# Electronic Supplementary Information

## Unveiling the High Reactivity of Experimental *Pseudodiradical* Azomethine Ylides within Molecular Electron Density Theory

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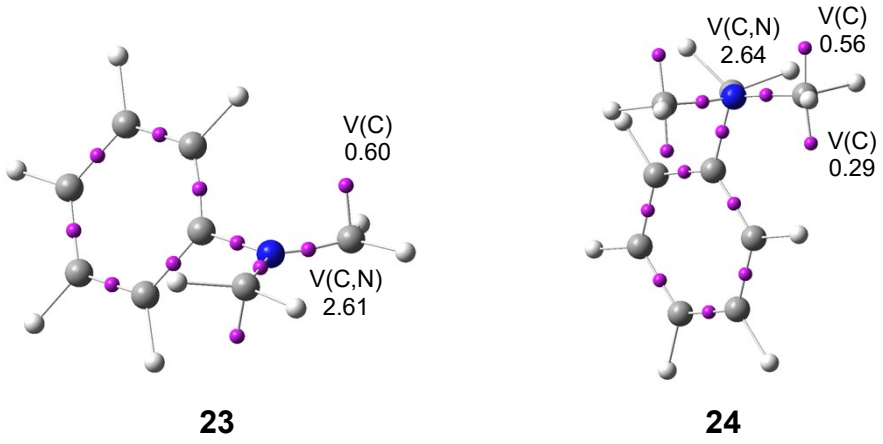



**23** **24**

**Figure S1.** ELF topological analysis of experimental non-stabilized *N*-phenyl and *N*-benzyl AYs **23** and **24**. Populations of the V(C) monosynaptic and V(C,N) disynaptic basins are given in average number of electrons, e.

**Table S1.** *ω*B97X-D/6-311G(d) total energies, in Hartree, of the stationary points involved in the 32CA reactions of AY **18** with styrene **25**, benzaldehyde **26**, and MFB **21**, in gas phase and in benzene.

| Structure | *Gas phase* | *Benzene* |
|---|---|---|
| **18** | -173.180313 | -173.182240 |
| **25** | -309.608774 | -309.610501 |
| **MC-I** | -482.802934 | -482.805255 |
| **TS-I-n** | -482.796095 | -482.798665 |
| **TS-I-x** | -482.796838 | -482.799795 |
| **CA-I-n** | -482.908875 | -482.910521 |
| **CA-I-x** | -482.905347 | -482.907293 |
| **26** | -345.535472 | -345.538400 |
| **MC-II** | -518.732018 | -518.735696 |
| **TS-II-n** | -518.730011 | -518.734516 |
| **TS-II-x** | -518.727332 | -518.731996 |
| **CA-II-n** | -518.801309 | -518.804111 |
| **CA-II-x** | -518.801415 | -518.804461 |
| **21** | -573.396588 | -573.400651 |
| **MC-III** | -746.595529 | -746.600707 |
| **TS-III-n** | -746.595013 | -746.600413 |
| **TS-III-x** | -746.592999 | -746.598060 |
| **TS-IV-n** | -746.582284 | -746.587436 |
| **TS-IV-x** | -746.577104 | -746.583584 |
| **CA-III-n** | -746.669846 | -746.673471 |
| **CA-III-x** | -746.669761 | -746.673476 |
| **CA-IV-n** | -746.633327 | -746.637862 |
| **CA-IVx** | -746.639417 | -746.643600 |

**Table S2.** $\omega$B97X-D/6-311G(d) absolute enthalpies (H, in Hartree), entropies (S, in cal·mol$^{-1}$K$^{-1}$), and Gibbs free energies (G, in Hartree), computed at 353.25 K in benzene, of the stationary points involved in the 32CA reactions of AY **18** with styrene **25**, benzaldehyde **26**, and MBF **21**.

