -4.98269767

H -3.17371317 -0.06086132 0.89605813

H 0.54263579 -0.84270705 -0.45531698

H 0.46666773 0.91445310 -0.39369510

H 1.54267483 2.90924110 -3.12007219

H 2.07376582 -0.02852264 2.09560381

H 1.53047337 0.02343450 4.53158801

H -0.82730041 0.08892011 5.28550177

H -2.69401937 0.10424390 3.63252908

H -3.14428063 -0.61094696 -1.50207343

H -1.79449081 -1.44280464 -3.38814824

H -0.43418154 1.84346915 -2.11165398

H 2.80881752 1.75593533 -4.94414503

H 2.02038361 -0.39950055 -5.87219947

**SP0 open form TCC B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.49806849

C 1.02531338 0.00000000 2.43201211

C 0.70098068 -0.04528264 3.79200067

C -0.63187079 -0.09918634 4.20489892

C -1.67605319 -0.10512009 3.27684791

C -1.32964854 -0.05089298 1.93275721

N -2.15802473 -0.03468171 0.80691193

C -1.44945330 0.05132237 -0.35471962

C -2.06083998 0.25596854 -1.57835162

C -1.47989399 0.43492325 -2.84772247

C -0.28837236 0.03121581 -3.45591289

C 0.05141015 0.67791183 -4.70289902

C 1.16775670 0.36115842 -5.41084019

C 2.02803332 -0.68352985 -4.93532449

C 1.73383705 -1.37539007 -3.80340663

C 0.54796155 -1.09319941 -3.00233548

O 0.26513837 -1.80943317 -2.02379684

H -3.16766347 -0.04824769 0.84339711

H 0.39673876 -0.94090963 -0.44962748

H 0.56914524 0.80903295 -0.48352457

H 1.40899154 0.88608463 -6.33587287

H 2.06789090 0.03430406 2.11103422

H 1.49677193 -0.04081641 4.53811580

H -0.86588065 -0.13749996 5.27004908

H -2.71771257 -0.14902784 3.59849745

H -3.13289579 0.47225682 -1.52727152

H -2.12180008 1.02756627 -3.51294800

H -0.61229187 1.46967927 -5.06209827

H 2.92615682 -0.93257132 -5.50646374

H 2.36664023 -2.18910776 -3.44476484

**SP0 MP2/cc-pvdz optimised geometry – form A**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51098740

C 1.03871753 0.00000000 2.44679918

C 0.71742655 0.04644124 3.81910519

C -0.62642263 0.10253984 4.23269828

C -1.67750308 0.11206267 3.29428646

C -1.34433256 0.05714471 1.93493956

N -2.20585455 0.11142838 0.81132332

C -1.45870838 -0.41729993 -0.31501305

C -1.97672365 0.06773277 -1.64192043

C -1.81156371 -0.69810904 -2.74916288

C -1.22563494 -2.03216367 -2.61941876

C -0.82008173 -2.82002785 -3.71675234

C -0.32551137 -4.11799890 -3.52273553

C -0.24829095 -4.64737206 -2.22020070

C -0.64789400 -3.87796216 -1.11558814

C -1.12633527 -2.57341317 -1.31406506

O -1.56085126 -1.86997880 -0.22034069

H -3.10494243 -0.36068773 0.92800209

H 0.71299013 -0.69426373 -0.47366225

H 0.18264861 1.01657430 -0.39511161

H -0.00959001 -4.71922328 -4.38099833

H 2.08391134 -0.04633965 2.12076821

H 1.51640665 0.03757458 4.56741093

H -0.86306860 0.13501954 5.30161908

H -2.72178087 0.15621587 3.62186731

H -2.41256698 1.07120384 -1.67508107

H -2.12681540 -0.34435269 -3.73763103

H -0.90103442 -2.40217105 -4.72708596

H 0.13406603 -5.66112568 -2.06103911

H -0.59665720 -4.26719597 -0.09403856

**SP0 MP2/cc-pvdz optimised geometry – form B**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51308439

C 1.04147110 0.00000000 2.44471891

C 0.72435842 0.03900152 3.81864288

C -0.61810886 0.08791268 4.23696731

C -1.67293474 0.09700670 3.30230063

C -1.34411030 0.05218803 1.94130740

N -2.19332581 0.11531857 0.81491320

C -1.44787064 -0.42164737 -0.31770112

C -2.03866575 0.06958829 -1.61105720

C -3.00380059 -0.65950370 -2.22658265

C -3.39097132 -1.95437603 -1.67062051

C -4.52232113 -2.68409174 -2.09496599

C -4.80756333 -3.94346057 -1.54965626

C -3.95011869 -4.49414630 -0.57660552

C -2.82130027 -3.78314294 -0.14090959

C -2.54473341 -2.51784433 -0.68382734

O -1.40235612 -1.87729923 -0.28604231

H -3.13491771 -0.26829974 0.91382239

H 0.70978278 -0.70125952 -0.46325619

H 0.18314984 1.01711008 -0.39096441

H -5.68874430 -4.49966908 -1.88447932

H 2.08583682 -0.04180292 2.11543642

H 1.52587165 0.02932218 4.56417338

H -0.85118059 0.11432817 5.30686811

H -2.71630627 0.13385206 3.63372442

H -1.72737884 1.05202458 -1.97988645

H -3.49963951 -0.29534822 -3.13389888

H -5.17524645 -2.25008891 -2.86131683

H -4.16574405 -5.47890331 -0.14887995

H -2.13969957 -4.18928917 0.61281864

**SP0 open form TTC MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51469036

C 1.04305571 0.00000000 2.44431335

C 0.72673252 0.00001057 3.81922931

C -0.61433819 0.00002662 4.24626435

C -1.67432526 0.00003258 3.31875992

C -1.33904023 0.00002190 1.95908890

N -2.17946782 0.00002457 0.83899827

C -1.48534992 -0.00001494 -0.34622972

C -2.08520526 -0.00005944 -1.59106884

C -1.31791984 -0.00009220 -2.78526104

C -1.78823520 -0.00013244 -4.09896462

C -0.81686230 -0.00016102 -5.17343857

C -1.19781170 -0.00020822 -6.49274386

C -2.60221700 -0.00023042 -6.83277371

C -3.57004658 -0.00020522 -5.85981365

C -3.24657682 -0.00015461 -4.42532962

O -4.15034713 -0.00013274 -3.56624931

H 2.08747334 -0.00001311 2.11371992

H 1.53094866 0.00001073 4.56151841

H -0.84187875 0.00003466 5.31717468

H -2.71720580 0.00004507 3.65210012

H -3.17492679 -0.00006910 -1.67508358

H -0.22172743 -0.00008053 -2.67441370

H 0.24719091 -0.00014341 -4.90366712

H -2.89520420 -0.00026813 -7.88951723

H -3.19439785 -0.00001703 0.88018699

H 0.50211345 -0.89018987 -0.41758092

H 0.50206276 0.89023014 -0.41756342

H -4.63610686 -0.00022185 -6.11102540

H -0.44577766 -0.00022911 -7.28789609

**SP0 open form TTT MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51439058

C 1.04406265 0.00000000 2.44283344

C 0.73014651 0.00000000 3.81832606

C -0.61017871 0.00000000 4.24723036

C -1.67144880 0.00000000 3.32095314

C -1.33824800 0.00000000 1.96080686

N -2.18175074 0.00000000 0.84244892

C -1.48534950 -0.00001475 -0.34546452

C -2.06112127 -0.00004079 -1.59805166

C -1.26688519 -0.00005465 -2.77944837

C -1.69699567 -0.00008067 -4.09864125

C -3.08885285 -0.00009860 -4.49547978

C -3.44496598 -0.00012413 -5.82117482

C -2.42690213 -0.00013364 -6.85312495

C -1.09268990 -0.00011762 -6.54096625

C -0.61982355 -0.00008995 -5.14498506

O 0.58920585 -0.00008275 -4.86759810

H 2.08774478 -0.00000432 2.11005251

H 1.53556854 0.00000000 4.55930015

H -0.83641485 0.00000000 5.31845405

H -2.71378193 0.00000000 3.65635786

H -3.15542161 -0.00005067 -1.66352908

H -0.17329115 -0.00004395 -2.66567907

H -3.86741675 -0.00009164 -3.72437021

H -2.73911397 -0.00015413 -7.90428055

H -3.19545272 -0.00004308 0.89250354

H 0.50233474 -0.88885822 -0.41982252

H 0.50231731 0.88887078 -0.41981829

H -0.32030646 -0.00012472 -7.31732117

H -4.50119114 -0.00013751 -6.10886284

**SP0 open form CTT MP2/cc-pvdz optimised structure**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51344439

C 1.04020713 0.00000000 2.44632223

C 0.72016020 0.00001141 3.82027415

C -0.62238074 0.00002939 4.24247722

C -1.67954588 0.00003648 3.31172414

C -1.34063326 0.00001637 1.95287191

N -2.18315793 0.00003771 0.83395746

C -1.48311401 -0.00005027 -0.35086709

C -2.01554160 -0.00015246 -1.62479552

C -3.41503962 -0.00018900 -1.88556296

C -4.06134903 -0.00027843 -3.11296973

C -3.37647310 -0.00033945 -4.38787688

C -4.08137913 -0.00042725 -5.56563309

C -5.53107457 -0.00046052 -5.55259003

C -6.23624061 -0.00040603 -4.37766501

C -5.56256588 -0.00031665 -3.06749824

O -6.20340820 -0.00027242 -2.00486063

H 2.08565992 -0.00001470 2.11882434

H 1.52204027 0.00000638 4.56508728

H -0.85364642 0.00003806 5.31262660

H -2.72354228 0.00005047 3.64156310

H -1.29691944 -0.00020610 -2.44976684

H -4.11193411 -0.00014582 -1.03365605

H -2.28100617 -0.00031498 -4.40893534

H -6.06840363 -0.00053096 -6.50842004

H -3.19667358 -0.00008940 0.88714481

H 0.49992071 -0.89030064 -0.42089250

H 0.49985954 0.89034436 -0.42087451

H -7.33122638 -0.00043091 -4.36373531

H -3.55335078 -0.00047284 -6.52453401

**SP0 open form CTC MP2/cc-pvtz optimised structure**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51249882

C 1.03849220 0.00000000 2.44761941

C 0.71619150 0.00000000 3.82092059

C -0.62687973 0.00000000 4.24188154

C -1.68251319 0.00000000 3.30945838

C -1.34072052 0.00000000 1.95139657

N -2.18147068 -0.00000000 0.82967178

C -1.48143397 -0.00000000 -0.35374494

C -1.99363211 -0.00000000 -1.63901934

C -3.38389074 -0.00000000 -1.93184449

C -3.99558073 -0.00000591 -3.18539504

C -5.44333144 -0.00000461 -3.24258939

C -6.12011975 -0.00001640 -4.43703620

C -5.38213461 -0.00003058 -5.68015224

C -4.01036013 -0.00003252 -5.69247147

C -3.20988659 -0.00002046 -4.45802374

O -1.96507091 -0.00002259 -4.50365313

H 2.08434517 0.00000000 2.12167375

H 1.51697638 0.00000000 4.56692340

H -0.85932412 0.00000000 5.31176105

H -2.72689170 0.00000000 3.63842739

H -1.28889478 -0.00000000 -2.47186678

H -4.08495005 0.00000670 -1.07999491

H -5.99537662 0.00000099 -2.29365007

H -5.93379369 -0.00003992 -6.62780524

H -3.19425514 0.00000888 0.88622103

H 0.49854569 -0.88933826 -0.42443644

H 0.49853439 0.88934574 -0.42443330

H -3.44445085 -0.00004323 -6.63015037

H -7.21443655 -0.00001515 -4.45471159

**SP0 open form CCC MP2/cc-pvtz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50466860

C 1.02172743 0.00000000 2.46181711

C 0.65795914 0.00468867 3.82301949

C -0.69730836 0.01051295 4.21696220

C -1.72735960 0.01075200 3.26056866

C -1.35492645 0.00407389 1.90886731

N -2.23224034 0.00018877 0.79598201

C -1.49336958 -0.00363090 -0.29305976

C -2.01403922 -0.04785385 -1.64985865

C -3.24067124 -0.45823123 -2.10050406

C -4.46300915 -0.92321414 -1.41962133

C -5.10352207 -2.04790095 -2.00713730

C -6.32380037 -2.53762112 -1.53400031

C -6.96832275 -1.86914743 -0.47509015

C -6.36806012 -0.74547334 0.10248285

C -5.12369038 -0.25327266 -0.34923673

O -4.65476035 0.88576100 0.22035858

H 2.07714649 -0.00244946 2.16846955

H 1.43963808 0.00453733 4.58993112

H -0.94782568 0.01490063 5.28278222

H -2.78356709 0.01511527 3.54704076

H -1.27225597 0.17998167 -2.42584601

H -3.31043058 -0.52585854 -3.19636047

H -4.60963157 -2.54428584 -2.85118161

H -7.93451439 -2.22459813 -0.10105854

H -3.72367602 0.66172109 0.50008669

H 0.49257289 -0.88732267 -0.43760434

H 0.48258549 0.89488458 -0.43468867

H -6.85127546 -0.20020955 0.91953635

H -6.78094475 -3.41647840 -1.99966116

**SP0 open form CCT MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51329480

C 1.03912722 0.00000000 2.44768148

C 0.71684085 0.01555584 3.82101519

C -0.62630131 0.03818061 4.24135555

C -1.68183427 0.04583049 3.30885031

C -1.34093776 0.02633829 1.95056140

N -2.18470842 0.04509508 0.83172816

C -1.48409572 -0.06151854 -0.34857195

C -1.99542859 -0.27321656 -1.61493391

C -3.37272926 -0.46120296 -1.96506000

C -4.50349267 0.11345312 -1.39607887

C -4.46546264 1.29923293 -0.56160648

C -5.61998246 1.84956519 -0.06025546

C -6.90832211 1.24988240 -0.35205524

C -7.01398864 0.16288265 -1.17870482

C -5.82979472 -0.47553069 -1.78692057

O -5.93635074 -1.45047492 -2.54314756

H -0.85871173 0.04884180 5.31125357

H 1.51756761 0.01010541 4.56712392

H 2.08502942 -0.01920685 2.12210971

H -2.72675557 0.06424120 3.63523893

H -1.24618574 -0.49457328 -2.38323249

H -3.58509358 -1.16980066 -2.77950200

H -7.98523948 -0.27586802 -1.43099159

H -3.50492349 1.80093216 -0.40164916

H -7.81197603 1.69874333 0.07689644

H -5.57814910 2.77078235 0.53034877

H -3.19742541 -0.04911456 0.87371031

H 0.54686229 -0.85460527 -0.43336204

H 0.45015593 0.92362882 -0.40782606

**SP0 open form TCT MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51369370

C 1.04440402 0.00000000 2.44263704

C 0.73153549 0.05263135 3.81697505

C -0.60782414 0.12291120 4.24426418

C -1.66794123 0.13986370 3.31706597

C -1.33668293 0.07741271 1.95752890

N -2.18266398 0.09822566 0.83841476

C -1.48064411 -0.11768501 -0.33699741

C -2.07515510 -0.52846126 -1.51279974

C -1.37054293 -0.84556511 -2.72199589

C -0.26667495 -0.19019258 -3.24642555

C 0.11654353 1.14764619 -2.84487043

C 1.21860606 1.75971455 -3.38661871

C 2.03124209 1.06884381 -4.37235264

C 1.68156968 -0.16868976 -4.84323954

C 0.48358442 -0.87907256 -4.35275122

O 0.15116911 -1.98349807 -4.80243218

H -3.18174228 -0.07595727 0.90177604

H 0.57092565 -0.82185752 -0.46774920

H 0.43730618 0.93936004 -0.38183130

H 1.46787572 2.79059297 -3.11420000

H 2.08700682 -0.05440181 2.11050094

H 1.53635502 0.04011000 4.55864209

H -0.83365545 0.16304214 5.31490479

H -2.70913797 0.19748182 3.65140338

H -3.13977947 -0.79419569 -1.46024926

H -1.71977000 -1.71404436 -3.30007460

H -0.54610037 1.69311461 -2.16360277

H 2.92149627 1.57042728 -4.77002093

H 2.26684563 -0.67718582 -5.61670018

**SP0 open form TCC MP2/cc-pvdz optimised geometry (NB. This only exists for SP0)**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.49947752

