# Supporting Information

for

# Substitution effect and effect of axle's flexibility at (pseudo-)rotaxanes

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## Geometry and structure data

# Appendix

## 0.1 H-bond geometry data

H-bond data is collected starting with the lower label number of the axles oxygens, from this the left and then the right is taken when the oxygen is oriented from above, after this the CH$\cdots$O bond in the middle is collected.

| subst. | label 1 | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(CH\cdots O)}$ | $a_{(CH\cdots O)}$ | label 2 | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(CH\cdots O)}$ | $a_{(CH\cdots O)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| NO2 | 12 | 227.2 | 158 | 234.8 | 155 | 229.4 | 169 | 15 | 239.5 | 152 | 224.2 | 162 | 229.1 | 172 |
| CF3 | 41 | 221.1 | 163 | 238.0 | 153 | 226.8 | 173 | 55 | 234.2 | 156 | 224.7 | 158 | 227.3 | 169 |
| Cl | 12 | 227.9 | 163 | 223.1 | 157 | 225.7 | 172 | 14 | 223.3 | 157 | 227.9 | 162 | 225.7 | 172 |
| SiH3 | 41 | 216.6 | 160 | 235.1 | 156 | 221.7 | 171 | 54 | 235.1 | 156 | 216.6 | 160 | 221.7 | 171 |
| H | 12 | 221.2 | 160 | 222.3 | 163 | 220.1 | 176 | 13 | 222.0 | 164 | 221.3 | 160 | 220.1 | 177 |
| p tBu | 69 | 226.5 | 164 | 221.3 | 159 | 224.2 | 174 | 76 | 221.0 | 160 | 226.9 | 164 | 224.3 | 174 |
| OH | 41 | 208.1 | 167 | 217.8 | 172 | 234.0 | 142 | 62 | 218.0 | 172 | 208.4 | 167 | 233.3 | 143 |
| NH2 | 41 | 222.0 | 165 | 215.4 | 162 | 216.6 | 178 | 54 | 215.3 | 162 | 222.3 | 165 | 216.6 | 177 |
| NO2 | 12 | 243.8 | 155 | 222.8 | 157 | 231.8 | 172 | 15 | 222.7 | 157 | 243.5 | 155 | 231.7 | 172 |
| OH | 12 | 226.2 | 159 | 223.0 | 160 | 223.9 | 171 | 14 | 226.1 | 162 | 221.6 | 160 | 222.0 | 177 |
| 2-Ph | 20 | 203.7 | 166 | 249.8 | 163 | 226.5 | 172 | 21 | 249.8 | 163 | 203.7 | 166 | 226.5 | 172 |

Table 1: Double bond

| subst. | label 1 | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(CH\cdots O)}$ | $a_{(CH\cdots O)}$ | label 2 | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(CH\cdots O)}$ | $a_{(CH\cdots O)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| NO2 | 41 | 246.2 | 155 | 221.5 | 156 | 227.0 | 174 | 46 | 217.8 | 161 | 241.9 | 154 | 225.9 | 176 |
| CF3 | 12 | 216.4 | 157 | 243.3 | 156 | 224.4 | 172 | 18 | 241.7 | 156 | 217.2 | 157 | 225.1 | 172 |
| Cl | 41 | 240.3 | 158 | 218.7 | 156 | 223.8 | 174 | 46 | 215.2 | 162 | 235.4 | 157 | 221.9 | 176 |
| SiH3 | 41 | 239.1 | 159 | 219.2 | 157 | 223.1 | 174 | 46 | 215.1 | 163 | 234.3 | 157 | 221.3 | 176 |
| H | 41 | 238.4 | 159 | 217.3 | 157 | 222.8 | 173 | 46 | 213.8 | 163 | 233.2 | 158 | 220.3 | 176 |
| tBu | 78 | 238.7 | 159 | 211.1 | 159 | 220.0 | 174 | 98 | 212.3 | 159 | 237.3 | 159 | 219.0 | 174 |
| OH | 41 | 239.8 | 161 | 215.8 | 158 | 222.8 | 174 | 46 | 213.9 | 164 | 230.2 | 158 | 218.9 | 178 |
| NH2 | 41 | 212.6 | 159 | 231.9 | 160 | 217.0 | 172 | 46 | 233.5 | 161 | 211.2 | 159 | 218.1 | 171 |
| NO2 | 11 | 240.1 | 155 | 225.2 | 156 | 227.8 | 177 | 23 | 213.8 | 155 | 262.5 | 149 | 230.5 | 171 |
| OH | 41 | 213.9 | 158 | 237.8 | 158 | 221.8 | 172 | 48 | 237.9 | 158 | 213.3 | 159 | 221.6 | 172 |
| 2-ph | 41 | 235.0 | 158 | 211.3 | 163 | 227.7 | 156 | 50 | 211.3 | 163 | 235.0 | 158 | 227.7 | 156 |

Table 2: Single bond

| | subst. | label 1 | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(CH\cdots O)}$ | $a_{(CH\cdots O)}$ | label 2 | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(CH\cdots O)}$ | $a_{(CH\cdots O)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | NO2 | 12 | 221.6 | 157 | 236.5 | 152 | 228.8 | 165 | 15 | 240.9 | 152 | 218.9 | 160 | 229.8 | 167 |
| p | H | 12 | 215.9 | 159 | 210.6 | 166 | 215.9 | 168 | 13 | 210.5 | 166 | 216.0 | 159 | 215.9 | 168 |
| | NH2 | 41 | 208.3 | 168 | 213.7 | 161 | 213.0 | 171 | 54 | 213.5 | 162 | 208.3 | 168 | 213.0 | 171 |
| | 2-ph | 20 | 201.6 | 165 | 242.6 | 158 | 220.1 | 169 | 21 | 242.7 | 158 | 201.5 | 165 | 220.0 | 169 |

Table 3: Double bond Cosmo (Chloroform 4.806 Dielektrizitätskonstante)

| | subst. | label 1 | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(CH\cdots O)}$ | $a_{(CH\cdots O)}$ | label 2 | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(NH\cdots O)}$ | $a_{(NH\cdots O)}$ | $R_{(CH\cdots O)}$ | $a_{(CH\cdots O)}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | NO2 | 41 | 248.1 | 153 | 216.2 | 154 | 226.0 | 169 | 46 | 212.0 | 160 | 247.1 | 152 | 226.8 | 171 |
| p | H | 41 | 234.1 | 159 | 211.7 | 157 | 220.7 | 167 | 46 | 211.6 | 162 | 228.4 | 159 | 219.1 | 171 |
| | NH2 | 41 | 208.8 | 159 | 218.4 | 163 | 213.5 | 165 | 46 | 218.3 | 163 | 208.9 | 159 | 213.4 | 165 |
| | 2-ph | 41 | 226.9 | 159 | 206.8 | 165 | 223.1 | 156 | 50 | 207.0 | 165 | 226.5 | 160 | 223.2 | 156 |

Table 4: Single bond Cosmo (Chloroform 4.806)

## 0.2 Gas phase results on the structures with the C–C axle

Table 5: Cartesian coordinates and total energy in a.u. of complex **3a@1**

E(RI-TPSS-D3/def2-TZVP)=-3125.071271770

| | | | |
|---|---|---|---|
| C | -4.7537372 | 1.1897337 | 0.2959751 |
| C | -4.0276960 | 0.0620943 | 0.6927430 |
| C | -4.6972972 | -1.1558679 | 0.8654380 |
| C | -6.0700522 | -1.2391037 | 0.6437989 |
| C | -6.7869868 | -0.1136356 | 0.2418172 |
| C | -6.1330795 | 1.1132058 | 0.0750797 |
| C | -2.5346512 | 0.0691819 | 0.8782682 |
| O | -1.8923135 | -0.9825600 | 0.9040394 |
| C | -6.9636989 | 2.2917994 | -0.3459145 |
| O | -8.0813913 | 2.1451032 | -0.8502234 |
| N | -1.9375638 | 1.2955074 | 0.9975546 |
| C | -0.4946982 | 1.4408843 | 0.8699998 |
| C | -0.0698294 | 1.8084577 | -0.5432165 |
| C | -0.8003609 | 1.3736840 | -1.6536947 |
| C | -0.4034925 | 1.7158613 | -2.9443095 |
| C | 0.7346284 | 2.4992629 | -3.1598752 |
| C | 1.4825127 | 2.9151022 | -2.0509767 |
| C | 1.0811197 | 2.5728514 | -0.7608695 |
| C | 1.1100964 | 2.9506154 | -4.5553602 |
| N | 0.5157026 | 4.2532882 | -4.8791104 |
| C | 1.1335651 | 5.4179659 | -4.5249358 |
| O | 2.2549705 | 5.4342303 | -4.0051093 |
| C | 0.3849942 | 6.6900911 | -4.8032805 |
| C | -0.9964192 | 6.7225921 | -5.0157883 |
| C | -1.6644815 | 7.9341537 | -5.2206931 |

| | | | |
|---|---|---|---|
| C | -0.9299610 | 9.1267587 | -5.2177636 |
| C | 0.4485265 | 9.1004623 | -5.0131813 |
| C | 1.1055695 | 7.8905595 | -4.7965594 |
| C | -3.1551780 | 8.0300543 | -5.3974852 |
| O | -3.7382460 | 9.1153788 | -5.3396111 |
| N | -3.8181011 | 6.8528414 | -5.6207781 |
| C | -5.2771595 | 6.7847600 | -5.6045164 |
| C | -5.8007779 | 6.2684432 | -4.2784636 |
| C | -5.4169723 | 6.8990761 | -3.0882840 |
| C | -5.8694311 | 6.4248471 | -1.8602998 |
| C | -6.7232429 | 5.3182580 | -1.7902368 |
| C | -7.1247272 | 4.6994755 | -2.9804754 |
| C | -6.6598481 | 5.1670696 | -4.2098126 |
| C | -7.1550574 | 4.7546580 | -0.4539488 |
| N | -6.4282641 | 3.5284656 | -0.1128396 |
| O | -3.0641254 | 4.0640980 | -0.0491510 |
| C | -2.3187594 | 4.6983950 | -0.8089146 |
| C | -2.4901921 | 4.6392552 | -2.3186512 |
| C | -3.5448362 | 3.6101748 | -2.6943357 |
| C | -3.5617044 | 3.3271016 | -4.1826586 |
| O | -2.8267367 | 3.9260681 | -4.9822290 |
| N | -1.2626828 | 5.4563279 | -0.3459509 |
| C | -0.3877489 | 6.1755605 | -1.2954230 |
| C | -0.8463330 | 5.3963762 | 1.0134834 |
| C | -1.7707348 | 5.3350344 | 2.0700865 |
| C | -1.3235166 | 5.2564547 | 3.3828202 |
| C | 0.0450347 | 5.2484971 | 3.6388315 |
| C | 0.9793744 | 5.3322649 | 2.6109709 |
| C | 0.5295938 | 5.4069368 | 1.2996425 |
| N | 0.5179797 | 5.1579977 | 5.0354958 |

| | | | |
|---|---|---|---|
| N | -4.4250436 | 2.3321557 | -4.5867541 |
| C | -4.4794486 | 1.9058203 | -5.9450525 |
| C | -4.5059379 | 2.8329615 | -6.9974619 |
| C | -4.5889164 | 2.3923600 | -8.3114964 |
| C | -4.6469630 | 1.0239879 | -8.5661487 |
| C | -4.6252710 | 0.0857610 | -7.5389050 |
| C | -4.5390330 | 0.5325360 | -6.2262611 |
| N | -4.7393531 | 0.5550406 | -9.9651726 |
| C | -5.2330665 | 1.5880754 | -3.5979534 |
| H | 1.0127657 | 10.0286727 | -5.0164109 |
| H | 2.1750116 | 7.8496473 | -4.6152470 |
| H | -1.5607636 | 5.7968476 | -4.9680256 |
| H | -1.4637096 | 10.0596666 | -5.3695574 |
| H | -3.3210783 | 5.9704051 | -5.5470676 |
| H | -0.4423386 | 4.2601857 | -5.2105872 |
| H | 0.7596410 | 2.2327615 | -5.3024159 |
| H | 2.1929542 | 3.0598357 | -4.6490627 |
| H | -5.6333062 | 7.8022293 | -5.7912805 |
| H | -5.6191251 | 6.1446388 | -6.4246249 |
| H | -0.9880015 | 1.3743589 | -3.7966455 |
| H | -1.6820044 | 0.7568865 | -1.5071081 |
| H | 1.6705616 | 2.9022424 | 0.0916892 |
| H | 2.3674902 | 3.5245396 | -2.2102565 |
| H | -4.7657621 | 7.7686010 | -3.1326285 |
| H | -5.5587880 | 6.9207833 | -0.9429997 |
| H | -7.7928833 | 3.8432290 | -2.9316759 |
| H | -6.9704554 | 4.6709307 | -5.1272004 |
| H | -0.1458391 | 2.2029121 | 1.5747324 |
| H | -0.0571459 | 0.4796180 | 1.1583057 |
| H | -8.2150663 | 4.4898164 | -0.4684464 |

| | | | |
|---|---|---|---|
| H | -6.9833422 | 5.4857850 | 0.3420343 |
| H | -2.4866704 | 2.1421039 | 0.8891655 |
| H | -5.4715621 | 3.6187295 | 0.2099611 |
| H | -4.2339559 | 2.1248570 | 0.1088963 |
| H | -6.5839262 | -2.1861222 | 0.7822057 |
| H | -7.8548621 | -0.1587132 | 0.0524814 |
| H | -4.1162919 | -2.0235758 | 1.1617694 |
| H | -1.5301592 | 4.3822762 | -2.7795676 |
| H | -4.5368936 | 3.9493063 | -2.3789176 |
| H | 1.2539512 | 5.4488241 | 0.4947337 |
| H | 2.0373151 | 5.3265414 | 2.8451611 |
| H | -2.0211322 | 5.2114492 | 4.2107229 |
| H | -2.8308171 | 5.3527587 | 1.8633748 |
| H | -4.5042261 | -0.1909585 | -5.4183671 |
| H | -4.6659425 | -0.9707507 | -7.7757487 |
| H | -4.6202805 | 3.0911561 | -9.1390314 |
| H | -4.4687525 | 3.8922813 | -6.7846760 |
| H | -0.9863903 | 6.5998711 | -2.0999212 |
| H | 0.0952252 | 6.9959829 | -0.7642876 |
| H | 0.3745421 | 5.5170822 | -1.7247427 |
| H | -6.0313455 | 1.0686019 | -4.1266282 |
| H | -4.6319624 | 0.8620799 | -3.0402713 |
| H | -5.6921582 | 2.2864135 | -2.8985698 |
| H | -3.3566483 | 2.6771888 | -2.1522641 |
| H | -2.7703627 | 5.6263006 | -2.7046405 |
| O | -0.3354054 | 5.0618804 | 5.9227071 |
| O | 1.7379307 | 5.1830580 | 5.2281114 |
| O | -4.8027769 | -0.6634852 | -10.1558896 |
| O | -4.7479599 | 1.4109724 | -10.8549863 |

Table 6: Cartesian coordinates and total energy in a.u. of complex **3b@1**

E(RI-TPSS-D3/def2-TZVP)=-3390.259594367

| | | | |
|---|---|---|---|
| C | -4.8467921 | 0.6542763 | -0.3364292 |
| C | -4.2873751 | -0.3909424 | 0.4137781 |
| C | -5.0382962 | -0.9818834 | 1.4376406 |
| C | -6.3170431 | -0.5175326 | 1.7330106 |
| C | -6.8564519 | 0.5406269 | 1.0049002 |
| C | -6.1210861 | 1.1158962 | -0.0351095 |
| N | -2.9673145 | -0.8700214 | 0.1588425 |
| C | -2.7058517 | -2.3071282 | 0.3764675 |
| C | -8.2217024 | 1.0883679 | 1.3145463 |
| F | -8.8504425 | 0.4026172 | 2.3012944 |
| C | -1.9289263 | 0.0036329 | -0.0682072 |
| O | -2.1095588 | 1.2184595 | -0.2449534 |
| C | -0.5336251 | -0.5953858 | -0.0500728 |
| C | 0.5212255 | 0.4956392 | -0.1304152 |
| C | 1.9239390 | -0.0745176 | -0.0498180 |
| N | 2.9446251 | 0.8342885 | -0.1988450 |
| C | 2.6563344 | 2.2657284 | -0.4233843 |
| O | 2.1328715 | -1.2865744 | 0.1183083 |
| C | 4.3004943 | 0.4060058 | -0.3251879 |
| C | 4.8408197 | -0.5652805 | 0.5287721 |
| C | 6.1670942 | -0.9500843 | 0.3846384 |
| C | 6.9682658 | -0.3716176 | -0.6042800 |
| C | 6.4375216 | 0.6006874 | -1.4488583 |
| C | 5.1072972 | 0.9866594 | -1.3102990 |
| C | 8.4027834 | -0.8060482 | -0.7215349 |

| | | | |
|---|---|---|---|
| F | 9.0500440 | -0.2012935 | -1.7484562 |
| F | 9.1082023 | -0.5282014 | 0.4119188 |
| F | 8.5091184 | -2.1506249 | -0.9167810 |
| F | -9.0373373 | 1.0593115 | 0.2231677 |
| F | -8.1629305 | 2.3918013 | 1.7109038 |
| N | -2.2090153 | 3.0650193 | 2.2738582 |
| C | -2.6657176 | 2.1890180 | 3.3459783 |
| C | -1.7726217 | 0.9704880 | 3.5006350 |
| C | -2.3201444 | -0.2964972 | 3.7226808 |
| C | -1.5034052 | -1.4190786 | 3.8498555 |
| C | -0.1119087 | -1.2970063 | 3.7488799 |
| C | 0.4376271 | -0.0264662 | 3.5482359 |
| C | -0.3806831 | 1.0942441 | 3.4281734 |
| C | 0.7685848 | -2.5273887 | 3.7953581 |
| N | 0.7877904 | -3.2385304 | 2.5126988 |
| C | -0.1055856 | -4.2351398 | 2.2386482 |
| O | -0.9370042 | -4.6195085 | 3.0683919 |
| C | -0.0069232 | -4.8646662 | 0.8790768 |
| C | 0.6284830 | -4.2411955 | -0.1990911 |
| C | 0.6935964 | -4.8623235 | -1.4498986 |
| C | 0.1055215 | -6.1219627 | -1.6188716 |
| C | -0.5325439 | -6.7464506 | -0.5490372 |
| C | -0.5973927 | -6.1205594 | 0.6945722 |
| C | 1.3222007 | -4.2130899 | -2.6522824 |
| O | 1.1024061 | -4.6321861 | -3.7921438 |
| N | 2.1341158 | -3.1406180 | -2.4073612 |
| C | 2.6099111 | -2.2830000 | -3.4873862 |
| C | 1.7530707 | -1.0392800 | -3.6357654 |
| C | 2.3326122 | 0.2270230 | -3.7568937 |
| C | 1.5412971 | 1.3684082 | -3.8812213 |

| | | | |
|---|---|---|---|
| C | 0.1446735 | 1.2656993 | -3.8719493 |
| C | -0.4352027 | -0.0027372 | -3.7643540 |
| C | 0.3572874 | -1.1423477 | -3.6525697 |
| C | -0.7126639 | 2.5121007 | -3.9201884 |
| N | -0.7575250 | 3.2026138 | -2.6274833 |
| C | 0.1163523 | 4.2086200 | -2.3259703 |
| O | 0.9645211 | 4.6065660 | -3.1319273 |
| C | -0.0287871 | 4.8338616 | -0.9685593 |
| C | 0.5291993 | 6.1025554 | -0.7716150 |
| C | 0.4166317 | 6.7298453 | 0.4677629 |
| C | -0.2362272 | 6.0938140 | 1.5215142 |
| C | -0.7909010 | 4.8206761 | 1.3410480 |
| C | -0.6787003 | 4.1982358 | 0.0940551 |
| C | -1.4303442 | 4.1593376 | 2.5314083 |
| O | -1.2443384 | 4.5862622 | 3.6740114 |
| H | -0.9843584 | -7.7248728 | -0.6854871 |
| H | 0.1539918 | -6.5846447 | -2.5997453 |
| H | 1.0328492 | -3.2414395 | -0.0741243 |
| H | -1.0997836 | -6.5837760 | 1.5379919 |
| H | 1.3880899 | -2.8746989 | 1.7809514 |
| H | 2.2215233 | -2.7679634 | -1.4671185 |
| H | 3.6501557 | -2.0040665 | -3.2906547 |
| H | 2.5765404 | -2.8851445 | -4.4005570 |
| H | 0.4036272 | -3.2369391 | 4.5418793 |
| H | 1.7987943 | -2.2531006 | 4.0421907 |
| H | 3.4164095 | 0.3182398 | -3.7546237 |
| H | 1.9961956 | 2.3511795 | -3.9755939 |
| H | -1.5194205 | -0.0992360 | -3.7708238 |
| H | -0.1072869 | -2.1226928 | -3.5850170 |
| H | -1.9351642 | -2.4030358 | 4.0132846 |

| | | | |
|---|---|---|---|
| H | -3.3997986 | -0.4031368 | 3.7944032 |
| H | 0.0632679 | 2.0756403 | 3.2839531 |
| H | 1.5185196 | 0.0869184 | 3.4845867 |
| H | -1.7390954 | 2.2598253 | -4.2035593 |
| H | -0.3132747 | 3.2288921 | -4.6420092 |
| H | -2.6606695 | 2.7883093 | 4.2619135 |
| H | -3.6949660 | 1.8768220 | 3.1399515 |
| H | -1.3723158 | 2.8291312 | -1.9130277 |
| H | -2.2734726 | 2.6917528 | 1.3319745 |
| H | -1.0566624 | 3.1891390 | -0.0390066 |
| H | 0.8429669 | 7.7182928 | 0.6136400 |
| H | -0.3209295 | 6.5572514 | 2.4995673 |
| H | 1.0439631 | 6.5747119 | -1.6024853 |
| H | -0.4145423 | -1.2918193 | -0.8877892 |
| H | 0.3688721 | 1.2123109 | 0.6839796 |
| H | -4.6204560 | -1.7937755 | 2.0227947 |
| H | -6.8864620 | -0.9730171 | 2.5356753 |
| H | -6.5518045 | 1.9251846 | -0.6166237 |
| H | -4.2862157 | 1.1001369 | -1.1455646 |
| H | 4.6966512 | 1.7354216 | -1.9796434 |
| H | 7.0559286 | 1.0511500 | -2.2172993 |
| H | 6.5868711 | -1.6986281 | 1.0496903 |
| H | 4.2253244 | -1.0095961 | 1.2991954 |
| H | -1.9427025 | -2.6548336 | -0.3197449 |
| H | -2.3750979 | -2.5122300 | 1.3994311 |
| H | -3.6258578 | -2.8565450 | 0.1745615 |
| H | 3.5636767 | 2.8328864 | -0.2161013 |
| H | 2.3318010 | 2.4604754 | -1.4499065 |
| H | 1.8799288 | 2.6029274 | 0.2643432 |
| H | 0.4156615 | 1.0611965 | -1.0626557 |

| | | | |
|---|---|---|---|
| H | -0.4038158 | -1.1825044 | 0.8655324 |

Table 7: Cartesian coordinates and total energy in a.u. of complex **3c@1**

E(RI-TPSS-D3/def2-TZVP)=-3635.082636617

| | | | |
|---|---|---|---|
| C | -4.7269338 | 1.1172264 | 0.2692051 |
| C | -4.0097508 | -0.0251824 | 0.6383571 |
| C | -4.6922078 | -1.2371154 | 0.8026703 |
| C | -6.0692428 | -1.2991171 | 0.6008610 |
| C | -6.7778932 | -0.1579474 | 0.2292807 |
| C | -6.1106131 | 1.0627652 | 0.0709085 |
| C | -2.5144880 | -0.0367872 | 0.8058918 |
| O | -1.8846100 | -1.0971511 | 0.8188545 |
| C | -6.9336106 | 2.2612763 | -0.3080864 |
| O | -8.0744848 | 2.1404119 | -0.7657015 |
| N | -1.9024848 | 1.1812612 | 0.9251132 |
| C | -0.4596992 | 1.3118766 | 0.7824027 |
| C | -0.0493622 | 1.6905652 | -0.6322269 |
| C | -0.7991815 | 1.2767575 | -1.7377060 |
| C | -0.4192802 | 1.6345822 | -3.0291802 |
| C | 0.7212916 | 2.4125031 | -3.2505077 |
| C | 1.4895783 | 2.8058784 | -2.1473324 |
| C | 1.1047076 | 2.4483933 | -0.8564433 |
| C | 1.0745693 | 2.8888306 | -4.6432827 |
| N | 0.4978333 | 4.2093281 | -4.9213341 |
| C | 1.1533034 | 5.3536399 | -4.5679454 |
| O | 2.2958286 | 5.3380445 | -4.0960533 |

| | | | |
|---|---|---|---|
| C | 0.4205629 | 6.6456773 | -4.7940041 |
| C | -0.9633900 | 6.7064080 | -4.9810715 |
| C | -1.6135463 | 7.9326304 | -5.1510105 |
| C | -0.8594311 | 9.1128088 | -5.1339990 |
| C | 0.5213608 | 9.0589177 | -4.9512311 |
| C | 1.1613765 | 7.8335726 | -4.7732718 |
| C | -3.1044145 | 8.0540290 | -5.3084481 |
| O | -3.6696174 | 9.1479220 | -5.2263141 |
| N | -3.7878232 | 6.8915328 | -5.5446492 |
| C | -5.2475351 | 6.8475735 | -5.5137082 |
| C | -5.7637262 | 6.3099849 | -4.1934054 |
| C | -5.3627126 | 6.9151238 | -2.9959232 |
| C | -5.8033098 | 6.4192604 | -1.7723076 |
| C | -6.6618110 | 5.3158666 | -1.7139924 |
| C | -7.0798943 | 4.7221295 | -2.9111255 |
| C | -6.6272910 | 5.2114655 | -4.1365275 |
| C | -7.0793215 | 4.7278074 | -0.3840441 |
| N | -6.3648835 | 3.4845875 | -0.0839942 |
| O | -3.0321439 | 3.9548500 | -0.0410562 |
| C | -2.2800533 | 4.6049364 | -0.7861571 |
| C | -2.4502797 | 4.5847419 | -2.2977940 |
| C | -3.5134906 | 3.5767424 | -2.7044975 |
| C | -3.5344273 | 3.3364113 | -4.2013140 |
| O | -2.8057032 | 3.9663418 | -4.9873007 |
| N | -1.2303930 | 5.3472984 | -0.3043662 |
| C | -0.3398803 | 6.0779428 | -1.2284100 |
| C | -0.8339326 | 5.2660018 | 1.0677342 |
| C | -1.7723142 | 5.2678252 | 2.1078690 |
| C | -1.3529018 | 5.1709493 | 3.4318328 |
| C | 0.0076324 | 5.0820148 | 3.7231024 |

| | | | |
|---|---|---|---|
| C | 0.9545975 | 5.0997928 | 2.7015154 |
| C | 0.5297529 | 5.1902297 | 1.3786302 |
| Cl | 0.5311272 | 4.9561163 | 5.3842758 |
| N | -4.3934839 | 2.3583266 | -4.6319273 |
| C | -4.4451242 | 1.9764684 | -6.0109723 |
| C | -4.5600238 | 2.9347982 | -7.0229918 |
| C | -4.6340963 | 2.5425622 | -8.3560566 |
| C | -4.6005974 | 1.1854913 | -8.6774572 |
| C | -4.4917289 | 0.2185208 | -7.6804041 |
| C | -4.4091872 | 0.6196925 | -6.3488449 |
| Cl | -4.6992614 | 0.6925051 | -10.3498194 |
| C | -5.2087585 | 1.5853001 | -3.6737032 |
| H | 1.1011874 | 9.9775140 | -4.9425008 |
| H | 2.2331390 | 7.7703278 | -4.6130185 |
| H | -1.5436100 | 5.7904120 | -4.9439566 |
| H | -1.3796391 | 10.0573779 | -5.2584440 |
| H | -3.3061250 | 5.9980841 | -5.4909518 |
| H | -0.4769626 | 4.2399358 | -5.2010062 |
| H | 0.6930156 | 2.1953012 | -5.3982717 |
| H | 2.1567666 | 2.9809938 | -4.7597146 |
| H | -5.5885601 | 7.8747791 | -5.6734897 |
| H | -5.6093839 | 6.2315211 | -6.3437281 |
| H | -1.0212891 | 1.3131545 | -3.8770975 |
| H | -1.6853291 | 0.6676067 | -1.5864856 |
| H | 1.7080824 | 2.7624759 | -0.0078939 |
| H | 2.3756383 | 3.4126438 | -2.3112648 |
| H | -4.7049501 | 7.7801323 | -3.0310848 |
| H | -5.4775050 | 6.8938481 | -0.8490044 |
| H | -7.7501058 | 3.8669008 | -2.8713332 |
| H | -6.9488647 | 4.7330004 | -5.0595270 |

| | | | |
|---|---|---|---|
| H | -0.0952226 | 2.0636933 | 1.4899203 |
| H | -0.0292340 | 0.3428415 | 1.0549736 |
| H | -8.1429577 | 4.4773755 | -0.3857445 |
| H | -6.8839775 | 5.4391790 | 0.4246229 |
| H | -2.4414047 | 2.0369262 | 0.8293697 |
| H | -5.3901963 | 3.5548777 | 0.1885597 |
| H | -4.1972673 | 2.0480348 | 0.0896843 |
| H | -6.5933007 | -2.2416942 | 0.7319738 |
| H | -7.8494920 | -0.1853516 | 0.0584974 |
| H | -4.1180223 | -2.1164299 | 1.0774324 |
| H | -1.4919435 | 4.3299650 | -2.7635357 |
| H | -4.5026680 | 3.9154715 | -2.3797490 |
| H | 1.2706390 | 5.1851569 | 0.5866928 |
| H | 2.0114692 | 5.0354755 | 2.9360523 |
| H | -2.0799882 | 5.1717566 | 4.2365311 |
| H | -2.8278250 | 5.3425127 | 1.8848703 |
| H | -4.3097627 | -0.1328323 | -5.5723110 |
| H | -4.4635920 | -0.8334680 | -7.9418904 |
| H | -4.7255346 | 3.2837757 | -9.1425038 |
| H | -4.5911988 | 3.9864211 | -6.7694169 |
| H | -0.9263258 | 6.5545012 | -2.0133644 |
| H | 0.1721926 | 6.8575900 | -0.6641573 |
| H | 0.4005213 | 5.4149739 | -1.6888579 |
| H | -5.9939815 | 1.0738296 | -4.2295708 |
| H | -4.6104143 | 0.8463159 | -3.1291962 |
| H | -5.6814865 | 2.2582878 | -2.9575680 |
| H | -3.3342618 | 2.6274712 | -2.1884927 |
| H | -2.7178173 | 5.5844563 | -2.6592173 |