| Structure | H | S | G |
|---|---|---|---|
| **18** | -173.078211 | 74.2 | -173.119988 |
| **25** | -309.467154 | 82.0 | -309.513336 |
| **MC-I** | -482.554237 | 123.8 | -482.623918 |
| **TS-I-n** | -482.548348 | 115.8 | -482.613526 |
| **TS-I-x** | -482.549728 | 116.1 | -482.615062 |
| **CA-I-n** | -482.654957 | 109.1 | -482.716400 |
| **CA-I-x** | -482.651830 | 110.4 | -482.713976 |
| **26** | -345.418068 | 84.1 | -345.465420 |
| **MC-II** | -518.508656 | 119.2 | -518.575767 |
| **TS-II-n** | -518.508140 | 112.9 | -518.571704 |
| **TS-II-x** | -518.505783 | 115.6 | -518.570840 |
| **CA-II-n** | -518.572723 | 108.4 | -518.633740 |
| **CA-II-x** | -518.573092 | 109.1 | -518.634486 |
| **21** | -573.231123 | 111.5 | -573.293872 |
| **MC-III** | -746.324313 | 142.8 | -746.404712 |
| **TS-III-n** | -746.324580 | 138.9 | -746.402790 |
| **TS-III-x** | -746.322592 | 140.5 | -746.401695 |
| **TS-IV-n** | -746.312135 | 136.5 | -746.388948 |
| **TS-IV-x** | -746.308510 | 138.9 | -746.386682 |
| **CA-III-n** | -746.392813 | 132.5 | -746.467377 |
| **CA-III-x** | -746.392793 | 133.7 | -746.468033 |
| **CA-IV-n** | -746.358674 | 131.1 | -746.432470 |
| **CA-IV-x** | -746.364407 | 132.8 | -746.439174 |

**Table S3.** C1–C(O)4 and C3–C5 distances, in angstroms Å, at the ωB97X-D/6-311G(d) optimized geometries of the TSs associated with the 32CA reactions of AY **18** with styrene **25**, benzaldehyde **26** and MFB **21**, in gas phase and in solvent.

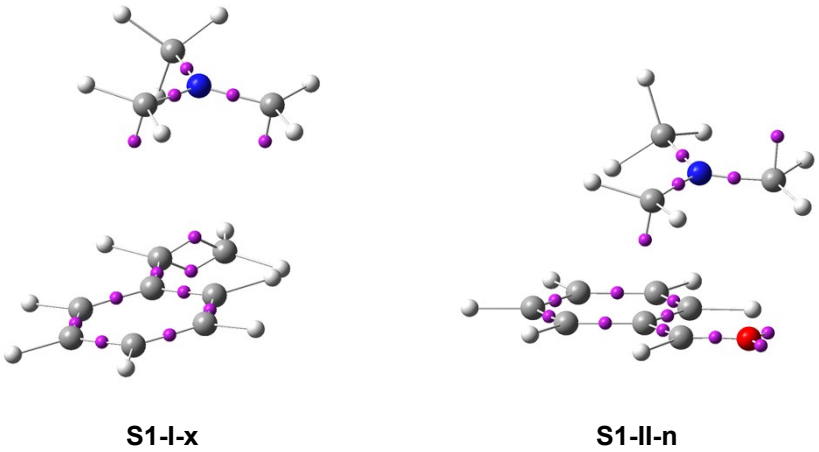
| | *Gas phase* | | *Benzene* | |
|---|---|---|---|---|
| Structure | C3–C5 | C1–C(O)4 | C3–C5 | C1–C(O)4 |
| **TS-I-n** | 2.514 | 2.402 | 2.523 | 2.401 |
| **TS-I-x** | 2.602 | 2.420 | 2.613 | 2.415 |
| **TS-II-n** | 2.238 | 2.571 | 2.291 | 2.661 |
| **TS-II-x** | 2.284 | 2.490 | 2.354 | 2.587 |
| **TS-III-n** | 2.576 | 2.834 | 2.358 | 2.672 |
| **TS-III-n** | 2.397 | 2.636 | 2.503 | 2.792 |
| **TS-IV-n** | 2.105 | 2.664 | 2.071 | 2.739 |
| **TS-IV-x** | 2.130 | 2.643 | 2.162 | 2.702 |