C 1.03306572 0.00000000 2.44555330

C 0.70063107 -0.06829051 3.81163890

C -0.64561698 -0.15399116 4.22512681

C -1.69430411 -0.16503954 3.28912923

C -1.34162679 -0.08467868 1.93413989

N -2.16559280 -0.06484733 0.80289834

C -1.44671180 0.06254142 -0.35746010

C -2.04666138 0.29695053 -1.59377426

C -1.42610785 0.53100828 -2.83860019

C -0.17448955 0.16867117 -3.37980782

C 0.23187918 0.86765023 -4.58160739

C 1.41635181 0.58904520 -5.22424180

C 2.26375942 -0.46265532 -4.73179203

C 1.89140344 -1.20427955 -3.63474937

C 0.64002271 -0.97609864 -2.91466891

O 0.28744630 -1.75298424 -1.98810159

H -3.18094365 -0.08082531 0.83316917

H 0.37650126 -0.96506555 -0.44620910

H 0.59765603 0.78098216 -0.50522812

H 1.70864501 1.15645294 -6.11354486

H 2.07955262 0.05815245 2.12767531

H 1.49514165 -0.05976986 4.56452429

H -0.88071058 -0.21060896 5.29292303

H -2.73924577 -0.23353834 3.60915679

H -3.12603328 0.49878023 -1.55834958

H -2.05122528 1.12052184 -3.52840170

H -0.41809963 1.67055519 -4.95158948

H 3.20854517 -0.68011619 -5.24384092

H 2.51306798 -2.02673004 -3.26397534

**Geometries – BIPS**

**BIPS B97XD/ccpvdz optimised geometry – form A**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51584781

C 1.04431832 0.00000000 2.42151983

C 0.75866799 0.05326826 3.79393277

C -0.56289416 0.10528208 4.22790234

C -1.62840536 0.10274082 3.31834228

C -1.32634091 0.05662465 1.96190710

N -2.20237919 0.06574079 0.87202625

C -1.48807008 -0.43474736 -0.28203108

C -2.06146657 0.08959970 -1.56946272

C -2.24342066 -0.68854952 -2.64119496

C -1.95197032 -2.11614311 -2.58069214

C -2.01741512 -2.97180478 -3.68480303

C -1.76822360 -4.33361839 -3.54853036

C -1.46020597 -4.85124428 -2.28832485

C -1.39174112 -4.01730337 -1.17589068

C -1.62876569 -2.65094920 -1.32463155

O -1.57042195 -1.88243844 -0.21160284

C -3.58712524 -0.31111593 1.05161392

C 1.01017789 -0.95587408 -0.63062861

C 0.25118864 1.43440212 -0.49656089

H -1.81812401 -4.99105668 -4.41724935

H 2.07927795 -0.04731037 2.07474180

H 1.57227010 0.04843399 4.52071951

H -0.77900020 0.13890504 5.29761051

H -2.65985892 0.12843269 3.67191914

H -2.29733659 1.15375356 -1.58861607

H -2.63261406 -0.27152954 -3.57310523

H -2.27169732 -2.55299349 -4.66154636

H -1.26595682 -5.91879110 -2.16932249

H -4.09758987 -0.27568202 0.07948797

H -4.08367538 0.40591607 1.72162027

H -3.69759887 -1.32792283 1.46911195

H 2.03296698 -0.58979340 -0.45342371

H 0.86245501 -1.01696663 -1.72060675

H 0.92823100 -1.96582884 -0.20931632

H 1.24141019 1.76991725 -0.15466944

H 0.23185466 1.48582667 -1.59619602

H -0.49833612 2.13296839 -0.09566495

H -1.15192901 -4.40239012 -0.18419896

**BIPS B97XD/ccpvdz optimised geometry – form B**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51622141

C 1.04639368 0.00000000 2.41948741

C 0.76359793 0.05615945 3.79215658

C -0.55709277 0.11160303 4.22861305

C -1.62411500 0.10909478 3.32099355

C -1.32524396 0.06071904 1.96365964

N -2.20297627 0.06428343 0.87419458

C -1.48229303 -0.44809414 -0.28033381

C -2.07889327 0.05186212 -1.56586344

C -2.79394257 -0.73518585 -2.37822123

C -3.01197174 -2.13770963 -2.05304775

C -3.85638370 -2.98537880 -2.77896859

C -4.02288004 -4.31469213 -2.40774801

C -3.33438490 -4.80875896 -1.29613569

C -2.49100233 -3.98335145 -0.55953419

C -2.33085500 -2.64980057 -0.93896456

O -1.46645998 -1.89551366 -0.22282613

C -3.58588786 -0.31126401 1.06815844

C 1.02123684 -0.94224531 -0.63332966

C 0.24808408 1.44048715 -0.48185374

H -4.68376563 -4.96645533 -2.98037885

H 2.08046884 -0.05025664 2.07053399

H 1.57853961 0.05070675 4.51743987

H -0.77124760 0.14769433 5.29861332

H -2.65456105 0.13686785 3.67725183

H -1.95104860 1.11116025 -1.78325819

H -3.24170874 -0.33217613 -3.28986738

H -4.38619777 -2.58436909 -3.64648596

H -3.45746846 -5.85144331 -0.99750587

H -4.11334667 -0.26164432 0.10634488

H -4.07146680 0.39860335 1.75359458

H -3.69333751 -1.33167278 1.48061845

H 2.03879194 -0.56001660 -0.45901099

H 0.86751822 -1.00350152 -1.72219505

H 0.95057064 -1.95338612 -0.21569257

H 1.21680095 1.78770182 -0.09395480

H 0.28365305 1.49892800 -1.58078130

H -0.52804311 2.12711391 -0.11200118

H -1.94450261 -4.34978442 0.31005499

**BIPS open form TTC B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51713475

C 1.05520169 0.00000000 2.41331816

C 0.78154059 0.00000000 3.78631782

C -0.53745482 0.00000000 4.23655347

C -1.61114589 0.00000000 3.34057451

C -1.31666215 0.00000000 1.98156887

N -2.18760551 0.00000000 0.88388395

C -1.50436619 0.00000000 -0.30227052

C -2.16559234 0.00000000 -1.50709518

C -1.54403788 -0.00000000 -2.77892015

C -2.16968142 -0.00000000 -4.01346952

C -1.34300455 -0.00000000 -5.19867104

C -1.86876939 -0.00000000 -6.44975470

C -3.29935845 -0.00000677 -6.61403496

C -4.13811957 -0.00000348 -5.54771094

C -3.64678599 0.00000711 -4.16794498

O -4.43826762 0.00000986 -3.21728201

H 2.08754380 -0.00000432 2.05654476

H 1.60192706 0.00000000 4.50497836

H -0.74275184 0.00000000 5.30831895

H -2.63626885 0.00000000 3.71133498

H -3.25398658 0.00000000 -1.52189650

H -0.45020390 0.00000739 -2.81597413

H -0.25739939 -0.00000000 -5.06099004

H -3.71192333 -0.00000670 -7.62645588

C -3.63055583 -0.00002534 0.96407757

C 0.68455402 -1.27331298 -0.52829981

C 0.68454300 1.27332002 -0.52829703

H -3.93948407 -0.00005130 2.01435026

H -4.04581858 0.89154074 0.47006680

H -4.04578712 -0.89158626 0.47003228

H 1.73117792 -1.29938145 -0.18857547

H 0.17919461 -2.17360729 -0.15008729

H 0.68002432 -1.31302788 -1.62609176

H 1.73117034 1.29939155 -0.18858137

H 0.68000187 1.31304213 -1.62608855

H 0.17918157 2.17360872 -0.15007313

H -5.22295168 -0.00000032 -5.66644731

H -1.22307861 -0.00000000 -7.32860769

**BIPS open form TTT B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51728714

C 1.05717312 0.00000000 2.41117928

C 0.78746676 -0.00000000 3.78489205

C -0.52991550 -0.00000000 4.23916060

C -1.60585228 -0.00000000 3.34557863

C -1.31436326 -0.00000000 1.98612585

N -2.18914725 -0.00000000 0.89001214

C -1.50659037 -0.00000000 -0.29962198

C -2.14564071 -0.00000864 -1.51397453

C -1.47558149 -0.00000895 -2.76599796

C -2.02121965 -0.00002995 -4.02747490

C -3.43726812 -0.00005655 -4.30771720

C -3.90431497 -0.00008789 -5.58092303

C -2.97716093 -0.00009516 -6.68931085

C -1.63519732 -0.00007144 -6.50177340

C -1.04844751 -0.00003694 -5.15716470

O 0.17036894 -0.00001528 -4.98048591

H 2.08829639 0.00000000 2.05123039

H 1.60999842 -0.00000000 4.50107174

H -0.73242689 -0.00000000 5.31143459

H -2.62978650 -0.00000000 3.72009881

H -3.23654275 -0.00001569 -1.51363737

H -0.38360949 0.00000642 -2.78025193

H -4.14296810 -0.00005245 -3.47382886

H -3.38105279 -0.00012063 -7.70526117

C -3.62856223 -0.00000000 0.98024618

C 0.68772525 -1.27291720 -0.52742652

C 0.68771842 1.27291980 -0.52742768

H -3.93177282 0.00001754 2.03223383

H -4.05022951 0.89458469 0.49505836

H -4.05022927 -0.89459932 0.49508687

H 1.72898225 -1.30078487 -0.17226655

H 0.17683052 -2.17425668 -0.15870855

H 0.70274289 -1.30550532 -1.62505980

H 1.72897576 1.30079212 -0.17226928

H 0.70273459 1.30550668 -1.62506117

H 0.17681952 2.17425631 -0.15871043

H -0.93400727 -0.00007690 -7.33786874

H -4.97644137 -0.00010782 -5.78176967

**BIPS open form CTT B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51215601

C 1.05037448 0.00000000 2.41396973

C 0.76863377 -0.00499002 3.78530460

C -0.55275957 -0.01290872 4.22748417

C -1.62136079 -0.01212158 3.32483428

C -1.31887492 0.00265601 1.96772326

N -2.19667319 0.01659264 0.86851049

C -1.50321870 -0.03160516 -0.31190561

C -1.97467238 -0.09658365 -1.59933922

C -3.31292701 -0.27142823 -2.04405674

C -3.77274331 -0.32104747 -3.33979513

C -2.94542051 -0.16771038 -4.51241436

C -3.47227992 -0.23101488 -5.76065240

C -4.88855103 -0.45605174 -5.93534810

C -5.72597667 -0.60644675 -4.88061267

C -5.23727171 -0.54794339 -3.49901213

O -5.99504351 -0.67700133 -2.53617036

H 2.08431502 0.00164084 2.06212277

H 1.58461547 -0.00792259 4.50896129

H -0.76467606 -0.02501560 5.29786728

H -2.64815059 -0.03271769 3.69021910

H -1.19480138 -0.04784169 -2.36196736

H -4.11310258 -0.41603380 -1.31699614

H -1.87409118 0.00519187 -4.38800416

H -5.28633919 -0.50402232 -6.95257050

C -3.62909732 0.15537215 1.01181376

C 0.70467967 -1.24641350 -0.55715905

C 0.64071863 1.28448074 -0.55277496

H -3.85450248 0.50470376 2.02579764

H -4.00702753 0.90337380 0.30142955

H -4.15532628 -0.79577691 0.83843602

H 1.76429129 -1.24421907 -0.25884715

H 0.23989658 -2.16609499 -0.17368860

H 0.65843792 -1.26734304 -1.65608766

H 1.69941394 1.33388828 -0.25526526

H 0.59155932 1.30677727 -1.65175860

H 0.13137862 2.17807080 -0.16379633

H -6.79613731 -0.77545315 -5.01086465

H -2.83789279 -0.11312092 -6.64012638

**BIPS open form CTC B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51172751

C 1.04785827 0.00000000 2.41656725

C 0.76259003 0.00196107 3.78735834

C -0.55919341 0.00646900 4.22850198

C -1.62609833 0.00573944 3.32348927

C -1.31893759 -0.00580174 1.96786925

N -2.19488652 -0.01888297 0.86596311

C -1.50105847 0.03413182 -0.31264327

C -1.95599131 0.09639239 -1.60749054

C -3.27276426 0.31353871 -2.08543545

C -3.67696900 0.36199059 -3.40910460

C -5.06760601 0.64119747 -3.68635124

C -5.55704163 0.70946302 -4.95020838

C -4.66792468 0.50050038 -6.06358950

C -3.34981692 0.23718235 -5.88097602

C -2.74842044 0.14557176 -4.54825889

O -1.54275544 -0.09615336 -4.41753173

H 2.08242444 0.00013025 2.06695770

H 1.57730063 0.00502792 4.51256559

H -0.77228864 0.01612524 5.29867129

H -2.65443245 0.02450473 3.68542298

H -1.19691812 0.01442082 -2.38474753

H -4.06802912 0.50783732 -1.36083308

H -5.73404089 0.79967251 -2.83288020

H -5.07273682 0.55811690 -7.07748975

C -3.62164430 -0.19166721 1.00269176

C 0.63272986 -1.28673339 -0.55881492

C 0.70471405 1.24251076 -0.56624337

H -3.84062311 -0.61277105 1.99144318

H -4.16623534 0.76000667 0.89606356

H -3.98190322 -0.89943389 0.24308174

H 1.69467111 -1.33544990 -0.27292484

H 0.12753039 -2.17927374 -0.16162154

H 0.56650162 -1.30720836 -1.65648645

H 1.76767152 1.23424830 -0.28006415

H 0.64115412 1.25805830 -1.66398718

H 0.24964347 2.16529165 -0.17793648

H -2.67073481 0.07904256 -6.72049120

H -6.61145935 0.92057104 -5.13179350

**BIPS open form CCC B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51143962

C 1.04250253 0.00000000 2.42298989

C 0.74380222 0.01729264 3.79037920

C -0.58148742 0.03455332 4.22398696

C -1.64131606 0.02857560 3.31195696

C -1.31858216 0.00477683 1.96233251

N -2.18550517 -0.03817662 0.85262565

C -1.49720093 0.01932262 -0.29942635

C -2.02721964 0.03488514 -1.58939467

C -3.21501820 0.61066913 -2.05286659

C -3.98627538 1.66949575 -1.54705747

C -5.23793002 1.95102738 -2.19714147

C -6.01655965 3.01649810 -1.85779532

C -5.55767631 3.92049996 -0.84744026

C -4.35783113 3.74002965 -0.23035453

C -3.49151258 2.60220788 -0.51865972

O -2.40424767 2.46941246 0.07470758

H 2.08019324 -0.00590060 2.08306388

H 1.55280083 0.02583742 4.52214273

H -0.80000093 0.05925020 5.29273540

H -2.67456234 0.06029036 3.65759420

H -1.38861448 -0.42439705 -2.34963795

H -3.54436060 0.23697974 -3.03106567

H -5.57018900 1.26412006 -2.98144215

H -6.18047425 4.77832219 -0.57977544

C -3.61107773 -0.21519165 0.98081558

C 0.67830549 -1.25749882 -0.56597809

C 0.63821708 1.28237214 -0.56135382

H -3.81310901 -0.81657199 1.87685435

H -4.13357186 0.75041765 1.05214920

H -3.98297979 -0.74766062 0.09678002

H 1.74007935 -1.26831464 -0.27695603

H 0.20736455 -2.17372724 -0.18049233

H 0.62967064 -1.27119683 -1.66512213

H 1.69377249 1.34248635 -0.25427123

H 0.59100292 1.27862474 -1.66078618

H 0.09451762 2.16480935 -0.19872180

H -3.99314938 4.43296604 0.53031215

H -6.97085309 3.19241044 -2.35573453

**BIPS open form CCT B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51413897

C 1.04899260 0.00000000 2.41751759

C 0.76523474 -0.01079912 3.78903049

C -0.55624777 -0.02356991 4.23153018

C -1.62423591 -0.02668822 3.32784819

C -1.31901780 -0.02075641 1.97165075

N -2.19990858 -0.03396143 0.87866736

C -1.50376595 0.04871208 -0.30458220

C -2.01213988 0.11656985 -1.57152997

C -3.33498706 0.43967480 -2.02623963

C -4.21054033 1.38210650 -1.54541388

C -3.86507605 2.37148060 -0.54551187

C -4.74405504 3.33183909 -0.16914680

C -6.06430775 3.37875967 -0.75887241

C -6.45303195 2.49792341 -1.71076568

C -5.56086641 1.43039804 -2.18254966

O -5.91642380 0.61934242 -3.03381200

H 2.08370588 0.00908876 2.06781692

H 1.58088196 -0.00476617 4.51316093