Table 8: Cartesian coordinates and total energy in a.u. of complex **3d@1**

E(RI-TPSS-D3/def2-TZVP)=-3297.275183438

| | | | |
|---|---|---|---|
| C | -4.7564519 | 1.2737280 | 0.3609315 |
| C | -4.0279531 | 0.1529453 | 0.7717149 |
| C | -4.6963926 | -1.0617621 | 0.9696481 |
| C | -6.0709174 | -1.1476759 | 0.7601460 |
| C | -6.7910000 | -0.0277826 | 0.3480893 |
| C | -6.1379295 | 1.1956259 | 0.1552026 |
| C | -2.5338451 | 0.1654169 | 0.9499554 |
| O | -1.8915953 | -0.8864280 | 1.0021914 |
| C | -6.9738189 | 2.3706191 | -0.2672961 |
| O | -8.1135558 | 2.2202901 | -0.7191540 |
| N | -1.9372391 | 1.3938830 | 1.0334937 |
| C | -0.4953698 | 1.5376259 | 0.8923888 |
| C | -0.0830307 | 1.8696447 | -0.5334908 |
| C | -0.8257385 | 1.4127444 | -1.6267868 |
| C | -0.4439158 | 1.7291909 | -2.9285295 |
| C | 0.6914415 | 2.5081993 | -3.1721531 |
| C | 1.4522397 | 2.9452801 | -2.0803238 |
| C | 1.0658750 | 2.6285108 | -0.7793181 |
| C | 1.0465992 | 2.9387088 | -4.5793513 |
| N | 0.4513925 | 4.2387606 | -4.9101145 |
| C | 1.0854885 | 5.4059744 | -4.5948718 |
| O | 2.2241739 | 5.4269298 | -4.1138368 |
| C | 0.3338814 | 6.6764394 | -4.8755644 |
| C | -1.0483741 | 6.7060010 | -5.0814049 |
| C | -1.7176963 | 7.9132393 | -5.3048418 |
| C | -0.9842982 | 9.1063671 | -5.3219129 |

| | | | |
|---|---|---|---|
| C | 0.3946548 | 9.0837354 | -5.1193860 |
| C | 1.0536643 | 7.8772648 | -4.8889086 |
| C | -3.2084774 | 8.0018654 | -5.4856180 |
| O | -3.7927727 | 9.0886396 | -5.4613946 |
| N | -3.8693787 | 6.8179973 | -5.6748246 |
| C | -5.3283001 | 6.7487753 | -5.6513283 |
| C | -5.8433752 | 6.2644179 | -4.3099429 |
| C | -5.4560419 | 6.9278305 | -3.1390955 |
| C | -5.8937125 | 6.4797914 | -1.8960829 |
| C | -6.7363173 | 5.3676351 | -1.7919353 |
| C | -7.1421341 | 4.7162516 | -2.9631511 |
| C | -6.6917540 | 5.1573688 | -4.2074715 |
| C | -7.1468829 | 4.8301872 | -0.4385059 |
| N | -6.4189199 | 3.6076398 | -0.0892987 |
| O | -3.0999946 | 4.1125796 | -0.0514333 |
| C | -2.3498630 | 4.7457832 | -0.8121018 |
| C | -2.5162281 | 4.6763623 | -2.3231883 |
| C | -3.5627542 | 3.6389582 | -2.6978183 |
| C | -3.5655611 | 3.3340192 | -4.1827915 |
| O | -2.8354595 | 3.9377686 | -4.9877458 |
| N | -1.3025696 | 5.5064113 | -0.3511905 |
| C | -0.4260871 | 6.2229557 | -1.2993944 |
| C | -0.8895880 | 5.4551868 | 1.0169238 |
| C | -1.8116819 | 5.4320799 | 2.0703410 |
| C | -1.3584776 | 5.3577684 | 3.3860981 |
| C | 0.0094944 | 5.3143244 | 3.7022386 |
| C | 0.9167050 | 5.3621762 | 2.6299171 |
| C | 0.4815835 | 5.4314726 | 1.3104892 |
| Si | 0.5959722 | 5.2060707 | 5.4815830 |
| N | -4.4069042 | 2.3251679 | -4.5768297 |

| | | | |
|---|---|---|---|
| C | -4.4407130 | 1.8758943 | -5.9357745 |
| C | -4.5431400 | 2.7823024 | -6.9969714 |
| C | -4.6044405 | 2.3118549 | -8.3045098 |
| C | -4.5716493 | 0.9363939 | -8.5994493 |
| C | -4.4716074 | 0.0465508 | -7.5183310 |
| C | -4.4030107 | 0.5043669 | -6.2035004 |
| Si | -4.6658409 | 0.3063692 | -10.3653296 |
| C | -5.2171150 | 1.5845437 | -3.5893429 |
| H | 0.9582226 | 10.0123428 | -5.1367129 |
| H | 2.1241528 | 7.8390543 | -4.7130379 |
| H | -1.6128530 | 5.7817744 | -5.0172916 |
| H | -1.5189012 | 10.0364304 | -5.4878515 |
| H | -3.3734203 | 5.9366486 | -5.5724401 |
| H | -0.5217717 | 4.2427259 | -5.1973042 |
| H | 0.6807075 | 2.2121054 | -5.3106191 |
| H | 2.1280607 | 3.0432950 | -4.6923109 |
| H | -5.6869098 | 7.7606567 | -5.8618756 |
| H | -5.6724016 | 6.0866738 | -6.4528416 |
| H | -1.0404116 | 1.3745819 | -3.7670444 |
| H | -1.7079764 | 0.8025465 | -1.4581898 |
| H | 1.6619556 | 2.9781835 | 0.0601959 |
| H | 2.3334443 | 3.5541852 | -2.2615939 |
| H | -4.8102608 | 7.7995664 | -3.2100613 |
| H | -5.5772171 | 6.9984303 | -0.9934567 |
| H | -7.7998292 | 3.8538391 | -2.8876736 |
| H | -7.0011252 | 4.6330853 | -5.1093563 |
| H | -0.1443039 | 2.3199409 | 1.5732078 |
| H | -0.0538371 | 0.5848938 | 1.2020428 |
| H | -8.2078208 | 4.5688073 | -0.4285130 |
| H | -6.9578112 | 5.5757578 | 0.3402857 |

| | | | |
|---|---|---|---|
| H | -2.4855779 | 2.2392849 | 0.9056173 |
| H | -5.4440937 | 3.6996847 | 0.1767144 |
| H | -4.2366301 | 2.2044528 | 0.1547866 |
| H | -6.5840983 | -2.0923202 | 0.9169943 |
| H | -7.8609614 | -0.0739852 | 0.1710782 |
| H | -4.1131445 | -1.9245076 | 1.2760356 |
| H | -1.5534255 | 4.4208783 | -2.7790108 |
| H | -4.5594330 | 3.9772933 | -2.3966848 |
| H | 1.2107759 | 5.4471389 | 0.5077443 |
| H | 1.9882789 | 5.3377046 | 2.8174907 |
| H | -2.0974047 | 5.3394768 | 4.1838596 |
| H | -2.8720975 | 5.4703044 | 1.8623595 |
| H | -4.3126453 | -0.2068794 | -5.3874734 |
| H | -4.4396463 | -1.0253955 | -7.6983243 |
| H | -4.6880660 | 3.0393740 | -9.1093319 |
| H | -4.5758980 | 3.8454426 | -6.7955650 |
| H | -1.0222797 | 6.6607368 | -2.0991964 |
| H | 0.0698590 | 7.0317365 | -0.7624463 |
| H | 0.3278253 | 5.5601468 | -1.7377574 |
| H | -5.9859409 | 1.0302438 | -4.1266120 |
| H | -4.6108135 | 0.8859722 | -3.0021434 |
| H | -5.7107436 | 2.2834509 | -2.9130932 |
| H | -3.3764951 | 2.7147181 | -2.1405258 |
| H | -2.7986019 | 5.6594725 | -2.7172347 |
| H | -0.5884381 | 5.1948991 | 6.3754927 |
| H | 1.3896540 | 3.9690475 | 5.6977488 |
| H | 1.4596279 | 6.3664743 | 5.8202338 |
| H | -4.6104695 | -1.1766445 | -10.3441767 |
| H | -5.9308963 | 0.7432365 | -11.0102497 |
| H | -3.5354097 | 0.8317489 | -11.1729251 |

Table 9: Cartesian coordinates and total energy in a.u. of complex **3e@1**

E(RI-TPSS-D3/def2-TZVP)=-2715.812036735

| | | | |
|---|---|---|---|
| C | -4.7245002 | 1.1105806 | 0.2691639 |
| C | -4.0062950 | -0.0316930 | 0.6363674 |
| C | -4.6894050 | -1.2418406 | 0.8104814 |
| C | -6.0683330 | -1.3017877 | 0.6208892 |
| C | -6.7783358 | -0.1601532 | 0.2531370 |
| C | -6.1100736 | 1.0586306 | 0.0847405 |
| C | -2.5099382 | -0.0433805 | 0.7939900 |
| O | -1.8804732 | -1.1044116 | 0.8094613 |
| C | -6.9337543 | 2.2591910 | -0.2865872 |
| O | -8.0821646 | 2.1415037 | -0.7260888 |
| N | -1.8975510 | 1.1748302 | 0.9029075 |
| C | -0.4552879 | 1.3059086 | 0.7560294 |
| C | -0.0489006 | 1.6790052 | -0.6612258 |
| C | -0.7989971 | 1.2578537 | -1.7636778 |
| C | -0.4234926 | 1.6131520 | -3.0572578 |
| C | 0.7134891 | 2.3948696 | -3.2834340 |
| C | 1.4826601 | 2.7949028 | -2.1831956 |
| C | 1.1016085 | 2.4408369 | -0.8903516 |
| C | 1.0602491 | 2.8722333 | -4.6774551 |
| N | 0.4898090 | 4.1972193 | -4.9462603 |
| C | 1.1580481 | 5.3364651 | -4.6001781 |
| O | 2.3094626 | 5.3133872 | -4.1506560 |
| C | 0.4279452 | 6.6332998 | -4.8077624 |

| | | | |
|---|---|---|---|
| C | -0.9568324 | 6.7002723 | -4.9854415 |
| C | -1.6039049 | 7.9295340 | -5.1437047 |
| C | -0.8459934 | 9.1071730 | -5.1218852 |
| C | 0.5355546 | 9.0473877 | -4.9464245 |
| C | 1.1727432 | 7.8186075 | -4.7823316 |
| C | -3.0949678 | 8.0557365 | -5.2965768 |
| O | -3.6558988 | 9.1522711 | -5.2157545 |
| N | -3.7828472 | 6.8953191 | -5.5283714 |
| C | -5.2426131 | 6.8565912 | -5.4955000 |
| C | -5.7579058 | 6.3165993 | -4.1758886 |
| C | -5.3549474 | 6.9189695 | -2.9777465 |
| C | -5.7936940 | 6.4204863 | -1.7545365 |
| C | -6.6519937 | 5.3169569 | -1.6974527 |
| C | -7.0709510 | 4.7251267 | -2.8951716 |
| C | -6.6205530 | 5.2172722 | -4.1202182 |
| C | -7.0677835 | 4.7261676 | -0.3682579 |
| N | -6.3560889 | 3.4802741 | -0.0744677 |
| O | -3.0370980 | 3.9391680 | -0.0406484 |
| C | -2.2812252 | 4.5932796 | -0.7793892 |
| C | -2.4431652 | 4.5760942 | -2.2921463 |
| C | -3.5059122 | 3.5710570 | -2.7064751 |
| C | -3.5255266 | 3.3397954 | -4.2048423 |
| O | -2.7990369 | 3.9793644 | -4.9860439 |
| N | -1.2370213 | 5.3360587 | -0.2905417 |
| C | -0.3381232 | 6.0637680 | -1.2083333 |
| C | -0.8550144 | 5.2606562 | 1.0885445 |
| C | -1.8072995 | 5.2928327 | 2.1148098 |
| C | -1.3961003 | 5.2032798 | 3.4432084 |
| C | -0.0432194 | 5.0913727 | 3.7661892 |
| C | 0.9048653 | 5.0791786 | 2.7439500 |

| | | | |
|---|---|---|---|
| C | 0.5043744 | 5.1621996 | 1.4115467 |
| H | 0.2686717 | 5.0213754 | 4.8038362 |
| N | -4.3788297 | 2.3616589 | -4.6414659 |
| C | -4.4291308 | 1.9885576 | -6.0255010 |
| C | -4.5752188 | 2.9546843 | -7.0253346 |
| C | -4.6461913 | 2.5633663 | -8.3603353 |
| C | -4.5803080 | 1.2129883 | -8.7082412 |
| C | -4.4400893 | 0.2509351 | -7.7087250 |
| C | -4.3596369 | 0.6349517 | -6.3706407 |
| H | -4.6398282 | 0.9136833 | -9.7502940 |
| C | -5.1903263 | 1.5781218 | -3.6892580 |
| H | 1.1183913 | 9.9640762 | -4.9333472 |
| H | 2.2453090 | 7.7504153 | -4.6295174 |
| H | -1.5401311 | 5.7863354 | -4.9521792 |
| H | -1.3637750 | 10.0542135 | -5.2375199 |
| H | -3.3054961 | 5.9992179 | -5.4724668 |
| H | -0.4908645 | 4.2336326 | -5.2049440 |
| H | 0.6683675 | 2.1833601 | -5.4314818 |
| H | 2.1420882 | 2.9582471 | -4.8016561 |
| H | -5.5803091 | 7.8854644 | -5.6515300 |
| H | -5.6076251 | 6.2438100 | -6.3265011 |
| H | -1.0270607 | 1.2880438 | -3.9026608 |
| H | -1.6828544 | 0.6463743 | -1.6084013 |
| H | 1.7040311 | 2.7622938 | -0.0439683 |
| H | 2.3655456 | 3.4052876 | -2.3509569 |
| H | -4.6960749 | 7.7831905 | -3.0120939 |
| H | -5.4656676 | 6.8922727 | -0.8305827 |
| H | -7.7396275 | 3.8686083 | -2.8563271 |
| H | -6.9416433 | 4.7394754 | -5.0437024 |
| H | -0.0906761 | 2.0623145 | 1.4584937 |

| | | | |
|---|---|---|---|
| H | -0.0230650 | 0.3385102 | 1.0317184 |
| H | -8.1320760 | 4.4784155 | -0.3676365 |
| H | -6.8682662 | 5.4349554 | 0.4417947 |
| H | -2.4364762 | 2.0311367 | 0.8092873 |
| H | -5.3773975 | 3.5475171 | 0.1852190 |
| H | -4.1944442 | 2.0393812 | 0.0810546 |
| H | -6.5929532 | -2.2430918 | 0.7590845 |
| H | -7.8516397 | -0.1856571 | 0.0929897 |
| H | -4.1143917 | -2.1213394 | 1.0830014 |
| H | -1.4829914 | 4.3201166 | -2.7534835 |
| H | -4.4954966 | 3.9078050 | -2.3808509 |
| H | 1.2491128 | 5.1354988 | 0.6232657 |
| H | 1.9625014 | 4.9981080 | 2.9780630 |
| H | -2.1432590 | 5.2277703 | 4.2313859 |
| H | -2.8575855 | 5.3840776 | 1.8723435 |
| H | -4.2365448 | -0.1162453 | -5.5957691 |
| H | -4.3854196 | -0.8027102 | -7.9665990 |
| H | -4.7606067 | 3.3197213 | -9.1316835 |
| H | -4.6310062 | 4.0016415 | -6.7556942 |
| H | -0.9180366 | 6.5501810 | -1.9924864 |
| H | 0.1799506 | 6.8345258 | -0.6375664 |
| H | 0.3976060 | 5.3969804 | -1.6709641 |
| H | -5.9660066 | 1.0590715 | -4.2513974 |
| H | -4.5871258 | 0.8437549 | -3.1436371 |
| H | -5.6738905 | 2.2437507 | -2.9729807 |
| H | -3.3273629 | 2.6189303 | -2.1956301 |
| H | -2.7061167 | 5.5771042 | -2.6532256 |

Table 10: Cartesian coordinates and total energy in a.u. of complex **3f@1**

E(RI-TPSS-D3/def2-TZVP)=-3030.504804719

| | | | |
|---|---|---|---|
| N | -6.0508616 | 2.0331519 | 1.4320260 |
| C | -7.1097832 | 3.0121625 | 1.6474866 |
| C | -7.4747399 | 3.7400594 | 0.3647750 |
| C | -7.7097168 | 5.1182914 | 0.3648749 |
| C | -8.0183129 | 5.7933466 | -0.8148732 |
| C | -8.0915334 | 5.0998574 | -2.0292256 |
| C | -7.8809542 | 3.7172096 | -2.0260861 |
| C | -7.5798544 | 3.0439634 | -0.8444578 |
| C | -8.3275187 | 5.8471430 | -3.3240051 |
| N | -7.1083795 | 6.5017472 | -3.8104979 |
| C | -6.8062289 | 7.7884239 | -3.4639445 |
| O | -7.5654042 | 8.4784230 | -2.7744703 |
| C | -5.5113434 | 8.3384611 | -3.9903939 |
| C | -4.4845220 | 7.5255934 | -4.4801552 |
| C | -3.2944150 | 8.0817075 | -4.9590248 |
| C | -3.1334057 | 9.4726712 | -4.9365812 |
| C | -4.1512055 | 10.2881595 | -4.4455466 |
| C | -5.3341883 | 9.7271853 | -3.9676732 |
| C | -2.1415653 | 7.2491848 | -5.4510127 |
| O | -1.0209591 | 7.7435553 | -5.6069917 |
| N | -2.4051289 | 5.9322272 | -5.7018447 |
| C | -1.3306033 | 4.9736484 | -5.9361935 |
| C | -0.9808584 | 4.2045212 | -4.6747994 |
| C | -0.8155972 | 2.8166906 | -4.7004951 |
| C | -0.5197455 | 2.1088268 | -3.5366153 |
| C | -0.3928209 | 2.7784084 | -2.3135806 |

| | | | |
|---|---|---|---|
| C | -0.5386196 | 4.1694717 | -2.2909027 |
| C | -0.8245045 | 4.8757605 | -3.4566408 |
| C | -0.1655898 | 1.9996630 | -1.0361374 |
| N | -1.3970726 | 1.3729048 | -0.5454285 |
| C | -1.7263464 | 0.0897981 | -0.8803174 |
| O | -0.9911299 | -0.6167992 | -1.5788991 |
| C | -3.0181059 | -0.4364522 | -0.3221350 |
| C | -4.0226416 | 0.3957287 | 0.1815183 |
| C | -5.2053607 | -0.1389038 | 0.7014657 |
| C | -5.3825516 | -1.5281290 | 0.7049725 |
| C | -4.3883286 | -2.3626891 | 0.1980031 |
| C | -3.2121703 | -1.8230373 | -0.3199700 |
| C | -6.3360284 | 0.7152439 | 1.2082481 |
| O | -7.4590146 | 0.2381385 | 1.3958501 |
| H | -4.0208706 | 11.3666497 | -4.4322916 |
| H | -2.1982444 | 9.8871582 | -5.2999478 |
| H | -4.5947484 | 6.4463882 | -4.4438226 |
| H | -6.1354479 | 10.3430925 | -3.5712804 |
| H | -6.4202299 | 5.9221859 | -4.2803243 |
| H | -3.3119679 | 5.5345767 | -5.4724357 |
| H | -1.6365682 | 4.2797875 | -6.7256408 |
| H | -0.4698137 | 5.5499218 | -6.2893582 |
| H | -9.0718827 | 6.6349557 | -3.1869935 |
| H | -8.6741820 | 5.1623097 | -4.1038251 |
| H | -0.9286328 | 2.2857039 | -5.6425732 |
| H | -0.4000028 | 1.0286686 | -3.5607845 |
| H | -0.4302725 | 4.7048763 | -1.3495394 |
| H | -0.9258936 | 5.9572390 | -3.4246947 |
| H | -8.1866601 | 6.8670519 | -0.8102918 |
| H | -7.6397888 | 5.6686225 | 1.2998913 |

| | | | |
|---|---|---|---|
| H | -7.4266772 | 1.9684771 | -0.8592594 |
| H | -7.9484567 | 3.1619252 | -2.9598249 |
| H | 0.2127621 | 2.6589640 | -0.2487753 |
| H | 0.5518417 | 1.1916425 | -1.1969740 |
| H | -7.9715398 | 2.4614869 | 2.0375655 |
| H | -6.7817560 | 3.7320975 | 2.4045234 |
| H | -2.0698007 | 1.9676609 | -0.0722301 |
| H | -5.1426600 | 2.4126725 | 1.1792137 |
| H | -3.9012977 | 1.4729191 | 0.1239350 |
| H | -4.5313727 | -3.4396356 | 0.2044013 |
| H | -6.3119135 | -1.9263011 | 1.1001397 |
| H | -2.4287431 | -2.4544630 | -0.7274449 |
| C | -3.3843154 | 1.0216966 | -6.5794228 |
| C | -4.3245432 | 1.8681272 | -5.9861394 |
| C | -5.2242379 | 2.5565538 | -6.8088021 |
| C | -5.1547711 | 2.4060411 | -8.1892066 |
| C | -4.2085744 | 1.5726104 | -8.8070739 |
| C | -3.3323206 | 0.8792838 | -7.9659709 |
| N | -4.3460444 | 1.9979052 | -4.5588287 |
| C | -4.0309633 | 0.7957948 | -3.7627878 |
| C | -4.4669848 | 3.2214340 | -3.9529698 |
| O | -4.7392133 | 4.2559818 | -4.5874528 |
| C | -4.2173304 | 3.2493552 | -2.4544676 |
| C | -4.2343136 | 4.6707418 | -1.9139599 |
| C | -4.0010402 | 4.6901585 | -0.4117947 |
| C | -4.4825137 | 6.3465927 | 5.9878978 |
| C | -4.1727759 | 1.4500208 | -10.3351737 |
| N | -4.1541546 | 5.9032965 | 0.2082734 |
| C | -4.2070526 | 6.0135450 | 1.6362177 |
| C | -3.3341867 | 5.3052495 | 2.4718655 |

| | | | |
|---|---|---|---|
| C | -3.4420425 | 5.4304507 | 3.8522865 |
| C | -4.4004126 | 6.2575540 | 4.4593300 |
| C | -4.4816336 | 7.1089566 | -0.5768743 |
| C | -5.2453076 | 6.9751949 | 3.6067121 |
| C | -5.1548120 | 6.8590381 | 2.2196667 |
| C | -3.0614260 | 0.5022746 | -10.8194473 |
| C | -5.5305958 | 0.9042291 | -10.8360132 |
| C | -3.9239311 | 2.8461046 | -10.9528345 |
| C | -5.6006511 | 7.2929789 | 6.4589565 |
| C | -4.7621781 | 4.9389312 | 6.5651036 |
| C | -3.1365101 | 6.8679842 | 6.5436685 |
| O | -3.7161337 | 3.6531400 | 0.2126338 |
| H | -5.8415176 | 7.4229232 | 1.5967909 |
| H | -6.0016476 | 7.6380969 | 4.0136210 |
| H | -2.7496220 | 4.8651714 | 4.4706229 |
| H | -2.5800755 | 4.6588065 | 2.0437987 |
| H | -2.6761523 | 0.4755537 | -5.9643306 |
| H | -2.5821257 | 0.2151503 | -8.3820222 |
| H | -5.8681720 | 2.9547283 | -8.7985333 |
| H | -5.9696155 | 3.2067125 | -6.3702907 |
| H | -3.9079839 | 7.1190399 | -1.5032030 |
| H | -5.5480452 | 7.1624140 | -0.8190556 |
| H | -4.1996144 | 7.9837976 | 0.0096786 |
| H | -4.2917587 | -0.0815104 | -4.3547687 |
| H | -2.9709809 | 0.7492298 | -3.4934045 |
| H | -4.6280887 | 0.7835545 | -2.8508026 |
| H | -3.2541281 | 2.7730367 | -2.2410932 |
| H | -5.1940378 | 5.1491745 | -2.1367728 |
| H | -3.0759944 | 0.4530449 | -11.9133519 |
| H | -2.0695190 | 0.8533786 | -10.5144260 |

| | | | |
|---|---|---|---|
| H | -3.2020891 | -0.5152288 | -10.4382767 |
| H | -3.9043145 | 2.7759760 | -12.0464937 |
| H | -4.7095391 | 3.5556515 | -10.6742510 |
| H | -2.9648112 | 3.2534073 | -10.6156385 |
| H | -5.5220369 | 0.8185944 | -11.9286594 |
| H | -5.7299568 | -0.0863853 | -10.4133602 |
| H | -6.3570568 | 1.5650307 | -10.5557789 |
| H | -4.8166397 | 4.9844981 | 7.6589379 |
| H | -5.7128376 | 4.5474571 | 6.1878173 |
| H | -3.9733207 | 4.2293501 | 6.2958490 |
| H | -3.1784255 | 6.9268037 | 7.6373440 |
| H | -2.3072038 | 6.2067517 | 6.2729674 |
| H | -2.9159901 | 7.8667234 | 6.1520662 |
| H | -5.6192018 | 7.3180976 | 7.5536523 |
| H | -5.4404458 | 8.3173641 | 6.1048037 |
| H | -6.5854652 | 6.9570820 | 6.1162260 |
| H | -3.4654290 | 5.2665294 | -2.4184568 |
| H | -4.9775596 | 2.6515702 | -1.9398839 |