**Table S4.** Most relevant ELF valence basin populations, IRC values and distances of the C–C forming bonds, at the IRC structures **S1** – **S8** defining the seven topological phases associated with the molecular mechanism along the more favorable *exo* stereoisomeric path of the 32CA reaction between AY **18** and styrene **25**. Distances are given in angstroms, Å, IRC coordinates in Å·amu$^{1/2}$, and electron populations in average number of electrons, e.

| Structures | **S1** | **S2** | **S3** | **S4** | **S5** | **S6** | **S7** | **S8** |
|---|---|---|---|---|---|---|---|---|
| Phases | | *I* | *II* | *III* | *IV* | *V* | *VI* | *VII* |
| d(C1–C4) | 2.875 | 2.444 | 2.381 | 2.193 | 2.151 | 2.069 | 1.712 | 1.542 |
| d(C3–C5) | 2.936 | 2.621 | 2.579 | 2.452 | 2.423 | 2.366 | 2.056 | 1.579 |
| IRC | -2.74 | 0.12 | 0.48 | 1.55 | 1.79 | 2.27 | 4.53 | 7.39 |
| V(C1,N2) | 2.64 | 2.51 | 2.42 | 2.17 | 2.12 | 2.03 | 1.77 | 1.71 |
| V(N2) | | 0.33 | 0.49 | 1.03 | 1.15 | 1.36 | 1.97 | 2.22 |
| V(N2,C3) | 2.70 | 2.60 | 2.54 | 2.33 | 2.28 | 2.20 | 1.94 | 1.74 |
| V(C4,C5) | 1.63 | 1.58 | 3.24 | 3.03 | 2.78 | 2.54 | 2.07 | 1.88 |
| V'(C4,C5) | 1.72 | 1.70 | | | | | | |
| V(C1) | 0.53 | 0.68 | 0.71 | 0.78 | 0.80 | | | |
| V(C3) | 0.45 | 0.52 | 0.53 | 0.57 | 0.59 | 0.60 | | |
| V(C4) | | | | 0.26 | 0.33 | | | |
| V(C5) | | | | | 0.17 | 0.37 | | |
| V(C1,C4) | | | | | | 1.27 | 1.69 | 1.88 |
| V(C3,C5) | | | | | | | 1.43 | 1.83 |

**Table S5.** Most relevant ELF valence basin populations, IRC values and distances of the C–C forming bonds, at the IRC structures **S1** – **S9** defining the eight topological phases associated with the molecular mechanism along the more favorable *endo* stereoisomeric path of the 32CA reaction between AY **18** and benzaldehyde **26**. Distances are given in angstroms, Å, IRC coordinates in Å·amu$^{1/2}$, and electron populations in average number of electrons, e.

| Structures | **S1** | **S2** | **S3** | **S4** | **S5** | **S6** | **S7** | **S8** | **S9** |
|---|---|---|---|---|---|---|---|---|---|
| Phases | *I* | *II* | *III* | *IV* | *V* | *VI* | *VII* | *VIII* | |
| d(C1–O4) | 2.876 | 2.786 | 2.551 | 2.518 | 2.382 | 2.022 | 1.807 | 1.776 | 1.445 |
| d(C3–C5) | 2.656 | 2.587 | 2.141 | 2.047 | 1.743 | 1.6 | 1.575 | 1.573 | 1.546 |
| IRC | -3.96 | -2.31 | 0.66 | 1.16 | 2.81 | 4.95 | 6.11 | 6.28 | 8.25 |
| V(C1,N2) | 2.83 | 2.88 | 3.27 | 3.34 | 2.97 | 2.45 | 2.24 | 2.21 | 1.85 |
| V(N2) | | | | | 0.69 | 1.52 | 1.81 | 1.84 | 2.12 |
| V(N2,C3) | 2.51 | 2.49 | 2.34 | 2.27 | 1.97 | 1.72 | 1.65 | 1.65 | 1.64 |
| V(O4,C5) | 2.31 | 2.30 | 2.05 | 1.92 | 1.62 | 1.44 | 1.38 | 1.37 | 1.28 |
| V(C1) | 0.27 | | | | | 0.15 | 0.29 | | |
| V(C3) | 0.83 | 0.86 | 0.99 | | | | | | |
| V(O4) | 2.60 | 2.70 | 2.78 | 2.77 | 2.94 | 2.97 | 2.71 | 2.70 | 2.44 |
| V'(O4) | 2.66 | 2.58 | 2.73 | 2.82 | 2.86 | 2.86 | 2.73 | 2.71 | 2.52 |
| V''(O4) | | | | | | | 0.34 | | |
| V(C5) | | | 0.12 | | | | | | |
| V(C1,O4) | | | | | | | | 0.68 | 1.26 |
| V(C3,C5) | | | | 1.26 | 1.63 | 1.83 | 1.88 | 1.88 | 1.93 |