H -0.76755388 -0.02546408 5.30218103

H -2.65459725 -0.02157113 3.68465114

H -1.29617478 -0.11782022 -2.36542045

H -3.68573396 -0.07267607 -2.92997970

H -2.85715963 2.35755521 -0.12530766

H -6.75418873 4.16042579 -0.42988329

C -3.59011871 -0.41085986 1.00207570

C 0.63136015 -1.29087713 -0.54849532

C 0.70750358 1.23848231 -0.56779339

H -3.71528259 -1.00175558 1.91923187

H -4.26169711 0.46109920 1.03193015

H -3.87347808 -1.02897277 0.13939597

H 1.68921842 -1.34899232 -0.24954376

H 0.11390617 -2.17929986 -0.15831936

H 0.58481369 -1.31450597 -1.64777297

H 1.77301516 1.22900243 -0.29094554

H 0.63581143 1.25864037 -1.66555838

H 0.25806126 2.16288908 -0.17643917

H -7.44318253 2.53779132 -2.16771508

H -4.45830120 4.09131867 0.55996819

**BIPS open form TCT B97XD/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51966161

C 1.05880426 0.00000000 2.41078175

C 0.79465467 -0.01245354 3.78651762

C -0.52087458 -0.02991639 4.24424555

C -1.59979324 -0.03602982 3.35337634

C -1.31385753 -0.02795585 1.99202132

N -2.19227398 -0.04822973 0.90683061

C -1.51320940 0.07834664 -0.29509019

C -2.15633703 0.40343524 -1.44933253

C -1.59062127 0.55073521 -2.77728793

C -0.98292717 -0.39589570 -3.54691961

C -0.98148762 -1.81135076 -3.22392296

C -0.44512480 -2.72161791 -4.06786243

C 0.16118715 -2.29479349 -5.31380760

C 0.18432951 -0.99654185 -5.69318962

C -0.38391839 0.05914160 -4.84379568

O -0.34749189 1.24164971 -5.16533067

H 2.08905542 0.01706562 2.04791820

H 1.61990577 -0.00341660 4.49962119

H -0.72013170 -0.03375340 5.31733740

H -2.62397924 -0.03881684 3.72768364

H -3.19493069 0.73794044 -1.36124322

H -1.70923887 1.52716460 -3.26513427

H -1.47250856 -2.12437454 -2.30085478

H 0.59514848 -3.05669469 -5.96665190

C -3.62531380 -0.00830980 1.01935431

C 0.67451465 -1.28710566 -0.50396067

C 0.72635609 1.23508220 -0.55425244

H -3.92991944 -0.42123439 1.98893657

H -4.02201826 1.01882861 0.93138637

H -4.07597060 -0.62560506 0.22812022

H 1.67761544 -1.36804721 -0.05791082

H 0.10228875 -2.18023845 -0.21194904

H 0.78668661 -1.27919115 -1.59512312

H 1.78276257 1.21703551 -0.24497275

H 0.69322546 1.25115504 -1.65340088

H 0.27241523 2.16222564 -0.17586455

H 0.62833348 -0.67457085 -6.63639204

H -0.48395814 -3.78664400 -3.83484221

**The BIPS TCC structure collapses to the closed form.**

**BIPS MP2/cc-pvdz optimised geometry – form A**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51613336

C 1.05211320 0.00000000 2.43480355

C 0.75177362 0.06439230 3.81287904

C -0.58481461 0.13564254 4.24369983

C -1.65241256 0.13843265 3.32125269

C -1.33838660 0.07898073 1.95622581

N -2.20937937 0.10560275 0.84763381

C -1.47567708 -0.46022445 -0.27328232

C -2.04232123 -0.01415893 -1.59117397

C -2.12788257 -0.85550197 -2.65226783

C -1.74703249 -2.25730860 -2.51007742

C -1.69086449 -3.16447934 -3.58886844

C -1.37626712 -4.51405958 -3.37535602

C -1.13162797 -4.97080487 -2.06582796

C -1.18499782 -4.08217574 -0.98033546

C -1.48143045 -2.72720301 -1.20268298

O -1.55131341 -1.91223082 -0.10717719

C -3.58437016 -0.34150235 1.03174849

C 1.03197723 -0.93036318 -0.63760597

C 0.20760471 1.44488375 -0.49365167

H -1.33035982 -5.20881134 -4.21967779

H 2.09232889 -0.06314105 2.09475330

H 1.56128341 0.05546860 4.54994627

H -0.80597483 0.17704078 5.31578609

H -2.68866353 0.18193943 3.67059302

H -2.34495935 1.03497384 -1.66337947

H -2.50548434 -0.50092278 -3.61887301

H -1.90050686 -2.79564554 -4.59991882

H -0.88994877 -6.02397603 -1.88743301

H -4.09245731 -0.32993867 0.05477473

H -4.10885643 0.35808688 1.70226871

H -3.64236554 -1.36317796 1.45250753

H 2.04729965 -0.53853506 -0.45164219

H 0.88645095 -0.98342067 -1.73123320

H 0.96919064 -1.94697881 -0.22127042

H 1.19456369 1.80387902 -0.15557422

H 0.17752816 1.49600746 -1.59632350

H -0.56474015 2.11529545 -0.08111708

H -0.99931395 -4.41580165 0.04553050

**BIPS MP2/cc-pvdz optimized geometry – form B**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51680213

C 1.05373628 0.00000000 2.43339754

C 0.75573103 0.06977084 3.81168004

C -0.57984116 0.14856496 4.24443316

C -1.64882597 0.15206376 3.32359604

C -1.33711914 0.08843404 1.95790097

N -2.20802799 0.10956312 0.84887519

C -1.47003101 -0.47193785 -0.27126599

C -2.06056378 -0.05339558 -1.58642149

C -2.85845084 -0.88603115 -2.30451922

C -3.13518240 -2.23307942 -1.82269031

C -4.08501416 -3.09642585 -2.41031479

C -4.29096107 -4.38594669 -1.90218338

C -3.53520068 -4.82801364 -0.79770619

C -2.58781856 -3.98337273 -0.19993465

C -2.39133833 -2.68788976 -0.70881360

O -1.41410535 -1.92460266 -0.13531850

C -3.59008481 -0.30385944 1.04959152

C 1.04017006 -0.91833620 -0.64175294

C 0.20798137 1.45156230 -0.47483831

H -5.03052536 -5.04749519 -2.36389327

H 2.09302471 -0.06906581 2.09177488

H 1.56635754 0.05949449 4.54749780

H -0.79913171 0.19467087 5.31671362

H -2.68414878 0.20051203 3.67489684

H -1.88022822 0.97302283 -1.91547643

H -3.31564508 -0.55001222 -3.24308753

H -4.65979306 -2.74012286 -3.27339039

H -3.68691696 -5.83580025 -0.39678835

H -4.11797068 -0.26724614 0.08453383

H -4.08431275 0.40136003 1.73753522

H -3.66950627 -1.32676620 1.46834563

H 2.05053425 -0.50647536 -0.47333260

H 0.87614095 -0.98108273 -1.73210475

H 0.99436767 -1.93259059 -0.22090439

H 1.16722103 1.82263339 -0.07663419

H 0.24870072 1.51326330 -1.57642721

H -0.59777604 2.10708492 -0.10458414

H -1.98819675 -4.30580278 0.65709357

**BIPS open form TTC MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51788666

C 1.06496706 0.00000000 2.42313493

C 0.78150968 0.00000000 3.80470985

C -0.55090622 0.00000000 4.25808255

C -1.63152929 0.00000000 3.35444199

C -1.32945256 0.00000000 1.98449237

N -2.19467577 -0.00000547 0.87768259

C -1.50038598 0.00001381 -0.30915043

C -2.16322042 0.00003316 -1.53013719

C -1.53393648 0.00003815 -2.80052622

C -2.17688082 0.00005748 -4.04283102

C -1.35226976 0.00005946 -5.23236700

C -1.89733625 0.00007784 -6.49367339

C -3.33208854 0.00009581 -6.65135908

C -4.16675759 0.00009490 -5.56098392

C -3.66393439 0.00007586 -4.18051794

O -4.45608523 0.00007566 -3.21445130

H 2.10197590 0.00000000 2.06864669

H 1.60129527 0.00000000 4.52994172

H -0.75714631 0.00000000 5.33340250

H -2.66081130 0.00000000 3.72466272

H -3.25492654 0.00004688 -1.54127707

H -0.43661785 0.00002596 -2.84172172

H -0.26237648 0.00004568 -5.10007118

H -3.75886954 0.00011043 -7.66152535

C -3.64527960 -0.00001255 0.94285768

C 0.68882919 -1.27510279 -0.52532902

C 0.68883692 1.27509722 -0.52532747

H -3.96006222 -0.00011472 1.99441729

H -4.05145292 0.89429380 0.44041994

H -4.05143997 -0.89423120 0.44025598

H 1.74037234 -1.29380048 -0.18898379

H 0.18336378 -2.17434323 -0.13564404

H 0.67386333 -1.31721637 -1.62615625

H 1.74038085 1.29378852 -0.18898336

H 0.67387204 1.31721263 -1.62615564

H 0.18337770 2.17434078 -0.13564234

H -5.25630931 0.00010848 -5.67325542

H -1.25198965 0.00007894 -7.37762627

**BIPS open form TTT MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51830411

C 1.06720338 0.00000000 2.42082332

C 0.78874713 -0.00000000 3.80342209

C -0.54204017 -0.00000000 4.26075440

C -1.62530319 -0.00000000 3.35996373

C -1.32746355 -0.00000000 1.98911713

N -2.19651685 0.00000000 0.88525488

C -1.50281472 -0.00000000 -0.30683111

C -2.13941251 -0.00000527 -1.53785226

C -1.45580693 -0.00000543 -2.78513293

C -2.01226643 -0.00001744 -4.05785536

C -3.43280927 -0.00003228 -4.32811038

C -3.90583632 -0.00004358 -5.61738353

C -2.98390433 -0.00004081 -6.73522793

C -1.62670037 -0.00002698 -6.54297171

C -1.03237607 -0.00001422 -5.19503987

O 0.19728845 -0.00000171 -5.02427647

H 2.10288352 0.00000000 2.06265300

H 1.61099414 -0.00000000 4.52584241

H -0.74544936 -0.00000000 5.33664787

H -2.65318801 -0.00000000 3.73440835

H -3.23414098 -0.00001435 -1.54202181

H -0.36067714 0.00000365 -2.79208837

H -4.13976862 -0.00003451 -3.49068451

H -3.38822735 -0.00005004 -7.75453758

C -3.64325580 0.00000000 0.96126699

C 0.69332360 -1.27443568 -0.52314713

C 0.69333014 1.27442833 -0.52315154

H -3.95194180 0.00002254 2.01476372

H -4.05704480 0.89687778 0.46781286

H -4.05704593 -0.89689622 0.46784945

H 1.73916653 -1.29466018 -0.16992074

H 0.18192217 -2.17481793 -0.14355462

H 0.69924193 -1.31021856 -1.62415071

H 1.73917263 1.29464883 -0.16992212

H 0.69925241 1.31020744 -1.62415519

H 0.18193350 2.17481607 -0.14356375

H -0.92673654 -0.00002484 -7.38523465

H -4.98349187 -0.00005478 -5.80999811

**BIPS open form CTT MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51338420

C 1.05821120 0.00000000 2.42615642

C 0.76457997 0.00150497 3.80591885

C -0.57095787 0.00258663 4.24898086

C -1.64528547 0.00519855 3.33694314

C -1.33231127 0.01396429 1.96940259

N -2.20407469 0.03259738 0.86351004

C -1.49986137 -0.02920139 -0.31946006

C -1.97639298 -0.10774382 -1.61883141

C -3.31462220 -0.31899823 -2.05620235

C -3.76953033 -0.37417170 -3.36878947

C -2.93583622 -0.16859601 -4.53205137

C -3.45998761 -0.24994251 -5.79897717

C -4.86525631 -0.54415616 -5.99236088

C -5.70708369 -0.74278286 -4.92882644

C -5.23188395 -0.66727006 -3.53680653

O -5.99986148 -0.83594138 -2.57558884

H 2.09761038 -0.00538612 2.07863894

H 1.57888220 -0.00349408 4.53730644

H -0.78527260 -0.00623545 5.32272500

H -2.67769749 -0.01415371 3.69779873

H -1.19263771 -0.04799504 -2.38188965

H -4.10613166 -0.50198489 -1.32258255

H -1.87291221 0.06220866 -4.39875144

H -5.25732001 -0.60619507 -7.01456238

C -3.63892100 0.21932548 0.99904779

C 0.70888956 -1.24615725 -0.55746554

C 0.64542245 1.28691535 -0.54862651

H -3.84098925 0.66759533 1.98285104

H -3.99197497 0.90983477 0.21792392

H -4.19311073 -0.73095823 0.91266481

H 1.77227148 -1.24049351 -0.25989067

H 0.24115725 -2.16647857 -0.17069171

H 0.65728174 -1.26409577 -1.65980133

H 1.70809390 1.33177428 -0.25159011

H 0.59096070 1.31004475 -1.65100193

H 0.13318022 2.17939223 -0.15243453

H -6.77055718 -0.96252494 -5.07060940

H -2.81938675 -0.09068033 -6.67229404

**BIPS open form CTC MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51275011

C 1.05523526 0.00000000 2.42934250

C 0.75722590 -0.00491651 3.80811289

C -0.57922928 -0.00990173 4.24930282

C -1.65121497 -0.01246365 3.33456457

C -1.33245991 -0.01665257 1.96871479

N -2.20185209 -0.03286959 0.85939322

C -1.49771961 0.02823795 -0.32001450

C -1.95645535 0.09261835 -1.62903083

C -3.27323088 0.33574246 -2.10273261

C -3.67204586 0.38499742 -3.44292580

C -5.05465861 0.70801646 -3.72535891

C -5.53554906 0.78337326 -5.01013425

C -4.64678135 0.53819984 -6.12112048

C -3.32441070 0.23030418 -5.91777986

C -2.73412448 0.12459489 -4.57602165

O -1.52783104 -0.16380028 -4.43243565

H 2.09549056 0.00713924 2.08478695

H 1.56967450 -0.00007744 4.54162191

H -0.79523911 -0.00446280 5.32270688

H -2.68523761 0.00363004 3.69153799

H -1.19082433 -0.00449137 -2.40278039

H -4.06557007 0.56304694 -1.37783521

H -5.72137023 0.89562367 -2.87343795

H -5.03860182 0.60186465 -7.14334646

C -3.63282559 -0.24066574 0.98739553

C 0.63958585 -1.28772340 -0.55593617

C 0.70522965 1.24403564 -0.56768095

H -3.83167816 -0.74050699 1.94735635

H -4.19646619 0.70792167 0.95177324

H -3.97381804 -0.89492940 0.17024020

H 1.70547552 -1.33026336 -0.27038389

H 0.13301549 -2.18030073 -0.15237082

H 0.56851431 -1.30827302 -1.65711215

H 1.77178511 1.23603668 -0.28179185

H 0.63672804 1.25482984 -1.66892454

H 0.24422095 2.16650602 -0.17738050

H -2.64369868 0.04379041 -6.75535025

H -6.58581135 1.02855899 -5.19647762

**BIPS open form CCC MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51232018

C 1.05232589 0.00000000 2.43350365

C 0.74522580 0.01444528 3.80948227

C -0.59352186 0.02590099 4.24757109

C -1.66076638 0.01570283 3.32893519

C -1.33065956 -0.00180813 1.96783708

N -2.19485825 -0.05106482 0.85249882

C -1.49386889 -0.00316450 -0.30578893

C -2.03938355 0.05448333 -1.59175621

C -3.27711811 0.59502854 -1.99784250

C -4.06693640 1.60148019 -1.39564881

C -5.35553699 1.87206727 -1.98867980

C -6.16734031 2.89284631 -1.54327638

C -5.71374199 3.74970803 -0.48437951

C -4.47034598 3.56876484 0.07977902

C -3.56100920 2.49518637 -0.32339756

O -2.43049505 2.37807521 0.21566169

H 2.09467742 -0.00223686 2.09565355

H 1.55431260 0.02549768 4.54686311

H -0.81176661 0.04900626 5.32015766

H -2.69827466 0.04625333 3.67394388

H -1.40334190 -0.36099650 -2.38462501

H -3.63083655 0.26133710 -2.98656595

H -5.69023465 1.22016862 -2.80597217

H -6.35875364 4.56432307 -0.13378181

C -3.61540497 -0.30456435 0.96335485

C 0.70176574 -1.24794843 -0.56532183