Table 11: Cartesian coordinates and total energy in a.u. of complex **3g@1**

E(RI-TPSS-D3/def2-TZVP)=-2866.339344806

| | | | |
|---|---|---|---|
| C | -4.7930534 | 1.2078977 | 0.2908928 |
| C | -4.0812937 | 0.0569663 | 0.6441037 |
| C | -4.7715839 | -1.1512403 | 0.8038085 |
| C | -6.1506924 | -1.2015047 | 0.6133527 |
| C | -6.8538748 | -0.0517840 | 0.2585902 |

| | | | |
|---|---|---|---|
| C | -6.1788935 | 1.1652585 | 0.1042040 |
| C | -2.5846408 | 0.0307986 | 0.8018295 |
| O | -1.9681049 | -1.0378446 | 0.8238407 |
| C | -6.9982268 | 2.3714504 | -0.2586154 |
| O | -8.1545998 | 2.2600701 | -0.6787882 |
| N | -1.9571340 | 1.2417326 | 0.9039762 |
| C | -0.5128995 | 1.3516843 | 0.7559196 |
| C | -0.1028570 | 1.7218929 | -0.6609090 |
| C | -0.8667971 | 1.3267927 | -1.7635354 |
| C | -0.4877353 | 1.6823453 | -3.0559345 |
| C | 0.6657425 | 2.4404873 | -3.2799410 |
| C | 1.4475390 | 2.8145738 | -2.1798332 |
| C | 1.0645317 | 2.4576914 | -0.8884759 |
| C | 1.0178334 | 2.9207412 | -4.6715294 |
| N | 0.4411653 | 4.2425979 | -4.9426903 |
| C | 1.0974061 | 5.3856944 | -4.5869610 |
| O | 2.2452075 | 5.3708922 | -4.1276420 |
| C | 0.3581265 | 6.6774061 | -4.7970641 |
| C | -1.0231070 | 6.7304606 | -5.0029047 |
| C | -1.6820841 | 7.9528646 | -5.1636255 |
| C | -0.9391624 | 9.1392775 | -5.1152854 |
| C | 0.4390042 | 9.0939153 | -4.9103421 |
| C | 1.0877990 | 7.8712132 | -4.7446723 |
| C | -3.1712247 | 8.0601930 | -5.3466843 |
| O | -3.7460081 | 9.1514345 | -5.2942794 |
| N | -3.8422326 | 6.8881886 | -5.5712696 |
| C | -5.3018864 | 6.8328294 | -5.5524678 |
| C | -5.8237029 | 6.3332364 | -4.2193222 |
| C | -5.4339936 | 6.9779722 | -3.0390549 |
| C | -5.8696413 | 6.5105513 | -1.8025415 |

| | | | |
|---|---|---|---|
| C | -6.7131576 | 5.3980569 | -1.7143803 |
| C | -7.1241298 | 4.7671366 | -2.8950932 |
| C | -6.6749661 | 5.2269797 | -4.1329717 |
| C | -7.1162699 | 4.8362639 | -0.3688328 |
| N | -6.4096924 | 3.5901429 | -0.0627556 |
| O | -3.0614134 | 4.0103334 | -0.0332883 |
| C | -2.3100035 | 4.6629534 | -0.7805256 |
| C | -2.5025155 | 4.6635271 | -2.2905564 |
| C | -3.5625337 | 3.6518613 | -2.6969714 |
| C | -3.5412528 | 3.3624850 | -4.1850516 |
| O | -2.8160257 | 3.9918393 | -4.9779334 |
| N | -1.2443243 | 5.3808567 | -0.3067151 |
| C | -0.3751631 | 6.1315106 | -1.2337545 |
| C | -0.8009513 | 5.2538056 | 1.0507425 |
| C | -1.6966182 | 5.2150043 | 2.1250558 |
| C | -1.2245339 | 5.0625423 | 3.4264708 |
| C | 0.1470657 | 4.9591923 | 3.6755431 |
| C | 1.0477755 | 5.0202699 | 2.6098266 |
| C | 0.5732127 | 5.1639314 | 1.3114612 |
| O | 0.6702199 | 4.8047725 | 4.9349979 |
| N | -4.3521729 | 2.3430427 | -4.5994807 |
| C | -4.3275310 | 1.8913523 | -5.9612851 |
| C | -4.4951771 | 2.7820681 | -7.0229407 |
| C | -4.4798960 | 2.3179752 | -8.3352594 |
| C | -4.3059894 | 0.9546313 | -8.5967417 |
| C | -4.1442436 | 0.0581805 | -7.5373753 |
| C | -4.1488362 | 0.5300047 | -6.2294494 |
| O | -4.2866536 | 0.4355339 | -9.8669868 |
| C | -5.1854751 | 1.5906288 | -3.6419856 |
| H | 1.0101783 | 10.0173929 | -4.8754388 |

| | | | |
|---|---|---|---|
| H | 2.1576998 | 7.8145322 | -4.5700015 |
| H | -1.5956138 | 5.8095671 | -4.9894990 |
| H | -1.4655293 | 10.0812993 | -5.2335196 |
| H | -3.3576596 | 5.9982924 | -5.4830265 |
| H | -0.5410742 | 4.2708176 | -5.1975011 |
| H | 0.6335344 | 2.2308820 | -5.4285901 |
| H | 2.0998281 | 3.0124850 | -4.7894014 |
| H | -5.6515360 | 7.8505368 | -5.7495898 |
| H | -5.6486436 | 6.1840981 | -6.3639428 |
| H | -1.1010704 | 1.3769696 | -3.9016504 |
| H | -1.7646995 | 0.7357364 | -1.6092710 |
| H | 1.6769641 | 2.7582389 | -0.0417696 |
| H | 2.3424099 | 3.4077752 | -2.3458098 |
| H | -4.7854930 | 7.8485487 | -3.0972329 |
| H | -5.5486499 | 7.0127622 | -0.8922822 |
| H | -7.7828278 | 3.9044337 | -2.8321461 |
| H | -6.9861050 | 4.7166955 | -5.0423710 |
| H | -0.1357905 | 2.1015493 | 1.4588897 |
| H | -0.0949577 | 0.3776670 | 1.0298385 |
| H | -8.1822467 | 4.5966064 | -0.3487759 |
| H | -6.9000829 | 5.5584661 | 0.4248976 |
| H | -2.4830112 | 2.1052423 | 0.7984521 |
| H | -5.4236765 | 3.6537448 | 0.1696793 |
| H | -4.2573851 | 2.1361401 | 0.1167224 |
| H | -6.6805459 | -2.1415210 | 0.7399292 |
| H | -7.9270952 | -0.0691337 | 0.0970554 |
| H | -4.2012143 | -2.0368849 | 1.0658662 |
| H | -1.5495182 | 4.4184379 | -2.7720777 |
| H | -4.5591076 | 4.0034417 | -2.4106718 |
| H | 1.2845345 | 5.1907572 | 0.4933003 |

| | | | |
|---|---|---|---|
| H | 2.1122458 | 4.9469560 | 2.8080061 |
| H | -1.9323790 | 5.0308083 | 4.2522872 |
| H | -2.7601004 | 5.2969270 | 1.9468219 |
| H | -4.0073409 | -0.1689986 | -5.4100226 |
| H | -4.0071252 | -0.9968872 | -7.7507502 |
| H | -4.6096868 | 3.0191193 | -9.1572210 |
| H | -4.6308975 | 3.8381491 | -6.8240376 |
| H | -0.9767145 | 6.6189304 | -2.0002632 |
| H | 0.1442584 | 6.9026764 | -0.6643385 |
| H | 0.3604142 | 5.4806786 | -1.7191127 |
| H | -5.9192533 | 1.0191794 | -4.2098445 |
| H | -4.5895710 | 0.9039259 | -3.0301009 |
| H | -5.7187840 | 2.2792904 | -2.9843157 |
| H | -3.4028307 | 2.7186511 | -2.1472448 |
| H | -2.7789010 | 5.6658130 | -2.6377628 |
| H | -0.0552685 | 4.7724650 | 5.5792179 |
| H | -4.4016604 | 1.1559823 | -10.5074296 |

Table 12: Cartesian coordinates and total energy in a.u. of complex **3h@1**

E(RI-TPSS-D3/def2-TZVP)=-2826.590231228

| | | | |
|---|---|---|---|
| C | -4.8171303 | 1.2018557 | 0.3166197 |
| C | -4.4609504 | -0.1248038 | 0.0561727 |
| C | -5.4155093 | -1.1353957 | 0.2223765 |
| C | -6.6989772 | -0.8178666 | 0.6639065 |
| C | -7.0441111 | 0.5052079 | 0.9328374 |
| C | -6.1015504 | 1.5266650 | 0.7625249 |

| | | | |
|---|---|---|---|
| C | -3.0852646 | -0.5254773 | -0.3954318 |
| O | -2.8684789 | -1.6332117 | -0.8995249 |
| C | -6.5416038 | 2.9432122 | 1.0163108 |
| O | -7.7384370 | 3.2320023 | 1.1093739 |
| N | -2.0884437 | 0.3836884 | -0.1798505 |
| C | -0.7011138 | 0.1036703 | -0.5611348 |
| C | -0.3627514 | 0.6439049 | -1.9337857 |
| C | -0.8035040 | -0.0218890 | -3.0839257 |
| C | -0.5643066 | 0.5185878 | -4.3465639 |
| C | 0.1262420 | 1.7250671 | -4.4927925 |
| C | 0.5914430 | 2.3743359 | -3.3436366 |
| C | 0.3458038 | 1.8410113 | -2.0807394 |
| C | 0.3614389 | 2.3324781 | -5.8639785 |
| N | 0.0429619 | 3.7560340 | -5.8808009 |
| C | 1.0150632 | 4.7062757 | -5.7445451 |
| O | 2.2194738 | 4.4397293 | -5.8044718 |
| C | 0.5422983 | 6.1150875 | -5.5081537 |
| C | -0.7610921 | 6.4186779 | -5.1043895 |
| C | -1.1487682 | 7.7398933 | -4.8621362 |
| C | -0.2084854 | 8.7670880 | -5.0069594 |
| C | 1.0933571 | 8.4708411 | -5.4071509 |
| C | 1.4709686 | 7.1526223 | -5.6556663 |
| C | -2.5414454 | 8.1165484 | -4.4437536 |
| O | -2.7905806 | 9.2245721 | -3.9554735 |
| N | -3.5150517 | 7.1837592 | -4.6645030 |
| C | -4.9094724 | 7.4305234 | -4.2842624 |
| C | -5.2217329 | 6.9161294 | -2.8954208 |
| C | -4.8119613 | 7.6350711 | -1.7656759 |
| C | -5.0191092 | 7.1180513 | -0.4879265 |
| C | -5.6434501 | 5.8807196 | -0.3046320 |

| | | | |
|---|---|---|---|
| C | -6.0806724 | 5.1791830 | -1.4333333 |
| C | -5.8696873 | 5.6905019 | -2.7117305 |
| C | -5.8395230 | 5.3042476 | 1.0871088 |
| N | -5.5485788 | 3.8760545 | 1.1248350 |
| O | -2.6621142 | 3.6168461 | 0.0383647 |
| C | -2.2424914 | 4.5134871 | -0.7173442 |
| C | -2.3631215 | 4.3974151 | -2.2282406 |
| C | -3.1669774 | 3.1688313 | -2.6250408 |
| C | -3.3041638 | 3.0581151 | -4.1343488 |
| O | -2.8725540 | 3.9448928 | -4.8951163 |
| N | -1.6748481 | 5.6639298 | -0.2422896 |
| C | -1.1805100 | 6.6965696 | -1.1721282 |
| C | -1.7117288 | 5.9935432 | 1.1536917 |
| C | -1.4306554 | 5.0500475 | 2.1488529 |
| C | -1.5039106 | 5.3994530 | 3.4917419 |
| C | -1.8483041 | 6.7028856 | 3.8875724 |
| C | -2.1020292 | 7.6511935 | 2.8839539 |
| C | -2.0370644 | 7.2987163 | 1.5407079 |
| N | -1.9975257 | 7.0278034 | 5.2367671 |
| N | -3.9046429 | 1.9218438 | -4.6026459 |
| C | -3.8994809 | 1.5973832 | -6.0004780 |
| C | -4.2012240 | 2.5464829 | -6.9836565 |
| C | -4.1665222 | 2.2018468 | -8.3293227 |
| C | -3.8408339 | 0.8975458 | -8.7385486 |
| C | -3.5623423 | -0.0554045 | -7.7458798 |
| C | -3.5885284 | 0.2927043 | -6.4001340 |
| N | -3.7328894 | 0.5761533 | -10.0925889 |
| C | -4.4127239 | 0.9004594 | -3.6676103 |
| H | 1.8177158 | 9.2719781 | -5.5251851 |
| H | 2.4824382 | 6.8983052 | -5.9571179 |

| | | | |
|---|---|---|---|
| H | -1.4694711 | 5.6140314 | -4.9342227 |
| H | -0.5218926 | 9.7860321 | -4.8019151 |
| H | -3.2694368 | 6.2448758 | -4.9634929 |
| H | -0.9348732 | 3.9935141 | -5.7349332 |
| H | -0.2516445 | 1.8198362 | -6.6122628 |
| H | 1.4138183 | 2.2450243 | -6.1514364 |
| H | -5.0617901 | 8.5111065 | -4.3405774 |
| H | -5.5504732 | 6.9428461 | -5.0252260 |
| H | -0.9239516 | 0.0022245 | -5.2331860 |
| H | -1.3477454 | -0.9567124 | -2.9756903 |
| H | 0.7050767 | 2.3636693 | -1.1960236 |
| H | 1.1498570 | 3.3014932 | -3.4418599 |
| H | -4.3135298 | 8.5914100 | -1.9017621 |
| H | -4.6842993 | 7.6770875 | 0.3822434 |
| H | -6.5904429 | 4.2276351 | -1.3093349 |
| H | -6.2064546 | 5.1261689 | -3.5795957 |
| H | -0.0478299 | 0.5496896 | 0.1954310 |
| H | -0.5846320 | -0.9825104 | -0.5332744 |
| H | -6.8786685 | 5.4210375 | 1.4107506 |
| H | -5.1892556 | 5.8207164 | 1.8008682 |
| H | -2.3095003 | 1.3260549 | 0.1273668 |
| H | -4.5798863 | 3.6175431 | 0.9564303 |
| H | -4.0997147 | 1.9941112 | 0.1274202 |
| H | -7.4341896 | -1.6063636 | 0.7988414 |
| H | -8.0409988 | 0.7758864 | 1.2668332 |
| H | -5.1273187 | -2.1587682 | 0.0026372 |
| H | -1.3659383 | 4.3469479 | -2.6793999 |
| H | -4.1591909 | 3.2146519 | -2.1631537 |
| H | -2.2514624 | 8.0520297 | 0.7895135 |
| H | -2.3638192 | 8.6709309 | 3.1564227 |

| | | | |
|---|---|---|---|
| H | -1.2888901 | 4.6480802 | 4.2481365 |
| H | -1.1603021 | 4.0395493 | 1.8727719 |
| H | -3.3570736 | -0.4636973 | -5.6567148 |
| H | -3.3122406 | -1.0750262 | -8.0293435 |
| H | -4.3975818 | 2.9568817 | -9.0772656 |
| H | -4.4576357 | 3.5575751 | -6.6957822 |
| H | -0.6516094 | 6.2315604 | -2.0045304 |
| H | -1.9945485 | 7.3117612 | -1.5701875 |
| H | -0.4785383 | 7.3318671 | -0.6312949 |
| H | -5.1088828 | 0.2608113 | -4.2103638 |
| H | -3.6056198 | 0.2876986 | -3.2527798 |
| H | -4.9511578 | 1.3754123 | -2.8464627 |
| H | -2.6894511 | 2.2617651 | -2.2392557 |
| H | -2.8366285 | 5.3024427 | -2.6235703 |
| H | -1.4920747 | 6.4377449 | 5.8864486 |
| H | -1.9035379 | 8.0105471 | 5.4626648 |
| H | -3.8373259 | -0.4055972 | -10.3182790 |
| H | -4.2555596 | 1.1697877 | -10.7251607 |

Table 13: Cartesian coordinates and total energy in a.u. of complex **3a′@1**

E(RI-TPSS-D3/def2-TZVP)=-3125.071518298

| | | | |
|---|---|---|---|
| C | -4.7570835 | 0.5814623 | -0.1830660 |
| C | -4.0682767 | 0.0474997 | 0.9121861 |
| C | -4.7163917 | -0.8409981 | 1.7703916 |
| C | -6.0362304 | -1.1769772 | 1.5053455 |
| C | -6.7447067 | -0.6628257 | 0.4220065 |

| | | | |
|---|---|---|---|
| C | -6.0871520 | 0.2300723 | -0.4195275 |
| N | -2.7206150 | 0.4369019 | 1.1714494 |
| C | -2.3862734 | 1.8739570 | 1.1043474 |
| H | -7.7741673 | -0.9583962 | 0.2605654 |
| C | -1.7589969 | -0.5100920 | 1.4333154 |
| O | -2.0177047 | -1.7237298 | 1.4428478 |
| C | -0.3680107 | 0.0331504 | 1.6825322 |
| C | 0.6582944 | -1.0737004 | 1.8612190 |
| C | 2.0647881 | -0.4974967 | 1.8625859 |
| N | 3.0970573 | -1.4106665 | 1.8692423 |
| C | 4.4421339 | -0.9981622 | 1.6404080 |
| C | 4.9528097 | 0.1711561 | 2.2146822 |
| C | 6.2643979 | 0.5303366 | 1.9314658 |
| C | 7.1041495 | -0.2243983 | 1.1177112 |
| C | 6.5901653 | -1.3979921 | 0.5742088 |
| C | 5.2738513 | -1.7828469 | 0.8270703 |
| H | 8.1184065 | 0.1058972 | 0.9310568 |
| O | 2.2622222 | 0.7252897 | 1.8235867 |
| C | 2.8204345 | -2.8608046 | 1.8865125 |
| N | 2.7734236 | 2.0583046 | -0.9156083 |
| C | 3.2945309 | 0.9530122 | -1.7071221 |
| C | 2.3406519 | -0.2298385 | -1.7478111 |
| C | 2.8326576 | -1.5379290 | -1.7993746 |
| C | 1.9677537 | -2.6303486 | -1.8322118 |
| C | 0.5805350 | -2.4369045 | -1.8074850 |
| C | 0.0875359 | -1.1286362 | -1.7775922 |
| C | 0.9551344 | -0.0389226 | -1.7510083 |
| C | -0.3582597 | -3.6228517 | -1.7370297 |
| N | -0.5104403 | -4.1093069 | -0.3609656 |
| C | 0.3611688 | -5.0181737 | 0.1662097 |

| | | | |
|---|---|---|---|
| O | 1.2512997 | -5.5437498 | -0.5123437 |
| C | 0.1847180 | -5.3584468 | 1.6178520 |
| C | -0.5344482 | -4.5495524 | 2.5030721 |
| C | -0.6344695 | -4.8801821 | 3.8580287 |
| C | -0.0030035 | -6.0389061 | 4.3266873 |
| C | 0.7106834 | -6.8523510 | 3.4484028 |
| C | 0.8135986 | -6.5125293 | 2.1008289 |
| C | -1.3455440 | -4.0144160 | 4.8618433 |
| O | -1.1733814 | -4.1702402 | 6.0739225 |
| N | -2.1741212 | -3.0542891 | 4.3542986 |
| C | -2.7729078 | -2.0289948 | 5.2054945 |
| C | -1.9834433 | -0.7339866 | 5.1569545 |
| C | -2.5912815 | 0.4851607 | 4.8408792 |
| C | -1.8491029 | 1.6665572 | 4.8050604 |
| C | -0.4747623 | 1.6484360 | 5.0733257 |
| C | 0.1330725 | 0.4279395 | 5.3901862 |
| C | -0.6106093 | -0.7478808 | 5.4358296 |
| C | 0.3430956 | 2.9189299 | 4.9753896 |
| N | 0.6132187 | 3.3016462 | 3.5862081 |
| C | -0.1710221 | 4.2048378 | 2.9269143 |
| O | -1.1450952 | 4.7448608 | 3.4618424 |
| C | 0.2242057 | 4.5248551 | 1.5137390 |
| C | 1.0037361 | 3.6684691 | 0.7287165 |
| C | 1.3321119 | 4.0059608 | -0.5887907 |
| C | 0.8717553 | 5.2181191 | -1.1186445 |
| C | 0.0956042 | 6.0747911 | -0.3409813 |
| C | -0.2377971 | 5.7281576 | 0.9669706 |
| C | 2.1002688 | 3.0927902 | -1.5054256 |
| O | 2.0995174 | 3.2702243 | -2.7262122 |
| H | 1.1941431 | -7.7524334 | 3.8174279 |

| | | | |
|---|---|---|---|
| H | -0.0794559 | -6.2735517 | 5.3836707 |
| H | -0.9747894 | -3.6251617 | 2.1424606 |
| H | 1.3797819 | -7.1218580 | 1.4032179 |
| H | -1.1640334 | -3.6166257 | 0.2379185 |
| H | -2.2179074 | -2.9002440 | 3.3527715 |
| H | -3.8101845 | -1.8685848 | 4.8963185 |
| H | -2.7757934 | -2.4364633 | 6.2207930 |
| H | 0.0253171 | -4.4566595 | -2.3295538 |
| H | -1.3517837 | -3.3518217 | -2.1053884 |
| H | -3.6582951 | 0.5135516 | 4.6301347 |
| H | -2.3277888 | 2.6121296 | 4.5631359 |
| H | 1.1983608 | 0.4012387 | 5.6108403 |
| H | -0.1317724 | -1.6866440 | 5.7026284 |
| H | 2.3577043 | -3.6442408 | -1.8560506 |
| H | 3.9078834 | -1.7012651 | -1.8131657 |
| H | 0.5532751 | 0.9700937 | -1.7363774 |
| H | -0.9880638 | -0.9617435 | -1.7686638 |
| H | 1.3035373 | 2.7949926 | 5.4843576 |
| H | -0.1912881 | 3.7574105 | 5.4288045 |
| H | 3.4607997 | 1.3421007 | -2.7168029 |
| H | 4.2590820 | 0.6387604 | -1.2944196 |
| H | 1.3731680 | 2.8381279 | 3.1027741 |
| H | 2.6840708 | 1.8904481 | 0.0818952 |
| H | 1.3115079 | 2.7079121 | 1.1323157 |
| H | -0.2553909 | 7.0147166 | -0.7572554 |
| H | 1.1255360 | 5.4578309 | -2.1463894 |
| H | -0.8550143 | 6.3724431 | 1.5853159 |
| H | 0.4706596 | -1.6153115 | 2.7956331 |
| H | -0.0743673 | 0.6751688 | 0.8456210 |
| H | 4.8888923 | -2.6902557 | 0.3750236 |

| | | | |
|---|---|---|---|
| H | 7.2140320 | -2.0171137 | -0.0628359 |
| N | 6.7917512 | 1.7790425 | 2.5429035 |
| H | 4.3585553 | 0.7924883 | 2.8662916 |
| H | -4.2508126 | 1.2677806 | -0.8551716 |
| H | -6.6092415 | 0.6511383 | -1.2728338 |
| N | -6.7184091 | -2.1089565 | 2.4389511 |
| H | -4.2158514 | -1.2571303 | 2.6310943 |
| H | 1.9868164 | -3.0715056 | 2.5551567 |
| H | 2.5823123 | -3.2422706 | 0.8884611 |
| H | 3.7018360 | -3.3741850 | 2.2728324 |
| H | -3.3151017 | 2.4428215 | 1.1109510 |
| H | -1.8080603 | 2.1626433 | 1.9834387 |
| H | -1.8173002 | 2.1189879 | 0.2014949 |
| H | -0.3895325 | 0.6784523 | 2.5680008 |
| H | 0.5714527 | -1.8068795 | 1.0514209 |
| O | 7.9647313 | 2.0758284 | 2.3049165 |
| O | 6.0251343 | 2.4401460 | 3.2487462 |
| O | -7.8803467 | -2.4264868 | 2.1789315 |
| O | -6.0799197 | -2.5044293 | 3.4197368 |

Table 14: Cartesian coordinates and total energy in a.u. of complex **3g′@1**

E(RI-TPSS-D3/def2-TZVP)=-2866.341199704

| | | | |
|---|---|---|---|
| C | -5.0393184 | 0.8204586 | 0.2009420 |
| C | -4.2119772 | -0.1896238 | 0.7065139 |
| C | -4.6811929 | -1.5060494 | 0.7404036 |
| C | -5.9527545 | -1.8271938 | 0.2564955 |

| | | | |
|---|---|---|---|
| C | -6.7671844 | -0.8087841 | -0.2537791 |
| C | -6.3090480 | 0.5070274 | -0.2811005 |
| C | -2.8492339 | 0.2004461 | 1.2025566 |
| O | -2.5711966 | 1.3753939 | 1.4669842 |
| C | -6.5151445 | -3.2213050 | 0.3047554 |
| O | -7.7227869 | -3.4281941 | 0.1516832 |
| N | -1.9340951 | -0.8072251 | 1.3133940 |
| C | -0.5772964 | -0.5581358 | 1.8085279 |
| C | -0.4686957 | -0.7793682 | 3.3019564 |
| C | -0.9921330 | 0.1641779 | 4.1949439 |
| C | -0.9683383 | -0.0759950 | 5.5677873 |
| C | -0.4128109 | -1.2512500 | 6.0817858 |
| C | 0.1332696 | -2.1812275 | 5.1898629 |
| C | 0.1003045 | -1.9487335 | 3.8169310 |
| C | -0.4006968 | -1.5229003 | 7.5751127 |
| N | -0.8431668 | -2.8787421 | 7.8809061 |
| C | 0.0505251 | -3.8889359 | 8.1004857 |
| O | 1.2594763 | -3.6861978 | 8.2493010 |
| C | -0.5159051 | -5.2814652 | 8.1475938 |
| C | -1.7926317 | -5.5965937 | 7.6735151 |
| C | -2.2657766 | -6.9116149 | 7.7057310 |
| C | -1.4376177 | -7.9263759 | 8.2004833 |
| C | -0.1628625 | -7.6189735 | 8.6729825 |
| C | 0.2994912 | -6.3045879 | 8.6467445 |
| C | -3.6326857 | -7.2955284 | 7.2164255 |
| O | -3.9164573 | -8.4690627 | 6.9518208 |
| N | -4.5442409 | -6.2841494 | 7.1099819 |
| C | -5.9019412 | -6.5268020 | 6.6137530 |
| C | -6.0063981 | -6.3102051 | 5.1192844 |
| C | -5.4938269 | -7.2636574 | 4.2304987 |

| | | | |
|---|---|---|---|
| C | -5.5126716 | -7.0283788 | 2.8567996 |
| C | -6.0518173 | -5.8478309 | 2.3374588 |
| C | -6.5873214 | -4.9078068 | 3.2251273 |
| C | -6.5597057 | -5.1357054 | 4.5990112 |
| C | -6.0587090 | -5.5833977 | 0.8426079 |
| N | -5.6192386 | -4.2281504 | 0.5309382 |
| O | -2.8035957 | -3.9903461 | 1.8204256 |
| C | -2.5597675 | -4.6947069 | 2.8146249 |
| N | -2.0204347 | -5.9520869 | 2.7109854 |
| C | -1.7625260 | -6.7634091 | 3.9169973 |
| C | -2.8734190 | -4.2188452 | 4.2227368 |
| C | -3.5868397 | -2.8760948 | 4.2049510 |
| C | -3.9087500 | -2.4021428 | 5.6113809 |
| O | -3.6626591 | -3.1022864 | 6.6081279 |
| N | -4.4610124 | -1.1502981 | 5.7103367 |
| C | -4.7182842 | -0.3423609 | 4.5018095 |
| C | -4.6486293 | -0.5181585 | 6.9823062 |
| C | -4.2712859 | 0.8231858 | 7.1366323 |
| C | -4.4539306 | 1.4475424 | 8.3676203 |
| C | -4.9999302 | 0.7566720 | 9.4472671 |
| C | -5.3794319 | -0.5784375 | 9.2779306 |
| C | -5.2115974 | -1.2183021 | 8.0492323 |
| O | -5.9375770 | -1.3260630 | 10.2853163 |
| C | -1.8520490 | -6.5884288 | 1.4385715 |
| C | -1.3081512 | -5.8925116 | 0.3587265 |
| C | -1.1606614 | -6.5376348 | -0.8698320 |
| C | -1.5411539 | -7.8738595 | -1.0272735 |
| C | -2.0667228 | -8.5607642 | 0.0649402 |
| C | -2.2289285 | -7.9314756 | 1.2962467 |
| O | -0.6210524 | -5.7932858 | -1.8897380 |

| | | | |
|---|---|---|---|
| H | -5.1339128 | 1.2487833 | 10.4081257 |
| H | -1.4232346 | -8.3698740 | -1.9882204 |
| H | 0.4737455 | -8.4081576 | 9.0629664 |
| H | 1.2929438 | -6.0442963 | 8.9985151 |
| H | -2.4084157 | -4.8188639 | 7.2327294 |
| H | -1.8148327 | -8.9442934 | 8.2044894 |
| H | -4.2562790 | -5.3191829 | 7.2343956 |
| H | -1.8166544 | -3.0870768 | 7.6768205 |
| H | -1.0504175 | -0.8094383 | 8.0922127 |
| H | 0.6133048 | -1.4284070 | 7.9765668 |
| H | -6.1494714 | -7.5586119 | 6.8741821 |
| H | -6.5807451 | -5.8541329 | 7.1468332 |
| H | -1.3911866 | 0.6554946 | 6.2523820 |
| H | -1.4287968 | 1.0776627 | 3.7995167 |
| H | 0.5205505 | -2.6858766 | 3.1351940 |
| H | 0.5891946 | -3.0887756 | 5.5764835 |
| H | -5.0689155 | -8.1808785 | 4.6299445 |
| H | -5.0983300 | -7.7678731 | 2.1756281 |
| H | -7.0310850 | -3.9958599 | 2.8348485 |
| H | -6.9717035 | -4.3906624 | 5.2772231 |
| H | 0.1051107 | -1.2244924 | 1.2720827 |
| H | -0.3369023 | 0.4761897 | 1.5513569 |
| H | -7.0709546 | -5.6832414 | 0.4378802 |
| H | -5.4050993 | -6.2978974 | 0.3318557 |
| H | -2.2178912 | -1.7735063 | 1.1895310 |
| H | -4.6467263 | -4.0160565 | 0.7353225 |
| H | -4.0668225 | -2.2798939 | 1.1900213 |
| H | -6.9448766 | 1.2925859 | -0.6795770 |
| H | -7.7566980 | -1.0737799 | -0.6130526 |
| H | -4.6653142 | 1.8395585 | 0.1958136 |

| | | | |
|---|---|---|---|
| H | -1.9460036 | -4.1371567 | 4.8007254 |
| H | -4.5112082 | -2.9563316 | 3.6220417 |
| H | -2.6525753 | -8.4754681 | 2.1328437 |
| H | -2.3620754 | -9.5998496 | -0.0477414 |
| H | -1.0019289 | -4.8598932 | 0.4535859 |
| H | -3.8322474 | 1.3693344 | 6.3092688 |
| H | -4.1588196 | 2.4855692 | 8.4902447 |
| H | -5.5168447 | -2.2503896 | 7.9439727 |
| H | -1.3043792 | -6.1476686 | 4.6915346 |
| H | -2.6807116 | -7.2078001 | 4.3142374 |
| H | -1.0625671 | -7.5549740 | 3.6503772 |
| H | -5.3998097 | 0.4639479 | 4.7714189 |
| H | -3.7968531 | 0.0824891 | 4.0912875 |
| H | -5.1973475 | -0.9544899 | 3.7365597 |
| H | -2.9686300 | -2.1240551 | 3.7021670 |
| H | -3.4896517 | -4.9694046 | 4.7300033 |
| H | -0.5556935 | -6.3464725 | -2.6847962 |
| H | -6.0152782 | -0.7762314 | 11.0815921 |