**S1-I-x** **S1-II-n**

**Figure S2.** ELF topological analysis of **S1** along the IRCs associated with the *exo* and *endo* steroisomeric reaction paths of the 32CA reactions of AY **18** with styrene **25** and benzaldeyde **26**, respectively, showing the orientation of the carbon *pseudoradical* centers.

Cartesian coordinates of the stationary points involved in the 32CA reaction between AY **18** and styrene **25**.

AY **18**

E = -173.168460572 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.717551 | -1.197831 | -0.009586 |
| 1 | 0.097918 | -2.078397 | -0.014957 |
| 1 | 1.794746 | -1.255224 | 0.032800 |
| 6 | 0.717596 | 1.197806 | -0.009538 |
| 1 | 0.098001 | 2.078398 | -0.014875 |
| 1 | 1.794794 | 1.255154 | 0.032844 |
| 6 | -1.332194 | 0.000021 | 0.007680 |
| 1 | -1.703510 | -0.886226 | -0.502572 |
| 1 | -1.666534 | -0.000076 | 1.044755 |
| 1 | -1.703485 | 0.886378 | -0.502400 |
| 7 | 0.139412 | -0.000001 | -0.025290 |

Styrene **25**

E = -309.595264231 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.349747 | -0.786408 | 0.087395 |
| 6 | 0.039610 | -0.851671 | 0.134792 |
| 6 | 0.799305 | 0.303931 | 0.042402 |
| 6 | 0.188553 | 1.554806 | -0.099809 |
| 6 | -1.207153 | 1.603237 | -0.145721 |
| 6 | -1.971159 | 0.446980 | -0.053392 |
| 1 | -1.941611 | -1.692733 | 0.159973 |
| 1 | 0.533885 | -1.811480 | 0.244667 |
| 1 | 1.880762 | 0.227438 | 0.081847 |
| 1 | -1.701591 | 2.564322 | -0.255727 |
| 1 | -3.053617 | 0.511233 | -0.091651 |
| 6 | 0.948056 | 2.814048 | -0.202497 |
| 6 | 2.269774 | 2.964618 | -0.178527 |
| 1 | 0.334518 | 3.707165 | -0.309260 |
| 1 | 2.717711 | 3.948286 | -0.263024 |
| 1 | 2.957309 | 2.131037 | -0.075497 |

**MC-I**

E = -482.777141673 a.u.

| | | | |
|---|---|---|---|
| 6 | -2.088428 | -0.170627 | 1.579361 |
| 6 | -2.719176 | -0.664976 | -0.668038 |
| 1 | -1.481624 | -0.471667 | 2.416750 |