C 0.63005374 1.29245962 -0.55429006

H -3.79509640 -0.87139524 1.88935260

H -4.20073766 0.63300105 0.96849257

H -3.92849467 -0.89812036 0.09073299

H 1.76964236 -1.23566464 -0.28538517

H 0.24655887 -2.17112781 -0.16950909

H 0.63938542 -1.26447076 -1.66730486

H 1.69065085 1.35562929 -0.25234306

H 0.57440878 1.29368928 -1.65705258

H 0.07946286 2.16863864 -0.17796414

H -4.10489016 4.22671219 0.87651623

H -7.14740435 3.05960184 -2.00176750

**BIPS open form CCT MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51510154

C 1.05832648 0.00000000 2.42817585

C 0.76491257 -0.01920417 3.80808188

C -0.57010669 -0.04479917 4.25291421

C -1.64462539 -0.05102443 3.34118240

C -1.33182499 -0.03526711 1.97408774

N -2.20712989 -0.05200339 0.87214654

C -1.50016977 0.03975220 -0.31037261

C -2.02442070 0.10576937 -1.58997148

C -3.35724097 0.44640448 -1.99688275

C -4.19829485 1.39764752 -1.42747934

C -3.75240624 2.36607071 -0.44524926

C -4.59151277 3.35990810 -0.00483109

C -5.95253566 3.44543080 -0.49753925

C -6.42557001 2.57041249 -1.44027467

C -5.59297833 1.47758772 -1.97593454

O -6.03352150 0.66799628 -2.80529134

H 2.09781020 0.01869218 2.08116705

H 1.57979097 -0.01033818 4.53888487

H -0.78270035 -0.05230153 5.32706534

H -2.67936714 -0.05151352 3.69684729

H -1.31791836 -0.15009880 -2.39084064

H -3.75371765 -0.02733613 -2.90748930

H -2.71051603 2.33181353 -0.10743615

H -6.60352757 4.24348369 -0.12096893

C -3.59758216 -0.45498157 0.97179512

C 0.63967321 -1.29199173 -0.54395948

C 0.70753070 1.23994278 -0.56999351

H -3.72871442 -1.01335855 1.91159740

H -4.28894090 0.40578387 0.94451552

H -3.83530882 -1.10910199 0.11697861

H 1.70215224 -1.34046231 -0.24697784

H 0.12350287 -2.18059435 -0.14418782

H 0.58644277 -1.31832214 -1.64639212

H 1.77736641 1.22925302 -0.29613987

H 0.62764563 1.25652459 -1.67085587

H 0.25469324 2.16450661 -0.17456424

H -7.44679360 2.64070549 -1.82979828

H -4.22882748 4.11187596 0.70371403

**BIPS TCT open form MP2/cc-pvdz optimised geometry**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.52100695

C 1.06899028 0.00000000 2.42126894

C 0.79440451 -0.02352884 3.80508716

C -0.53417684 -0.06259763 4.26612690

C -1.61945826 -0.07585156 3.36702338

C -1.32436608 -0.05372412 1.99568819

N -2.19758351 -0.08572361 0.90002924

C -1.51277886 0.08008757 -0.29755982

C -2.16273704 0.48533793 -1.44830936

C -1.58485097 0.63030971 -2.76441452

C -0.91842801 -0.33573104 -3.49715699

C -0.95887581 -1.74778271 -3.16266396

C -0.42205875 -2.68199702 -4.01104130

C 0.22973805 -2.27331410 -5.24229775

C 0.28968996 -0.95802206 -5.62044734

C -0.25884346 0.11451661 -4.77181789

O -0.15466765 1.31125409 -5.07438893

H 2.10382151 0.03515864 2.06192374

H 1.61882257 -0.00823274 4.52499652

H -0.73412144 -0.07447415 5.34273593

H -2.64815596 -0.09405813 3.73924347

H -3.18268344 0.87378268 -1.32471348

H -1.72863688 1.59048643 -3.28543063

H -1.50010382 -2.05150809 -2.26016340

H 0.65798443 -3.04467915 -5.89350398

C -3.63699372 -0.01852739 1.01332033

C 0.69285292 -1.28922863 -0.48398237

C 0.72965840 1.23635242 -0.55397328

H -3.94941581 -0.51134096 1.94603990

H -4.00827388 1.02435954 1.01432857

H -4.08957280 -0.55426751 0.16345360

H 1.69881455 -1.34425782 -0.03180685

H 0.12776069 -2.18459690 -0.17373912

H 0.79997443 -1.29641409 -1.57892435

H 1.78875090 1.21313136 -0.24195281

H 0.69091828 1.25206974 -1.65598112

H 0.27185579 2.16294309 -0.17032450

H 0.76729542 -0.64778576 -6.55573207

H -0.50577904 -3.74886300 -3.77947781

**The TCC open form collapses to the closed form**

**Geometries - nitroBIPS**

**nitroBIPS B97XD/cc-pvdz optimized geometry – form A**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51603655

C 1.04508773 0.00000000 2.42113073

C 0.75874445 0.05373810 3.79302312

C -0.56279546 0.10683353 4.22732968

C -1.62851749 0.10484740 3.31813511

C -1.32538311 0.05756398 1.96254779

N -2.20227184 0.06571217 0.87044810

C -1.48840144 -0.43008870 -0.27870583

C -2.06052232 0.08256244 -1.56996992

C -2.25635521 -0.70091474 -2.63448447

C -1.98397407 -2.13195633 -2.56058974

C -2.07924311 -2.99046793 -3.65244448

C -1.84799851 -4.34895217 -3.47641155

C -1.53485625 -4.88267995 -2.22744200

C -1.44115091 -4.03425149 -1.13478397

C -1.65375055 -2.66148548 -1.29923678

O -1.56074335 -1.88943756 -0.20551371

C -3.59017468 -0.30169149 1.04847364

C 1.00800924 -0.95689313 -0.63283490

C 0.25065104 1.43409046 -0.49831517

N -1.94479088 -5.24299430 -4.63396273

O -2.22096847 -4.74463948 -5.71048194

O -1.74318064 -6.42932142 -4.44935303

H 2.08003057 -0.04746529 2.07465363

H 1.57216191 0.04867772 4.51984258

H -0.77851582 0.14107047 5.29694061

H -2.65980776 0.13205111 3.67183314

H -2.28512217 1.14874170 -1.59900528

H -2.64415549 -0.28985748 -3.56884805

H -2.33684890 -2.61448864 -4.64227761

H -1.36473936 -5.95370641 -2.13240594

H -4.08120488 0.41749558 1.71973718

H -4.10135005 -0.25985320 0.07697113

H -3.70771424 -1.31805361 1.46501160

H 2.03058973 -0.58800873 -0.46235364

H 0.93248703 -1.96541975 -0.20678536

H 0.85692759 -1.02063699 -1.72237629

H 1.24039429 1.76915541 -0.15539133

H 0.23381666 1.48504524 -1.59801331

H -0.49870634 2.13316130 -0.09825126

H -1.19706180 -4.41165515 -0.14199258

**nitroBIPS B97XD/cc-pvtz optimized geometry** **– form B**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51649541

C 1.04629922 0.00000000 2.42042371

C 0.76158412 0.05592675 3.79238160

C -0.55935176 0.11144604 4.22835820

C -1.62570750 0.10942863 3.32017763

C -1.32432981 0.06056955 1.96412551

N -2.20337086 0.06301750 0.87268490

C -1.48396653 -0.44062747 -0.27768723

C -2.07917982 0.05534522 -1.56400405

C -2.76347683 -0.73448088 -2.39826984

C -2.94963769 -2.14722036 -2.09641504

C -3.74503326 -2.99971874 -2.85912871

C -3.86521258 -4.33304762 -2.49144379

C -3.20559952 -4.84874654 -1.37591654

C -2.41311447 -4.00721296 -0.61169527

C -2.28330874 -2.65973567 -0.96818834

O -1.47523784 -1.89975456 -0.21528546

C -3.58702975 -0.31235746 1.06430488

C 1.01710392 -0.94556615 -0.63545562

C 0.24946319 1.43933087 -0.48493493

N -4.70617754 -5.22091417 -3.29978042

O -5.27084267 -4.73919072 -4.26545976

O -4.78945091 -6.38594225 -2.95651152

H 2.08067130 -0.04971955 2.07270947

H 1.57592024 0.05048198 4.51818502

H -0.77383880 0.14752594 5.29813916

H -2.65638436 0.13803922 3.67544321

H -1.97226387 1.12014828 -1.76499857

H -3.20854469 -0.33131167 -3.31036566

H -4.27407225 -2.63663927 -3.73994190

H -3.32669895 -5.90105937 -1.12462319

H -4.07279770 0.39681084 1.74969086

H -4.11436322 -0.26074443 0.10241258

H -3.69457387 -1.33259438 1.47706989

H 2.03520513 -0.56272339 -0.46756120

H 0.95124876 -1.95518727 -0.21304725

H 0.85948434 -1.01017455 -1.72362958

H 1.22112052 1.78346156 -0.10227833

H 0.27984511 1.49642090 -1.58406835

H -0.52203631 2.12903681 -0.11131460

H -1.88097199 -4.37039800 0.26720315

**nitroBIPS open form TTC B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51618497

C 1.05396694 0.00000000 2.41478464

C 0.77435910 -0.00000000 3.78581295

C -0.54574861 -0.00000000 4.23433424

C -1.61695518 -0.00000000 3.33607747

C -1.31497722 -0.00000000 1.97988184

N -2.18538365 0.00000000 0.87458417

C -1.50335154 -0.00000000 -0.29969558

C -2.16961259 -0.00000000 -1.51254411

C -1.54780191 0.00000000 -2.77007606

C -2.18091881 -0.00001197 -4.01326197

C -1.35356597 -0.00000955 -5.17609892

C -1.89727501 -0.00002827 -6.42492510

C -3.31722731 -0.00005108 -6.62101442

C -4.14744991 -0.00005433 -5.55008438

C -3.65669200 -0.00003526 -4.16909463

O -4.44415827 -0.00003888 -3.21700163

H 2.08735132 0.00000000 2.06186863

H 1.59244815 -0.00000000 4.50698301

H -0.75258991 -0.00000000 5.30555695

H -2.64324319 -0.00000000 3.70323986

H -3.25807095 0.00000000 -1.52688196

H -0.45470934 0.00000739 -2.81105008

H -0.26677838 0.00000134 -5.07714937

H -3.69623855 -0.00006542 -7.64252223

C -3.63116454 0.00000000 0.95752532

C 0.68213280 -1.27458719 -0.52987294

C 0.68213337 1.27458680 -0.52987313

H -3.93594407 0.00000545 2.00860662

H -4.04475376 0.89225036 0.46496764

H -4.04475373 -0.89225664 0.46497691

H 1.72738324 -1.30169408 -0.18732671

H 0.17529357 -2.17515433 -0.15443234

H 0.68211639 -1.31195881 -1.62757178

H 1.72738263 1.30169491 -0.18732592

H 0.68211860 1.31195718 -1.62757155

H 0.17529297 2.17515466 -0.15443419

H -5.23145029 -0.00007150 -5.67114412

N -1.01842588 -0.00002507 -7.58619369

O -1.54132043 -0.00006145 -8.68853604

O 0.18748145 0.00001200 -7.39630433

**nitroBIPS open form TTT B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51636438

C 1.05606300 0.00000000 2.41252457

C 0.78064460 0.00000000 3.78435387

C -0.53799981 0.00000000 4.23662878

C -1.61156999 0.00000000 3.34093415

C -1.31306522 0.00000000 1.98399704

N -2.18708992 -0.00000000 0.88071031

C -1.50569554 -0.00000000 -0.29705504

C -2.14997866 -0.00000000 -1.51874802

C -1.48158678 -0.00000000 -2.75670745

C -2.02878569 -0.00000000 -4.02924000

C -3.43124958 -0.00000632 -4.28723913

C -3.89076479 -0.00000588 -5.56757545

C -2.99771891 0.00000087 -6.69512347

C -1.65757146 0.00000703 -6.50368513

C -1.06260384 0.00000712 -5.16173400

O 0.15485687 0.00001271 -4.98540401

H 2.08827303 0.00000000 2.05632666

H 1.60091158 0.00000000 4.50304709

H -0.74221633 0.00000000 5.30836544

H -2.63664279 0.00000000 3.71185049

H -3.24063266 -0.00000000 -1.51749729

H -0.38938671 -0.00000000 -2.77396649

H -4.15972762 -0.00001160 -3.47647990

H -3.43457756 0.00000083 -7.69322483

C -3.63002509 -0.00000000 0.97284645

C 0.68539851 -1.27417567 -0.52864625

C 0.68540096 1.27417533 -0.52864595

H -3.92956004 0.00000000 2.02545692

H -4.04974507 0.89508451 0.48905583

H -4.04974568 -0.89508149 0.48905019

H 1.72553630 -1.30304938 -0.17123718

H 0.17326270 -2.17556714 -0.16199748

H 0.70366837 -1.30533487 -1.62621200

H 1.72553875 1.30304662 -0.17123369

H 0.70367502 1.30533413 -1.62621138

H 0.17326692 2.17556786 -0.16199896

H -0.96283852 0.00001220 -7.34441808

N -5.32942400 -0.00001242 -5.80507849

O -5.70908846 -0.00001184 -6.96410827

O -6.07336269 -0.00001811 -4.83699834

**nitroBIPS open form CTT B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51055714

C 1.05165550 0.00000000 2.41188550

C 0.76871503 -0.00000582 3.78185149

C -0.55286241 -0.00001151 4.22493026

C -1.62131714 -0.00001156 3.32297699

C -1.31689598 -0.00000572 1.96706097

N -2.19437896 0.00000219 0.85890249

C -1.50142444 -0.00003116 -0.31036727

C -1.96527603 -0.00007051 -1.61232543

C -3.29437797 -0.00019536 -2.07634542

C -3.73386644 -0.00025044 -3.39168170

C -2.86463734 -0.00016341 -4.52166620

C -3.38057117 -0.00023333 -5.78060655

C -4.79821722 -0.00039498 -6.02090881

C -5.66594613 -0.00048270 -4.98161169

C -5.20929923 -0.00041817 -3.58701633

O -5.99616097 -0.00049198 -2.64053950

H 2.08534285 0.00000000 2.06009630

H 1.58423423 -0.00000591 4.50592644

H -0.76451300 -0.00002142 5.29520229

H -2.64674656 -0.00002513 3.69205666

H -1.17203289 -0.00003431 -2.36231494

H -4.12743965 -0.00028426 -1.37307858

H -1.78070599 -0.00004073 -4.40774917

H -5.14078721 -0.00044328 -7.05526579

C -3.63568807 0.00008746 0.99194136

C 0.67075223 -1.26699988 -0.55709639

C 0.67072091 1.26701713 -0.55709666

H -3.90046872 0.00029716 2.05334235

H -4.07116925 0.89487039 0.52392454

H -4.07126901 -0.89481461 0.52424065

H 1.72919246 -1.28981625 -0.25698458

H 0.18364348 -2.17436666 -0.17187258

H 0.62701674 -1.28722963 -1.65594943

H 1.72916115 1.28985875 -0.25698620

H 0.62698389 1.28724438 -1.65595027

H 0.18359067 2.17437135 -0.17187324

H -6.74483821 -0.00060551 -5.14114795

N -2.47119063 -0.00014188 -6.92050486

O -2.96586930 -0.00021321 -8.03539482

O -1.27051636 -0.00000480 -6.70004548

**nitroBIPS open CTC form B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51069716

C 1.04656054 0.00000000 2.41797301

C 0.75540664 -0.00496791 3.78674791

C -0.56767039 -0.01247729 4.22575094

C -1.63210408 -0.01132674 3.31859899

C -1.31759725 0.00296169 1.96568632

N -2.19220606 0.01598337 0.85552468

C -1.49904123 -0.03170183 -0.31045571

C -1.95420119 -0.08753750 -1.61626763

C -3.25528360 -0.33173269 -2.08532861

C -3.65685075 -0.39755755 -3.42099096

C -5.02733943 -0.69844412 -3.68088281

C -5.50019391 -0.78183691 -4.95556372

C -4.64184247 -0.57476554 -6.08478608

C -3.33106987 -0.28966372 -5.89342940

C -2.73191932 -0.17656831 -4.56038215

O -1.53226956 0.08482961 -4.42568619

H 2.08218305 0.00157155 2.07223451

H 1.56766541 -0.00809931 4.51459433

H -0.78268997 -0.02444730 5.29528133

H -2.66132756 -0.03165675 3.67739067

H -1.19573497 0.01428821 -2.39194597

H -4.05121466 -0.53634002 -1.36523825