## 0.3 Gas phase results on the structures with the C=C axle

Table 15: Cartesian coordinates and total energy in a.u. of complex **2a@1**

E(RI-TPSS-D3/def2-TZVP)=-3123.834770161

| | | | |
|---|---|---|---|
| C | -5.1227283 | -1.1830483 | 0.4686801 |
| C | -4.2667596 | -0.4025756 | -0.3208438 |
| C | -4.7702363 | 0.7108669 | -1.0079034 |

| | | | |
|---|---|---|---|
| C | -6.1156103 | 1.0373855 | -0.9127898 |
| C | -6.9488278 | 0.2456090 | -0.1252714 |
| C | -6.4712821 | -0.8621956 | 0.5681030 |
| N | -2.8940781 | -0.7660450 | -0.4423681 |
| C | -1.9100978 | 0.1858325 | -0.2889497 |
| C | -0.5155016 | -0.2931380 | -0.4372182 |
| C | 0.4941898 | 0.3862512 | 0.1183340 |
| C | 1.8843895 | -0.1247594 | 0.0257348 |
| O | 2.1192469 | -1.3125280 | -0.2561815 |
| N | -8.3841173 | 0.5907820 | -0.0259262 |
| O | -9.0987157 | -0.1353812 | 0.6713420 |
| O | -2.1702414 | 1.3708362 | -0.0179345 |
| N | 2.8814948 | 0.7809850 | 0.3193981 |
| C | 4.2280101 | 0.3637695 | 0.5185742 |
| C | 4.8364138 | -0.5941935 | -0.3075199 |
| C | 6.1573195 | -0.9628847 | -0.0845863 |
| C | 6.8623391 | -0.3730176 | 0.9607986 |
| C | 6.2817389 | 0.5837051 | 1.7885317 |
| C | 4.9621209 | 0.9509051 | 1.5624317 |
| N | 8.2692930 | -0.7648631 | 1.1926377 |
| O | 8.7544752 | -1.6191484 | 0.4451729 |
| O | 8.8703215 | -0.2115336 | 2.1186275 |
| O | -8.7759903 | 1.5829201 | -0.6470947 |
| N | 0.8694179 | -3.1873364 | -2.6567444 |
| C | 0.9633231 | -2.4605087 | -3.9257657 |
| C | 0.1537836 | -1.1813297 | -3.9131112 |
| C | 0.7782192 | 0.0665859 | -3.8170630 |
| C | 0.0270609 | 1.2371715 | -3.7664399 |
| C | -1.3714857 | 1.1862805 | -3.8027627 |
| C | -1.9967117 | -0.0607963 | -3.8943119 |

| | | | |
|---|---|---|---|
| C | -1.2447101 | -1.2340884 | -3.9571147 |
| C | -2.1739618 | 2.4710826 | -3.7383398 |
| N | -1.7979878 | 3.2838713 | -2.5844755 |
| C | -0.9511436 | 4.3523110 | -2.7149021 |
| O | -0.6275576 | 4.8098792 | -3.8133778 |
| C | -0.0229006 | -4.2081264 | -2.4802018 |
| O | -0.7855095 | -4.5787457 | -3.3784406 |
| C | -0.0137576 | -4.8720991 | -1.1336172 |
| C | -0.5835467 | -6.1466036 | -1.0276319 |
| C | -0.5982367 | -6.8053477 | 0.2006546 |
| C | -0.0599532 | -6.1959219 | 1.3322922 |
| C | 0.5069913 | -4.9186205 | 1.2413190 |
| C | 0.5203522 | -4.2633298 | 0.0064898 |
| C | 1.0263860 | -4.2873590 | 2.5031519 |
| N | 1.8670676 | -3.2202327 | 2.3432715 |
| C | 2.2451349 | -2.3734351 | 3.4686595 |
| C | 1.3938573 | -1.1191626 | 3.5495793 |
| C | 0.0064458 | -1.1913605 | 3.3806686 |
| C | -0.7759496 | -0.0418550 | 3.4510296 |
| C | -0.1951573 | 1.2064121 | 3.6972030 |
| C | 1.1911052 | 1.2788249 | 3.8835488 |
| C | 1.9736672 | 0.1273845 | 3.8035166 |
| C | -1.0348722 | 2.4662482 | 3.7111061 |
| N | -0.9257945 | 3.2153066 | 2.4543405 |
| C | 0.0145687 | 4.1906339 | 2.2864835 |
| O | 0.7972040 | 4.5125684 | 3.1876760 |
| O | 0.7003447 | -4.7153267 | 3.6131069 |
| C | -0.4280674 | 4.9481385 | -1.4374968 |
| C | -0.5002649 | 4.2919457 | -0.2046589 |
| C | 0.0449920 | 4.8680241 | 0.9468469 |

| | | | |
|---|---|---|---|
| C | 0.6787649 | 6.1132981 | 0.8570471 |
| C | 0.7464867 | 6.7760416 | -0.3670750 |
| C | 0.2011769 | 6.1971641 | -1.5112915 |
| H | -1.0333677 | -7.7977479 | 0.2760283 |
| H | -1.0073422 | -6.5984482 | -1.9190838 |
| H | 0.9060031 | -3.2496248 | -0.0586399 |
| H | -0.0747047 | -6.6844922 | 2.3016027 |
| H | 2.0444212 | -2.8492950 | 1.4157520 |
| H | 1.4398758 | -2.8620616 | -1.8839100 |
| H | 2.0186529 | -2.2423784 | -4.1161977 |
| H | 0.5987063 | -3.1407171 | -4.6998821 |
| H | 2.1179397 | -2.9821704 | 4.3693154 |
| H | 3.3031155 | -2.1064270 | 3.3775813 |
| H | 1.8647194 | 0.1217185 | -3.7883009 |
| H | 0.5240878 | 2.2020133 | -3.7053082 |
| H | -3.0831413 | -0.1161317 | -3.9274373 |
| H | -1.7347768 | -2.2007205 | -4.0434312 |
| H | -0.4608034 | -2.1552534 | 3.1991061 |
| H | -1.8533835 | -0.1132729 | 3.3135531 |
| H | 1.6456566 | 2.2457537 | 4.0831236 |
| H | 3.0502369 | 0.1951486 | 3.9459274 |
| H | -3.2462936 | 2.2506632 | -3.6981694 |
| H | -1.9865974 | 3.0905959 | -4.6202954 |
| H | -0.7081520 | 3.1392099 | 4.5076968 |
| H | -2.0900617 | 2.2219837 | 3.8636495 |
| H | -1.9464159 | 2.8707326 | -1.6690070 |
| H | -1.5151634 | 2.9264838 | 1.6814437 |
| H | -0.9427625 | 3.3013744 | -0.1453151 |
| H | 1.2305963 | 7.7463283 | -0.4301439 |
| H | 1.1108828 | 6.5387281 | 1.7574648 |

| | | | |
|---|---|---|---|
| H | 0.2578995 | 6.6876853 | -2.4779399 |
| C | -2.5618669 | -2.1976648 | -0.6218190 |
| H | -0.3067984 | -1.1948395 | -1.0015353 |
| H | 0.2819904 | 1.2798082 | 0.6946882 |
| C | 2.5722464 | 2.2124030 | 0.5416461 |
| H | -4.7320741 | -2.0328808 | 1.0193316 |
| H | -7.1498018 | -1.4474726 | 1.1772774 |
| H | -6.5303978 | 1.8855059 | -1.4445378 |
| H | -4.1086968 | 1.3076343 | -1.6212387 |
| H | 4.4953571 | 1.6846355 | 2.2106155 |
| H | 6.8598928 | 1.0189975 | 2.5949451 |
| H | 6.6509544 | -1.6917378 | -0.7164039 |
| H | 4.2805942 | -1.0382676 | -1.1208079 |
| H | -3.4902670 | -2.7474794 | -0.7669714 |
| H | -1.9545024 | -2.3285390 | -1.5198943 |
| H | -2.0325358 | -2.6006275 | 0.2452052 |
| H | 3.4851491 | 2.7851086 | 0.3788294 |
| H | 1.8327815 | 2.5454013 | -0.1868048 |
| H | 2.2022449 | 2.3982474 | 1.5540799 |

Table 16: Cartesian coordinates and total energy in a.u. of complex **2b@1**

E(RI-TPSS-D3/def2-TZVP)=-3389.022865141

| | | | |
|---|---|---|---|
| C | -0.0001890 | 6.1290970 | -1.2404001 |
| C | -0.5576513 | 4.8487156 | -1.1350477 |
| C | -0.5637388 | 4.2060649 | 0.1066252 |
| C | -0.0319216 | 4.8308627 | 1.2391854 |

| | | | |
|---|---|---|---|
| C | 0.5284009 | 6.1082359 | 1.1185338 |
| C | 0.5362487 | 6.7541041 | -0.1165322 |
| C | -1.0749180 | 4.2024653 | -2.3905813 |
| O | -0.7646152 | 4.6323413 | -3.5045839 |
| C | -0.0136283 | 4.1828641 | 2.5938270 |
| O | 0.7400694 | 4.5798080 | 3.4884310 |
| N | -1.8938234 | 3.1204519 | -2.2214464 |
| C | -2.2665003 | 2.2667809 | -3.3421633 |
| C | -1.3948675 | 1.0266774 | -3.4356965 |
| C | -0.0171873 | 1.1016494 | -3.2024706 |
| C | 0.7785311 | -0.0381530 | -3.2854493 |
| C | 0.2200749 | -1.2796712 | -3.6061161 |
| C | -1.1554870 | -1.3538346 | -3.8588633 |
| C | -1.9505768 | -0.2120489 | -3.7697522 |
| C | 1.0682093 | -2.5337333 | -3.6157473 |
| N | 0.9566873 | -3.2774884 | -2.3558471 |
| C | 0.0029685 | -4.2380119 | -2.1789123 |
| O | -0.7769791 | -4.5659588 | -3.0804099 |
| C | -0.0435077 | -4.8933053 | -0.8283976 |
| C | 0.5148899 | -4.3101153 | 0.3128979 |
| C | 0.4333423 | -4.9442108 | 1.5564432 |
| C | -0.2224884 | -6.1778794 | 1.6522574 |
| C | -0.7839095 | -6.7628857 | 0.5187640 |
| C | -0.7036691 | -6.1230135 | -0.7168583 |
| C | 0.9795955 | -4.3401796 | 2.8206416 |
| O | 0.6729118 | -4.7883407 | 3.9283498 |
| N | 1.8283694 | -3.2771339 | 2.6671371 |
| C | 2.2327786 | -2.4587723 | 3.8073443 |
| C | 1.4139229 | -1.1859163 | 3.9017364 |
| C | 0.0157139 | -1.2548031 | 3.9019378 |

| | | | |
|---|---|---|---|
| C | -0.7488721 | -0.0936262 | 3.9679006 |
| C | -0.1382765 | 1.1622505 | 4.0456455 |
| C | 1.2601396 | 1.2325610 | 4.0603835 |
| C | 2.0251782 | 0.0689606 | 3.9795719 |
| C | -0.9627245 | 2.4317153 | 4.0588920 |
| N | -0.8878669 | 3.1487701 | 2.7828442 |
| O | 2.1805565 | -1.4122536 | 0.0968759 |
| C | 1.9007699 | -0.2341672 | 0.3836256 |
| N | 2.8614256 | 0.7440094 | 0.4940562 |
| C | 4.2299177 | 0.4380765 | 0.2248542 |
| C | 4.8481013 | -0.6690064 | 0.8204605 |
| C | 6.1865440 | -0.9323748 | 0.5637703 |
| C | 6.9187306 | -0.0965441 | -0.2860081 |
| C | 6.3068747 | 1.0055371 | -0.8789123 |
| C | 4.9634220 | 1.2702493 | -0.6265304 |
| C | 8.3678910 | -0.4098819 | -0.5406632 |
| F | 9.0996282 | -0.3835406 | 0.6086272 |
| C | 0.5014945 | 0.2110427 | 0.5759916 |
| C | -0.5039403 | -0.4568313 | -0.0005125 |
| C | -1.8903600 | 0.0665144 | 0.0762297 |
| O | -2.1133224 | 1.2522895 | 0.3822547 |
| N | -2.8897636 | -0.8120815 | -0.2747256 |
| C | -4.2119674 | -0.3574038 | -0.5573176 |
| C | -4.8977927 | -0.9263494 | -1.6389541 |
| C | -6.1821458 | -0.4995088 | -1.9618397 |
| C | -6.7937391 | 0.4969311 | -1.2031364 |
| C | -6.1208891 | 1.0528883 | -0.1121828 |
| C | -4.8389969 | 0.6306478 | 0.2166194 |
| C | -8.1693445 | 1.0023425 | -1.5403155 |
| F | -8.1404109 | 2.3020512 | -1.9519039 |

| | | | |
|---|---|---|---|
| F | -9.0000452 | 0.9628631 | -0.4612592 |
| F | -8.7626952 | 0.2877430 | -2.5287494 |
| F | 8.5280688 | -1.6562453 | -1.0670470 |
| F | 8.9473713 | 0.4634207 | -1.4013696 |
| H | -1.2895888 | -7.7208937 | 0.5991523 |
| H | -1.1458436 | -6.5545219 | -1.6094936 |
| H | 0.9768418 | -3.3299490 | 0.2367053 |
| H | -0.2861848 | -6.6517451 | 2.6267993 |
| H | 1.9603404 | -2.8673756 | 1.7471925 |
| H | 1.5333213 | -2.9722366 | -1.5794166 |
| H | 2.1229738 | -2.2839013 | -3.7620951 |
| H | 0.7496842 | -3.2107862 | -4.4118827 |
| H | 2.0890854 | -3.0798112 | 4.6963819 |
| H | 3.2986631 | -2.2202198 | 3.7229927 |
| H | 1.8473762 | 0.0345788 | -3.0928304 |
| H | 0.4328085 | 2.0590053 | -2.9561852 |
| H | -3.0189369 | -0.2814881 | -3.9621020 |
| H | -1.5937905 | -2.3160635 | -4.1101587 |
| H | -0.4706436 | -2.2255845 | 3.8524324 |
| H | -1.8348985 | -0.1623174 | 3.9611858 |
| H | 1.7400016 | 2.2054805 | 4.1328141 |
| H | 3.1114068 | 0.1379767 | 3.9829431 |
| H | -3.3183397 | 1.9796041 | -3.2399643 |
| H | -2.1605948 | 2.8771974 | -4.2446686 |
| H | -0.5988148 | 3.1228504 | 4.8235140 |
| H | -2.0136395 | 2.2025239 | 4.2607345 |
| H | -2.0626063 | 2.7499835 | -1.2917447 |
| H | -1.4440911 | 2.7958563 | 2.0114152 |
| H | -0.9414768 | 3.1902619 | 0.1831753 |
| H | 0.9647655 | 7.7485125 | -0.2033252 |

| | | | |
|---|---|---|---|
| H | 0.9508433 | 6.5719530 | 2.0044878 |
| H | 0.0088947 | 6.6072418 | -2.2149946 |
| C | -2.5991206 | -2.2454047 | -0.5015658 |
| H | -0.2881576 | -1.3325547 | -0.6024048 |
| H | 0.2853069 | 1.0971814 | 1.1613443 |
| C | 2.5023811 | 2.1622863 | 0.7160067 |
| H | -4.4236391 | -1.6908932 | -2.2442597 |
| H | -6.7021153 | -0.9376942 | -2.8065842 |
| H | -6.6070220 | 1.8139232 | 0.4902019 |
| H | -4.3266944 | 1.0595445 | 1.0654431 |
| H | 4.4849600 | 2.1189463 | -1.1046618 |
| H | 6.8724141 | 1.6504365 | -1.5421034 |
| H | 6.6687924 | -1.7861636 | 1.0294331 |
| H | 4.2813044 | -1.3122285 | 1.4804448 |
| H | -1.8682992 | -2.5919101 | 0.2290181 |
| H | -3.5215648 | -2.8056666 | -0.3465690 |
| H | -2.2255187 | -2.4333657 | -1.5125719 |
| H | 3.4217301 | 2.7218858 | 0.8820145 |
| H | 1.9676948 | 2.5855218 | -0.1387367 |
| H | 1.8899520 | 2.2543273 | 1.6145057 |

Table 17: Cartesian coordinates and total energy in a.u. of complex **2c@1**

E(RI-TPSS-D3/def2-TZVP)=-3633.846602797

| | | | |
|---|---|---|---|
| C | -5.1788402 | -0.9637269 | 0.4661218 |
| C | -4.2660855 | -0.2821163 | -0.3442614 |
| C | -4.6988953 | 0.8030762 | -1.1119673 |

| | | | |
|---|---|---|---|
| C | -6.0301649 | 1.2034752 | -1.0724518 |
| C | -6.9314815 | 0.5116669 | -0.2624006 |
| C | -6.5151638 | -0.5730522 | 0.5071546 |
| N | -2.9025087 | -0.7148368 | -0.3969144 |
| C | -1.8899400 | 0.1889802 | -0.1924287 |
| C | -0.5131509 | -0.3537667 | -0.2434966 |
| C | 0.5131957 | 0.3532202 | 0.2433406 |
| C | 1.8900338 | -0.1894244 | 0.1920806 |
| O | 2.1141205 | -1.3933901 | -0.0398762 |
| Cl | -8.6033439 | 1.0104636 | -0.2138232 |
| O | -2.1139235 | 1.3929153 | 0.0395855 |
| N | 2.9025545 | 0.7144349 | 0.3963243 |
| C | 4.2661467 | 0.2817272 | 0.3439024 |
| C | 4.6989239 | -0.8032266 | 1.1119626 |
| C | 6.0302078 | -1.2035747 | 1.0727045 |
| C | 6.9315961 | -0.5119366 | 0.2625784 |
| C | 6.5153146 | 0.5725363 | -0.5073480 |
| C | 5.1789602 | 0.9631400 | -0.4665663 |
| Cl | 8.6034723 | -1.0106895 | 0.2142969 |
| N | 1.1084336 | -3.1261783 | -2.5259248 |
| C | 1.3279998 | -2.3381162 | -3.7396558 |
| C | 0.5028471 | -1.0684485 | -3.7528410 |
| C | 1.1067951 | 0.1866997 | -3.6310421 |
| C | 0.3396651 | 1.3483638 | -3.6233390 |
| C | -1.0546188 | 1.2796821 | -3.7277424 |
| C | -1.6599401 | 0.0245393 | -3.8380645 |
| C | -0.8914832 | -1.1388737 | -3.8586994 |
| C | -1.8749346 | 2.5541107 | -3.7070882 |
| N | -1.5937350 | 3.3529701 | -2.5167555 |
| C | -0.7338238 | 4.4174806 | -2.5642493 |

| | | | |
|---|---|---|---|
| O | -0.3260041 | 4.8933937 | -3.6270010 |
| C | 0.2042858 | -4.1486445 | -2.4916022 |
| O | -0.4408431 | -4.4949825 | -3.4872161 |
| C | 0.0408142 | -4.8503389 | -1.1736083 |
| C | -0.6000214 | -6.0953072 | -1.1660131 |
| C | -0.7781903 | -6.7823367 | 0.0337818 |
| C | -0.3305560 | -6.2321560 | 1.2335268 |
| C | 0.3066174 | -4.9850973 | 1.2403318 |
| C | 0.4816032 | -4.3020226 | 0.0337341 |
| C | 0.7336223 | -4.4175564 | 2.5644271 |
| N | 1.5937541 | -3.3531844 | 2.5169330 |
| C | 1.8752497 | -2.5546273 | 3.7074288 |
| C | 1.0552600 | -1.2799874 | 3.7281953 |
| C | -0.3390850 | -1.3484402 | 3.6244390 |
| C | -1.1059981 | -0.1866293 | 3.6321311 |
| C | -0.5017505 | 1.0684331 | 3.7532855 |
| C | 0.8926389 | 1.1386263 | 3.8585501 |
| C | 1.6608697 | -0.0249326 | 3.8379041 |
| C | -1.3266973 | 2.3382350 | 3.7401698 |
| N | -1.1074666 | 3.1261941 | 2.5263008 |
| C | -0.2033434 | 4.1486454 | 2.4915627 |
| O | 0.4428579 | 4.4943875 | 3.4866927 |
| O | 0.3263581 | -4.8938929 | 3.6272087 |
| C | -0.3075507 | 4.9855344 | -1.2401435 |
| C | -0.4815179 | 4.3020633 | -0.0336125 |
| C | -0.0411279 | 4.8508193 | 1.1736975 |
| C | 0.5982033 | 6.0965490 | 1.1661711 |
| C | 0.7752613 | 6.7839671 | -0.0335735 |
| C | 0.3280820 | 6.2333834 | -1.2332844 |
| H | -1.2691225 | -7.7514074 | 0.0335409 |

| | | | |
|---|---|---|---|
| H | -0.9485522 | -6.5012190 | -2.1106365 |
| H | 0.9287143 | -3.3123485 | 0.0370265 |
| H | -0.4686439 | -6.7446497 | 2.1804361 |
| H | 1.8063846 | -2.9206598 | 1.6229625 |
| H | 1.5670210 | -2.8047819 | -1.6787232 |
| H | 2.3939408 | -2.0996784 | -3.8029628 |
| H | 1.0583338 | -2.9813035 | -4.5813769 |
| H | 1.6318984 | -3.1891240 | 4.5644444 |
| H | 2.9449868 | -2.3217198 | 3.7459780 |
| H | 2.1898448 | 0.2537655 | -3.5472281 |
| H | 0.8205891 | 2.3201985 | -3.5432926 |
| H | -2.7430749 | -0.0445823 | -3.9198900 |
| H | -1.3649520 | -2.1118088 | -3.9647896 |
| H | -0.8202266 | -2.3202080 | 3.5449067 |
| H | -2.1890982 | -0.2535243 | 3.5488359 |
| H | 1.3663364 | 2.1115019 | 3.9641440 |
| H | 2.7440551 | 0.0440115 | 3.9192061 |
| H | -2.9446144 | 2.3210027 | -3.7457199 |
| H | -1.6316117 | 3.1885028 | -4.5642065 |
| H | -1.0566527 | 2.9814708 | 4.5817491 |
| H | -2.3926470 | 2.0999675 | 3.8038724 |
| H | -1.8076388 | 2.9213710 | -1.6226570 |
| H | -1.5681704 | 2.8062901 | 1.6797169 |
| H | -0.9272100 | 3.3117156 | -0.0369072 |
| H | 1.2649928 | 7.7536447 | -0.0333046 |
| H | 0.9465539 | 6.5027025 | 2.1107534 |
| H | 0.4653773 | 6.7461875 | -2.1801421 |
| C | -2.6385397 | -2.1581030 | -0.5917994 |
| H | -0.3233479 | -1.3243537 | -0.6859120 |
| H | 0.3233598 | 1.3237737 | 0.6858194 |

| | | | |
|---|---|---|---|
| C | 2.6384133 | 2.1577083 | 0.5909320 |
| H | -4.8468456 | -1.7971892 | 1.0783713 |
| H | -7.2246631 | -1.0985314 | 1.1367966 |
| H | -6.3709713 | 2.0419849 | -1.6699735 |
| H | -3.9938955 | 1.3302715 | -1.7422552 |
| H | 4.8470036 | 1.7964050 | -1.0791089 |
| H | 7.2248540 | 1.0978797 | -1.1370507 |
| H | 6.3709701 | -2.0419380 | 1.6704561 |
| H | 3.9938729 | -1.3303043 | 1.7423027 |
| H | -3.5928735 | -2.6525581 | -0.7670086 |
| H | -2.0112820 | -2.3122062 | -1.4732463 |
| H | -2.1578444 | -2.6022920 | 0.2836644 |
| H | 3.5927399 | 2.6524269 | 0.7653911 |
| H | 2.1570257 | 2.6014663 | -0.2843623 |
| H | 2.0116632 | 2.3119493 | 1.4727266 |

Table 18: Cartesian coordinates and total energy in a.u. of complex **2d@1**

E(RI-TPSS-D3/def2-TZVP)=-3296.040016287

| | | | |
|---|---|---|---|
| C | -0.1816330 | 6.1587515 | -1.5699167 |
| C | -0.7465092 | 4.8891567 | -1.3975342 |
| C | -0.6202082 | 4.2493253 | -0.1609080 |
| C | 0.0518988 | 4.8635443 | 0.9003869 |
| C | 0.6196810 | 6.1292162 | 0.7114824 |
| C | 0.4945091 | 6.7736366 | -0.5179702 |
| C | -1.4167443 | 4.2502290 | -2.5838134 |
| O | -1.2507887 | 4.6924498 | -3.7239423 |

| | | | |
|---|---|---|---|
| C | 0.2094727 | 4.2176121 | 2.2474007 |
| O | 1.0666282 | 4.6024459 | 3.0507365 |
| N | -2.2027449 | 3.1623230 | -2.3228611 |
| C | -2.6894268 | 2.2995440 | -3.3934569 |
| C | -1.8324976 | 1.0555590 | -3.5484888 |
| C | -0.4366822 | 1.1456250 | -3.5114294 |
| C | 0.3497885 | 0.0027684 | -3.6273212 |
| C | -0.2355046 | -1.2573373 | -3.7854171 |
| C | -1.6314663 | -1.3472221 | -3.8466931 |
| C | -2.4174736 | -0.2017701 | -3.7256617 |
| C | 0.6147568 | -2.5087631 | -3.8330751 |
| N | 0.6572031 | -3.2040621 | -2.5417393 |
| C | -0.2102052 | -4.2175532 | -2.2478445 |
| O | -1.0679081 | -4.6024203 | -3.0505745 |
| C | -0.0511306 | -4.8638349 | -0.9011939 |
| C | 0.6201943 | -4.2488830 | 0.1601714 |
| C | 0.7481955 | -4.8892196 | 1.3963655 |
| C | 0.1857157 | -6.1599318 | 1.5682960 |
| C | -0.4897009 | -6.7754994 | 0.5162845 |
| C | -0.6165127 | -6.1306442 | -0.7127722 |
| C | 1.4177874 | -4.2497013 | 2.5826680 |
| O | 1.2519187 | -4.6918150 | 3.7228496 |
| N | 2.2031632 | -3.1613833 | 2.3216021 |
| C | 2.6895018 | -2.2982551 | 3.3920410 |
| C | 1.8320345 | -1.0546292 | 3.5470867 |
| C | 0.4362750 | -1.1451155 | 3.5092217 |
| C | -0.3506293 | -0.0025703 | 3.6253176 |
| C | 0.2341698 | 1.2576395 | 3.7843647 |
| C | 1.6300816 | 1.3479367 | 3.8464321 |
| C | 2.4165127 | 0.2027954 | 3.7252659 |

| | | | |
|---|---|---|---|
| C | -0.6165038 | 2.5087962 | 3.8320398 |
| N | -0.6584913 | 3.2044751 | 2.5408971 |
| O | 2.1230523 | -1.3453604 | -0.2381322 |
| C | 1.9075347 | -0.1470004 | 0.0261596 |
| N | 2.9182492 | 0.7642097 | 0.2217097 |
| C | 4.2765836 | 0.3546776 | 0.3966247 |
| C | 4.8536513 | -0.6756419 | -0.3589356 |
| C | 6.1791497 | -1.0364748 | -0.1333015 |
| C | 6.9739447 | -0.3961716 | 0.8333488 |
| C | 6.3794332 | 0.6441866 | 1.5656269 |
| C | 5.0553265 | 1.0186587 | 1.3541311 |
| Si | 8.7556072 | -0.9036673 | 1.1369877 |
| C | 0.5247602 | 0.3613761 | 0.2038643 |
| C | -0.5249362 | -0.3609894 | -0.2056585 |
| C | -1.9077223 | 0.1472513 | -0.0275629 |
| O | -2.1233841 | 1.3456800 | 0.2363580 |
| N | -2.9183753 | -0.7642118 | -0.2219918 |
| C | -4.2769620 | -0.3547895 | -0.3954571 |
| C | -5.0563082 | -1.0177542 | -1.3531303 |
| C | -6.3807392 | -0.6434297 | -1.5628869 |
| C | -6.9748764 | 0.3957836 | -0.8286711 |
| C | -6.1794200 | 1.0350614 | 0.1381160 |
| C | -4.8536067 | 0.6743266 | 0.3620121 |
| Si | -8.7568607 | 0.9031967 | -1.1305781 |
| H | -0.9225164 | -7.7621524 | 0.6556229 |
| H | -1.1482620 | -6.5872375 | -1.5416689 |
| H | 1.0083096 | -3.2422034 | 0.0356398 |
| H | 0.2825798 | -6.6379956 | 2.5382040 |
| H | 2.2468672 | -2.7774704 | 1.3821683 |
| H | 1.3023217 | -2.8581405 | -1.8393758 |

| | | | |
|---|---|---|---|
| H | 1.6432014 | -2.2610589 | -4.1132021 |
| H | 0.2129025 | -3.2216318 | -4.5574682 |
| H | 2.6704144 | -2.8983733 | 4.3071352 |
| H | 3.7265439 | -2.0152910 | 3.1824141 |
| H | 1.4341088 | 0.0892689 | -3.5877922 |
| H | 0.0347060 | 2.1168704 | -3.3883159 |
| H | -3.5012170 | -0.2839729 | -3.7627871 |
| H | -2.0918737 | -2.3234033 | -3.9773309 |
| H | -0.0347442 | -2.1164375 | 3.3853333 |
| H | -1.4349011 | -0.0894139 | 3.5851615 |
| H | 2.0901028 | 2.3241953 | 3.9778215 |
| H | 3.5002090 | 0.2853186 | 3.7630244 |
| H | -3.7266161 | 2.0170469 | -3.1839522 |
| H | -2.6699655 | 2.8997539 | -4.3084761 |
| H | -0.2152375 | 3.2215515 | 4.5568612 |
| H | -1.6450182 | 2.2607034 | 4.1115696 |
| H | -2.2459524 | 2.7778553 | -1.3836246 |
| H | -1.3023994 | 2.8578833 | 1.8377533 |
| H | -1.0105151 | 3.2435747 | -0.0358479 |
| H | 0.9291452 | 7.7594389 | -0.6576592 |
| H | 1.1519038 | 6.5852940 | 1.5403570 |
| H | -0.2772770 | 6.6364747 | -2.5401117 |
| C | -2.6223007 | -2.2060943 | -0.3780558 |
| H | -0.3544573 | -1.2967489 | -0.7254705 |
| H | 0.3540994 | 1.2971133 | 0.7236525 |
| C | 2.6221512 | 2.2061241 | 0.3774618 |
| H | -4.6257103 | -1.8154551 | -1.9499903 |
| H | -6.9549845 | -1.1725904 | -2.3196262 |
| H | -6.5994458 | 1.8347206 | 0.7449645 |
| H | -4.2703797 | 1.1826727 | 1.1166271 |

| | | | |
|---|---|---|---|
| H | 4.6244350 | 1.8171810 | 1.9496648 |
| H | 6.9530920 | 1.1741027 | 2.3222829 |
| H | 6.5994089 | -1.8371835 | -0.7386038 |
| H | 4.2710364 | -1.1848638 | -1.1134078 |
| H | -9.3511627 | -0.0185111 | -2.1303574 |
| H | -8.8273313 | 2.2954864 | -1.6436117 |
| H | -9.5375161 | 0.8390206 | 0.1310728 |
| H | 9.3473140 | 0.0142872 | 2.1417351 |
| H | 8.8255791 | -2.2980427 | 1.6443782 |
| H | 9.5390350 | -0.8338958 | -0.1226675 |
| H | -1.8273585 | -2.4960625 | 0.3087250 |
| H | -3.5195579 | -2.7644035 | -0.1099826 |
| H | -2.3329945 | -2.4566707 | -1.4028242 |
| H | 3.5194650 | 2.7644025 | 0.1094927 |
| H | 1.8273866 | 2.4959521 | -0.3095705 |
| H | 2.3325861 | 2.4568717 | 1.4021190 |