| | | | |
|---|---|---|---|
| 1 | -2.754991 | 0.676280 | 1.630570 |
| 1 | -2.595685 | -1.352875 | -1.488073 |
| 1 | -3.423544 | 0.150666 | -0.702809 |
| 7 | -2.052404 | -0.886754 | 0.460278 |
| 6 | -1.101747 | -2.010298 | 0.431514 |
| 1 | -0.231405 | -1.722080 | -0.155208 |
| 1 | -0.800746 | -2.258099 | 1.445789 |
| 1 | -1.587791 | -2.872416 | -0.023139 |
| 6 | -0.412725 | 1.940676 | -0.019476 |
| 6 | -1.309450 | 2.226137 | -0.961820 |
| 1 | -2.090622 | 2.958072 | -0.783925 |
| 1 | -1.321213 | 1.734518 | -1.927852 |
| 6 | 0.680225 | 0.958610 | -0.134325 |
| 6 | 1.077013 | 0.412974 | -1.357519 |
| 6 | 1.336270 | 0.523251 | 1.020601 |
| 6 | 2.078097 | -0.547162 | -1.420918 |
| 1 | 0.596254 | 0.743064 | -2.272139 |
| 6 | 2.336177 | -0.436885 | 0.963581 |
| 1 | 1.036881 | 0.933586 | 1.979888 |
| 6 | 2.708823 | -0.982102 | -0.260246 |
| 1 | 2.370933 | -0.953779 | -2.383547 |
| 1 | 2.824798 | -0.762209 | 1.876450 |
| 1 | 3.492062 | -1.731270 | -0.310536 |
| 1 | -0.479635 | 2.449337 | 0.939253 |

**TS-I-n**

E = -482.796094720 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.505802 | -1.469984 | -0.156852 |
| 6 | 1.419578 | -1.435337 | -1.170542 |
| 1 | 2.170118 | -2.210819 | -1.250196 |
| 1 | 1.257803 | -0.854230 | -2.070010 |
| 6 | 1.703020 | -0.008097 | 1.501309 |
| 6 | 3.089009 | 0.103793 | -0.387099 |
| 1 | 0.991297 | 0.500594 | 2.132948 |
| 1 | 2.216112 | -0.885902 | 1.863295 |
| 1 | 3.485503 | 0.736297 | -1.168236 |
| 1 | 3.686198 | -0.727668 | -0.043731 |
| 7 | 2.269415 | 0.678043 | 0.508615 |
| 6 | 1.613948 | 1.924400 | 0.103678 |
| 1 | 0.797595 | 1.697816 | -0.583400 |
| 1 | 1.216092 | 2.424863 | 0.984547 |

| | | | |
|---|---|---|---|
| 1 | 2.343220 | 2.572786 | -0.379992 |
| 6 | -0.771770 | -0.729402 | -0.132914 |
| 6 | -1.211849 | 0.065880 | -1.197967 |
| 6 | -1.612203 | -0.829546 | 0.983425 |
| 6 | -2.417044 | 0.753171 | -1.134521 |
| 1 | -0.610799 | 0.142633 | -2.097534 |
| 6 | -2.819840 | -0.151602 | 1.046248 |
| 1 | -1.298568 | -1.446574 | 1.820282 |
| 6 | -3.229044 | 0.653562 | -0.011549 |
| 1 | -2.729261 | 1.362279 | -1.976294 |
| 1 | -3.446052 | -0.250924 | 1.926471 |
| 1 | -4.171566 | 1.186760 | 0.034984 |
| 1 | 0.588765 | -2.255237 | 0.587274 |

**TS-I-x**

E = -482.796837602 a.u.

| | | | |
|---|---|---|---|
| 6 | -3.538572 | 0.064101 | -0.609695 |
| 6 | -2.693801 | 1.167865 | -0.611718 |
| 6 | -1.434571 | 1.092661 | -0.032509 |
| 6 | -0.984454 | -0.089107 | 0.570171 |
| 6 | -1.846372 | -1.192293 | 0.557608 |
| 6 | -3.105037 | -1.118381 | -0.020616 |
| 1 | -4.521251 | 0.124043 | -1.063170 |
| 1 | -3.016849 | 2.096062 | -1.071002 |
| 1 | -0.790047 | 1.964962 | -0.053246 |
| 1 | -1.517222 | -2.121460 | 1.012786 |
| 1 | -3.752266 | -1.988817 | -0.011063 |
| 6 | 0.346080 | -0.204945 | 1.186624 |
| 1 | 0.616671 | -1.197865 | 1.530404 |
| 6 | 1.131722 | 0.850633 | 1.533271 |
| 1 | 0.780206 | 1.872248 | 1.459393 |
| 1 | 1.999704 | 0.700761 | 2.163808 |
| 6 | 1.483644 | -0.828137 | -1.069166 |
| 6 | 2.469346 | 1.217195 | -0.450107 |
| 1 | 1.622880 | -1.889564 | -1.204955 |
| 1 | 0.627705 | -0.332225 | -1.498731 |
| 1 | 3.390365 | 1.723347 | -0.201842 |
| 1 | 1.672208 | 1.775025 | -0.919106 |
| 7 | 2.540912 | -0.093871 | -0.730635 |
| 6 | 3.697667 | -0.810645 | -0.194842 |
| 1 | 3.523835 | -1.026271 | 0.862614 |