H -5.71952512 -0.86567968 -2.85395062

H -5.07365999 -0.65433699 -7.08195253

C -3.62380827 0.16704259 0.99129290

C 0.69896205 -1.24535274 -0.56901743

C 0.63206298 1.28651087 -0.56172816

H -3.84875720 0.58161364 1.98077432

H -3.99256712 0.87124816 0.23301417

H -4.14913950 -0.79425513 0.88171929

H 1.76177130 -1.23847391 -0.28372050

H 0.24314668 -2.16734734 -0.17988910

H 0.63477302 -1.25989273 -1.66660824

H 1.69293172 1.33357729 -0.27314848

H 0.57022557 1.30465191 -1.65950686

H 0.12760747 2.18043746 -0.16696566

H -2.65560591 -0.12840087 -6.73451115

N -6.90633505 -1.08845144 -5.17648241

O -7.29345328 -1.15722715 -6.33143473

O -7.61957200 -1.25931656 -4.20028622

**nitroBIPS open CCC form B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51063954

C 1.03973063 0.00000000 2.42626710

C 0.73257851 -0.01115099 3.79113412

C -0.59452206 -0.02156549 4.22151271

C -1.65064034 -0.01567213 3.30596601

C -1.31731892 0.00013704 1.95995981

N -2.18158951 0.03367897 0.84073668

C -1.49434184 -0.03931079 -0.29555778

C -2.03283560 -0.03974830 -1.60390761

C -3.14103764 -0.70657273 -2.08385762

C -3.86296024 -1.81304397 -1.55613120

C -5.08473342 -2.15089736 -2.18700678

C -5.80366793 -3.25224741 -1.79983424

C -5.31786754 -4.12640925 -0.78867619

C -4.11952912 -3.86952131 -0.19641146

C -3.31516342 -2.69851357 -0.51798824

O -2.23083081 -2.49168678 0.06191161

H 2.07900018 0.00048202 2.09211802

H 1.53806184 -0.01969413 4.52661848

H -0.81604814 -0.04048819 5.28948800

H -2.68582334 -0.04015179 3.64611472

H -1.44509262 0.52431942 -2.33327952

H -3.46216733 -0.39212781 -3.08409952

H -5.48496755 -1.52342498 -2.98495201

H -5.91771625 -4.99539583 -0.51973289

C -3.61758542 0.13362060 0.96959488

C 0.67057289 -1.25824037 -0.57681993

C 0.64066874 1.28192896 -0.56113380

H -3.85110111 0.78786547 1.81938350

H -4.02803128 0.56719114 0.05066898

H -4.06422609 -0.85921919 1.12453068

H 1.73200458 -1.27797190 -0.28664248

H 0.16547612 -2.16035615 -0.20895606

H 0.60713844 -1.25098196 -1.67520036

H 1.69925123 1.32135866 -0.26487424

H 0.59913314 1.29579636 -1.66030849

H 0.14207202 2.18316951 -0.17507477

H -3.71506338 -4.53076255 0.57139828

N -7.07168450 -3.54239700 -2.44850667

O -7.68008173 -4.53610303 -2.08367798

O -7.46264086 -2.78012237 -3.31926619

**nitroBIPS open CCT form B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51240383

C 1.04493562 0.00000000 2.42174983

C 0.74866881 0.01271363 3.78947745

C -0.57559131 0.02566180 4.22641988

C -1.63778225 0.02083836 3.31730523

C -1.31685384 -0.00003050 1.96696121

N -2.19272699 -0.02313952 0.86024311

C -1.50131614 0.03839695 -0.30503324

C -2.00721609 0.07212054 -1.59389943

C -3.25616653 0.50463906 -2.09176438

C -4.14597165 1.45801862 -1.60632195

C -3.82794038 2.36248125 -0.55181265

C -4.70633588 3.33799753 -0.18738437

C -5.97047865 3.50472772 -0.84971085

C -6.31455468 2.68337751 -1.86976516

C -5.43929119 1.59764471 -2.33159140

O -5.76006806 0.84556660 -3.24856346

H 2.08213299 -0.00412907 2.08052277

H 1.55912280 0.02110703 4.51932213

H -0.79179003 0.04771409 5.29544500

H -2.67048628 0.05022524 3.66495979

H -1.30156602 -0.26765505 -2.35740577

H -3.55685237 0.09708101 -3.06443969

H -2.86521300 2.31869157 -0.04274845

H -6.62411902 4.30891910 -0.51277136

C -3.60253612 -0.31208845 0.99623190

C 0.64704604 -1.27903202 -0.55779965

C 0.68221591 1.25614277 -0.56458325

H -3.74415127 -0.95954998 1.87149745

H -4.20037205 0.60421890 1.11749909

H -3.95035702 -0.83604155 0.09734695

H 1.70301075 -1.32310594 -0.25177741

H 0.14083720 -2.17818944 -0.17778819

H 0.61198276 -1.29361260 -1.65729949

H 1.74752566 1.26170464 -0.28866706

H 0.60687793 1.27894825 -1.66186787

H 0.21857795 2.17008214 -0.16533112

H -7.26446538 2.79495907 -2.39411840

N -4.34151355 4.24680833 0.88924896

O -5.11594649 5.15192231 1.15167971

O -3.28871370 4.04940559 1.47809568

**nitroBIPS TCT form B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51812678

C 1.05787287 0.00000000 2.41250329

C 0.78580707 -0.00631666 3.78514597

C -0.53115098 -0.02085333 4.24229937

C -1.60671988 -0.02861108 3.34907398

C -1.30939685 -0.02334066 1.99162476

N -2.18689108 -0.03784989 0.89623210

C -1.51833773 0.05335564 -0.29198551

C -2.18742359 0.42209056 -1.44538262

C -1.72659280 0.43473261 -2.78720460

C -1.01233199 -0.53593638 -3.46416695

C -0.90906858 -1.87514604 -2.97906428

C -0.26081551 -2.82127873 -3.70780396

C 0.32743249 -2.52276075 -4.98733511

C 0.22592394 -1.27868635 -5.51100040

C -0.46048977 -0.18778762 -4.80476397

O -0.55254449 0.94307655 -5.27174926

H 2.08972389 0.01227414 2.05530513

H 1.60849118 0.00339511 4.50110092

H -0.73150490 -0.02264944 5.31481197

H -2.63275125 -0.03094968 3.71757933

H -3.16151816 0.89674186 -1.29409963

H -2.01884052 1.29280477 -3.40557407

H -1.39346654 -2.15877357 -2.04624108

H 0.83195006 -3.32933872 -5.51879460

C -3.62431325 -0.03066830 1.02083634

C 0.74755353 -1.25034962 -0.49856441

C 0.67159619 1.26903400 -0.55255978

H -3.91031820 -0.52280570 1.95850165

H -4.03079589 0.99470361 1.01751955

H -4.06623396 -0.59199462 0.18654408

H 1.72270909 -1.30276026 0.00800212

H 0.20330199 -2.17987558 -0.27989345

H 0.93417103 -1.19313331 -1.57741357

H 1.73148004 1.28502352 -0.25703747

H 0.61949739 1.28746623 -1.65093876

H 0.18977601 2.17678065 -0.16181985

H 0.64955274 -1.03524810 -6.48609861

N -0.18673987 -4.18005855 -3.18987476

O 0.33834602 -5.02538014 -3.89432105

O -0.64153795 -4.39672565 -2.07626358

**nitroBIPS MP2/cc-pvdz optimised – form A**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51633234

C 1.05266119 0.00000000 2.43445019

C 0.75182438 0.06556400 3.81222177

C -0.58460287 0.13847428 4.24330496

C -1.65250852 0.14188180 3.32123605

C -1.33767288 0.08048239 1.95694435

N -2.20948028 0.10677308 0.84672813

C -1.47648671 -0.45556086 -0.27068486

C -2.04112746 -0.01471239 -1.59047233

C -2.13471175 -0.85562578 -2.65056653

C -1.76594866 -2.26060219 -2.50222273

C -1.72661094 -3.16312101 -3.58083758

C -1.42541937 -4.50595906 -3.33637078

C -1.17823606 -4.98775784 -2.04191752

C -1.21877401 -4.08904769 -0.96868067

C -1.49826794 -2.72893990 -1.19314454

O -1.54594633 -1.91492334 -0.10481691

C -3.58687675 -0.33441699 1.02961912

C 1.02920421 -0.93240469 -0.63933040

C 0.20911137 1.44440116 -0.49524954

N -1.37970859 -5.44586540 -4.47368714

O -1.60002173 -4.98781937 -5.59741967

O -1.12411700 -6.62608839 -4.22396344

H 2.09286930 -0.06361581 2.09472904

H 1.56127246 0.05647723 4.54921774

H -0.80541808 0.18120206 5.31528821

H -2.68859240 0.18735246 3.67062897

H -2.33598706 1.03627681 -1.66655603

H -2.50953033 -0.50309143 -3.61828751

H -1.93341673 -2.82823227 -4.60061746

H -0.95164395 -6.04545710 -1.89315763

H -4.10748843 0.36602522 1.70187196

H -4.09627742 -0.31742160 0.05336380

H -3.64956294 -1.35648978 1.44871859

H 2.04480620 -0.53914866 -0.45942801

H 0.97109452 -1.94747143 -0.21847853

H 0.88062880 -0.98820768 -1.73256374

H 1.19604743 1.80178246 -0.15600836

H 0.18167307 1.49534593 -1.59803507

H -0.56233239 2.11630183 -0.08364212

H -1.03219686 -4.42260307 0.05670525

**nitroBIPS MP2/cc-pvdz optimised – form B**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51693586

C 1.05413492 0.00000000 2.43321930

C 0.75557282 0.07104485 3.81114051

C -0.57985054 0.15124837 4.24416498

C -1.64904735 0.15513297 3.32362846

C -1.33623076 0.08922358 1.95879592

N -2.20876556 0.10871604 0.84816401

C -1.47139437 -0.46625518 -0.26890162

C -2.06142840 -0.04881363 -1.58400860

C -2.84723704 -0.88057815 -2.31510808

C -3.11188831 -2.23446548 -1.84403620

C -4.04406178 -3.09536730 -2.45426305

C -4.21890630 -4.38315677 -1.94222056

C -3.48537673 -4.85246936 -0.84056860

C -2.56011034 -3.99608461 -0.23286697

C -2.37347485 -2.69088983 -0.72545705

O -1.41977463 -1.92647561 -0.13119231

C -3.59009956 -0.30830283 1.04811868

C 1.03712573 -0.92107785 -0.64317732

C 0.21046316 1.45096192 -0.47620095

N -5.19981601 -5.27972705 -2.58574527

O -5.83092010 -4.83392606 -3.54697199

O -5.32253836 -6.41423095 -2.11838342

H 2.09342536 -0.06941169 2.09196632

H 1.56609786 0.06087089 4.54694070

H -0.79888647 0.19876700 5.31630263

H -2.68418806 0.20553329 3.67500043

H -1.88887056 0.98173563 -1.90413701

H -3.30375782 -0.54347360 -3.25286389

H -4.62634428 -2.76946172 -3.32008248

H -3.65020448 -5.86806160 -0.47513423

H -4.08476097 0.39282356 1.73935708

H -4.12053184 -0.26768342 0.08452587

H -3.66661081 -1.33267566 1.46397546

H 2.04805961 -0.51042696 -0.47650252

H 0.99238830 -1.93493751 -0.22109984

H 0.87266503 -0.98407648 -1.73348015

H 1.17123955 1.81909918 -0.07939312

H 0.25047059 1.51231846 -1.57784739

H -0.59227721 2.10936313 -0.10454339

H -1.96660573 -4.32075271 0.62719309

**nitroBIPS open form TTC MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51693245

C 1.06339650 0.00000000 2.42460126

C 0.77457080 -0.00000000 3.80458217

C -0.55892245 -0.00000000 4.25630737

C -1.63747149 -0.00000000 3.35079998

C -1.32826907 -0.00000000 1.98317755

N -2.19256427 0.00000000 0.87010222

C -1.49927960 -0.00000000 -0.30794856

C -2.16410781 -0.00000000 -1.53303962

C -1.53144590 0.00000000 -2.79439691

C -2.17565575 0.00000000 -4.04005069

C -1.34483568 0.00000000 -5.21391583

C -1.90308558 0.00000000 -6.46578834

C -3.32827418 0.00000000 -6.65811356

C -4.15684160 0.00000000 -5.56484113

C -3.65991298 0.00000000 -4.18120031

O -4.45334737 0.00000000 -3.21723507

H 2.10144133 0.00000000 2.07383644

H 1.59236204 -0.00000000 4.53199200

H -0.76660379 -0.00000000 5.33114393

H -2.66770843 -0.00000000 3.71792372

H -3.25577663 0.00000000 -1.54761945

H -0.43453198 0.00000000 -2.83483780

H -0.25482017 -0.00000000 -5.11177443

H -3.72140570 0.00000000 -7.67748564

C -3.64594867 0.00000000 0.93694927

C 0.68782431 -1.27614382 -0.52576093

C 0.68782709 1.27614218 -0.52576265

H -3.95806719 0.00001970 1.98890566

H -4.04966665 0.89498065 0.43523443

H -4.04966711 -0.89499736 0.43526555

H 1.73806411 -1.29483157 -0.18638111

H 0.18136153 -2.17579521 -0.13836665

H 0.67719559 -1.31662027 -1.62649824

H 1.73806622 1.29482743 -0.18638074

H 0.67719855 1.31661773 -1.62649908

H 0.18136595 2.17579478 -0.13836894

H -5.24539247 0.00000000 -5.68327069

N -1.02732846 -0.00000000 -7.64681366

O -1.57451850 -0.00002519 -8.75462937

O 0.19247697 0.00002506 -7.46310747

**nitroBIPS TTT open form MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51739513

C 1.06557404 0.00000000 2.42237480

C 0.78162739 -0.00010617 3.80340640

C -0.55038010 -0.00024503 4.25862935

C -1.63145458 -0.00022200 3.35581776

C -1.32665123 0.00001044 1.98718632

N -2.19450798 0.00028433 0.87732932

C -1.50172985 -0.00020080 -0.30566912

C -2.14132024 -0.00090746 -1.54010762

C -1.45926475 -0.00091356 -2.77944553

C -2.01758521 -0.00165718 -4.05521294

C -3.43294369 -0.00247892 -4.30287255

C -3.89859799 -0.00317862 -5.59017308

C -3.01426740 -0.00309174 -6.73167279

C -1.65822104 -0.00234614 -6.53990132

C -1.04813389 -0.00153941 -5.19725537

O 0.18177658 -0.00082361 -5.03638180

H 2.10239290 0.00003123 2.06804326

H 1.60172478 -0.00013901 4.52819727

H -0.75553864 -0.00043489 5.33399069

H -2.66036851 -0.00051651 3.72690031

H -3.23592234 -0.00161632 -1.54582218

H -0.36410011 -0.00025583 -2.78798924

H -4.15560157 -0.00259016 -3.48245969

H -3.45359846 -0.00364026 -7.73190115

C -3.64465795 0.00046918 0.95398333

C 0.69226506 -1.27534016 -0.52358487

C 0.69186154 1.27555592 -0.52361965

H -3.95117831 0.00439246 2.00767659

H -4.05538034 0.89619416 0.45784843

H -4.05574402 -0.89857766 0.46413175

H 1.73710297 -1.29574305 -0.16815670

H 0.18004192 -2.17599875 -0.14587747

H 0.70087349 -1.30980169 -1.62452071

H 1.73671426 1.29627103 -0.16825253

H 0.70038477 1.31000237 -1.62455898

H 0.17938764 2.17606141 -0.14588287

H -0.96831827 -0.00229391 -7.39001685

N -5.35212083 -0.00391591 -5.82556555

O -5.73237086 -0.00375900 -7.00083224

O -6.09800013 -0.00462355 -4.84295026

**nitroBIPS CTT open form MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51234131

C 1.05668889 0.00000000 2.42742178

C 0.75820401 -0.00295662 3.80562628

C -0.57835003 -0.00673825 4.24700852

C -1.65074310 -0.00387595 3.33325803

C -1.33127467 0.00913048 1.96803533

N -2.20163688 0.02774527 0.85516439

C -1.49801609 -0.02479613 -0.31876253

C -1.97079029 -0.09016788 -1.62531921

C -3.29914807 -0.30262332 -2.06732843

C -3.74641395 -0.36326532 -3.38603616

C -2.89410302 -0.17002901 -4.52651452

C -3.41767223 -0.25340783 -5.78877216

C -4.81398206 -0.52964565 -6.02971782

C -5.66153521 -0.71669148 -4.97021556