Table 19: Cartesian coordinates and total energy in a.u. of complex **2e@1**

E(RI-TPSS-D3/def2-TZVP)=-2714.577052918

| | | | |
|---|---|---|---|
| C | -5.0358483 | -0.7409196 | -1.4780077 |
| C | -4.2719947 | -0.2314802 | -0.4213814 |
| C | -4.8255314 | 0.7211379 | 0.4407709 |
| C | -6.1305492 | 1.1621918 | 0.2347899 |
| C | -6.8924844 | 0.6612060 | -0.8217871 |
| C | -6.3414273 | -0.2949363 | -1.6742559 |
| N | -2.9343914 | -0.7119867 | -0.2336481 |

| | | | |
|---|---|---|---|
| C | -1.9007858 | 0.1735013 | -0.0518945 |
| C | -0.5360816 | -0.3999187 | -0.0315739 |
| C | 0.5343775 | 0.4020126 | 0.0296840 |
| C | 1.8989704 | -0.1717273 | 0.0503384 |
| O | 2.0894784 | -1.3988519 | -0.0683044 |
| O | -2.0916263 | 1.4006314 | 0.0662945 |
| N | 2.9327622 | 0.7133630 | 0.2331358 |
| C | 4.2700649 | 0.2322850 | 0.4214724 |
| C | 4.8236509 | -0.7204115 | -0.4405817 |
| C | 6.1283371 | -1.1621368 | -0.2339719 |
| C | 6.8899384 | -0.6617482 | 0.8231288 |
| C | 6.3388849 | 0.2945256 | 1.6754463 |
| C | 5.0336311 | 0.7411878 | 1.4785684 |
| N | 0.8739287 | -3.1782297 | -2.4477683 |
| C | 0.9865875 | -2.4554715 | -3.7164805 |
| C | 0.1456771 | -1.1970293 | -3.7375172 |
| C | 0.7375814 | 0.0675040 | -3.6694785 |
| C | -0.0428428 | 1.2204098 | -3.6473875 |
| C | -1.4393429 | 1.1339264 | -3.6862092 |
| C | -2.0311502 | -0.1300780 | -3.7575972 |
| C | -1.2506573 | -1.2849319 | -3.7891767 |
| C | -2.2831442 | 2.3939116 | -3.6356713 |
| N | -1.8935693 | 3.2511109 | -2.5194285 |
| C | -1.0327692 | 4.2993928 | -2.6919933 |
| O | -0.7165604 | 4.7239277 | -3.8073255 |
| C | -0.0006566 | -4.2158390 | -2.2933794 |
| O | -0.7109899 | -4.6243559 | -3.2191448 |
| C | -0.0403038 | -4.8618235 | -0.9366885 |
| C | -0.6982660 | -6.0916612 | -0.8129222 |
| C | -0.7592760 | -6.7303928 | 0.4249160 |

| | | | |
|---|---|---|---|
| C | -0.1785547 | -6.1466200 | 1.5494565 |
| C | 0.4788823 | -4.9150089 | 1.4408031 |
| C | 0.5391791 | -4.2830454 | 0.1960095 |
| C | 1.0415369 | -4.2985812 | 2.6921582 |
| N | 1.8989780 | -3.2479120 | 2.5173165 |
| C | 2.2880212 | -2.3889228 | 3.6322982 |
| C | 1.4406535 | -1.1313226 | 3.6836640 |
| C | 0.0444512 | -1.2213130 | 3.6427534 |
| C | -0.7390162 | -0.0704659 | 3.6655978 |
| C | -0.1505128 | 1.1954850 | 3.7364526 |
| C | 1.2455344 | 1.2868897 | 3.7904859 |
| C | 2.0290311 | 0.1341116 | 3.7581750 |
| C | -0.9945356 | 2.4518609 | 3.7152086 |
| N | -0.8800174 | 3.1765575 | 2.4477442 |
| C | -0.0054553 | 4.2146696 | 2.2966411 |
| O | 0.7012267 | 4.6234758 | 3.2250729 |
| O | 0.7293876 | -4.7239457 | 3.8083128 |
| C | -0.4718117 | 4.9143778 | -1.4391713 |
| C | -0.5383670 | 4.2832959 | -0.1942573 |
| C | 0.0396017 | 4.8604718 | 0.9400195 |
| C | 0.7020025 | 6.0880912 | 0.8178138 |
| C | 0.7692486 | 6.7259962 | -0.4201284 |
| C | 0.1902904 | 6.1436221 | -1.5463096 |
| H | 7.9060907 | -1.0115458 | 0.9786254 |
| H | -7.9089005 | 1.0104621 | -0.9767795 |
| H | -1.2648494 | -7.6878605 | 0.5135211 |
| H | -1.1518609 | -6.5248079 | -1.6989734 |
| H | 1.0137262 | -3.3107235 | 0.1157712 |
| H | -0.2281790 | -6.6193542 | 2.5254556 |
| H | 2.0484400 | -2.8617996 | 1.5899669 |

| | | | |
|---|---|---|---|
| H | 1.3584163 | -2.7828639 | -1.6468959 |
| H | 2.0415485 | -2.2093558 | -3.8755555 |
| H | 0.6652007 | -3.1491402 | -4.4975537 |
| H | 2.1592218 | -2.9830325 | 4.5418242 |
| H | 3.3464751 | -2.1284828 | 3.5302458 |
| H | 1.8224084 | 0.1506465 | -3.6348335 |
| H | 0.4311136 | 2.1977279 | -3.6050985 |
| H | -3.1154685 | -0.2085274 | -3.7907966 |
| H | -1.7151065 | -2.2659532 | -3.8547479 |
| H | -0.4270154 | -2.1997255 | 3.5980819 |
| H | -1.8235709 | -0.1563817 | 3.6290934 |
| H | 1.7073737 | 2.2689872 | 3.8582055 |
| H | 3.1130900 | 0.2153242 | 3.7931649 |
| H | -3.3425326 | 2.1365681 | -3.5356086 |
| H | -2.1509448 | 2.9882050 | -4.5445722 |
| H | -0.6770253 | 3.1451531 | 4.4981715 |
| H | -2.0493238 | 2.2028993 | 3.8709237 |
| H | -2.0458775 | 2.8649045 | -1.5925962 |
| H | -1.3607953 | 2.7804094 | 1.6449680 |
| H | -1.0168132 | 3.3128243 | -0.1150885 |
| H | 1.2783771 | 7.6816879 | -0.5075433 |
| H | 1.1541858 | 6.5201058 | 1.7051394 |
| H | 0.2447626 | 6.6156648 | -2.5223813 |
| C | -2.7031588 | -2.1656523 | -0.3926642 |
| H | -0.3838947 | -1.4701389 | -0.0890880 |
| H | 0.3823085 | 1.4722601 | 0.0871796 |
| C | 2.7018263 | 2.1669279 | 0.3933817 |
| H | -4.6081032 | -1.4769513 | -2.1517968 |
| H | -6.9234110 | -0.6939236 | -2.5000089 |
| H | -6.5548937 | 1.8996847 | 0.9099046 |

| | | | |
|---|---|---|---|
| H | -4.2368225 | 1.1103552 | 1.2618092 |
| H | 4.6059238 | 1.4773284 | 2.1522493 |
| H | 6.9206143 | 0.6930949 | 2.5015806 |
| H | 6.5526943 | -1.8996911 | -0.9090120 |
| H | 4.2352284 | -1.1091562 | -1.2620440 |
| H | -3.6712368 | -2.6629613 | -0.3586483 |
| H | -2.2125564 | -2.3949269 | -1.3428825 |
| H | -2.0990498 | -2.5459752 | 0.4332188 |
| H | 3.6699626 | 2.6641269 | 0.3592419 |
| H | 2.0973668 | 2.5480026 | -0.4318801 |
| H | 2.2116788 | 2.3955076 | 1.3440173 |

Table 20: Cartesian coordinates and total energy in a.u. of complex **2f@1**

E(RI-TPSS-D3/def2-TZVP)=-3029.268726161

| | | | |
|---|---|---|---|
| C | 0.3676077 | 6.1989916 | -1.2122111 |
| C | -0.2985275 | 4.9671156 | -1.2130586 |
| C | -0.4863254 | 4.2926332 | -0.0036956 |
| C | -0.0302989 | 4.8345974 | 1.2007901 |
| C | 0.6389274 | 6.0644808 | 1.1871982 |
| C | 0.8310564 | 6.7425772 | -0.0155166 |
| C | -0.7418937 | 4.4056840 | -2.5345836 |
| O | -0.3437667 | 4.8856374 | -3.5997769 |
| C | -0.2051388 | 4.1413793 | 2.5221489 |
| O | 0.4279220 | 4.4993361 | 3.5217896 |
| N | -1.6037576 | 3.3436294 | -2.4832389 |
| C | -1.8987346 | 2.5520548 | -3.6753019 |

| | | | |
|---|---|---|---|
| C | -1.0753905 | 1.2800450 | -3.7137097 |
| C | 0.3198999 | 1.3519800 | -3.6270468 |
| C | 1.0897075 | 0.1922393 | -3.6459822 |
| C | 0.4870718 | -1.0639325 | -3.7624431 |
| C | -0.9082796 | -1.1374749 | -3.8513470 |
| C | -1.6792902 | 0.0238207 | -3.8187451 |
| C | 1.3149360 | -2.3318851 | -3.7561523 |
| N | 1.1014825 | -3.1208617 | -2.5420566 |
| C | 0.1989070 | -4.1443982 | -2.5064714 |
| C | 0.0259192 | -4.8372729 | -1.1847298 |
| C | -0.6446041 | -6.0664219 | -1.1693531 |
| C | -0.8341657 | -6.7442232 | 0.0339390 |
| C | -0.3667468 | -6.2011573 | 1.2293584 |
| C | 0.3006013 | -4.9699461 | 1.2284118 |
| C | 0.4855209 | -4.2956640 | 0.0184988 |
| C | 0.7487877 | -4.4091550 | 2.5486327 |
| O | 0.3559281 | -4.8908450 | 3.6150056 |
| O | -0.4384408 | -4.4998926 | -3.5042652 |
| N | 1.6091501 | -3.3459118 | 2.4946386 |
| C | 1.9060947 | -2.5536689 | 3.6858672 |
| C | 1.0804525 | -1.2832155 | 3.7257788 |
| C | -0.3149654 | -1.3580495 | 3.6438987 |
| C | -1.0869982 | -0.1997839 | 3.6628869 |
| C | -0.4864937 | 1.0577982 | 3.7747605 |
| C | 0.9089804 | 1.1342488 | 3.8590854 |
| C | 1.6821907 | -0.0255788 | 3.8264068 |
| C | -1.3169769 | 2.3240394 | 3.7683775 |
| H | -1.3496478 | -7.7005386 | 0.0398595 |
| H | -1.0071730 | -6.4669561 | -2.1110010 |
| H | 0.9569452 | -3.3175948 | 0.0162358 |

| | | | |
|---|---|---|---|
| H | -0.5120344 | -6.7066718 | 2.1789527 |
| H | 1.8077061 | -2.9045567 | 1.6012234 |
| H | 1.5451996 | -2.7832162 | -1.6925927 |
| H | 2.3800909 | -2.0907467 | -3.8236004 |
| H | 1.0427717 | -2.9750054 | -4.5970728 |
| H | 1.6792848 | -3.1940805 | 4.5429132 |
| H | 2.9750132 | -2.3154453 | 3.7070026 |
| H | 2.1733356 | 0.2615820 | -3.5723519 |
| H | 0.7994899 | 2.3246333 | -3.5494533 |
| H | -2.7633699 | -0.0477554 | -3.8832646 |
| H | -1.3811969 | -2.1113412 | -3.9510598 |
| H | -0.7928851 | -2.3317923 | 3.5696343 |
| H | -2.1706953 | -0.2714083 | 3.5927671 |
| H | 1.3803888 | 2.1092007 | 3.9554446 |
| H | 2.7663339 | 0.0482681 | 3.8872642 |
| H | -2.9680334 | 2.3158949 | -3.6996916 |
| H | -1.6682900 | 3.1922461 | -4.5315671 |
| H | -1.0471446 | 2.9672012 | 4.6100257 |
| H | -2.3816992 | 2.0805825 | 3.8345272 |
| H | -1.8090775 | 2.9048868 | -1.5901311 |
| H | -1.5443913 | 2.7751779 | 1.7045926 |
| H | -0.9567371 | 3.3140308 | -0.0028843 |
| H | 1.3455249 | 7.6994457 | -0.0199776 |
| H | 0.9986322 | 6.4652438 | 2.1298409 |
| H | 0.5152384 | 6.7044952 | -2.1614485 |
| N | -1.1035657 | 3.1141487 | 2.5550956 |
| O | 2.1132388 | -1.3983976 | -0.0629215 |
| C | 1.8930066 | -0.1925175 | 0.1699993 |
| N | 2.9053858 | 0.7113497 | 0.3580937 |
| C | 2.6403700 | 2.1538355 | 0.5551254 |

| | | | |
|---|---|---|---|
| C | 0.5168160 | 0.3504753 | 0.2407376 |
| C | -0.5187141 | -0.3552996 | -0.2275646 |
| C | -1.8945633 | 0.1889446 | -0.1590069 |
| O | -2.1139634 | 1.3945933 | 0.0760077 |
| N | -2.9074761 | -0.7131045 | -0.3527564 |
| C | -2.6437798 | -2.1555753 | -0.5517311 |
| C | -4.2747045 | -0.2848160 | -0.3007597 |
| C | -5.1837755 | -0.9594284 | 0.5134475 |
| C | -6.5259879 | -0.5789717 | 0.5354487 |
| C | -6.9978240 | 0.4834535 | -0.2430438 |
| C | -6.0607031 | 1.1540025 | -1.0476475 |
| C | -4.7223707 | 0.7837585 | -1.0825956 |
| C | -8.4667149 | 0.9235748 | -0.2504078 |
| C | 4.2730447 | 0.2855193 | 0.2982649 |
| C | 4.7275260 | -0.7818559 | 1.0778317 |
| C | 6.0663363 | -1.1496099 | 1.0345112 |
| C | 6.9971281 | -0.4777839 | 0.2236399 |
| C | 6.5184715 | 0.5834405 | -0.5523274 |
| C | 5.1757425 | 0.9614226 | -0.5219726 |
| C | 8.4668028 | -0.9154041 | 0.2216607 |
| C | -9.3361453 | 0.0733731 | 0.6924652 |
| C | -8.5610799 | 2.4001320 | 0.1996136 |
| C | -9.0309880 | 0.7892166 | -1.6843611 |
| C | 9.3289080 | -0.0633298 | -0.7262632 |
| C | 9.0398988 | -0.7807447 | 1.6520789 |
| C | 8.5607431 | -2.3916022 | -0.2296530 |
| H | -0.3368886 | -1.3277444 | -0.6692303 |
| H | 0.3349572 | 1.3230906 | 0.6819764 |
| H | -4.8462905 | -1.7805680 | 1.1401862 |
| H | -7.2028623 | -1.1276612 | 1.1813702 |

| | | | |
|---|---|---|---|
| H | -6.3819065 | 1.9832499 | -1.6719954 |
| H | -4.0226993 | 1.3146087 | -1.7166639 |
| H | 4.8327910 | 1.7816211 | -1.1469875 |
| H | 7.1901979 | 1.1330359 | -1.2028202 |
| H | 6.3930292 | -1.9780106 | 1.6571380 |
| H | 4.0328731 | -1.3138871 | 1.7164484 |
| H | -3.6015372 | -2.6522624 | -0.6984096 |
| H | -2.0392001 | -2.3112198 | -1.4490537 |
| H | -2.1390888 | -2.5963352 | 0.3118168 |
| H | 3.5977545 | 2.6516533 | 0.7004401 |
| H | 2.1344879 | 2.5930042 | -0.3085673 |
| H | 2.0363034 | 2.3100056 | 1.4526671 |
| H | -10.3718181 | 0.4263376 | 0.6495751 |
| H | -9.3324163 | -0.9834781 | 0.4031823 |
| H | -9.0005638 | 0.1509157 | 1.7325111 |
| H | -10.0806667 | 1.1037810 | -1.7062055 |
| H | -8.4775906 | 1.4116654 | -2.3946070 |
| H | -8.9748450 | -0.2493810 | -2.0277520 |
| H | -9.6069046 | 2.7281992 | 0.1944679 |
| H | -8.1658789 | 2.5226140 | 1.2136869 |
| H | -7.9968141 | 3.0609316 | -0.4658463 |
| H | 10.3654826 | -0.4143390 | -0.6896932 |
| H | 8.9872346 | -0.1412918 | -1.7642970 |
| H | 9.3249027 | 0.9934499 | -0.4367301 |
| H | 10.0903921 | -1.0929184 | 1.6669435 |
| H | 8.9835532 | 0.2574742 | 1.9965851 |
| H | 8.4925019 | -1.4049548 | 2.3654243 |
| H | 9.6070157 | -2.7182577 | -0.2304425 |
| H | 8.0009997 | -3.0534929 | 0.4385367 |
| H | 8.1601223 | -2.5140395 | -1.2416029 |

Table 21: Cartesian coordinates and total energy in a.u. of complex **2g@1**

E(RI-TPSS-D3/def2-TZVP)=-2865.106176949

| | | | |
|---|---|---|---|
| C | -0.4728078 | -5.6877397 | -1.5919420 |
| C | 0.5354128 | -4.7379591 | -1.3845441 |
| C | 0.7841340 | -4.2825428 | -0.0865723 |
| C | 0.0082608 | -4.7193109 | 0.9907370 |
| C | -0.9986172 | -5.6673276 | 0.7682985 |
| C | -1.2277420 | -6.1551852 | -0.5168642 |
| C | 1.2405569 | -4.1910503 | -2.5965636 |
| O | 1.0545733 | -4.6755700 | -3.7162698 |
| C | 0.1627464 | -4.1737407 | 2.3824267 |
| O | -0.4510797 | -4.6654983 | 3.3352546 |
| N | 2.0418243 | -3.1018636 | -2.3858013 |
| C | 2.4675505 | -2.2577160 | -3.5008212 |
| C | 1.5499656 | -1.0565141 | -3.6440487 |
| C | 2.0617243 | 0.2413450 | -3.7312999 |
| C | 1.2103548 | 1.3423940 | -3.8129798 |
| C | -0.1791937 | 1.1676305 | -3.7976297 |
| C | -0.6906153 | -0.1311027 | -3.7270781 |
| C | 0.1610837 | -1.2304099 | -3.6554482 |
| C | -1.0979767 | 2.3709926 | -3.7850213 |
| N | -1.0034703 | 3.0965239 | -2.5154769 |
| C | -0.1715051 | 4.1742241 | -2.3831962 |
| C | -0.0085584 | 4.7180236 | -0.9918935 |
| C | -0.7844861 | 4.2862653 | 0.0873695 |

| | | | |
|---|---|---|---|
| C | -0.5271433 | 4.7373211 | 1.3851566 |
| C | 0.4896220 | 5.6783923 | 1.5904569 |
| C | 1.2444072 | 6.1415025 | 0.5133801 |
| C | 1.0066755 | 5.6575912 | -0.7717133 |
| C | -1.2328670 | 4.1944238 | 2.5985672 |
| N | -2.0376590 | 3.1075280 | 2.3893530 |
| C | -2.4671039 | 2.2670255 | 3.5059408 |
| C | -1.5542241 | 1.0625313 | 3.6503679 |
| C | -2.0698789 | -0.2344470 | 3.7265879 |
| C | -1.2217775 | -1.3380938 | 3.8074842 |
| C | 0.1682307 | -1.1667769 | 3.8022861 |
| C | 0.6834284 | 0.1310193 | 3.7426500 |
| C | -0.1649911 | 1.2329131 | 3.6720944 |
| C | 1.0840974 | -2.3723668 | 3.7902678 |
| N | 0.9930457 | -3.0954607 | 2.5191754 |
| O | 0.4376626 | 4.6657308 | -3.3390850 |
| O | -1.0446631 | 4.6799705 | 3.7174702 |
| O | -2.1290815 | 1.3185143 | -0.1190735 |
| C | -1.8983341 | 0.0949125 | -0.0129741 |
| C | -0.5149958 | -0.4240578 | -0.0337233 |
| C | 0.5183041 | 0.4267902 | 0.0406010 |
| C | 1.9014650 | -0.0926999 | 0.0181747 |
| N | 2.9038060 | 0.8258362 | -0.1657851 |
| C | 4.2477962 | 0.3942067 | -0.4109786 |
| C | 4.8559582 | -0.5937884 | 0.3705081 |
| C | 6.1614386 | -0.9927781 | 0.1008993 |
| C | 6.8769846 | -0.4088489 | -0.9497343 |
| C | 6.2783548 | 0.5857317 | -1.7276517 |
| C | 4.9736433 | 0.9791895 | -1.4574157 |
| O | 8.1635078 | -0.7624081 | -1.2644207 |

| | | | |
|---|---|---|---|
| N | -2.9009821 | -0.8245678 | 0.1644832 |
| C | -4.2457830 | -0.3943111 | 0.4075568 |
| C | -4.8520309 | 0.5968099 | -0.3714494 |
| C | -6.1584893 | 0.9940670 | -0.1039896 |
| C | -6.8768845 | 0.4052665 | 0.9419686 |
| C | -6.2801465 | -0.5924432 | 1.7173315 |
| C | -4.9744762 | -0.9841794 | 1.4492566 |
| O | -8.1644779 | 0.7569295 | 1.2543914 |
| O | 2.1321411 | -1.3160155 | 0.1279427 |
| H | -2.0065595 | -6.8939594 | -0.6843146 |
| H | -0.6489764 | -6.0345855 | -2.6054124 |
| H | 1.5946395 | -3.5859398 | 0.0897788 |
| H | -1.5869911 | -6.0003074 | 1.6177052 |
| H | 1.3132075 | -2.5943266 | 1.6922697 |
| H | 2.0283313 | -2.6379318 | -1.4792442 |
| H | 3.4981911 | -1.9296488 | -3.3310072 |
| H | 2.4405043 | -2.8839347 | -4.3972523 |
| H | 0.8104808 | -3.0838870 | 4.5727004 |
| H | 2.1237818 | -2.0630447 | 3.9406417 |
| H | 3.1391524 | 0.3890045 | -3.7298911 |
| H | 1.6153847 | 2.3492386 | -3.8811466 |
| H | -1.7684260 | -0.2833346 | -3.7211998 |
| H | -0.2534379 | -2.2337817 | -3.6045385 |
| H | -1.6297394 | -2.3443001 | 3.8676492 |
| H | -3.1476400 | -0.3793305 | 3.7169468 |
| H | 0.2521008 | 2.2356510 | 3.6297686 |
| H | 1.7616372 | 0.2804712 | 3.7448199 |
| H | -2.1375139 | 2.0589585 | -3.9306600 |
| H | -0.8290143 | 3.0815706 | -4.5698705 |
| H | -2.4373769 | 2.8946437 | 4.4012587 |

| | | | |
|---|---|---|---|
| H | -3.4990726 | 1.9429919 | 3.3364821 |
| H | -1.3174529 | 2.5950312 | -1.6863325 |
| H | -2.0231570 | 2.6408961 | 1.4840924 |
| H | -1.6023793 | 3.5978946 | -0.0874033 |
| H | 2.0298205 | 6.8736405 | 0.6791923 |
| H | 0.6721524 | 6.0222954 | 2.6038119 |
| H | 1.5947294 | 5.9870680 | -1.6227163 |
| C | -2.6147928 | -2.2692127 | 0.3089037 |
| H | -0.3137031 | -1.4875449 | -0.0817243 |
| H | 0.3172072 | 1.4903445 | 0.0883961 |
| C | 2.6170430 | 2.2697743 | -0.3161332 |
| H | -4.5164116 | -1.7492601 | 2.0679503 |
| H | -6.8431187 | -1.0452992 | 2.5267815 |
| H | -6.6216332 | 1.7643009 | -0.7172155 |
| H | -4.3038819 | 1.0595821 | -1.1814805 |
| H | 4.5140776 | 1.7417568 | -2.0780527 |
| H | 6.8391148 | 1.0348335 | -2.5407244 |
| H | 6.6260795 | -1.7605301 | 0.7160975 |
| H | 4.3099966 | -1.0528152 | 1.1841421 |
| H | 8.4612663 | -1.4605411 | -0.6587336 |
| H | -8.4607876 | 1.4574662 | 0.6507711 |
| H | -1.9665749 | -2.6119700 | -0.4989757 |
| H | -2.1468854 | -2.4927870 | 1.2718756 |
| H | -3.5588840 | -2.8064380 | 0.2318455 |
| H | 3.5615628 | 2.8072774 | -0.2469945 |
| H | 2.1439674 | 2.4882929 | -1.2777339 |
| H | 1.9733189 | 2.6169145 | 0.4935097 |