| | | | |
|---|---|---|---|
| 1 | 3.834385 | -1.741492 | -0.742630 |
| 1 | 4.589379 | -0.195333 | -0.302948 |

**CA-I-n**

E = -482.881840853 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.481619 | -0.532619 | 1.102578 |
| 6 | -2.852042 | 0.557498 | -0.421284 |
| 1 | -0.884531 | -1.445999 | 1.143268 |
| 1 | -1.804705 | -0.314147 | 2.125084 |
| 1 | -3.482083 | 0.442018 | -1.305958 |
| 1 | -3.367530 | 1.242336 | 0.263308 |
| 7 | -2.657722 | -0.728045 | 0.247906 |
| 6 | -2.516357 | -1.828412 | -0.689596 |
| 1 | -1.692999 | -1.711883 | -1.417225 |
| 1 | -2.347884 | -2.757226 | -0.140224 |
| 1 | -3.444690 | -1.946628 | -1.253758 |
| 6 | -0.663821 | 0.680515 | 0.544984 |
| 6 | -1.443166 | 1.078120 | -0.724588 |
| 1 | -1.403483 | 2.152522 | -0.917307 |
| 1 | -1.029368 | 0.573109 | -1.602625 |
| 6 | 0.805415 | 0.417144 | 0.319540 |
| 6 | 1.235234 | -0.646218 | -0.478117 |
| 6 | 1.773128 | 1.239765 | 0.892470 |
| 6 | 2.585672 | -0.876910 | -0.697197 |
| 1 | 0.502687 | -1.307465 | -0.932870 |
| 6 | 3.128549 | 1.013419 | 0.677382 |
| 1 | 1.461866 | 2.072549 | 1.517119 |
| 6 | 3.540081 | -0.046210 | -0.119075 |
| 1 | 2.895807 | -1.709620 | -1.320421 |
| 1 | 3.863289 | 1.667826 | 1.135427 |
| 1 | 4.596507 | -0.226645 | -0.288002 |
| 1 | -0.749065 | 1.502236 | 1.263326 |

**CA-I-x**

E = -482.882999500 a.u.

| | | | |
|---|---|---|---|
| 6 | -3.597875 | 0.063947 | -0.293538 |
| 6 | -2.712964 | 1.052611 | -0.711589 |
| 6 | -1.353015 | 0.917404 | -0.472186 |
| 6 | -0.845834 | -0.203346 | 0.190625 |
| 6 | -1.743943 | -1.185730 | 0.601661 |
| 6 | -3.108232 | -1.056348 | 0.363772 |

| | | | |
|---|---|---|---|
| 1 | -4.661680 | 0.168532 | -0.479312 |
| 1 | -3.085041 | 1.932599 | -1.226504 |
| 1 | -0.673340 | 1.697804 | -0.804636 |
| 1 | -1.370898 | -2.065781 | 1.118450 |
| 1 | -3.789123 | -1.833679 | 0.695542 |
| 6 | 0.636449 | -0.358124 | 0.422440 |
| 1 | 0.789013 | -1.242856 | 1.046865 |
| 6 | 1.339581 | 0.855073 | 1.088422 |
| 1 | 0.651429 | 1.681487 | 1.275627 |
| 1 | 1.759336 | 0.567046 | 2.055087 |
| 6 | 1.441202 | -0.540993 | -0.901349 |
| 6 | 2.456370 | 1.243647 | 0.090640 |
| 1 | 1.517322 | -1.586068 | -1.208784 |
| 1 | 0.940988 | 0.003040 | -1.709925 |
| 1 | 3.357131 | 1.630212 | 0.572060 |
| 1 | 2.093870 | 2.017293 | -0.595343 |
| 7 | 2.757791 | 0.045576 | -0.690106 |
| 6 | 3.665049 | -0.854206 | 0.005325 |
| 1 | 3.309605 | -1.186045 | 0.996787 |
| 1 | 3.833195 | -1.743663 | -0.606125 |
| 1 | 4.630414 | -0.361629 | 0.142890 |

Cartesian coordinates of the stationary points involved in the 32CA reaction between AY **18** and benzaldehyde **26**.