C -5.20601984 -0.64491309 -3.56990076

O -5.98602008 -0.80632422 -2.61843720

H 2.09695664 -0.00215920 2.08316010

H 1.57059939 -0.00759710 4.53905565

H -0.79416851 -0.01870597 5.32022429

H -2.68377376 -0.02551056 3.69178994

H -1.18521114 -0.01553788 -2.38499439

H -4.09853171 -0.48039356 -1.34120159

H -1.82823510 0.04528046 -4.41293870

H -5.16449127 -0.58335887 -7.06301730

C -3.64155376 0.18590459 0.98688062

C 0.70210330 -1.25043017 -0.55872071

C 0.64860568 1.28456038 -0.55192314

H -3.85710366 0.60284776 1.98072766

H -4.00131302 0.89037301 0.22140908

H -4.17309937 -0.77358264 0.87038902

H 1.76516121 -1.24768121 -0.26104536

H 0.23170854 -2.16910157 -0.17116917

H 0.65104897 -1.26744299 -1.66088613

H 1.71067851 1.32432452 -0.25325959

H 0.59767233 1.30547489 -1.65423767

H 0.14027721 2.18012376 -0.15776653

H -6.72440531 -0.92643978 -5.12825644

N -2.53040463 -0.05193138 -6.94684127

O -3.04162726 -0.13264957 -8.06847199

O -1.33919956 0.18290990 -6.72960802

**nitroBIPS CTC open form MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51173696

C 1.05338208 0.00000000 2.43102479

C 0.74965752 0.00079604 3.80803928

C -0.58811435 0.00144901 4.24687978

C -1.65775886 0.00455512 3.33006956

C -1.33165017 0.01267123 1.96672384

N -2.19918514 0.02933428 0.85030433

C -1.49572841 -0.02574593 -0.31943165

C -1.95295087 -0.08174573 -1.63485072

C -3.25948742 -0.34376428 -2.10656240

C -3.65139061 -0.40086925 -3.45238349

C -5.02323645 -0.73548150 -3.72526525

C -5.48244926 -0.81189304 -5.01438020

C -4.62077433 -0.56733259 -6.13978972

C -3.30423775 -0.24867311 -5.92424976

C -2.71430274 -0.13615985 -4.58183496

O -1.51104229 0.16006447 -4.43547008

H 2.09476180 -0.00457970 2.09045710

H 1.55976716 -0.00400719 4.54404596

H -0.80610024 -0.00716670 5.31964987

H -2.69266596 -0.01371000 3.68384564

H -1.18875493 0.03193916 -2.40774150

H -4.05319274 -0.57902999 -1.38642712

H -5.71289828 -0.93196974 -2.89802840

H -5.03684789 -0.64280476 -7.14718883

C -3.63632762 0.20852021 0.97585323

C 0.70053285 -1.24693319 -0.56911369

C 0.64059095 1.28690036 -0.55825836

H -3.84655096 0.69402145 1.93993931

H -3.98598655 0.86368731 0.16340895

H -4.17594426 -0.75264379 0.92818001

H 1.76672362 -1.24036714 -0.28289932

H 0.23815349 -2.16854025 -0.17845554

H 0.63248822 -1.25693442 -1.67025443

H 1.70578622 1.32622159 -0.27085235

H 0.57274336 1.30585112 -1.65947050

H 0.13614544 2.18135475 -0.15633836

H -2.62617243 -0.05834920 -6.76266885

N -6.89128033 -1.15335277 -5.25925324

O -7.25972224 -1.21704516 -6.43683969

O -7.61681143 -1.35440145 -4.28188711

**nitroBIPS CCC open form MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51129952

C 1.04920177 0.00000000 2.43637286

C 0.73421108 -0.00925364 3.81023202

C -0.60635264 -0.01440781 4.24459555

C -1.67032699 -0.00371170 3.32278581

C -1.33020006 0.00692082 1.96481246

N -2.19067988 0.05017888 0.84128632

C -1.49134058 -0.01445820 -0.30505670

C -2.03702942 -0.05495127 -1.60301901

C -3.22890723 -0.65911467 -2.02277196

C -3.97780981 -1.70430137 -1.41582259

C -5.24834784 -2.01339269 -2.00238350

C -5.99888937 -3.07255947 -1.54516934

C -5.52315694 -3.93372890 -0.50980569

C -4.28118780 -3.69745159 0.03618502

C -3.42597520 -2.57805386 -0.35665994

O -2.30152449 -2.40823782 0.18335452

H 2.09310135 -0.00291303 2.10409973

H 1.53991129 -0.02056922 4.55120058

H -0.82763005 -0.03265966 5.31642944

H -2.70934284 -0.02765305 3.66330838

H -1.42874994 0.42722358 -2.37903598

H -3.58028609 -0.35704347 -3.02163749

H -5.64220042 -1.39144516 -2.81240770

H -6.14679047 -4.76948998 -0.18374115

C -3.62493494 0.23470699 0.95140361

C 0.65506354 -1.27468670 -0.56632268

C 0.67342397 1.26762967 -0.56083640

H -3.82735458 0.83727592 1.84930875

H -3.97404612 0.76396148 0.05264017

H -4.14821147 -0.73532028 1.01233617

H 1.71913856 -1.30823831 -0.27327844

H 0.13167570 -2.16649110 -0.18942344

H 0.59148938 -1.27128962 -1.66836435

H 1.73927329 1.27615027 -0.27470350

H 0.61693668 1.28506639 -1.66282596

H 0.19713843 2.17954195 -0.16362991

H -3.88182110 -4.35051470 0.82003957

N -7.31252439 -3.33924083 -2.14912793

O -7.94888719 -4.30520745 -1.71504274

O -7.70113725 -2.58698385 -3.04667336

**nitroBIPS CCT open form MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51334423

C 1.05443925 0.00000000 2.43152967

C 0.75088180 0.01397795 3.80855636

C -0.58658223 0.02543877 4.24897580

C -1.65683317 0.01815172 3.33349901

C -1.33090315 -0.00306687 1.97081227

N -2.20014985 -0.03813958 0.85776819

C -1.49704386 0.01906853 -0.31292953

C -2.02355170 0.03228709 -1.60505340

C -3.30245877 0.46708014 -2.04273366

C -4.10230182 1.47369674 -1.48867299

C -3.59733546 2.41534255 -0.52779863

C -4.38221417 3.45730599 -0.10870029

C -5.72387263 3.65587610 -0.59976951

C -6.23618956 2.79285887 -1.53339086

C -5.47801155 1.63809329 -2.05217580

O -5.96199994 0.85114468 -2.87894726

H 2.09604494 -0.00246751 2.09140504

H 1.56169613 0.02436645 4.54375489

H -0.80285544 0.04881026 5.32183433

H -2.69294181 0.04773440 3.68294606

H -1.33843446 -0.33129554 -2.38198757

H -3.69549213 0.03893086 -2.97706722

H -2.56815321 2.34593221 -0.16467728

H -6.29759238 4.50791193 -0.22725532

C -3.61745188 -0.32287699 0.96295814

C 0.67485871 -1.26609576 -0.55982464

C 0.66578942 1.27166759 -0.55765740

H -3.79415179 -0.85642416 1.90868457

H -4.22720993 0.59773860 0.92329068

H -3.90811754 -0.95849699 0.11089360

H 1.73672158 -1.28539279 -0.25894541

H 0.18496948 -2.17558105 -0.17440257

H 0.63107426 -1.27849990 -1.66260602

H 1.73626042 1.28753886 -0.28762629

H 0.57808206 1.29860251 -1.65770778

H 0.18814934 2.17631853 -0.14467708

H -7.24655643 2.93028007 -1.93271810

N -3.82227260 4.43164645 0.84052968

O -4.53746993 5.38941823 1.15334112

O -2.68320047 4.23093495 1.27164581

**nitroBIPS TCT open form MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51843387

C 1.06621838 0.00000000 2.42376971

C 0.78278881 0.00899685 3.80482334

C -0.54811058 0.00569031 4.26450188

C -1.62977906 -0.00531729 3.36304156

C -1.32243325 -0.01381339 1.99489365

N -2.19342684 -0.04631841 0.89249567

C -1.51795913 0.00525897 -0.30195109

C -2.18768443 0.36431330 -1.47675490

C -1.70817157 0.26372645 -2.81052598

C -0.99105473 -0.80018482 -3.35471362

C -0.95981950 -2.08680752 -2.71348032

C -0.30511666 -3.13002232 -3.30835641

C 0.35241854 -2.99726700 -4.58688791

C 0.30986380 -1.80052437 -5.25335382

C -0.37632822 -0.61339526 -4.70801457

O -0.41012828 0.46781801 -5.31156917

H 2.10345820 0.00597071 2.07115898

H 1.60453177 0.02124158 4.52776968

H -0.74985806 0.01581103 5.34047892

H -2.66062287 0.00223828 3.72904651

H -3.14968320 0.87752085 -1.34497498

H -1.97383032 1.06320170 -3.51919136

H -1.50426922 -2.24517046 -1.77892004

H 0.85443729 -3.87169499 -5.00870969

C -3.63870626 -0.03112359 1.00753445

C 0.83453917 -1.19506929 -0.50184324

C 0.60547205 1.31325786 -0.53889722

H -3.92944226 -0.53918641 1.93882643

H -4.03732786 0.99968974 1.01625998

H -4.06827777 -0.57638102 0.15300873

H 1.82148390 -1.15889998 -0.00796786

H 0.36356727 -2.16280156 -0.26601462

H 0.99160146 -1.13006791 -1.58879724

H 1.66744545 1.37956566 -0.24424647

H 0.53908798 1.33460879 -1.64016890

H 0.07127531 2.18838793 -0.13292378

H 0.78725735 -1.68250697 -6.23165808

N -0.30876730 -4.43874266 -2.64449349

O 0.10696002 -5.40494040 -3.29235921

O -0.71513103 -4.49253060 -1.47830341

**Geometries - dinitroBIPS**

**dinitroBIPS B97XD/cc-pvdz optimised form A**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51615880

C 1.04618430 0.00000000 2.42029906

C 0.75935547 0.05408340 3.79186308

C -0.56200493 0.10751922 4.22758049

C -1.62841264 0.10573079 3.31892604

C -1.32369892 0.05738000 1.96445069

N -2.20259878 0.06437925 0.87000618

C -1.49149369 -0.41940533 -0.27485009

C -2.06679886 0.08328022 -1.56700473

C -2.27548041 -0.70641437 -2.62404317

C -2.00603013 -2.13923840 -2.55012563

C -2.13190112 -2.99195665 -3.63965236

C -1.92054525 -4.35753913 -3.47670521

C -1.59103195 -4.90011776 -2.24443351

C -1.43769622 -4.04255974 -1.16532167

C -1.64732466 -2.65812554 -1.28602198

O -1.56854373 -1.89274162 -0.20614238

C -3.59442919 -0.28913962 1.04634429

C 1.00608476 -0.96036029 -0.63263204

C 0.25019690 1.43428734 -0.49917414

N -2.06360937 -5.24992781 -4.63360136

O -2.37341580 -4.74220061 -5.69520467

O -1.87918625 -6.43763565 -4.45213534

H 2.08114957 -0.05102393 2.07396696

H 1.57324332 0.04602241 4.51862642

H -0.77710173 0.14045164 5.29764265

H -2.66002140 0.13127520 3.67306925

H -2.28480627 1.15104593 -1.60468698

H -2.66885736 -0.30056918 -3.55846214

H -2.40768899 -2.60800260 -4.62194422

H -1.44733285 -5.97293668 -2.12661083

H -4.07553431 0.42978107 1.72531333

H -4.10797179 -0.23252621 0.07630321

H -3.72194983 -1.30758211 1.45575114

H 2.02849992 -0.59372702 -0.45432690

H 0.92161144 -1.96923090 -0.20879314

H 0.86320925 -1.01115861 -1.72504704

H 1.24284645 1.76575970 -0.16048658

H 0.22954868 1.48575594 -1.59937059

H -0.49514186 2.13579617 -0.09445619

N -1.03429395 -4.64016992 0.11560916

O -1.52171195 -5.71950211 0.39102491

O -0.26132021 -4.01752502 0.81499476

**dinitroBIPS B97XD/cc-pvdz optimised – form B**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51615635

C 1.04651912 0.00000000 2.41961020

C 0.76057788 0.05202495 3.79096808

C -0.56029666 0.10269031 4.22751690

C -1.62684080 0.10041847 3.31966645

C -1.32284661 0.05434651 1.96524983

N -2.20301585 0.06245703 0.87148602

C -1.49123966 -0.41531497 -0.27629490

C -2.06747362 0.09160606 -1.56649950

C -2.25664411 -0.69215556 -2.63111571

C -1.96034716 -2.12006964 -2.56835268

C -2.05504360 -2.96171165 -3.66865618

C -1.81603411 -4.32421624 -3.51877697

C -1.48757368 -4.87296528 -2.29012526

C -1.36744827 -4.02617201 -1.19753970

C -1.60827656 -2.64568852 -1.30494510

O -1.56623276 -1.88871418 -0.21706358

C -3.59179675 -0.30326271 1.04975493

C 1.00123585 -0.96723958 -0.62911104

C 0.25572382 1.43207119 -0.50190394

N -1.92524833 -5.20541650 -4.68747652

O -2.22472589 -4.69009240 -5.74846630

O -1.70934523 -6.38966132 -4.51910319

H 2.08094071 -0.04932907 2.07270601

H 1.57455783 0.04421209 4.51697566

H -0.77461210 0.13349193 5.29735488

H -2.65791674 0.12385823 3.67406985

H -2.30237734 1.15555342 -1.59571827

H -2.65135136 -0.28574786 -3.56418449

H -2.32650171 -2.57259050 -4.64965559

H -1.31787169 -5.94248360 -2.18229393

H -4.07928297 0.41358580 1.72572357

H -4.10616410 -0.25549571 0.08016079

H -3.70916976 -1.32081206 1.46292643

H 2.02522439 -0.60765194 -0.44836722

H 0.90829077 -1.97436975 -0.20328343

H 0.86148926 -1.01914699 -1.72140645

H 1.24880489 1.76081650 -0.16318398

H 0.23622482 1.48177874 -1.60178416

H -0.48698848 2.13701664 -0.09950981

N -0.95838069 -4.63241437 0.07709635

O -1.36119702 -5.75838597 0.29928696

O -0.22693614 -3.99052100 0.80335274

**dinitroBIPS TTC open form B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51536253

C 1.05333472 0.00000000 2.41546416

C 0.76984127 0.00000000 3.78512791

C -0.55115308 0.00012332 4.23253278

C -1.62080362 0.00006682 3.33302489

C -1.31401714 -0.00026878 1.97843524

N -2.18385430 -0.00055427 0.86767672

C -1.50221840 0.00141628 -0.29765221

C -2.17304429 0.00594583 -1.51726946

C -1.55204985 0.00110433 -2.76466998

C -2.18173578 -0.00415536 -4.02066029

C -1.34846479 0.00162008 -5.16638821

C -1.87796269 0.00521436 -6.42817248

C -3.28131749 -0.01311947 -6.63359250

C -4.11633221 -0.05547337 -5.56256558

C -3.65805265 -0.00960489 -4.16233698

O -4.42888666 0.05504634 -3.20786348

C -3.63239780 -0.00075659 0.95248752

C 0.67898763 -1.27656388 -0.53051636

C 0.68183959 1.27462709 -0.53116510

N -0.99052024 0.02163921 -7.58254922

O 0.21184485 0.03923305 -7.37525423

O -1.50373224 0.01671714 -8.68749672

H 2.08745624 0.00005954 2.06518852

H 1.58642590 0.00011928 4.50794729

H -0.75917256 0.00040635 5.30335955

H -2.64758657 0.00067370 3.69841805

H -3.26105766 0.01496315 -1.52712402

H -0.45931505 -0.00139859 -2.80488461

H -0.26248831 0.00811149 -5.05880123

H -3.68123556 -0.00064536 -7.64675033

H -3.93447969 -0.01706838 2.00383378

H -4.04437087 0.89951122 0.47463588

H -4.04488117 -0.88585599 0.44769594

H 1.72338435 -1.30503345 -0.18630372

H 0.17054321 -2.17660416 -0.15611611

H 0.68117638 -1.31311873 -1.62813208

H 1.72646164 1.30082469 -0.18740856

H 0.68372089 1.31079263 -1.62880657

H 0.17563208 2.17598904 -0.15696922

N -5.55273433 -0.14107048 -5.84254224

O -5.96771820 0.45853479 -6.82126854

O -6.22674807 -0.82732257 -5.1037592

**dinitroBIPS TTT open structure B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51560437

C 1.05569401 0.00000000 2.41296335