Table 22: Cartesian coordinates and total energy in a.u. of complex **2h@1**

E(RI-TPSS-D3/def2-TZVP)=-2825.356495064

| | | | |
|---|---|---|---|
| C | 0.5965606 | 6.0869796 | -0.7675173 |
| C | -0.0267454 | 4.8436479 | -0.9295037 |
| C | -0.6704579 | 4.2570732 | 0.1637530 |
| C | -0.7105496 | 4.8956663 | 1.4059873 |
| C | -0.0889982 | 6.1420157 | 1.5521172 |
| C | 0.5578726 | 6.7321891 | 0.4677586 |
| C | 0.0337416 | 4.1959666 | -2.2849791 |
| O | 0.7871275 | 4.6249381 | -3.1668775 |
| C | -1.3460038 | 4.2747520 | 2.6204603 |
| O | -1.1462069 | 4.7351298 | 3.7487326 |
| N | -0.8034566 | 3.1372860 | -2.4925377 |
| C | -0.8336626 | 2.4262810 | -3.7732807 |
| C | 0.0389145 | 1.1897727 | -3.7654429 |
| C | 1.4332482 | 1.3112125 | -3.7975271 |
| C | 2.2410665 | 0.1773453 | -3.7234147 |
| C | 1.6795051 | -1.0986481 | -3.6257656 |
| C | 0.2853373 | -1.2191312 | -3.6144265 |
| C | -0.5227635 | -0.0874983 | -3.6808634 |
| C | 2.5547845 | -2.3331499 | -3.5126437 |
| N | 2.1248490 | -3.1895748 | -2.4111560 |
| C | 1.3267835 | -4.2787293 | -2.6268605 |
| O | 1.1191746 | -4.7381686 | -3.7541468 |
| C | 0.6931286 | -4.8957225 | -1.4093827 |
| C | 0.6667957 | -4.2589890 | -0.1658229 |
| C | 0.0246892 | -4.8413489 | 0.9306369 |
| C | -0.6101657 | -6.0791336 | 0.7707876 |

| | | | |
|---|---|---|---|
| C | -0.5851677 | -6.7226261 | -0.4657497 |
| C | 0.0596259 | -6.1362969 | -1.5534613 |
| C | -0.0234726 | -4.1941244 | 2.2868811 |
| O | -0.7700775 | -4.6225750 | 3.1748001 |
| N | 0.8159125 | -3.1358537 | 2.4878052 |
| C | 0.8510156 | -2.4206608 | 3.7661709 |
| C | -0.0275013 | -1.1883297 | 3.7586382 |
| C | -1.4210385 | -1.3163826 | 3.8010641 |
| C | -2.2348497 | -0.1870004 | 3.7250557 |
| C | -1.6804057 | 1.0911201 | 3.6148239 |
| C | -0.2870042 | 1.2183099 | 3.5936238 |
| C | 0.5271915 | 0.0911315 | 3.6623212 |
| C | -2.5634254 | 2.3201007 | 3.5001108 |
| N | -2.1363290 | 3.1806750 | 2.4009881 |
| O | 2.1126981 | -1.3647400 | 0.1408180 |
| C | 1.9031454 | -0.1405262 | -0.0095927 |
| N | 2.9271034 | 0.7545883 | -0.1884152 |
| C | 4.2740823 | 0.2996543 | -0.3630472 |
| C | 4.8377989 | -0.6809018 | 0.4624968 |
| C | 6.1478101 | -1.0962097 | 0.2666869 |
| C | 6.9399813 | -0.5478597 | -0.7572467 |
| C | 6.3714888 | 0.4425645 | -1.5755550 |
| C | 5.0601826 | 0.8565526 | -1.3793082 |
| N | 8.2731600 | -0.9223471 | -0.9083076 |
| C | 0.5313420 | 0.4061127 | -0.0367450 |
| C | -0.5289687 | -0.4123388 | 0.0250288 |
| C | -1.9003745 | 0.1356373 | 0.0005279 |
| O | -2.1086821 | 1.3597244 | -0.1524613 |
| N | -2.9249271 | -0.7574926 | 0.1864327 |
| C | -4.2701305 | -0.3001156 | 0.3679856 |

| | | | |
|---|---|---|---|
| C | -5.0520601 | -0.8559950 | 1.3881028 |
| C | -6.3611523 | -0.4388439 | 1.5922256 |
| C | -6.9318068 | 0.5537956 | 0.7781198 |
| C | -6.1441761 | 1.1007027 | -0.2500733 |
| C | -4.8363307 | 0.6823199 | -0.4537523 |
| N | -8.2630242 | 0.9317862 | 0.9373539 |
| H | -1.0735652 | -7.6860741 | -0.5824511 |
| H | 0.0788426 | -6.6136854 | -2.5283123 |
| H | 1.1243221 | -3.2814125 | -0.0592775 |
| H | -1.1133037 | -6.5145877 | 1.6284754 |
| H | 1.3261632 | -2.7213189 | 1.7123348 |
| H | 2.1882881 | -2.7766030 | -1.4841947 |
| H | 3.5983054 | -2.0414870 | -3.3539683 |
| H | 2.4941732 | -2.9405322 | -4.4206870 |
| H | 0.5179493 | -3.1301908 | 4.5276654 |
| H | 1.8905709 | -2.1443465 | 3.9708910 |
| H | 3.3234255 | 0.2819845 | -3.7360479 |
| H | 1.8745136 | 2.3021099 | -3.8737363 |
| H | -1.6056405 | -0.1968041 | -3.6615105 |
| H | -0.1660775 | -2.2059509 | -3.5515220 |
| H | -1.8569229 | -2.3089146 | 3.8859880 |
| H | -3.3165505 | -0.2968520 | 3.7459434 |
| H | 0.1593710 | 2.2067128 | 3.5209335 |
| H | 1.6093601 | 0.2057082 | 3.6348727 |
| H | -1.8731612 | 2.1555365 | -3.9856299 |
| H | -0.4925511 | 3.1369874 | -4.5301822 |
| H | -2.5095769 | 2.9267934 | 4.4091020 |
| H | -3.6045053 | 2.0214336 | 3.3383178 |
| H | -1.3214749 | 2.7239793 | -1.7216635 |
| H | -2.1951339 | 2.7688810 | 1.4731672 |

| | | | |
|---|---|---|---|
| H | -1.1179825 | 3.2749426 | 0.0559512 |
| H | 1.0371337 | 7.7000210 | 0.5860923 |
| H | -0.1187289 | 6.6207669 | 2.5260440 |
| H | 1.1015316 | 6.5254208 | -1.6225992 |
| C | -2.6769136 | -2.2070111 | 0.3529708 |
| H | -0.3589498 | -1.4763210 | 0.1280082 |
| H | 0.3610317 | 1.4700285 | -0.1396318 |
| C | 2.6781519 | 2.2043949 | -0.3512011 |
| H | -4.6337030 | -1.6152300 | 2.0416936 |
| H | -6.9465208 | -0.8855179 | 2.3921792 |
| H | -6.5671085 | 1.8603458 | -0.9033654 |
| H | -4.2509019 | 1.1214572 | -1.2508182 |
| H | 4.6435038 | 1.6142703 | -2.0358029 |
| H | 6.9603259 | 0.8900053 | -2.3725348 |
| H | 6.5688705 | -1.8544046 | 0.9228680 |
| H | 4.2486897 | -1.1209334 | 1.2564208 |
| H | 8.6775761 | -0.7582861 | -1.8220371 |
| H | 8.5223003 | -1.8294806 | -0.5339048 |
| H | -8.5119510 | 1.8397731 | 0.5648780 |
| H | -8.6624128 | 0.7683499 | 1.8533971 |
| H | -2.0067353 | -2.5700744 | -0.4275648 |
| H | -2.2525757 | -2.4345018 | 1.3352035 |
| H | -3.6302550 | -2.7222793 | 0.2438628 |
| H | 3.6309494 | 2.7200266 | -0.2392710 |
| H | 2.2551877 | 2.4344148 | -1.3333935 |
| H | 2.0064438 | 2.5647618 | 0.4293329 |

Table 23: Cartesian coordinates and total energy in a.u. of complex **2a′@1**

E(RI-TPSS-D3/def2-TZVP)=-3123.835720823

| | | | |
|---|---|---|---|
| C | -5.1931071 | -1.0085134 | 0.6139446 |
| C | -4.2668425 | -0.3523588 | -0.2042149 |
| C | -4.6800679 | 0.7108343 | -1.0071694 |
| C | -6.0136998 | 1.0907679 | -0.9689608 |
| C | -6.9573031 | 0.4553850 | -0.1653808 |
| C | -6.5296642 | -0.6068446 | 0.6261802 |
| N | -2.9057495 | -0.7811166 | -0.2424796 |
| C | -1.9002370 | 0.1449666 | -0.0846171 |
| C | -0.5189005 | -0.3762623 | -0.1895966 |
| C | 0.5194468 | 0.3772818 | 0.1884095 |
| C | 1.9007975 | -0.1440729 | 0.0838609 |
| O | 2.1397201 | -1.3429783 | -0.1463598 |
| N | -6.4452405 | 2.2130910 | -1.8409185 |
| O | -5.5911518 | 2.7355384 | -2.5643047 |
| O | -2.1391576 | 1.3440154 | 0.1450533 |
| N | 2.9063711 | 0.7818151 | 0.2429624 |
| C | 4.2673963 | 0.3529793 | 0.2050715 |
| C | 4.6798129 | -0.7118292 | 1.0063224 |
| C | 6.0134266 | -1.0918386 | 0.9686131 |
| C | 6.9578782 | -0.4549823 | 0.1671919 |
| C | 6.5310666 | 0.6088311 | -0.6226869 |
| C | 5.1945312 | 1.0105850 | -0.6109651 |
| N | 6.4439333 | -2.2160198 | 1.8386795 |
| O | 5.5886737 | -2.7409490 | 2.5588911 |
| O | -7.6291172 | 2.5504869 | -1.7904247 |
| O | 7.6281601 | -2.5524336 | 1.7898619 |

| | | | |
|---|---|---|---|
| N | 0.9489269 | -3.0326059 | -2.5740203 |
| C | 1.1113174 | -2.2245960 | -3.7834175 |
| C | 0.2860830 | -0.9551892 | -3.7497990 |
| C | 0.8989796 | 0.2990573 | -3.6751268 |
| C | 0.1380540 | 1.4641654 | -3.6425578 |
| C | -1.2607023 | 1.4021519 | -3.6760705 |
| C | -1.8744972 | 0.1476770 | -3.7398793 |
| C | -1.1121599 | -1.0201115 | -3.7820599 |
| C | -2.0719027 | 2.6832140 | -3.6283222 |
| N | -1.7371080 | 3.4766663 | -2.4464483 |
| C | -0.8096686 | 4.4787642 | -2.4976704 |
| O | -0.3635685 | 4.9200948 | -3.5604203 |
| C | 0.0629321 | -4.0698059 | -2.5231614 |
| O | -0.6271664 | -4.3957606 | -3.4953435 |
| C | -0.0305058 | -4.8097826 | -1.2193161 |
| C | -0.6826818 | -6.0488649 | -1.2174745 |
| C | -0.8137691 | -6.7693709 | -0.0313851 |
| C | -0.3115062 | -6.2557775 | 1.1626017 |
| C | 0.3415692 | -5.0171560 | 1.1752156 |
| C | 0.4747857 | -4.3023090 | -0.0184983 |
| C | 0.8091867 | -4.4785658 | 2.4976950 |
| N | 1.7370498 | -3.4768863 | 2.4467201 |
| C | 2.0717369 | -2.6831403 | 3.6283835 |
| C | 1.2604078 | -1.4021396 | 3.6755965 |
| C | -0.1383484 | -1.4643793 | 3.6422115 |
| C | -0.8994544 | -0.2993754 | 3.6745295 |
| C | -0.2867527 | 0.9549706 | 3.7491506 |
| C | 1.1114801 | 1.0200985 | 3.7814552 |
| C | 1.8740045 | -0.1475746 | 3.7394369 |
| C | -1.1121980 | 2.2242692 | 3.7825941 |

| | | | |
|---|---|---|---|
| N | -0.9496821 | 3.0324680 | 2.5733362 |
| C | -0.0638093 | 4.0698404 | 2.5230090 |
| O | 0.6255425 | 4.3960300 | 3.4956519 |
| O | 0.3621482 | -4.9192356 | 3.5603244 |
| C | -0.3414707 | 5.0172945 | -1.1753564 |
| C | -0.4750125 | 4.3026735 | 0.0184055 |
| C | 0.0303947 | 4.8098586 | 1.2192546 |
| C | 0.6831764 | 6.0486170 | 1.2174040 |
| C | 0.8147097 | 6.7689355 | 0.0312381 |
| C | 0.3122191 | 6.2555891 | -1.1627718 |
| H | 7.9871199 | -0.7922298 | 0.1749054 |
| H | -7.9865968 | 0.7924847 | -0.1728180 |
| H | -1.3137954 | -7.7337594 | -0.0375637 |
| H | -1.0798968 | -6.4224281 | -2.1561616 |
| H | 0.9356901 | -3.3183761 | -0.0027820 |
| H | -0.4201930 | -6.7897938 | 2.1014286 |
| H | 2.0048187 | -3.0910954 | 1.5483353 |
| H | 1.4557133 | -2.7339731 | -1.7464472 |
| H | 2.1730579 | -1.9824286 | -3.8908056 |
| H | 0.8073424 | -2.8570954 | -4.6218050 |
| H | 1.8491627 | -3.3132497 | 4.4939818 |
| H | 3.1446169 | -2.4703423 | 3.6219068 |
| H | 1.9854026 | 0.3629273 | -3.6526336 |
| H | 0.6263019 | 2.4345540 | -3.6035897 |
| H | -2.9603188 | 0.0826338 | -3.7763549 |
| H | -1.5946886 | -1.9916851 | -3.8569901 |
| H | -0.6264460 | -2.4348724 | 3.6039296 |
| H | -1.9858632 | -0.3633997 | 3.6517582 |
| H | 1.5938820 | 1.9917551 | 3.8561051 |
| H | 2.9598014 | -0.0823752 | 3.7763941 |

| | | | |
|---|---|---|---|
| H | -3.1447852 | 2.4704360 | -3.6218517 |
| H | -1.8494284 | 3.3135871 | -4.4937553 |
| H | -0.8085734 | 2.8567550 | 4.6211138 |
| H | -2.1739163 | 1.9818881 | 3.8897270 |
| H | -2.0033865 | 3.0896035 | -1.5480925 |
| H | -1.4552498 | 2.7330469 | 1.7452364 |
| H | -0.9363583 | 3.3190120 | 0.0027057 |
| H | 1.3152392 | 7.7330688 | 0.0373836 |
| H | 1.0804436 | 6.4220811 | 2.1561104 |
| H | 0.4211808 | 6.7895331 | -2.1016099 |
| C | -2.6317713 | -2.2234559 | -0.4323433 |
| H | -0.3368497 | -1.3662628 | -0.5895673 |
| H | 0.3373918 | 1.3674635 | 0.5879146 |
| C | 2.6323367 | 2.2240173 | 0.4337849 |
| H | -4.8665921 | -1.8266429 | 1.2492128 |
| H | -7.2387500 | -1.1218791 | 1.2664356 |
| H | -3.9873249 | 1.2263360 | -1.6555424 |
| H | 4.8687239 | 1.8298894 | -1.2450746 |
| H | 7.2408048 | 1.1250746 | -1.2612425 |
| H | 3.9864514 | -1.2285910 | 1.6530164 |
| H | -3.5860070 | -2.7363029 | -0.5433974 |
| H | -2.0556367 | -2.3812237 | -1.3477611 |
| H | -2.0947100 | -2.6452606 | 0.4204523 |
| H | 3.5864679 | 2.7366170 | 0.5468998 |
| H | 2.0966478 | 2.6467792 | -0.4194034 |
| H | 2.0548250 | 2.3809713 | 1.3484566 |

Table 24: Cartesian coordinates and total energy in a.u. of complex **2g′@1**

E(RI-TPSS-D3/def2-TZVP)=-2865.105273388

| | | | |
|---|---|---|---|
| C | -5.1630982 | -0.9412418 | -0.6510490 |
| C | -4.2874462 | -0.2880863 | 0.2240436 |
| C | -4.7399925 | 0.7442674 | 1.0424054 |
| C | -6.0787646 | 1.1298396 | 0.9849899 |
| C | -6.9667663 | 0.4841370 | 0.1178525 |
| C | -6.4989850 | -0.5484190 | -0.6925959 |
| N | -2.9180814 | -0.7049279 | 0.2994552 |
| C | -1.9105102 | 0.2185926 | 0.1832311 |
| C | -0.5316004 | -0.3103112 | 0.2867902 |
| C | 0.5146930 | 0.4317799 | -0.0936496 |
| C | 1.8830081 | -0.1374350 | -0.0598735 |
| O | 2.0736630 | -1.3475329 | 0.1712117 |
| O | -6.4593703 | 2.1490989 | 1.8212421 |
| O | -2.1371914 | 1.4275765 | -0.0188316 |
| N | 2.9100576 | 0.7296183 | -0.3406039 |
| C | 4.2430400 | 0.2453139 | -0.5414230 |
| C | 4.8107725 | -0.6667948 | 0.3475358 |
| C | 6.1109268 | -1.1221203 | 0.1236768 |
| C | 6.8476597 | -0.6691330 | -0.9751389 |
| C | 6.2710317 | 0.2533693 | -1.8459838 |
| C | 4.9742783 | 0.7161525 | -1.6410792 |
| O | 6.6104149 | -2.0175362 | 1.0358537 |
| N | 1.8290988 | -3.2279445 | -2.4107585 |
| C | 2.1756851 | -2.3771181 | -3.5439586 |
| C | 1.2939638 | -1.1435000 | -3.6121915 |
| C | 1.8470277 | 0.1239025 | -3.8161494 |

| | | | |
|---|---|---|---|
| C | 1.0382117 | 1.2578874 | -3.8714575 |
| C | -0.3484919 | 1.1467560 | -3.7085957 |
| C | -0.9023681 | -0.1215141 | -3.5106530 |
| C | -0.0933993 | -1.2542423 | -3.4668042 |
| C | -1.2145631 | 2.3889441 | -3.6958529 |
| N | -1.0443669 | 3.1622657 | -2.4626685 |
| C | -0.1308630 | 4.1726593 | -2.3778620 |
| O | 0.5443077 | 4.5356019 | -3.3483433 |
| C | 1.0097520 | -4.3123619 | -2.5570888 |
| O | 0.6932142 | -4.7631538 | -3.6620439 |
| C | 0.4987859 | -4.9352289 | -1.2875143 |
| C | -0.0788871 | -6.2085768 | -1.3638794 |
| C | -0.6078811 | -6.8062130 | -0.2213896 |
| C | -0.5710582 | -6.1409881 | 1.0031858 |
| C | 0.0093012 | -4.8701046 | 1.0944256 |
| C | 0.5318403 | -4.2737916 | -0.0568450 |
| C | 0.0321230 | -4.2005133 | 2.4392069 |
| N | 0.8957002 | -3.1510739 | 2.5768656 |
| C | 1.0162577 | -2.4156164 | 3.8365114 |
| C | 0.2117525 | -1.1331475 | 3.8352270 |
| C | -1.1871930 | -1.1800855 | 3.8270418 |
| C | -1.9328506 | -0.0016675 | 3.7952999 |
| C | -1.2998835 | 1.2447403 | 3.7847126 |
| C | 0.0993839 | 1.2897239 | 3.7965780 |
| C | 0.8438645 | 0.1138024 | 3.8174108 |
| C | -2.0911006 | 2.5371923 | 3.7359687 |
| N | -1.7262033 | 3.3380966 | 2.5687438 |
| C | -0.8328984 | 4.3693368 | 2.6650572 |
| O | -0.4488325 | 4.8163937 | 3.7496440 |
| O | -0.6796653 | -4.5974963 | 3.3681922 |

| | | | |
|---|---|---|---|
| C | 0.0103768 | 4.8417895 | -1.0397026 |
| C | -0.5040085 | 4.2955013 | 0.1394512 |
| C | -0.3336438 | 4.9413160 | 1.3671472 |
| C | 0.3696055 | 6.1514691 | 1.4101124 |
| C | 0.8861239 | 6.7021544 | 0.2386400 |
| C | 0.7145258 | 6.0507492 | -0.9817544 |
| H | 7.8594712 | -1.0306793 | -1.1446619 |
| H | -8.0107291 | 0.7868138 | 0.0775135 |
| H | -1.0525844 | -7.7953663 | -0.2851435 |
| H | -0.1089210 | -6.7029536 | -2.3299354 |
| H | 0.9323233 | -3.2658705 | -0.0028659 |
| H | -0.9846804 | -6.5845538 | 1.9035826 |
| H | 1.4132454 | -2.7951414 | 1.7790255 |
| H | 1.9946072 | -2.8348811 | -1.4889723 |
| H | 3.2274197 | -2.0836232 | -3.4623959 |
| H | 2.0526506 | -2.9911582 | -4.4413514 |
| H | 0.6649872 | -3.0906096 | 4.6216350 |
| H | 2.0756814 | -2.1984222 | 4.0065098 |
| H | 2.9241449 | 0.2217018 | -3.9326029 |
| H | 1.4724888 | 2.2411117 | -4.0337055 |
| H | -1.9790496 | -0.2219354 | -3.3854552 |
| H | -0.5394105 | -2.2342714 | -3.3197351 |
| H | -1.6842490 | -2.1468891 | 3.8544625 |
| H | -3.0197677 | -0.0529701 | 3.7874468 |
| H | 0.6009507 | 2.2541696 | 3.7947476 |
| H | 1.9309915 | 0.1638216 | 3.8257360 |
| H | -2.2712858 | 2.1183803 | -3.7804408 |
| H | -0.9504958 | 3.0539764 | -4.5216666 |
| H | -1.8785568 | 3.1574398 | 4.6111897 |
| H | -3.1663902 | 2.3318496 | 3.7114688 |

| | | | |
|---|---|---|---|
| H | -1.5149305 | 2.8122749 | -1.6329603 |
| H | -1.9210385 | 2.9251836 | 1.6615757 |
| H | -1.0084517 | 3.3348598 | 0.1058607 |
| H | 1.4281061 | 7.6429329 | 0.2771022 |
| H | 0.5036040 | 6.6344857 | 2.3729778 |
| H | 1.1180182 | 6.4563191 | -1.9043852 |
| C | -2.6451224 | -2.1520412 | 0.4462361 |
| H | -0.3566436 | -1.3088992 | 0.6681004 |
| H | 0.3415580 | 1.4270711 | -0.4845538 |
| C | 2.6736944 | 2.1743168 | -0.5600645 |
| H | -4.8017244 | -1.7340592 | -1.2981642 |
| H | -7.1843629 | -1.0476135 | -1.3710673 |
| H | -4.0672575 | 1.2509734 | 1.7208171 |
| H | 4.5308771 | 1.4241303 | -2.3325758 |
| H | 6.8383379 | 0.6098788 | -2.7006672 |
| H | 4.2608744 | -1.0308741 | 1.2046253 |
| H | -7.4074644 | 2.3215427 | 1.7037747 |
| H | 7.5183053 | -2.2527100 | 0.7853639 |
| H | -3.6014671 | -2.6647219 | 0.5340848 |
| H | -2.1027531 | -2.5487967 | -0.4158828 |
| H | -2.0737473 | -2.3398753 | 1.3589562 |
| H | 3.6339824 | 2.6834195 | -0.4885580 |
| H | 2.2338789 | 2.3691559 | -1.5430081 |
| H | 2.0203459 | 2.5709449 | 0.2182114 |

## 0.4 COSMO results on selected structures

Table 25: Cartesian coordinates and total energy in a.u. of complex **3a@1**

E(RI-TPSS-D3/def2-TZVP)=

| | | | |
|---|---|---|---|
| C | -4.7555616 | 1.1516193 | 0.3380627 |
| C | -4.0239531 | 0.0462900 | 0.7853146 |
| C | -4.6951958 | -1.1503891 | 1.0683015 |
| C | -6.0768308 | -1.2345867 | 0.9090590 |
| C | -6.8004514 | -0.1296909 | 0.4636158 |
| C | -6.1441132 | 1.0758661 | 0.1849405 |
| C | -2.5279135 | 0.0650273 | 0.9276062 |
| O | -1.8779558 | -0.9885970 | 0.9728751 |
| C | -6.9800338 | 2.2401039 | -0.2647992 |
| O | -8.1206706 | 2.0760640 | -0.7206540 |
| N | -1.9371912 | 1.2903119 | 0.9989668 |
| C | -0.4948856 | 1.4577542 | 0.8788278 |
| C | -0.0679513 | 1.8205966 | -0.5347012 |
| C | -0.7885785 | 1.3761467 | -1.6477682 |
| C | -0.3865553 | 1.7175449 | -2.9379685 |
| C | 0.7459713 | 2.5109102 | -3.1477867 |
| C | 1.4827764 | 2.9366747 | -2.0348281 |
| C | 1.0780273 | 2.5950904 | -0.7456354 |
| C | 1.1289286 | 2.9585895 | -4.5427409 |
| N | 0.5420160 | 4.2659530 | -4.8663889 |
| C | 1.1725355 | 5.4326156 | -4.5652132 |
| O | 2.3084608 | 5.4596230 | -4.0684148 |
| C | 0.4275133 | 6.6995120 | -4.8735351 |
| C | -0.9608336 | 6.7332477 | -5.0357609 |
| C | -1.6249040 | 7.9369654 | -5.2956238 |
| C | -0.8800942 | 9.1197939 | -5.3911564 |

| | | | |
|---|---|---|---|
| C | 0.5044406 | 9.0930111 | -5.2302152 |
| C | 1.1581349 | 7.8910087 | -4.9643028 |
| C | -3.1183932 | 8.0302458 | -5.4438861 |
| O | -3.6960205 | 9.1264612 | -5.4291867 |
| N | -3.7876545 | 6.8538983 | -5.5960505 |
| C | -5.2469756 | 6.7745317 | -5.5826575 |
| C | -5.7652658 | 6.2426188 | -4.2606018 |
| C | -5.3739764 | 6.8518895 | -3.0619614 |
| C | -5.8342684 | 6.3696534 | -1.8393397 |
| C | -6.7011428 | 5.2719054 | -1.7856282 |
| C | -7.1028726 | 4.6692164 | -2.9841056 |
| C | -6.6337968 | 5.1472526 | -4.2081141 |
| C | -7.1491775 | 4.7060915 | -0.4554611 |
| N | -6.4279151 | 3.4753420 | -0.1133546 |
| O | -3.0527591 | 3.9860288 | -0.0673648 |
| C | -2.3224704 | 4.6543419 | -0.8128580 |
| C | -2.4883901 | 4.6175459 | -2.3233708 |
| C | -3.5287601 | 3.5817105 | -2.7177289 |
| C | -3.5573439 | 3.3355170 | -4.2117934 |
| O | -2.8406721 | 3.9685797 | -5.0031659 |
| N | -1.2889326 | 5.4309212 | -0.3335448 |
| C | -0.4217038 | 6.1786601 | -1.2688738 |
| C | -0.8932396 | 5.3723648 | 1.0301877 |
| C | -1.8361632 | 5.2958805 | 2.0700339 |
| C | -1.4112907 | 5.2152924 | 3.3889905 |
| C | -0.0449969 | 5.2194500 | 3.6670578 |
| C | 0.9071181 | 5.3199452 | 2.6547356 |
| C | 0.4780307 | 5.3979806 | 1.3377232 |
| N | 0.4026473 | 5.1250369 | 5.0619271 |
| N | -4.4074189 | 2.3372885 | -4.6308362 |

| | | | |
|---|---|---|---|
| C | -4.4780135 | 1.9517575 | -5.9991535 |
| C | -4.5429177 | 2.9117715 | -7.0206135 |
| C | -4.6428582 | 2.5131163 | -8.3457907 |
| C | -4.6773351 | 1.1507277 | -8.6423723 |
| C | -4.6171368 | 0.1798013 | -7.6449492 |
| C | -4.5165026 | 0.5862588 | -6.3211164 |
| N | -4.7862772 | 0.7274773 | -10.0452648 |
| C | -5.1813073 | 1.5445417 | -3.6505291 |
| H | 1.0756760 | 10.0132561 | -5.3093480 |
| H | 2.2339315 | 7.8567992 | -4.8244038 |
| H | -1.5300225 | 5.8170670 | -4.9132990 |
| H | -1.4030632 | 10.0503460 | -5.5873314 |
| H | -3.2859824 | 5.9719341 | -5.5339673 |
| H | -0.4001054 | 4.2754104 | -5.2403921 |
| H | 0.7734127 | 2.2449153 | -5.2901646 |
| H | 2.2128081 | 3.0572845 | -4.6344569 |
| H | -5.6166245 | 7.7876252 | -5.7638451 |
| H | -5.5818632 | 6.1385347 | -6.4078192 |
| H | -0.9624000 | 1.3665595 | -3.7920136 |
| H | -1.6695303 | 0.7564720 | -1.5080062 |
| H | 1.6593339 | 2.9340657 | 0.1082879 |
| H | 2.3654149 | 3.5516382 | -2.1859635 |
| H | -4.7066003 | 7.7099540 | -3.0892699 |
| H | -5.5181527 | 6.8506452 | -0.9164214 |
| H | -7.7768344 | 3.8167212 | -2.9528765 |
| H | -6.9476807 | 4.6644404 | -5.1310371 |
| H | -0.1668682 | 2.2329980 | 1.5783807 |
| H | -0.0367666 | 0.5118085 | 1.1831133 |
| H | -8.2104156 | 4.4489097 | -0.4795258 |
| H | -6.9799287 | 5.4323283 | 0.3445867 |

| | | | |
|---|---|---|---|
| H | -2.4968893 | 2.1319764 | 0.8963193 |
| H | -5.4798281 | 3.5678367 | 0.2339784 |
| H | -4.2359211 | 2.0651724 | 0.0637636 |
| H | -6.5920125 | -2.1640025 | 1.1331800 |
| H | -7.8764527 | -0.1812143 | 0.3308414 |
| H | -4.1171804 | -2.0046336 | 1.4062762 |
| H | -1.5231861 | 4.3805751 | -2.7845282 |
| H | -4.5230136 | 3.8972114 | -2.3852958 |
| H | 1.2166200 | 5.4553138 | 0.5471373 |
| H | 1.9628214 | 5.3219928 | 2.8972788 |
| H | -2.1283861 | 5.1621697 | 4.1992297 |
| H | -2.8935160 | 5.3089023 | 1.8490592 |
| H | -4.4534280 | -0.1626274 | -5.5390103 |
| H | -4.6388990 | -0.8712606 | -7.9058892 |
| H | -4.7067062 | 3.2432861 | -9.1434558 |
| H | -4.5273954 | 3.9648422 | -6.7780316 |
| H | -1.0309415 | 6.6310639 | -2.0501310 |
| H | 0.0701884 | 6.9796217 | -0.7183011 |
| H | 0.3315683 | 5.5285322 | -1.7258891 |
| H | -5.9729001 | 1.0184626 | -4.1817131 |
| H | -4.5498137 | 0.8202243 | -3.1259643 |
| H | -5.6462467 | 2.2142146 | -2.9266685 |
| H | -3.3209879 | 2.6384741 | -2.2015805 |
| H | -2.7794821 | 5.6075379 | -2.6923480 |
| O | -0.4580709 | 4.9955028 | 5.9421820 |
| O | 1.6188966 | 5.1787263 | 5.2884141 |
| O | -4.8340014 | -0.4859645 | -10.2853913 |
| O | -4.8257070 | 1.6057428 | -10.9165356 |

Table 26: Cartesian coordinates and total energy in a.u. of complex **2a@1**

E(RI-TPSS-D3/def2-TZVP)=

| | | | |
|---|---|---|---|
| C | -5.1532638 | -1.1035438 | 0.4702363 |
| C | -4.2888563 | -0.3486441 | -0.3351533 |
| C | -4.7780554 | 0.7548785 | -1.0490747 |
| C | -6.1185886 | 1.0997817 | -0.9637044 |
| C | -6.9611950 | 0.3346733 | -0.1573739 |
| C | -6.4970511 | -0.7644403 | 0.5615990 |
| N | -2.9202492 | -0.7270646 | -0.4442594 |
| C | -1.9292899 | 0.2176026 | -0.3087417 |
| C | -0.5401831 | -0.2773608 | -0.4475398 |
| C | 0.4744740 | 0.3862111 | 0.1170047 |
| C | 1.8579613 | -0.1420001 | 0.0275977 |
| O | 2.0769378 | -1.3373972 | -0.2380984 |
| N | -8.3835476 | 0.6976987 | -0.0661502 |
| O | -9.1196793 | -0.0077564 | 0.6348819 |
| O | -2.1765596 | 1.4114345 | -0.0587452 |
| N | 2.8653089 | 0.7543782 | 0.3034299 |
| C | 4.2113501 | 0.3207453 | 0.4615867 |
| C | 4.7896409 | -0.6116932 | -0.4136316 |
| C | 6.1094969 | -1.0029996 | -0.2337015 |
| C | 6.8414586 | -0.4590329 | 0.8205762 |
| C | 6.2896240 | 0.4743871 | 1.6957636 |
| C | 4.9708905 | 0.8640518 | 1.5101057 |
| N | 8.2394121 | -0.8729687 | 1.0089528 |
| O | 8.7055425 | -1.7170677 | 0.2335403 |
| O | 8.8795997 | -0.3549021 | 1.9328707 |
| O | -8.7710567 | 1.6899042 | -0.6955666 |

| | | | |
|---|---|---|---|
| N | 0.8693226 | -3.2544750 | -2.6322233 |
| C | 0.9728783 | -2.5316669 | -3.9039613 |
| C | 0.1910360 | -1.2353953 | -3.8822111 |
| C | 0.8450434 | -0.0039508 | -3.7658969 |
| C | 0.1197246 | 1.1835216 | -3.7116697 |
| C | -1.2789087 | 1.1661919 | -3.7693471 |
| C | -1.9342408 | -0.0648254 | -3.8751688 |
| C | -1.2079676 | -1.2545737 | -3.9364742 |
| C | -2.0570150 | 2.4666913 | -3.7200132 |
| N | -1.6798087 | 3.2783597 | -2.5651538 |
| C | -0.8716378 | 4.3687795 | -2.6726460 |
| O | -0.5292589 | 4.8392299 | -3.7667809 |
| C | 0.0188917 | -4.3021839 | -2.4530669 |
| O | -0.7246241 | -4.7165095 | -3.3541780 |
| C | 0.0466895 | -4.9525461 | -1.0999473 |
| C | -0.4478108 | -6.2575771 | -0.9826874 |
| C | -0.4228290 | -6.9067734 | 0.2507640 |
| C | 0.0854460 | -6.2592599 | 1.3755937 |
| C | 0.5764843 | -4.9514127 | 1.2734135 |
| C | 0.5433087 | -4.3037040 | 0.0347004 |
| C | 1.0830873 | -4.2817865 | 2.5192113 |
| N | 1.8666575 | -3.1838013 | 2.3360323 |
| C | 2.2511652 | -2.3063726 | 3.4360660 |
| C | 1.3677572 | -1.0741472 | 3.5198603 |
| C | -0.0154880 | -1.1698629 | 3.3319838 |
| C | -0.8226672 | -0.0371881 | 3.4158502 |
| C | -0.2685015 | 1.2169569 | 3.6914918 |
| C | 1.1149099 | 1.3124547 | 3.8917470 |
| C | 1.9217406 | 0.1789051 | 3.8018692 |
| C | -1.1333607 | 2.4598769 | 3.7169109 |

| | | | |
|---|---|---|---|
| N | -1.0001605 | 3.2384264 | 2.4794748 |
| C | -0.1062002 | 4.2560672 | 2.3576937 |
| O | 0.6168320 | 4.6183996 | 3.2979282 |
| O | 0.7966762 | -4.7168614 | 3.6437766 |
| C | -0.4149116 | 4.9900294 | -1.3827422 |
| C | -0.5024322 | 4.3298440 | -0.1527944 |
| C | -0.0424888 | 4.9355645 | 1.0204126 |
| C | 0.5255228 | 6.2142724 | 0.9549251 |
| C | 0.6134931 | 6.8791004 | -0.2669898 |
| C | 0.1494369 | 6.2712188 | -1.4323988 |
| H | -0.7993448 | -7.9219374 | 0.3348357 |
| H | -0.8426293 | -6.7487322 | -1.8665048 |
| H | 0.8686275 | -3.2699187 | -0.0400539 |
| H | 0.1062445 | -6.7507495 | 2.3432499 |
| H | 2.0308561 | -2.8304433 | 1.3982883 |
| H | 1.4523287 | -2.9339551 | -1.8665401 |
| H | 2.0313100 | -2.3364434 | -4.0976415 |
| H | 0.5914334 | -3.2016586 | -4.6782212 |
| H | 2.1741994 | -2.8966163 | 4.3540567 |
| H | 3.2973131 | -2.0117668 | 3.3068741 |
| H | 1.9315778 | 0.0253351 | -3.7213656 |
| H | 0.6418909 | 2.1330960 | -3.6258693 |
| H | -3.0208045 | -0.0949034 | -3.9196920 |
| H | -1.7252143 | -2.2062696 | -4.0298412 |
| H | -0.4652271 | -2.1350739 | 3.1167254 |
| H | -1.8962602 | -0.1279012 | 3.2630343 |
| H | 1.5545969 | 2.2819801 | 4.1098919 |
| H | 2.9947722 | 0.2670809 | 3.9570155 |
| H | -3.1328143 | 2.2671595 | -3.6871182 |
| H | -1.8532895 | 3.0736314 | -4.6064338 |

| | | | |
|---|---|---|---|
| H | -0.8439757 | 3.1170979 | 4.5400257 |
| H | -2.1869883 | 2.1926984 | 3.8307178 |
| H | -1.8784450 | 2.8853960 | -1.6494209 |
| H | -1.5670235 | 2.9554350 | 1.6874697 |
| H | -0.8952899 | 3.3178483 | -0.1109761 |
| H | 1.0465106 | 7.8739973 | -0.3112709 |
| H | 0.8908936 | 6.6713660 | 1.8691531 |
| H | 0.2196818 | 6.7730815 | -2.3921991 |
| C | -2.5978863 | -2.1671355 | -0.5759188 |
| H | -0.3397715 | -1.1799922 | -1.0130403 |
| H | 0.2729948 | 1.2817248 | 0.6937784 |
| C | 2.5754454 | 2.1888607 | 0.5371664 |
| H | -4.7757505 | -1.9461750 | 1.0399119 |
| H | -7.1752981 | -1.3324156 | 1.1866647 |
| H | -6.5155758 | 1.9403844 | -1.5197772 |
| H | -4.1131326 | 1.3303214 | -1.6788798 |
| H | 4.5279828 | 1.5811052 | 2.1924858 |
| H | 6.8817264 | 0.8768958 | 2.5085877 |
| H | 6.5751293 | -1.7115893 | -0.9079408 |
| H | 4.2157052 | -1.0160176 | -1.2356504 |
| H | -3.5292876 | -2.7166736 | -0.6970078 |
| H | -1.9949719 | -2.3295173 | -1.4723628 |
| H | -2.0683045 | -2.5396274 | 0.3041950 |
| H | 3.5000765 | 2.7481032 | 0.4014714 |
| H | 1.8576636 | 2.5414082 | -0.2042883 |
| H | 2.1884564 | 2.3636476 | 1.5453923 |

Table 27: Cartesian coordinates and total energy in a.u. of complex **3e@1**

E(RI-TPSS-D3/def2-TZVP)=

| | | | |
|---|---|---|---|
| C | -4.7312587 | 1.0705960 | 0.3112350 |
| C | -4.0037757 | -0.0593733 | 0.6976325 |
| C | -4.6867875 | -1.2480380 | 0.9860835 |
| C | -6.0765764 | -1.2972235 | 0.8946978 |
| C | -6.7965273 | -0.1645982 | 0.5169219 |
| C | -6.1269653 | 1.0321960 | 0.2318753 |
| C | -2.5032463 | -0.0658721 | 0.7776494 |
| O | -1.8683024 | -1.1306240 | 0.7908267 |
| C | -6.9541337 | 2.2326406 | -0.1319488 |
| O | -8.1395800 | 2.1168650 | -0.4765636 |
| N | -1.8928304 | 1.1495342 | 0.8345762 |
| C | -0.4522587 | 1.2982250 | 0.6753555 |
| C | -0.0619578 | 1.6690036 | -0.7463968 |
| C | -0.8014664 | 1.2178306 | -1.8441881 |
| C | -0.4358433 | 1.5717261 | -3.1421380 |
| C | 0.6799601 | 2.3817752 | -3.3744127 |
| C | 1.4371709 | 2.8130532 | -2.2772194 |
| C | 1.0672565 | 2.4615892 | -0.9806975 |
| C | 1.0174874 | 2.8571377 | -4.7714992 |
| N | 0.4727623 | 4.1980491 | -5.0173207 |
| C | 1.1845930 | 5.3264342 | -4.7528473 |
| O | 2.3712751 | 5.2928363 | -4.3928692 |
| C | 0.4665845 | 6.6321643 | -4.9443752 |
| C | -0.9264409 | 6.7171033 | -5.0189704 |
| C | -1.5638699 | 7.9474157 | -5.2054830 |
| C | -0.7886557 | 9.1105821 | -5.2995216 |

| | | | |
|---|---|---|---|
| C | 0.6010605 | 9.0348534 | -5.2151827 |
| C | 1.2294811 | 7.8033214 | -5.0356648 |
| C | -3.0587782 | 8.0797146 | -5.2908414 |
| O | -3.6102314 | 9.1876175 | -5.2151805 |
| N | -3.7586893 | 6.9246938 | -5.4654746 |
| C | -5.2183349 | 6.8772195 | -5.4165100 |
| C | -5.7148169 | 6.3173226 | -4.0980567 |
| C | -5.2866601 | 6.8888309 | -2.8938053 |
| C | -5.7256698 | 6.3811106 | -1.6738138 |
| C | -6.6073028 | 5.2952400 | -1.6284398 |
| C | -7.0430042 | 4.7282418 | -2.8323531 |
| C | -6.5956227 | 5.2314709 | -4.0541967 |
| C | -7.0343040 | 4.7035609 | -0.3031239 |
| N | -6.3412785 | 3.4429852 | -0.0225826 |
| O | -3.0566886 | 3.8618680 | -0.0455137 |
| C | -2.2985270 | 4.5434302 | -0.7598575 |
| C | -2.4274790 | 4.5439695 | -2.2755155 |
| C | -3.4816558 | 3.5457860 | -2.7248534 |
| C | -3.4934186 | 3.3515053 | -4.2282067 |
| O | -2.7748855 | 4.0246680 | -4.9917197 |
| N | -1.2860359 | 5.3007878 | -0.2381143 |
| C | -0.3680382 | 6.0481464 | -1.1215697 |
| C | -0.9671000 | 5.2405057 | 1.1592404 |
| C | -1.9672971 | 5.3253836 | 2.1348613 |
| C | -1.6241758 | 5.2549345 | 3.4842101 |
| C | -0.2908597 | 5.1085638 | 3.8736107 |
| C | 0.7053367 | 5.0414645 | 2.8991131 |
| C | 0.3715488 | 5.1061788 | 1.5464231 |
| H | -0.0310771 | 5.0535088 | 4.9266625 |
| N | -4.3282067 | 2.3743230 | -4.6907996 |

| | | | |
|---|---|---|---|
| C | -4.3654778 | 2.0377373 | -6.0858051 |
| C | -4.5689611 | 3.0244311 | -7.0546578 |
| C | -4.6205968 | 2.6710897 | -8.4020921 |
| C | -4.4786711 | 1.3363477 | -8.7895677 |
| C | -4.2834707 | 0.3530116 | -7.8187262 |
| C | -4.2219411 | 0.7003572 | -6.4687016 |
| H | -4.5230798 | 1.0653318 | -9.8402651 |
| C | -5.1281281 | 1.5486240 | -3.7632201 |
| H | 1.1970709 | 9.9395266 | -5.2918069 |
| H | 2.3102410 | 7.7299296 | -4.9666341 |
| H | -1.5202214 | 5.8180021 | -4.8924173 |
| H | -1.2907722 | 10.0629330 | -5.4373873 |
| H | -3.2774756 | 6.0282550 | -5.4499409 |
| H | -0.5159700 | 4.2555028 | -5.2418008 |
| H | 0.5959754 | 2.1839139 | -5.5226730 |
| H | 2.0984967 | 2.9161224 | -4.9144367 |
| H | -5.5701251 | 7.9029612 | -5.5581796 |
| H | -5.5865463 | 6.2723803 | -6.2508507 |
| H | -1.0303471 | 1.2217654 | -3.9836511 |
| H | -1.6721401 | 0.5880297 | -1.6861536 |
| H | 1.6615382 | 2.8084151 | -0.1389449 |
| H | 2.3059340 | 3.4432801 | -2.4460829 |
| H | -4.6056132 | 7.7362337 | -2.9147756 |
| H | -5.3798703 | 6.8315862 | -0.7461338 |
| H | -7.7264155 | 3.8828516 | -2.8086495 |
| H | -6.9347200 | 4.7751345 | -4.9816562 |
| H | -0.0966864 | 2.0656295 | 1.3698181 |
| H | 0.0018026 | 0.3435784 | 0.9580713 |
| H | -8.1028242 | 4.4776284 | -0.3011075 |
| H | -6.8204007 | 5.4021564 | 0.5114435 |

| | | | |
|---|---|---|---|
| H | -2.4407268 | 2.0038647 | 0.7612445 |
| H | -5.3547746 | 3.4978192 | 0.2123202 |
| H | -4.2035880 | 1.9775074 | 0.0322563 |
| H | -6.6014825 | -2.2205362 | 1.1219277 |
| H | -7.8791768 | -0.1875714 | 0.4433286 |
| H | -4.1127920 | -2.1224278 | 1.2762153 |
| H | -1.4569223 | 4.2933213 | -2.7181096 |
| H | -4.4749569 | 3.8700632 | -2.3974278 |
| H | 1.1517124 | 5.0425545 | 0.7950753 |
| H | 1.7471646 | 4.9318097 | 3.1860800 |
| H | -2.4066238 | 5.3215745 | 4.2349631 |
| H | -3.0017516 | 5.4449685 | 1.8391056 |
| H | -4.0579788 | -0.0654795 | -5.7161430 |
| H | -4.1711338 | -0.6877495 | -8.1083656 |
| H | -4.7799643 | 3.4423925 | -9.1503563 |
| H | -4.6871576 | 4.0580284 | -6.7538314 |
| H | -0.9354876 | 6.5698477 | -1.8930960 |
| H | 0.1547669 | 6.7907245 | -0.5198633 |
| H | 0.3619835 | 5.3844885 | -1.5970584 |
| H | -5.8820232 | 1.0197021 | -4.3447612 |
| H | -4.5077035 | 0.8202930 | -3.2297305 |
| H | -5.6366379 | 2.1881515 | -3.0393181 |
| H | -3.3022949 | 2.5817594 | -2.2377868 |
| H | -2.6813152 | 5.5502324 | -2.6273947 |

Table 28: Cartesian coordinates and total energy in a.u. of complex **2e@1**

E(RI-TPSS-D3/def2-TZVP)=

| | | | |
|---|---|---|---|
| C | -5.0898500 | -0.4499762 | -1.3286415 |
| C | -4.2829866 | -0.0538323 | -0.2577042 |
| C | -4.7697438 | 0.8482606 | 0.6930087 |
| C | -6.0616110 | 1.3540862 | 0.5647418 |
| C | -6.8714327 | 0.9639157 | -0.5049568 |
| C | -6.3829618 | 0.0588128 | -1.4481342 |
| N | -2.9586342 | -0.5949059 | -0.1366334 |
| C | -1.8920389 | 0.2508285 | -0.0089174 |
| C | -0.5527602 | -0.3755987 | 0.0407416 |
| C | 0.5516176 | 0.3763423 | -0.0401479 |
| C | 1.8908541 | -0.2502248 | 0.0093808 |
| O | 2.0331456 | -1.4910311 | -0.0440290 |
| O | -2.0344569 | 1.4916128 | 0.0444125 |
| N | 2.9575824 | 0.5953235 | 0.1367693 |
| C | 4.2818804 | 0.0539682 | 0.2571209 |
| C | 4.7680179 | -0.8478429 | -0.6941741 |
| C | 6.0598217 | -1.3540318 | -0.5666749 |
| C | 6.8702121 | -0.9643909 | 0.5027984 |
| C | 6.3823449 | -0.0595443 | 1.4465345 |
| C | 5.0892460 | 0.4494859 | 1.3278842 |
| N | 1.0595011 | -3.2572681 | -2.4007899 |
| C | 1.2321033 | -2.5011424 | -3.6416724 |
| C | 0.3819075 | -1.2482640 | -3.6578693 |
| C | 0.9662897 | 0.0208277 | -3.6071139 |
| C | 0.1758688 | 1.1687839 | -3.6043378 |
| C | -1.2196100 | 1.0716370 | -3.6505814 |

| | | | |
|---|---|---|---|
| C | -1.8043462 | -0.1980216 | -3.6869868 |
| C | -1.0138995 | -1.3465793 | -3.6934747 |
| C | -2.0751210 | 2.3243918 | -3.6588939 |
| N | -1.7358634 | 3.2150069 | -2.5519898 |
| C | -0.9449798 | 4.3117845 | -2.7057916 |
| O | -0.5958958 | 4.7357706 | -3.8178587 |
| C | 0.3087354 | -4.3894188 | -2.3292585 |
| O | -0.2345340 | -4.8952260 | -3.3233772 |
| C | 0.1966327 | -5.0262503 | -0.9720858 |
| C | -0.3116243 | -6.3282297 | -0.8816640 |
| C | -0.4040722 | -6.9587049 | 0.3593229 |
| C | 0.0086375 | -6.3016214 | 1.5180906 |
| C | 0.5189805 | -4.9995217 | 1.4409509 |
| C | 0.5940242 | -4.3709280 | 0.1959368 |
| C | 0.9466105 | -4.3114531 | 2.7064199 |
| N | 1.7364063 | -3.2139333 | 2.5521975 |
| C | 2.0757286 | -2.3231309 | 3.6588847 |
| C | 1.2195581 | -1.0708079 | 3.6510650 |
| C | -0.1758438 | -1.1685610 | 3.6042078 |
| C | -0.9668171 | -0.0209693 | 3.6070937 |
| C | -0.3830342 | 1.2483701 | 3.6586060 |
| C | 1.0127183 | 1.3473060 | 3.6949694 |
| C | 1.8036886 | 0.1991166 | 3.6883057 |
| C | -1.2337391 | 2.5009017 | 3.6420675 |
| N | -1.0606576 | 3.2572299 | 2.4013400 |
| C | -0.3084370 | 4.3884234 | 2.3300270 |
| O | 0.2354271 | 4.8934386 | 3.3242324 |
| O | 0.5982186 | -4.7356428 | 3.8185933 |
| C | -0.5170389 | 4.9992768 | -1.4401337 |
| C | -0.5933121 | 4.3706781 | -0.1952065 |

| | | | |
|---|---|---|---|
| C | -0.1953699 | 5.0253419 | 0.9729824 |
| C | 0.3146323 | 6.3266642 | 0.8828450 |
| C | 0.4081593 | 6.9571862 | -0.3580379 |
| C | -0.0050560 | 6.3007523 | -1.5169887 |
| H | 7.8766534 | -1.3614359 | 0.5972047 |
| H | -7.8778640 | 1.3608390 | -0.5999703 |
| H | -0.7950306 | -7.9700341 | 0.4223387 |
| H | -0.6241302 | -6.8320384 | -1.7909254 |
| H | 0.9442576 | -3.3462168 | 0.1406089 |
| H | -0.0567986 | -6.7825355 | 2.4891318 |
| H | 1.9459762 | -2.8624212 | 1.6215777 |
| H | 1.4318917 | -2.8264629 | -1.5570255 |
| H | 2.2905986 | -2.2422146 | -3.7456579 |
| H | 0.9552229 | -3.1709520 | -4.4591631 |
| H | 1.9235066 | -2.8913523 | 4.5807958 |
| H | 3.1350168 | -2.0576950 | 3.5872989 |
| H | 2.0499468 | 0.1129874 | -3.5731197 |
| H | 0.6456816 | 2.1487469 | -3.5703141 |
| H | -2.8877241 | -0.2874096 | -3.7186229 |
| H | -1.4787723 | -2.3290943 | -3.7317741 |
| H | -0.6452012 | -2.1487237 | 3.5695355 |
| H | -2.0504173 | -0.1135975 | 3.5725361 |
| H | 1.4770785 | 2.3300235 | 3.7340111 |
| H | 2.8870179 | 0.2889965 | 3.7203372 |
| H | -3.1346008 | 2.0596088 | -3.5878260 |
| H | -1.9219825 | 2.8924688 | -4.5807364 |
| H | -0.9577437 | 3.1707649 | 4.4598011 |
| H | -2.2922082 | 2.2415757 | 3.7452337 |
| H | -1.9462759 | 2.8636687 | -1.6215004 |
| H | -1.4327409 | 2.8264517 | 1.5574179 |

| | | | |
|---|---|---|---|
| H | -0.9449139 | 3.3464525 | -0.1400667 |
| H | 0.8003665 | 7.9680458 | -0.4208154 |
| H | 0.6277060 | 6.8298642 | 1.7922511 |
| H | 0.0611056 | 6.7817633 | -2.4879325 |
| C | -2.7932625 | -2.0585490 | -0.2867362 |
| H | -0.4505321 | -1.4494743 | 0.1341178 |
| H | 0.4495008 | 1.4502098 | -0.1336760 |
| C | 2.7925444 | 2.0589520 | 0.2873228 |
| H | -4.7087128 | -1.1472353 | -2.0687413 |
| H | -7.0041581 | -0.2502755 | -2.2837920 |
| H | -6.4377207 | 2.0517112 | 1.3075053 |
| H | -4.1407216 | 1.1468457 | 1.5237338 |
| H | 4.7084999 | 1.1463934 | 2.0685114 |
| H | 7.0040062 | 0.2491923 | 2.2819717 |
| H | 6.4353893 | -2.0515918 | -1.3097799 |
| H | 4.1385451 | -1.1459462 | -1.5247353 |
| H | -3.7854171 | -2.5040436 | -0.3309167 |
| H | -2.2472009 | -2.3046746 | -1.2016359 |
| H | -2.2733387 | -2.4732218 | 0.5804724 |
| H | 3.7848332 | 2.5041930 | 0.3309934 |
| H | 2.2722233 | 2.4739737 | -0.5794792 |
| H | 2.2470968 | 2.3049858 | 1.2026078 |

Table 29: Cartesian coordinates and total energy in a.u. of complex **3h@1**

E(RI-TPSS-D3/def2-TZVP)=

| | | | |
|---|---|---|---|
| C | -4.8624773 | 1.2100872 | 0.4056991 |

| | | | |
|---|---|---|---|
| C | -4.4402222 | -0.1215845 | 0.3644963 |
| C | -5.3528144 | -1.1382012 | 0.6731843 |
| C | -6.6603910 | -0.8173419 | 1.0369331 |
| C | -7.0679362 | 0.5147180 | 1.0979958 |
| C | -6.1656574 | 1.5402107 | 0.7878001 |
| C | -3.0294598 | -0.5088265 | 0.0202601 |
| O | -2.7362859 | -1.6765854 | -0.2785467 |
| C | -6.6427391 | 2.9635883 | 0.8583813 |
| O | -7.8527844 | 3.2358273 | 0.8832966 |
| N | -2.0991657 | 0.4807129 | 0.1009864 |
| C | -0.6858533 | 0.2590621 | -0.2184117 |
| C | -0.3479447 | 0.7481288 | -1.6105084 |
| C | -0.7346746 | 0.0066003 | -2.7339604 |
| C | -0.4976153 | 0.4935678 | -4.0184592 |
| C | 0.1347309 | 1.7262851 | -4.2121222 |
| C | 0.5368081 | 2.4573543 | -3.0889967 |
| C | 0.2963220 | 1.9744408 | -1.8040282 |
| C | 0.3876116 | 2.2570731 | -5.6122105 |
| N | 0.0897243 | 3.6812280 | -5.7192896 |
| C | 1.0574578 | 4.6364770 | -5.6706976 |
| O | 2.2674820 | 4.3639541 | -5.6937579 |
| C | 0.5805888 | 6.0598230 | -5.5979502 |
| C | -0.7235034 | 6.3892651 | -5.2184497 |
| C | -1.1456525 | 7.7208786 | -5.1748408 |
| C | -0.2320229 | 8.7381013 | -5.4784197 |
| C | 1.0764285 | 8.4179001 | -5.8395970 |
| C | 1.4838826 | 7.0859263 | -5.9031207 |
| C | -2.5572339 | 8.1074273 | -4.8331445 |
| O | -2.8511948 | 9.2747069 | -4.5332262 |
| N | -3.4872468 | 7.1179206 | -4.9174286 |

| | | | |
|---|---|---|---|
| C | -4.9011175 | 7.3386840 | -4.5996505 |
| C | -5.2397392 | 6.8503766 | -3.2074638 |
| C | -4.8563004 | 7.5941524 | -2.0843622 |
| C | -5.0930423 | 7.1076846 | -0.7996519 |
| C | -5.7216540 | 5.8731542 | -0.6053366 |
| C | -6.1207754 | 5.1399584 | -1.7281099 |
| C | -5.8807321 | 5.6224435 | -3.0133433 |
| C | -5.9736374 | 5.3430007 | 0.7951645 |
| N | -5.6751249 | 3.9191212 | 0.9030505 |
| O | -2.7511692 | 3.5844029 | 0.0603631 |
| C | -2.3181408 | 4.4978980 | -0.6720836 |
| C | -2.4326641 | 4.4300442 | -2.1841378 |
| C | -3.1525853 | 3.1694499 | -2.6338345 |
| C | -3.2687858 | 3.1019407 | -4.1457351 |
| O | -2.8351166 | 4.0147723 | -4.8786282 |
| N | -1.7383855 | 5.6190623 | -0.1607832 |
| C | -1.2654216 | 6.7042523 | -1.0419817 |
| C | -1.6976232 | 5.8337733 | 1.2596897 |
| C | -1.1798797 | 4.8646654 | 2.1241350 |
| C | -1.1574360 | 5.0853373 | 3.4959754 |
| C | -1.6455890 | 6.2868281 | 4.0439246 |
| C | -2.1458972 | 7.2635323 | 3.1647519 |
| C | -2.1745742 | 7.0345331 | 1.7926937 |
| N | -1.6917017 | 6.4752460 | 5.4245265 |
| N | -3.8510997 | 1.9818127 | -4.6564258 |
| C | -3.8944628 | 1.7673540 | -6.0768690 |
| C | -4.4111710 | 2.7377823 | -6.9404746 |
| C | -4.4366681 | 2.5170416 | -8.3122501 |
| C | -3.9528071 | 1.3141685 | -8.8609783 |
| C | -3.4533608 | 0.3362760 | -7.9826346 |

| | | | |
|---|---|---|---|
| C | -3.4215409 | 0.5653381 | -6.6106574 |
| N | -3.9099437 | 1.1254106 | -10.2416335 |
| C | -4.3250160 | 0.8974990 | -3.7746751 |
| H | 1.7796671 | 9.2101085 | -6.0797927 |
| H | 2.4980000 | 6.8230377 | -6.1877017 |
| H | -1.4088913 | 5.6018522 | -4.9224033 |
| H | -0.5642787 | 9.7705698 | -5.4332605 |
| H | -3.2019341 | 6.1568722 | -5.0889581 |
| H | -0.8920229 | 3.9393028 | -5.6417388 |
| H | -0.2268529 | 1.7122668 | -6.3358826 |
| H | 1.4389155 | 2.1298461 | -5.8870756 |
| H | -5.0821913 | 8.4115555 | -4.6931096 |
| H | -5.5036259 | 6.8122120 | -5.3459162 |
| H | -0.8089031 | -0.0892210 | -4.8818689 |
| H | -1.2355846 | -0.9483918 | -2.5953406 |
| H | 0.6061752 | 2.5610496 | -0.9417779 |
| H | 1.0382989 | 3.4126930 | -3.2192230 |
| H | -4.3579859 | 8.5504157 | -2.2234264 |
| H | -4.7843420 | 7.6922572 | 0.0634816 |
| H | -6.6195308 | 4.1832420 | -1.5974438 |
| H | -6.1882350 | 5.0341330 | -3.8752807 |
| H | -0.0820520 | 0.7843267 | 0.5276850 |
| H | -0.5056117 | -0.8140536 | -0.1260695 |
| H | -7.0248779 | 5.4698870 | 1.0704984 |
| H | -5.3591333 | 5.8886804 | 1.5181708 |
| H | -2.3838370 | 1.4418824 | 0.2728345 |
| H | -4.6934116 | 3.6611218 | 0.8245261 |
| H | -4.1779622 | 1.9968413 | 0.1058521 |
| H | -7.3628322 | -1.6090473 | 1.2810781 |
| H | -8.0813854 | 0.7781696 | 1.3844219 |

| | | | |
|---|---|---|---|
| H | -5.0204304 | -2.1707094 | 0.6299998 |
| H | -1.4340909 | 4.4682715 | -2.6320737 |
| H | -4.1506651 | 3.1309349 | -2.1848463 |
| H | -2.5712397 | 7.8013478 | 1.1340366 |
| H | -2.5227042 | 8.2033677 | 3.5605306 |
| H | -0.7541409 | 4.3204477 | 4.1553121 |
| H | -0.7963019 | 3.9340585 | 1.7219135 |
| H | -3.0255874 | -0.2024517 | -5.9526951 |
| H | -3.0797188 | -0.6045744 | -8.3790017 |
| H | -4.8391793 | 3.2829053 | -8.9709299 |
| H | -4.7915392 | 3.6694498 | -6.5376784 |
| H | -0.6374577 | 6.2997165 | -1.8394621 |
| H | -2.1015118 | 7.2525055 | -1.4877862 |
| H | -0.6645214 | 7.3870838 | -0.4429384 |
| H | -4.9273743 | 0.2154194 | -4.3730978 |
| H | -3.4893527 | 0.3481875 | -3.3293600 |
| H | -4.9517617 | 1.3030707 | -2.9767723 |
| H | -2.6208076 | 2.2807926 | -2.2755441 |
| H | -2.9640357 | 5.3186220 | -2.5432379 |
| H | -1.0292693 | 5.9264498 | 5.9612391 |
| H | -1.7165586 | 7.4411608 | 5.7317290 |
| H | -3.8887935 | 0.1593689 | -10.5487291 |
| H | -4.5715724 | 1.6762883 | -10.7771923 |