C 0.77685080 0.00016685 3.78348081

C -0.54247769 0.00031730 4.23523004

C -1.61477697 0.00035294 3.33861446

C -1.31175261 0.00033220 1.98323237

N -2.18551760 0.00052673 0.87462738

C -1.50522068 -0.00057182 -0.29474333

C -2.15289072 -0.00292528 -1.52358729

C -1.47762573 -0.00360014 -2.74653847

C -2.01043614 -0.00729139 -4.03529410

C -3.39967942 -0.01383155 -4.30570480

C -3.85290878 -0.03140830 -5.59478679

C -2.95403188 -0.03028855 -6.69832204

C -1.61467717 0.00975696 -6.48282769

C -1.00928111 -0.01599616 -5.13720045

O 0.19400017 -0.07513880 -4.92187327

C -3.63064370 0.00091952 0.96866748

C 0.68566554 -1.27467437 -0.52906814

C 0.68405224 1.27575367 -0.52853320

N -5.28751221 -0.04644053 -5.85120289

O -5.65199987 -0.05564782 -7.01330119

O -6.03732564 -0.04884881 -4.88817736

H 2.08851508 -0.00020271 2.05907914

H 1.59586551 0.00012675 4.50353497

H -0.74734726 0.00036524 5.30666077

H -2.64030517 0.00026068 3.70802888

H -3.24348796 -0.00573985 -1.52364718

H -0.38572482 -0.00433349 -2.75365859

H -4.13653279 -0.00940481 -3.50234446

H -3.34661327 -0.05604891 -7.71411252

H -3.92770788 0.00756823 2.02162226

H -4.04868376 0.89373611 0.48061651

H -4.04898957 -0.89761548 0.49136901

H 1.72332921 -1.30429066 -0.16546585

H 0.17146964 -2.17672337 -0.16707460

H 0.71212545 -1.30340896 -1.62647314

H 1.72185967 1.30642383 -0.16548094

H 0.70983034 1.30474797 -1.62590010

H 0.16895757 2.17710405 -0.16611235

N -0.74942437 0.07478280 -7.66478851

O -1.12719581 -0.51058161 -8.66682433

O 0.26610456 0.73106056 -7.57591987

**dinitroBIPS CTT structure B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51036021

C 1.04815677 0.00000000 2.41632689

C 0.75662764 0.00906954 3.78433866

C -0.56674922 0.02080921 4.22342857

C -1.63129227 0.01935198 3.31717930

C -1.31638516 0.00120412 1.96465837

N -2.19250173 -0.01210011 0.85158539

C -1.49986384 0.02638264 -0.30788395

C -1.97100203 0.07888490 -1.61474555

C -3.28550409 0.28406703 -2.04280274

C -3.76300905 0.35258390 -3.35335606

C -2.94271940 0.19779611 -4.49568646

C -3.47912749 0.29157861 -5.74939378

C -4.86706165 0.53232473 -5.94790422

C -5.69468852 0.65181850 -4.87863750

C -5.22328030 0.61142017 -3.48125937

O -5.93742669 0.80140506 -2.50502066

C -3.63074514 -0.12420626 0.99358910

C 0.64085654 -1.28334424 -0.55823631

C 0.69337310 1.25210770 -0.56201468

N -2.61529094 0.13818501 -6.91307824

O -3.13209465 0.22180402 -8.01286754

O -1.42793835 -0.06447384 -6.71715326

H 2.08381990 -0.00413090 2.07091982

H 1.56871157 0.01200643 4.51220003

H -0.78159313 0.03573103 5.29279400

H -2.65967996 0.04146928 3.67737469

H -1.18986067 -0.00269292 -2.37280865

H -4.08316679 0.44727287 -1.31698324

H -1.87296441 0.00653377 -4.40939257

H -5.26019405 0.61377428 -6.96062077

H -3.86261567 -0.46105235 2.00931097

H -4.13205328 0.83793847 0.81216552

H -4.01843138 -0.87017211 0.28691157

H 1.69841392 -1.32751515 -0.25838395

H 0.13563448 -2.18004993 -0.17140207

H 0.59739196 -1.30263317 -1.65708151

H 1.75267032 1.25356327 -0.26496728

H 0.64692564 1.27069839 -1.66060967

H 0.22619961 2.17005325 -0.17742674

N -7.12269765 0.83405465 -5.15626921

O -7.42133043 1.46781056 -6.15558526

O -7.90935496 0.31690496 -4.39213830

**dinitroBIPS CTC structure** **B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51004097

C 1.04510993 0.00000000 2.41966222

C 0.74882508 0.00534227 3.78684422

C -0.57534087 0.01297756 4.22416389

C -1.63765873 0.01134215 3.31507733

C -1.31666478 -0.00306890 1.96435555

N -2.19017371 -0.01578549 0.84839298

C -1.49717776 0.03263561 -0.30798315

C -1.95529497 0.08679682 -1.62189014

C -3.23848613 0.38665872 -2.07791589

C -3.65510826 0.47606529 -3.41828246

C -5.00600504 0.82947806 -3.65472935

C -5.50089785 0.93369893 -4.92656940

C -4.67079852 0.71196379 -6.05510230

C -3.35857380 0.40979506 -5.87375629

C -2.73568648 0.21449416 -4.55200092

O -1.57568019 -0.16263787 -4.40811667

C -3.62342624 -0.16682250 0.98477785

C 0.62795104 -1.28882693 -0.56320915

C 0.69740179 1.24500396 -0.57304427

N -6.89908677 1.28497044 -5.12914497

O -7.58943937 1.46571507 -4.13899618

O -7.29635106 1.37725272 -6.27716160

H 2.08167112 -0.00159930 2.07737037

H 1.55906868 0.00862834 4.51687437

H -0.79182477 0.02523602 5.29322501

H -2.66810614 0.03146157 3.67020097

H -1.20149400 -0.05443831 -2.39562431

H -4.01809882 0.63068852 -1.35235199

H -5.68092534 1.02011721 -2.81860768

H -5.08613656 0.79297386 -7.05879030

H -3.84342215 -0.62237759 1.95719458

H -4.14251787 0.80137246 0.91908833

H -3.99639843 -0.83650980 0.19842497

H 1.68803779 -1.33661389 -0.27304454

H 0.12219216 -2.18213567 -0.16891206

H 0.56942708 -1.30649917 -1.66101737

H 1.76036788 1.23658582 -0.28957028

H 0.63213995 1.25754119 -1.67048444

H 0.24387808 2.16810394 -0.18396502

N -2.53737536 0.26216932 -7.07911065

O -3.06821757 -0.23404572 -8.05970886

O -1.39723976 0.67298502 -7.03213824

**dinitroBIPS CCC structure** **B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50938020

C 1.03616324 0.00000000 2.43033833

C 0.71788835 0.03509016 3.79148987

C -0.61190713 0.07463956 4.21565074

C -1.66300219 0.06930593 3.29599929

C -1.31581969 0.02263677 1.95517716

N -2.17927551 -0.00864457 0.82938660

C -1.49409645 0.03230424 -0.29636471

C -2.00832163 0.05628589 -1.63028203

C -3.02164860 0.80261636 -2.17031461

C -3.81793884 1.86720596 -1.63338585

C -4.96672408 2.24403141 -2.34529526

C -5.82952180 3.20809898 -1.85890089

C -5.60592211 3.81277623 -0.60818794

C -4.48318452 3.47467282 0.09287649

C -3.43169328 2.60134778 -0.42374146

O -2.32096567 2.50311395 0.11319800

C -3.61916665 -0.06689088 0.99393379

C 0.65615871 -1.26874329 -0.57118079

C 0.64996304 1.27492617 -0.56893091

N -7.01633065 3.56125277 -2.61872742

O -7.19255662 3.00637079 -3.69185145

O -7.76853328 4.39305166 -2.13951253

H 2.07762189 -0.01621114 2.10404085

H 1.51855169 0.04382941 4.53225728

H -0.83747747 0.11980510 5.28172821

H -2.70015507 0.12734168 3.62429073

H -1.42447769 -0.54537419 -2.33169136

H -3.23999780 0.56778528 -3.21820887

H -5.21697961 1.75975326 -3.29061250

H -6.33075702 4.51712033 -0.20162845

H -3.85543311 -0.88962248 1.68277472

H -3.97039775 0.88686926 1.41528542

H -4.09015019 -0.25083902 0.02406877

H 1.71349990 -1.29669760 -0.27001776

H 0.16823922 -2.17963119 -0.19439886

H 0.62150995 -1.27373349 -1.67051294

H 1.70759927 1.31286333 -0.26851329

H 0.59638766 1.27133041 -1.66764729

H 0.12777097 2.16683099 -0.19924972

N -4.35416760 3.97586779 1.45615306

O -4.71958033 5.11219135 1.69114123

O -3.92854046 3.19609459 2.29471343

**dinitroBIPS CCT structure B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51130138

C 1.04269576 0.00000000 2.42403932

C 0.73932611 0.02238166 3.78940655

C -0.58651543 0.04553840 4.22324605

C -1.64559364 0.04025276 3.31141915

C -1.31603241 0.00900065 1.96406728

N -2.18850525 -0.01577630 0.84848666

C -1.49843651 0.03413889 -0.30378511

C -2.00951386 0.05126009 -1.60655940

C -3.20668702 0.56245964 -2.11072135

C -4.06787633 1.55368307 -1.60470768

C -3.69946761 2.43775906 -0.56974042

C -4.54372891 3.44149007 -0.16819479

C -5.79943056 3.64381198 -0.79834625

C -6.17037930 2.84634585 -1.83444950

C -5.36735768 1.70367077 -2.31178630

O -5.73119438 0.91064926 -3.16892317

C -3.61172434 -0.23586297 0.98683731

C 0.65271620 -1.27344989 -0.56475828

C 0.66915230 1.26453055 -0.56505339

N -4.13312776 4.32482685 0.90965539

O -4.87161707 5.24962543 1.19825387

O -3.07514044 4.08141624 1.47307807

H 2.08120410 -0.01009503 2.08774494

H 1.54674766 0.03071112 4.52249977

H -0.80517253 0.07555357 5.29135993

H -2.67925511 0.07621512 3.65514040

H -1.32925460 -0.36887266 -2.35239068

H -3.50795578 0.20057495 -3.10061234

H -2.72494789 2.36816613 -0.08652252

H -6.45415898 4.44541818 -0.45866891

H -3.78038359 -0.88942915 1.85204622

H -4.15237208 0.71210241 1.12899571

H -3.99088946 -0.72250137 0.08041586

H 1.70769420 -1.31189157 -0.25593276

H 0.15156715 -2.17785634 -0.19076336

H 0.62238563 -1.28103958 -1.66423362

H 1.73513818 1.27532033 -0.29328476

H 0.58831228 1.28923466 -1.66171892

H 0.20250108 2.17429415 -0.15959954

N -7.44567998 3.15336244 -2.48807427

O -8.34393349 3.58835096 -1.78451066

O -7.51304095 2.98328559 -3.68632661

**dinitroBIPS TCT structure B97XD/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51687903

C 1.05567515 0.00000000 2.41537367

C 0.77557422 -0.00734706 3.78546872

C -0.54323228 -0.02429093 4.24003019

C -1.61506254 -0.03307418 3.34368689

C -1.30767017 -0.02479682 1.98928785

N -2.18350416 -0.03391504 0.88552283

C -1.51856992 0.03859096 -0.28983136

C -2.19589458 0.41952786 -1.45492381

C -1.77865225 0.33990185 -2.78742112

C -1.02938121 -0.66760061 -3.40450633

C -0.95221419 -1.96729645 -2.85774300

C -0.27392722 -2.95937878 -3.51322693

C 0.33844313 -2.72436831 -4.77387009

C 0.22955454 -1.50602314 -5.36624602

C -0.43776532 -0.35185938 -4.73160562

O -0.46573815 0.78033878 -5.19114369

C -3.62412637 -0.02481723 1.01558765

C 0.77233174 -1.23663840 -0.49765014

C 0.64622152 1.28121418 -0.55838079

N -0.20117221 -4.28204950 -2.91780839

O 0.33935576 -5.16482148 -3.55921154

O -0.67531409 -4.42886350 -1.79948430

H 2.08918466 0.01346320 2.06393530

H 1.59517190 0.00293371 4.50487100

H -0.74599269 -0.02797055 5.31183837

H -2.64284068 -0.03852836 3.70690322

H -3.12386279 0.97430247 -1.28842838

H -2.12231431 1.13032879 -3.46533194

H -1.46705122 -2.20660885 -1.92842954

H 0.87544916 -3.53092026 -5.27211817

H -3.90675916 -0.56270416 1.92866151

H -4.01656887 1.00346002 1.06801890

H -4.07084253 -0.53878859 0.15519025

H 1.74674656 -1.26659471 0.01149385

H 0.24825011 -2.17766069 -0.27944480

H 0.96042131 -1.17296239 -1.57539245

H 1.70608226 1.31493868 -0.26574206

H 0.58904910 1.29373702 -1.65661192

H 0.15065149 2.18221654 -0.16912973

N 0.81634958 -1.35793712 -6.70061382

O 1.82451315 -2.00274094 -6.94258526

O 0.24553555 -0.62811457 -7.48233497

**dinitroBIPS MP2/cc-pvdz optimised – form A**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51670800

C 1.05369488 0.00000000 2.43344581

C 0.75291276 0.06554042 3.81082665

C -0.58292376 0.13838337 4.24360534

C -1.65167794 0.14156397 3.32266305

C -1.33589466 0.07921082 1.95944285

N -2.21018793 0.10370559 0.84721867

C -1.47728645 -0.44832119 -0.26663151

C -2.04762196 -0.02052955 -1.58783443

C -2.13867583 -0.86662623 -2.64376766

C -1.74559004 -2.26574712 -2.49720671

C -1.70322509 -3.16024980 -3.58112317

C -1.38759994 -4.50187766 -3.34951717

C -1.12308540 -4.98947036 -2.06637299

C -1.14121370 -4.08033236 -1.00546872

C -1.45374719 -2.71825092 -1.18490915

O -1.54489697 -1.91825082 -0.10322293

C -3.58758999 -0.33890451 1.03051978

C 1.02723281 -0.93863390 -0.63467955

C 0.20827176 1.44357085 -0.49866620

N -1.35170589 -5.44093502 -4.49082385

O -1.60514853 -4.98036879 -5.60561135

O -1.07056900 -6.61520727 -4.24559034

H 2.09335162 -0.06711239 2.09352486

H 1.56272604 0.05348974 4.54725145

H -0.80264656 0.17924873 5.31576519

H -2.68758294 0.18505685 3.67267543

H -2.35188418 1.02738987 -1.66969581

H -2.52125317 -0.52367831 -3.61146366

H -1.92534672 -2.82080214 -4.59598255

H -0.89561822 -6.04307934 -1.89614250

H -4.10592053 0.35830833 1.70754890

H -4.10059814 -0.31704331 0.05618815

H -3.64837930 -1.36246447 1.44603236

H 2.04237978 -0.54716253 -0.44833989

H 0.95938022 -1.95014916 -0.20742721

H 0.88782688 -0.98820249 -1.72987437

H 1.19629804 1.79964229 -0.16176240

H 0.18018290 1.49293503 -1.60168083

H -0.56104169 2.11775525 -0.08655327

N -0.80673127 -4.59241065 0.33261824

O -1.32382702 -5.66300086 0.65964766

O -0.01740269 -3.92640160 1.00753328

**dinitroBIPS MP2/cc-pvdz optimised - form B**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51703510

C 1.05625463 0.00000000 2.43110241

C 0.75949154 0.06597925 3.80918347

C -0.57511838 0.14042191 4.24574565

C -1.64612464 0.14423762 3.32763237

C -1.33398500 0.08350561 1.96303163

N -2.21231233 0.10200632 0.85235291

C -1.47512985 -0.45203354 -0.26699510

C -2.07041617 -0.03469616 -1.57826481

C -2.85002207 -0.86794415 -2.31403475

C -3.10185439 -2.22935157 -1.85636055

C -4.03567730 -3.08266671 -2.47289899

C -4.21735078 -4.37348400 -1.97185025

C -3.49290143 -4.85348368 -0.87486153

C -2.55117683 -4.00393248 -0.29228054

C -2.34430954 -2.68482286 -0.74738704

O -1.41716819 -1.92185476 -0.13954446

C -3.58519389 -0.34266279 1.05581538

C 1.02563368 -0.93954882 -0.63722453

C 0.22279753 1.44680115 -0.48173604

N -5.20767396 -5.26276570 -2.61564465

O -5.84423319 -4.80155206 -3.56493371