Table 30: Cartesian coordinates and total energy in a.u. of complex **2h@1**

E(RI-TPSS-D3/def2-TZVP)=

| | | | |
|---|---|---|---|
| C | 0.2080306 | 6.2922227 | -0.8401249 |
| C | -0.2995183 | 4.9913328 | -0.9487280 |
| C | -0.7299296 | 4.3330122 | 0.2056552 |
| C | -0.6885537 | 4.9571665 | 1.4543992 |
| C | -0.1793506 | 6.2586113 | 1.5496515 |
| C | 0.2671324 | 6.9184231 | 0.4050438 |
| C | -0.3771822 | 4.3602852 | -2.3112809 |
| O | 0.1615922 | 4.8913366 | -3.2952061 |
| C | -1.1495669 | 4.2654226 | 2.7064042 |
| O | -0.8614071 | 4.7094508 | 3.8285119 |
| N | -1.0915806 | 3.2064612 | -2.4016324 |
| C | -1.2292897 | 2.4622915 | -3.6544116 |
| C | -0.3389459 | 1.2381139 | -3.6778593 |
| C | 1.0532029 | 1.3817740 | -3.7019525 |
| C | 1.8805541 | 0.2597579 | -3.6861733 |
| C | 1.3369298 | -1.0280774 | -3.6535738 |
| C | -0.0550978 | -1.1705681 | -3.6261846 |
| C | -0.8823890 | -0.0492940 | -3.6367739 |
| C | 2.2323151 | -2.2524909 | -3.6366356 |
| N | 1.8914245 | -3.1480324 | -2.5338574 |
| C | 1.1387365 | -4.2688199 | -2.7061922 |
| O | 0.8452140 | -4.7124890 | -3.8270703 |
| C | 0.6801191 | -4.9585129 | -1.4521779 |
| C | 0.7279590 | -4.3338917 | -0.2038898 |
| C | 0.2997103 | -4.9903390 | 0.9523652 |
| C | -0.2119074 | -6.2898585 | 0.8462764 |
| C | -0.2773539 | -6.9165055 | -0.3983468 |
| C | 0.1667341 | -6.2584962 | -1.5449271 |
| C | 0.3830712 | -4.3583705 | 2.3141376 |

| | | | |
|---|---|---|---|
| O | -0.1535885 | -4.8876289 | 3.3002004 |
| N | 1.0995965 | -3.2056162 | 2.4012704 |
| C | 1.2390474 | -2.4586996 | 3.6522543 |
| C | 0.3447712 | -1.2373389 | 3.6759867 |
| C | -1.0468974 | -1.3856694 | 3.7009612 |
| C | -1.8780396 | -0.2664932 | 3.6843480 |
| C | -1.3388268 | 1.0231752 | 3.6500989 |
| C | 0.0526946 | 1.1703189 | 3.6223317 |
| C | 0.8838268 | 0.0518611 | 3.6336513 |
| C | -2.2385577 | 2.2444391 | 3.6318655 |
| N | -1.8979050 | 3.1422009 | 2.5308717 |
| O | 2.0759712 | -1.4383788 | 0.0676698 |
| C | 1.8974751 | -0.1992466 | -0.0001595 |
| N | 2.9406567 | 0.6723657 | -0.1273618 |
| C | 4.2840326 | 0.1756893 | -0.2046124 |
| C | 4.7832054 | -0.7033693 | 0.7622320 |
| C | 6.0907411 | -1.1637281 | 0.6862405 |
| C | 6.9408263 | -0.7571059 | -0.3610532 |
| C | 6.4293272 | 0.1263436 | -1.3293867 |
| C | 5.1185537 | 0.5820924 | -1.2506858 |
| N | 8.2711485 | -1.1616504 | -0.3957754 |
| C | 0.5440621 | 0.3888426 | 0.0367485 |
| C | -0.5426392 | -0.3916012 | -0.0402565 |
| C | -1.8957148 | 0.1973489 | -0.0030880 |
| O | -2.0732171 | 1.4366000 | -0.0715735 |
| N | -2.9395895 | -0.6732052 | 0.1253427 |
| C | -4.2823441 | -0.1749726 | 0.2037663 |
| C | -5.1162605 | -0.5799428 | 1.2508700 |
| C | -6.4261975 | -0.1220433 | 1.3311270 |
| C | -6.9374595 | 0.7621063 | 0.3633129 |

| | | | |
|---|---|---|---|
| C | -6.0880865 | 1.1670136 | -0.6852179 |
| C | -4.7813772 | 0.7046057 | -0.7627038 |
| N | -8.2669880 | 1.1690657 | 0.3997680 |
| H | -0.6722389 | -7.9255235 | -0.4737005 |
| H | 0.1228139 | -6.7366152 | -2.5185728 |
| H | 1.0824513 | -3.3118429 | -0.1362831 |
| H | -0.5486292 | -6.7944461 | 1.7464229 |
| H | 1.4588801 | -2.7483212 | 1.5644529 |
| H | 2.0473503 | -2.7738072 | -1.6005726 |
| H | 3.2804952 | -1.9530974 | -3.5386756 |
| H | 2.1216509 | -2.8290319 | -4.5592497 |
| H | 0.9825742 | -3.1471344 | 4.4607089 |
| H | 2.2872103 | -2.1630937 | 3.7636592 |
| H | 2.9607931 | 0.3843356 | -3.7022069 |
| H | 1.4860455 | 2.3791098 | -3.7331676 |
| H | -1.9627426 | -0.1764184 | -3.6115946 |
| H | -0.4932925 | -2.1651747 | -3.5953634 |
| H | -1.4762903 | -2.3844437 | 3.7332072 |
| H | -2.9578385 | -0.3946649 | 3.7007517 |
| H | 0.4875700 | 2.1663371 | 3.5904035 |
| H | 1.9637344 | 0.1826770 | 3.6078332 |
| H | -2.2780334 | 2.1702361 | -3.7699009 |
| H | -0.9679304 | 3.1514805 | -4.4606634 |
| H | -2.1325390 | 2.8205139 | 4.5553290 |
| H | -3.2853776 | 1.9412866 | 3.5308461 |
| H | -1.4535081 | 2.7482852 | -1.5664547 |
| H | -2.0499696 | 2.7681284 | 1.5968445 |
| H | -1.0810374 | 3.3099151 | 0.1362968 |
| H | 0.6588607 | 7.9285271 | 0.4823530 |
| H | -0.1403911 | 6.7363727 | 2.5236889 |

| | | | |
|---|---|---|---|
| H | 0.5464385 | 6.7983137 | -1.7387897 |
| C | -2.7326653 | -2.1302309 | 0.2852200 |
| H | -0.4118846 | -1.4634642 | -0.1221309 |
| H | 0.4128917 | 1.4606410 | 0.1186802 |
| C | 2.7325699 | 2.1293701 | -0.2860208 |
| H | -4.7409047 | -1.2530511 | 2.0162236 |
| H | -7.0599284 | -0.4468483 | 2.1525439 |
| H | -6.4630383 | 1.8453486 | -1.4476392 |
| H | -4.1431758 | 1.0276979 | -1.5774212 |
| H | 4.7430159 | 1.2547629 | -2.0163432 |
| H | 7.0635925 | 0.4523458 | -2.1499205 |
| H | 6.4658152 | -1.8416379 | 1.4489771 |
| H | 4.1445378 | -1.0276156 | 1.5761228 |
| H | 8.7223395 | -1.1216232 | -1.3025093 |
| H | 8.4855302 | -2.0181997 | 0.1018542 |
| H | -8.4804020 | 2.0260920 | -0.0974621 |
| H | -8.7170875 | 1.1297708 | 1.3070714 |
| H | -2.2172500 | -2.5423143 | -0.5864247 |
| H | -2.1639669 | -2.3519475 | 1.1924062 |
| H | -3.7118934 | -2.6004052 | 0.3534704 |
| H | 3.7113902 | 2.6003811 | -0.3542589 |
| H | 2.1634780 | 2.3513415 | -1.1928927 |
| H | 2.2170666 | 2.5404108 | 0.5860783 |

Table 31: Cartesian coordinates and total energy in a.u. of complex **5@1**

E(RI-TPSS-D3/def2-TZVP)=

| | | | |
|---|---|---|---|
| C | 0.9376645 | 6.2330610 | -1.9313735 |
| C | 0.4360462 | 4.9305369 | -1.8179329 |
| C | 0.0869630 | 4.4406239 | -0.5562806 |
| C | 0.2082249 | 5.2413602 | 0.5823330 |
| C | 0.7099198 | 6.5421182 | 0.4552618 |
| C | 1.0704820 | 7.0337013 | -0.7979263 |
| C | 0.2877057 | 4.1184676 | -3.0735538 |
| O | 0.8838020 | 4.4344472 | -4.1153568 |
| C | -0.1717321 | 4.7570441 | 1.9516969 |
| O | 0.2424983 | 5.3205020 | 2.9754902 |
| N | -1.0086692 | 3.6860488 | 1.9907696 |
| C | -1.4829188 | 3.0890341 | 3.2328895 |
| C | -0.8817620 | 1.7216029 | 3.4825465 |
| C | 0.4938951 | 1.5141241 | 3.3350474 |
| C | 1.0491658 | 0.2600340 | 3.5770652 |
| C | 0.2448985 | -0.8160922 | 3.9683358 |
| C | -1.1308687 | -0.6067427 | 4.1214161 |
| C | -1.6873487 | 0.6489176 | 3.8785216 |
| C | 0.8366820 | -2.1952928 | 4.1567022 |
| N | 0.5607203 | -3.0593681 | 3.0064356 |
| C | -0.2912066 | -4.1169384 | 3.0726355 |
| C | -0.4384750 | -4.9297041 | 1.8173959 |
| C | -0.0888495 | -4.4400003 | 0.5558423 |
| C | -0.2084315 | -5.2412731 | -0.5825704 |
| C | -0.7091152 | -6.5424028 | -0.4553168 |
| C | -1.0705316 | -7.0336857 | 0.7977480 |
| C | -0.9392806 | -6.2325162 | 1.9310075 |
| C | 0.1727813 | -4.7573685 | -1.9517511 |
| O | -0.2391682 | -5.3221433 | -2.9757544 |

| | | | |
|---|---|---|---|
| O | -0.8896723 | -4.4310615 | 4.1136231 |
| N | 1.0085743 | -3.6855069 | -1.9903114 |
| C | 1.4833203 | -3.0881222 | -3.2320563 |
| C | 0.8816338 | -1.7209726 | -3.4819080 |
| C | 1.6870663 | -0.6478107 | -3.8769312 |
| C | 1.1302478 | 0.6076368 | -4.1200220 |
| C | -0.2457829 | 0.8162537 | -3.9683185 |
| C | -1.0499054 | -0.2603106 | -3.5779820 |
| C | -0.4942477 | -1.5141690 | -3.3355934 |
| C | -0.8379732 | 2.1952268 | -4.1570339 |
| N | -0.5622245 | 3.0593728 | -3.0067782 |
| O | -1.7210300 | 1.7371365 | -0.4986966 |
| C | -1.8332698 | 0.6178111 | 0.0453230 |
| C | -0.6383840 | -0.2879454 | 0.2944488 |
| C | 0.6398407 | 0.2877522 | -0.2950395 |
| C | 1.8345901 | -0.6183151 | -0.0462326 |
| N | 3.0484597 | -0.1579882 | -0.4347516 |
| C | 4.2512605 | -0.9529168 | -0.0960905 |
| N | -3.0470324 | 0.1576006 | 0.4345190 |
| C | -4.2500467 | 0.9520711 | 0.0954939 |
| O | 1.7219267 | -1.7380553 | 0.4969497 |
| H | -1.4566602 | -8.0446183 | 0.8918743 |
| H | -0.8119387 | -7.1512055 | -1.3479543 |
| H | 0.2459988 | -3.4120384 | 0.4559739 |
| H | -1.2183535 | -6.6008512 | 2.9132104 |
| H | 0.9851837 | -2.7870503 | 2.1217630 |
| H | 1.3464993 | -3.2743251 | -1.1249658 |
| H | 2.5739790 | -3.0170044 | -3.1956628 |
| H | 1.2100395 | -3.7796736 | -4.0347170 |
| H | 0.4089174 | -2.6918488 | 5.0300294 |

| | | | |
|---|---|---|---|
| H | 1.9218983 | -2.1267221 | 4.2871890 |
| H | 2.7590664 | -0.7959605 | -3.9857824 |
| H | 1.7672857 | 1.4371971 | -4.4177916 |
| H | -2.1202990 | -0.1087320 | -3.4578091 |
| H | -1.1280415 | -2.3375602 | -3.0187552 |
| H | -1.7679370 | -1.4358388 | 4.4204650 |
| H | -2.7591730 | 0.7975373 | 3.9884322 |
| H | 1.1277849 | 2.3371404 | 3.0174253 |
| H | 2.1193513 | 0.1078790 | 3.4557881 |
| H | -1.9231561 | 2.1263115 | -4.2876865 |
| H | -0.4102202 | 2.6917735 | -5.0303746 |
| H | -1.2086380 | 3.7805213 | 4.0352799 |
| H | -2.5736349 | 3.0185834 | 3.1972144 |
| H | -0.9848081 | 2.7853968 | -2.1216953 |
| H | -1.3497285 | 3.2768498 | 1.1257606 |
| H | -0.2489784 | 3.4130187 | -0.4564800 |
| H | 1.4572779 | 8.0443912 | -0.8919632 |
| H | 0.8143039 | 7.1503311 | 1.3481230 |
| H | 1.2161946 | 6.6015715 | -2.9136638 |
| C | -3.2330936 | -1.1244478 | 1.1197535 |
| C | 3.2347177 | 1.1244688 | -1.1193187 |
| C | 3.4373304 | 2.3186412 | -0.1993021 |
| H | 4.0995763 | 1.0161699 | -1.7811304 |
| H | 2.3788454 | 1.3029804 | -1.7749912 |
| C | -3.4366278 | -2.3191130 | 0.2005439 |
| H | -2.3765181 | -1.3027185 | 1.7746729 |
| H | -4.0975136 | -1.0154929 | 1.7820524 |
| C | 4.5367353 | -2.0703880 | -1.0799370 |
| H | 5.0872214 | -0.2488656 | -0.0591196 |
| H | 4.1027369 | -1.3684146 | 0.9033251 |

| | | | |
|---|---|---|---|
| C | -4.5356006 | 2.0700525 | 1.0787357 |
| H | -4.1017187 | 1.3669741 | -0.9041929 |
| H | -5.0858891 | 0.2478533 | 0.0590493 |
| C | -4.1955341 | 3.3907147 | 0.7634215 |
| C | -4.4579717 | 4.4268998 | 1.6609272 |
| C | -5.0624771 | 4.1525147 | 2.8890333 |
| C | -5.4087778 | 2.8379325 | 3.2122054 |
| C | -5.1509415 | 1.8053720 | 2.3098028 |
| H | -3.7153581 | 3.6003993 | -0.1883582 |
| H | -4.1821702 | 5.4458357 | 1.4046203 |
| H | -5.2629023 | 4.9571582 | 3.5908773 |
| H | -5.8844245 | 2.6178319 | 4.1638782 |
| H | -5.4420192 | 0.7883948 | 2.5622974 |
| C | 5.1519998 | -1.8051126 | -2.3109188 |
| C | 5.4095487 | -2.8371939 | -3.2139415 |
| C | 5.0631369 | -4.1519224 | -2.8914411 |
| C | 4.4587717 | -4.4269064 | -1.6634055 |
| C | 4.1965402 | -3.3911747 | -0.7653102 |
| H | 5.4432297 | -0.7880415 | -2.5628518 |
| H | 5.8850743 | -2.6166485 | -4.1655761 |
| H | 5.2633704 | -4.9562231 | -3.5937345 |
| H | 4.1828037 | -5.4459355 | -1.4076454 |
| H | 3.7162571 | -3.6013035 | 0.1863128 |
| C | 3.5802599 | 3.5894701 | -0.7714326 |
| C | 3.7504055 | 4.7124012 | 0.0343684 |
| C | 3.7739421 | 4.5828531 | 1.4250129 |
| C | 3.6371141 | 3.3212925 | 2.0006270 |
| C | 3.4720802 | 2.1944886 | 1.1905181 |
| H | 3.5396154 | 3.7033463 | -1.8526414 |
| H | 3.8400266 | 5.6928933 | -0.4226631 |

| | | | |
|---|---|---|---|
| H | 3.8825262 | 5.4613565 | 2.0537239 |
| H | 3.6508339 | 3.2108027 | 3.0814716 |
| H | 3.3607269 | 1.2146781 | 1.6460963 |
| C | -3.4705032 | -2.1960265 | -1.1893654 |
| C | -3.6363800 | -3.3233295 | -1.9986233 |
| C | -3.7749162 | -4.5842607 | -1.4220427 |
| C | -3.7522169 | -4.7127351 | -0.0312844 |
| C | -3.5812845 | -3.5893083 | 0.7736331 |
| H | -3.3577751 | -1.2167324 | -1.6457001 |
| H | -3.6494446 | -3.2136596 | -3.0795542 |
| H | -3.8843154 | -5.4631405 | -2.0500901 |
| H | -3.8431387 | -5.6927360 | 0.4265370 |
| H | -3.5414600 | -3.7025462 | 1.8549805 |
| H | -0.5193953 | -0.4352487 | 1.3739689 |
| H | 0.8448618 | 1.2761514 | 0.1318525 |
| H | -0.8433404 | -1.2763987 | -0.1323547 |
| H | 0.5207636 | 0.4352402 | -1.3745347 |

Table 32: Cartesian coordinates and total energy in a.u. of complex **4@1**

E(RI-TPSS-D3/def2-TZVP)=

| | | | |
|---|---|---|---|
| C | 0.6100719 | 6.0440195 | -0.7324363 |
| C | 0.0043800 | 5.1813265 | -1.6503815 |
| C | -0.0613066 | 3.8140276 | -1.3622546 |
| C | 0.4796760 | 3.3142777 | -0.1794644 |
| C | 1.0889761 | 4.1805026 | 0.7311124 |
| C | 1.1523027 | 5.5462984 | 0.4539107 |

| | | | |
|---|---|---|---|
| C | -0.5275408 | 5.7217443 | -2.9628383 |
| N | -1.8785494 | 5.2348132 | -3.2851823 |
| C | -2.9885313 | 5.8112433 | -2.4895979 |
| C | -3.7093597 | 6.9382995 | -3.2020669 |
| C | -4.9298721 | 6.7009133 | -3.8461185 |
| C | -5.6016249 | 7.7352999 | -4.4991075 |
| C | -5.0566066 | 9.0207875 | -4.5203620 |
| C | -3.8414758 | 9.2685891 | -3.8772711 |
| C | -3.1764991 | 8.2342164 | -3.2172964 |
| C | -2.1871892 | 4.2784864 | -4.1988831 |
| C | -1.0774010 | 3.5747212 | -4.8839909 |
| C | -1.3229339 | 2.5097589 | -5.6566873 |
| C | -0.2131462 | 1.8059178 | -6.3417409 |
| O | 0.9840578 | 2.0993336 | -6.1143048 |
| O | -3.3843916 | 3.9846032 | -4.4256973 |
| N | -0.5217475 | 0.8500475 | -7.2559562 |
| C | -1.8728028 | 0.3637107 | -7.5793217 |
| C | -2.4026172 | 0.9036399 | -8.8928078 |
| C | -3.0028678 | 0.0401540 | -9.8135573 |
| C | -3.5425170 | 0.5375438 | -11.0012480 |
| C | -3.4820819 | 1.9037744 | -11.2768845 |
| C | -2.8782624 | 2.7708426 | -10.3634305 |
| C | -2.3397805 | 2.2714057 | -9.1793910 |
| C | 0.5883707 | 0.2735306 | -8.0512912 |
| C | 1.3083074 | -0.8542873 | -7.3391437 |
| C | 0.7746789 | -2.1499009 | -7.3247115 |
| C | 1.4388292 | -3.1849665 | -6.6649997 |
| C | 2.6539181 | -2.9381871 | -6.0214255 |
| C | 3.1997218 | -1.6530184 | -6.0419274 |
| C | 2.5287705 | -0.6179211 | -6.6946185 |

| | | | |
|---|---|---|---|
| N | 1.6576596 | 0.2124886 | -3.3831303 |
| C | 0.7909352 | -0.9652066 | -3.3738426 |
| C | -0.6757508 | -0.5832672 | -3.3944461 |
| C | -1.5441483 | -1.1076672 | -4.3561604 |
| C | -2.8861656 | -0.7290273 | -4.3830307 |
| C | -3.3829356 | 0.1965792 | -3.4580839 |
| C | -2.5158448 | 0.7127805 | -2.4897761 |
| C | -1.1805146 | 0.3201564 | -2.4529841 |
| C | -4.8197203 | 0.6643544 | -3.5461163 |
| N | -5.0436882 | 1.4917631 | -4.7346018 |
| C | -5.6558585 | 1.0106983 | -5.8496530 |
| O | -6.0967896 | -0.1478283 | -5.9176340 |
| C | -5.8074168 | 1.9638062 | -7.0030445 |
| C | -6.6427095 | 1.5808210 | -8.0605700 |
| C | -6.8316815 | 2.4294178 | -9.1495299 |
| C | -6.1821593 | 3.6605579 | -9.2004661 |
| C | -5.3390170 | 4.0548227 | -8.1545578 |
| C | -5.1549798 | 3.1995263 | -7.0640606 |
| C | -4.6105693 | 5.3602412 | -8.2899766 |
| N | -4.0577286 | 5.8718733 | -7.1579812 |
| C | -3.1914397 | 7.0499117 | -7.1671171 |
| C | -1.7246076 | 6.6684434 | -7.1463843 |
| C | -1.2196598 | 5.7644808 | -8.0872395 |
| C | 0.1156672 | 5.3719279 | -8.0500185 |
| C | 0.9826398 | 5.8888279 | -7.0819718 |
| C | 0.4857737 | 6.8151838 | -6.1578375 |
| C | -0.8562891 | 7.1936657 | -6.1850461 |
| C | 2.4193702 | 5.4210167 | -6.9934540 |
| N | 2.6431200 | 4.5933495 | -5.8051022 |
| C | 3.2556360 | 5.0739257 | -4.6900266 |

| | | | |
|---|---|---|---|
| O | 3.6957692 | 6.2327091 | -4.6212935 |
| O | -4.5192409 | 5.9308070 | -9.3885273 |
| C | 3.4089293 | 4.1197228 | -3.5377903 |
| C | 2.7552263 | 2.8847076 | -3.4762720 |
| C | 2.9413168 | 2.0280645 | -2.3871799 |
| C | 3.7878193 | 2.4202347 | -1.3432095 |
| C | 4.4385876 | 3.6507060 | -1.3946368 |
| C | 4.2475010 | 4.5007095 | -2.4821365 |
| C | 2.2119836 | 0.7231844 | -2.2514159 |
| O | 2.1214783 | 0.1521415 | -1.1530594 |
| H | 5.0908061 | 3.9527037 | -0.5803960 |
| H | 3.9104864 | 1.7559075 | -0.4939583 |
| H | 2.0601243 | 2.6050081 | -4.2620160 |
| H | 4.7400641 | 5.4665146 | -2.5319891 |
| H | 2.2141137 | 3.6688150 | -5.8155834 |
| H | 1.7213951 | 0.7254111 | -4.2563024 |
| H | 1.0355695 | -1.5831066 | -4.2411014 |
| H | 1.0332223 | -1.5263848 | -2.4669504 |
| H | 3.1037122 | 6.2693619 | -6.9207718 |
| H | 2.6815796 | 4.8309155 | -7.8768321 |
| H | -1.1634176 | -1.8112163 | -5.0931287 |
| H | -3.5555214 | -1.1417279 | -5.1342728 |
| H | -2.8890179 | 1.4304460 | -1.7622922 |
| H | -0.5168695 | 0.7180877 | -1.6908067 |
| H | 1.1550751 | 7.2285485 | -5.4069109 |
| H | -1.2371404 | 7.8976489 | -5.4485551 |
| H | -1.8831344 | 5.3660660 | -8.8492981 |
| H | 0.4889093 | 4.6537393 | -8.7769527 |
| H | -5.0816462 | 1.2546311 | -2.6627738 |
| H | -5.5040312 | -0.1840481 | -3.6184202 |

| | | | |
|---|---|---|---|
| H | -3.4339470 | 7.6111315 | -8.0739231 |
| H | -3.4363959 | 7.6675975 | -6.2998033 |
| H | -4.6134301 | 2.4157431 | -4.7247646 |
| H | -4.1218726 | 5.3593180 | -6.2846457 |
| H | -4.4623662 | 3.4808098 | -6.2767120 |
| H | -7.4812190 | 2.1258230 | -9.9653153 |
| H | -6.3030303 | 4.3237578 | -10.0508491 |
| H | -7.1343636 | 0.6145416 | -8.0110486 |
| H | -1.8297792 | -0.7288741 | -7.6131328 |
| H | -2.5459957 | 0.6118871 | -6.7585205 |
| H | 0.1449117 | 5.4747304 | -3.7846183 |
| H | -0.5712526 | 6.8142757 | -2.9282147 |
| H | 0.1435932 | -0.0792325 | -8.9856853 |
| H | 1.2868538 | 1.0810926 | -8.2780406 |
| H | -3.6865004 | 5.0034636 | -2.2620309 |
| H | -2.5434737 | 6.1648002 | -1.5556395 |
| H | -5.3465787 | 5.6978984 | -3.8354822 |
| H | -6.5459571 | 7.5354860 | -4.9974559 |
| H | -5.5759344 | 9.8253112 | -5.0332617 |
| H | -3.4152696 | 10.2679656 | -3.8827954 |
| H | -2.2440050 | 8.4432137 | -2.6982410 |
| H | -0.1577645 | -2.3581118 | -7.8441728 |
| H | 1.0120602 | -4.1841082 | -6.6600612 |
| H | 3.1726199 | -3.7432639 | -5.5087636 |
| H | 4.1439984 | -1.4539918 | -5.5431599 |
| H | 2.9460295 | 0.3848756 | -6.7046107 |
| H | -3.0536124 | -1.0248194 | -9.5976600 |
| H | -4.0091447 | -0.1422087 | -11.7088086 |
| H | -3.9075026 | 2.2945910 | -12.1968081 |
| H | -2.8504901 | 3.8373987 | -10.5659606 |

| | | | |
|---|---|---|---|
| H | -1.8754542 | 2.9497524 | -8.4677691 |
| H | -0.5298296 | 3.1362286 | -2.0716356 |
| H | 0.4494979 | 2.2480365 | 0.0243440 |
| H | 1.5163321 | 3.7893766 | 1.6500046 |
| H | 1.6232094 | 6.2254202 | 1.1592462 |
| H | 0.6630528 | 7.1086434 | -0.9495008 |
| H | -2.3477111 | 2.1828204 | -5.7801191 |
| H | -0.0526329 | 3.9016904 | -4.7605104 |