O -5.32526822 -6.40026721 -2.15689166

H 2.09480882 -0.06848330 2.08810852

H 1.57135006 0.05353060 4.54332991

H -0.79207674 0.18159614 5.31841175

H -2.68061284 0.18870806 3.68145695

H -1.90644157 0.99905437 -1.89283209

H -3.31265937 -0.52956631 -3.24790210

H -4.61807277 -2.74608020 -3.33434567

H -3.65712690 -5.85867009 -0.48317109

H -4.08598899 0.33747164 1.76281280

H -4.12595682 -0.29517922 0.09818339

H -3.63842114 -1.37455317 1.45749010

H 2.04152274 -0.54669809 -0.45873916

H 0.95516315 -1.95414939 -0.21918509

H 0.87221053 -0.99328266 -1.72987929

H 1.18924555 1.80576444 -0.09066685

H 0.25866689 1.50449876 -1.58381756

H -0.57034631 2.11569547 -0.10762406

N -1.76398312 -4.52112015 0.83618506

O -2.38471610 -5.14611539 1.70004118

O -0.54976107 -4.30740935 0.81647731

**dinitroBIPS TTC structure MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51608339

C 1.06189950 0.00000000 2.42601186

C 0.76814299 0.00128040 3.80455052

C -0.56646724 0.00296468 4.25455141

C -1.64308735 0.00254652 3.34738450

C -1.32756550 -0.00055423 1.98167470

N -2.19084902 -0.00380262 0.86343335

C -1.49797103 0.00351353 -0.30669660

C -2.16670998 0.01600705 -1.53575416

C -1.53575035 0.00995802 -2.79084144

C -2.18095554 0.00942054 -4.04331033

C -1.34776417 0.00870214 -5.20918580

C -1.89770907 0.00635848 -6.46693713

C -3.31252690 -0.00488020 -6.66110405

C -4.13076377 -0.04032597 -5.56309678

C -3.66194100 0.00934310 -4.16313490

O -4.44618611 0.07352065 -3.19919975

C -3.64721572 -0.00536621 0.93279762

C 0.68270189 -1.27930624 -0.52653237

C 0.68982928 1.27484717 -0.52722986

N -1.02060550 0.01569322 -7.64665428

O 0.19768222 0.03450989 -7.45552512

O -1.56611402 0.00356200 -8.75411726

H 2.10093722 -0.00018177 2.07869737

H 1.58400864 0.00178587 4.53407105

H -0.77557810 0.00556711 5.32893809

H -2.67422485 0.00685226 3.71152739

H -3.25796487 0.03391082 -1.54759809

H -0.43925716 -0.00020963 -2.83215288

H -0.25844277 0.01146357 -5.10121459

H -3.73118671 0.00545882 -7.66980331

H -3.95563945 -0.07847081 1.98296275

H -4.05027120 0.92145556 0.49311433

H -4.04804641 -0.86582676 0.37355775

H 1.73214103 -1.30104221 -0.18558383

H 0.17305237 -2.17765402 -0.14035181

H 0.67380187 -1.31850000 -1.62721355

H 1.73971224 1.29047459 -0.18734218

H 0.68012685 1.31394260 -1.62789634

H 0.18590229 2.17631709 -0.14087060

N -5.57775555 -0.11166358 -5.80047653

O -6.05065636 0.64244475 -6.65606162

O -6.20285326 -0.94190654 -5.13730577

**dinitroBIPS TTT structure MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51664985

C 1.06452966 0.00000000 2.42340587

C 0.77641422 -0.00017809 3.80314213

C -0.55647222 -0.00036402 4.25727329

C -1.63603249 -0.00024229 3.35323743

C -1.32561814 0.00018513 1.98635721

N -2.19265178 0.00087970 0.87139165

C -1.50109043 -0.00021747 -0.30404528

C -2.14344403 -0.00297491 -1.54311207

C -1.45440598 -0.00388859 -2.77017038

C -1.99817916 -0.00724166 -4.05871743

C -3.40620189 -0.00442458 -4.31868596

C -3.86587758 -0.00984820 -5.60944476

C -2.97461567 -0.01080013 -6.73351743

C -1.62598602 0.02041382 -6.51362574

C -1.00047896 -0.02019048 -5.17018239

O 0.22051893 -0.08829729 -4.98870777

C -3.64531380 0.00138776 0.95001425

C 0.69224241 -1.27633539 -0.52330217

C 0.69146476 1.27673920 -0.52320555

N -5.31579377 -0.01451674 -5.86190229

O -5.68142976 -0.01075307 -7.04083252

O -6.06863131 -0.02151437 -4.88485200

H 2.10214611 -0.00000923 2.07194026

H 1.59498480 -0.00029036 4.52959413

H -0.76258726 -0.00073577 5.33228755

H -2.66561750 -0.00078429 3.72209709

H -3.23782315 -0.00611971 -1.55153405

H -0.35964997 -0.00563115 -2.76620283

H -4.13450510 0.00189657 -3.50326993

H -3.37419064 -0.02835404 -7.74984978

H -3.94898206 0.01102601 2.00416041

H -4.05378019 0.89532582 0.45023873

H -4.05459660 -0.90076640 0.46574619

H 1.73490255 -1.29711719 -0.16232447

H 0.17803649 -2.17727443 -0.14901266

H 0.70786675 -1.30958581 -1.62410660

H 1.73445153 1.29783890 -0.16321766

H 0.70594465 1.30984348 -1.62398921

H 0.17721355 2.17749236 -0.14854586

N -0.74680762 0.07939583 -7.68822065

O -1.01380924 -0.66555393 -8.63546985

O 0.17778220 0.89267141 -7.63717850

**dinitroBIPS CTT structure MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51150367

C 1.05502675 0.00000000 2.42899781

C 0.75145934 0.00581264 3.80568951

C -0.58623898 0.01253750 4.24505668

C -1.65657759 0.00926383 3.32945330

C -1.33057093 -0.00632972 1.96637219

N -2.19967511 -0.02524529 0.84776422

C -1.49635810 0.02239540 -0.31790468

C -1.96928821 0.08128284 -1.63092774

C -3.28901377 0.31699722 -2.06292722

C -3.75107411 0.38146764 -3.38305926

C -2.91350931 0.16569311 -4.52394073

C -3.43854994 0.25268140 -5.78679185

C -4.82307838 0.54799793 -6.01554416

C -5.65246057 0.72155528 -4.94285883

C -5.20332093 0.69673842 -3.53093566

O -5.94894590 0.93907593 -2.57438655

C -3.64274284 -0.17231471 0.98004800

C 0.64985146 -1.28358713 -0.55411623

C 0.69708920 1.25340407 -0.56007657

N -2.56468903 0.03625431 -6.95134440

O -3.08586457 0.11462239 -8.06754658

O -1.37474257 -0.20794121 -6.73844767

H 2.09630703 0.00026469 2.08831547

H 1.56179837 0.01049383 4.54132862

H -0.80372227 0.02669051 5.31773983

H -2.69051369 0.03254315 3.68490181

H -1.18628385 -0.01469105 -2.39052674

H -4.07746851 0.51901406 -1.33158861

H -1.85161325 -0.07013894 -4.41357070

H -5.20616915 0.62401323 -7.03551723

H -3.85941620 -0.59390771 1.97123776

H -4.16232474 0.79400022 0.87051049

H -4.00752479 -0.86793491 0.20921044

H 1.71135932 -1.32032469 -0.25400222

H 0.14374559 -2.18096553 -0.16133957

H 0.60168991 -1.30305973 -1.65640304

H 1.76000333 1.25245295 -0.26272412

H 0.64559784 1.26998906 -1.66208086

H 0.22516508 2.17095024 -0.17174693

N -7.07496285 0.96221923 -5.21582522

O -7.35350575 1.76634895 -6.10985261

O -7.87754950 0.31701259 -4.53857989

**dinitroBIPS CTC structure MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51096692

C 1.05156012 0.00000000 2.43286746

C 0.74254188 -0.00004055 3.80831264

C -0.59641338 -0.00018273 4.24523908

C -1.66394745 -0.00380104 3.32655438

C -1.33092294 -0.01197163 1.96544595

N -2.19692499 -0.02778889 0.84331544

C -1.49378675 0.02521749 -0.31788436

C -1.95295762 0.07429534 -1.63904608

C -3.24548587 0.38057373 -2.10292846

C -3.64490224 0.45343549 -3.45266548

C -5.00169992 0.83363655 -3.71281013

C -5.47150740 0.93111026 -4.99893266

C -4.62739602 0.67212136 -6.12164740

C -3.31592164 0.34435631 -5.90111757

C -2.70937660 0.15355121 -4.56734744

O -1.54091943 -0.24454476 -4.41616919

C -3.63708014 -0.19799769 0.96797648

C 0.63869009 -1.28817754 -0.55979747

C 0.69827664 1.24752511 -0.57241618

N -6.87148914 1.31040141 -5.23672503

O -7.58548660 1.51591763 -4.25206142

O -7.23958959 1.39822782 -6.41182491

H 2.09395614 0.00419722 2.09598936

H 1.55055672 0.00479244 4.54655908

H -0.81596214 0.00872693 5.31752576

H -2.69995878 0.01400110 3.67685593

H -1.19424745 -0.07511422 -2.41123578

H -4.02595067 0.64963209 -1.38034436

H -5.67779695 1.04922549 -2.87932751

H -5.02196020 0.74534528 -7.13744084

H -3.84771735 -0.70378050 1.92118707

H -4.16435529 0.77030146 0.94425951

H -3.99182011 -0.83008443 0.13998202

H 1.70325267 -1.32613903 -0.27100395

H 0.13464971 -2.18299512 -0.15829112

H 0.57376885 -1.30662471 -1.66100843

H 1.76431750 1.24041007 -0.28670259

H 0.63030297 1.25549003 -1.67343879

H 0.23675209 2.16978070 -0.18232894

N -2.46148483 0.14584152 -7.07829884

O -2.91765955 -0.53300678 -8.00316261

O -1.35962387 0.69808037 -7.05578012

**dinitroBIPS CCC structure MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.50938020

C 1.03616324 0.00000000 2.43033833

C 0.71788835 0.03509016 3.79148987

C -0.61190713 0.07463956 4.21565074

C -1.66300219 0.06930593 3.29599929

C -1.31581969 0.02263677 1.95517716

N -2.17927551 -0.00864457 0.82938660

C -1.49409645 0.03230424 -0.29636471

C -2.00832163 0.05628589 -1.63028203

C -3.02164860 0.80261636 -2.17031461

C -3.81793884 1.86720596 -1.63338585

C -4.96672408 2.24403141 -2.34529526

C -5.82952180 3.20809898 -1.85890089

C -5.60592211 3.81277623 -0.60818794

C -4.48318452 3.47467282 0.09287649

C -3.43169328 2.60134778 -0.42374146

O -2.32096567 2.50311395 0.11319800

C -3.61916665 -0.06689088 0.99393379

C 0.65615871 -1.26874329 -0.57118079

C 0.64996304 1.27492617 -0.56893091

N -7.01633065 3.56125277 -2.61872742

O -7.19255662 3.00637079 -3.69185145

O -7.76853328 4.39305166 -2.13951253

H 2.07762189 -0.01621114 2.10404085

H 1.51855169 0.04382941 4.53225728

H -0.83747747 0.11980510 5.28172821

H -2.70015507 0.12734168 3.62429073

H -1.42447769 -0.54537419 -2.33169136

H -3.23999780 0.56778528 -3.21820887

H -5.21697961 1.75975326 -3.29061250

H -6.33075702 4.51712033 -0.20162845

H -3.85543311 -0.88962248 1.68277472

H -3.97039775 0.88686926 1.41528542

H -4.09015019 -0.25083902 0.02406877

H 1.71349990 -1.29669760 -0.27001776

H 0.16823922 -2.17963119 -0.19439886

H 0.62150995 -1.27373349 -1.67051294

H 1.70759927 1.31286333 -0.26851329

H 0.59638766 1.27133041 -1.66764729

H 0.12777097 2.16683099 -0.19924972

N -4.35416760 3.97586779 1.45615306

O -4.71958033 5.11219135 1.69114123

O -3.92854046 3.19609459 2.29471343

**dinitroBIPS CCT structure MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51095774

C 1.05002592 0.00000000 2.43515130

C 0.73518086 0.03878805 3.80825548

C -0.60496010 0.07823248 4.24252986

C -1.67021821 0.07093079 3.32269519

C -1.33035703 0.02441132 1.96459920

N -2.19441961 -0.02027884 0.84022833

C -1.49224457 0.01622154 -0.31385017

C -2.03735100 -0.02248147 -1.62097068

C -3.24803706 0.55424075 -2.02084280

C -3.86714632 1.64634042 -1.35946470

C -3.08755712 2.56068182 -0.59671670

C -3.68955596 3.60440820 0.06964706

C -5.09661006 3.82563420 -0.02127219

C -5.85174067 3.00328006 -0.82148489

C -5.32561027 1.82850083 -1.55363582

O -6.02434321 1.02531964 -2.18756285

C -3.63334306 -0.17466474 0.95572190

C 0.68159650 -1.25555251 -0.57618090

C 0.65357176 1.28610406 -0.54822889

N -2.85894270 4.54479365 0.82644324

O -3.42702417 5.50185102 1.36161649

O -1.64631491 4.31306590 0.89791656

H 2.09375543 -0.02001024 2.10328867

H 1.54104913 0.04859560 4.54880664

H -0.82532528 0.12161738 5.31365246

H -2.70772162 0.11993165 3.66492867

H -1.42902172 -0.54201303 -2.37224074

H -3.74613596 0.18246282 -2.92766657

H -1.99882284 2.47004949 -0.57842331

H -5.56093927 4.65582619 0.51621815

H -3.84790209 -0.70221714 1.89599466

H -4.13758478 0.80810678 0.93355081

H -3.99363093 -0.76087688 0.09586563

H 1.74032650 -1.27172826 -0.26618115

H 0.19501210 -2.17440042 -0.20920455

H 0.65008968 -1.24858234 -1.67903349

H 1.73161643 1.28231728 -0.31134675

H 0.53172018 1.33974378 -1.64405223

H 0.20181456 2.18338466 -0.09203321

N -7.28087653 3.31270602 -0.94382841

O -7.89001753 3.60042804 0.09168643

O -7.75496502 3.27735602 -2.08083320

**dinitroBIPS TCT structure MP2/cc-pvdz optimised**

C 0.00000000 0.00000000 0.00000000

C 0.00000000 0.00000000 1.51717958

C 1.06377099 0.00000000 2.42648825

C 0.77262385 0.00225413 3.80526122

C -0.56005891 -0.01040440 4.26257930

C -1.63856539 -0.02320368 3.35860181

C -1.32103593 -0.02171174 1.99330576

N -2.18980548 -0.04527834 0.88330089

C -1.51727209 -0.00316924 -0.30008912

C -2.19164168 0.37609221 -1.48042340

C -1.74310071 0.20947940 -2.80240204

C -0.99597558 -0.87661498 -3.28856702

C -1.00738841 -2.13454454 -2.60998538

C -0.32805006 -3.20578460 -3.13363499

C 0.37404462 -3.11472415 -4.37680511

C 0.33750416 -1.94132971 -5.08343938

C -0.32312487 -0.70370897 -4.60709965

O -0.27432896 0.38308308 -5.19404069

C -3.63862190 -0.03156212 1.00231988

C 0.84651224 -1.19020769 -0.49695627

C 0.59269107 1.31725081 -0.54638297

N -0.34887023 -4.48368036 -2.41866163

O 0.09913154 -5.47306525 -3.00560791

O -0.80115429 -4.48690023 -1.26708860

H 2.10251353 0.01146621 2.07933020

H 1.59141007 0.01538067 4.53148312

H -0.76376533 -0.00729776 5.33799652

H -2.67108992 -0.02483291 3.71953437

H -3.11308721 0.95689803 -1.34088188

H -2.03994253 0.95875281 -3.55152652

H -1.59715924 -2.25925282 -1.69772675

H 0.90839702 -3.98278945 -4.77032035

H -3.92604405 -0.58776747 1.90646003

H -4.02463482 1.00074835 1.06943808

H -4.07047109 -0.52766597 0.12069826

H 1.83123635 -1.14118560 -0.00024515

H 0.38259288 -2.16007975 -0.25671715

H 1.00473068 -1.12643621 -1.58349512

H 1.65329230 1.39300265 -0.25043807

H 0.52738076 1.32911334 -1.64785436

H 0.05111539 2.19098601 -0.14695962

N 1.00886339 -1.91627463 -6.38836372

O 2.11835567 -2.45248382 -6.46632217

O 0.39401935 -1.37632028 -7.31005017

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