Benzaldehyde **26**
E = -345.525718314 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.295825 | -0.770560 | 0.087413 |
| 6 | 0.093839 | -0.778563 | 0.129129 |
| 6 | 0.791783 | 0.418052 | 0.030841 |
| 6 | 0.102008 | 1.620233 | -0.108864 |
| 6 | -1.293010 | 1.623696 | -0.150286 |
| 6 | -1.989334 | 0.429909 | -0.052232 |
| 1 | -1.843305 | -1.704199 | 0.164015 |
| 1 | 0.630037 | -1.714948 | 0.237914 |
| 1 | 1.878179 | 0.420361 | 0.062602 |
| 1 | -1.810012 | 2.570786 | -0.259569 |
| 1 | -3.073532 | 0.429252 | -0.084093 |
| 6 | 0.854058 | 2.893530 | -0.213174 |
| 1 | 1.959408 | 2.787498 | -0.170054 |
| 8 | 0.349278 | 3.979393 | -0.335847 |

**MC-II**

E = -518.711052755 a.u.

| | | | |
|---|---|---|---|
| 6 | 2.018771 | 0.066473 | 1.407093 |
| 6 | 2.445119 | 0.816001 | -0.812603 |
| 1 | 1.609792 | 0.373617 | 2.357681 |
| 1 | 2.818806 | -0.657058 | 1.356401 |
| 1 | 2.167876 | 1.512583 | -1.586200 |
| 1 | 3.150408 | 0.019564 | -0.989538 |
| 7 | 1.880388 | 0.916164 | 0.375076 |
| 6 | 0.940843 | 2.027241 | 0.590146 |
| 1 | 0.030921 | 1.639886 | 1.045655 |
| 1 | 1.406872 | 2.759201 | 1.250123 |
| 1 | 0.691778 | 2.488660 | -0.361492 |
| 1 | 0.731448 | -2.334040 | 0.980776 |
| 8 | 1.366437 | -1.945809 | -0.898497 |
| 6 | 0.608090 | -1.780020 | 0.030857 |
| 6 | -0.590865 | -0.904323 | -0.046507 |
| 6 | -0.847444 | -0.199807 | -1.220961 |
| 6 | -1.444218 | -0.762750 | 1.047066 |
| 6 | -1.940348 | 0.655701 | -1.292705 |
| 1 | -0.177904 | -0.339261 | -2.062004 |
| 6 | -2.537188 | 0.088040 | 0.975002 |
| 1 | -1.235057 | -1.310574 | 1.962104 |
| 6 | -2.782026 | 0.803493 | -0.195912 |
| 1 | -2.140398 | 1.204758 | -2.207205 |
| 1 | -3.199902 | 0.197580 | 1.827095 |
| 1 | -3.636705 | 1.469807 | -0.253508 |

**TS-II-n**

E = -518.730010747 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.791310 | -0.141506 | 1.332471 |
| 6 | 2.727825 | 0.565128 | -0.708886 |
| 1 | 1.255676 | 0.217112 | 2.201723 |
| 1 | 2.610801 | -0.829218 | 1.492806 |
| 1 | 2.702643 | 1.271633 | -1.523279 |
| 1 | 3.380490 | -0.291083 | -0.723656 |
| 7 | 1.986184 | 0.783731 | 0.346042 |
| 6 | 1.136515 | 1.980735 | 0.393152 |
| 1 | 0.131014 | 1.692304 | 0.695430 |
| 1 | 1.556255 | 2.682483 | 1.115199 |

| | | | |
|---|---|---|---|
| 1 | 1.094335 | 2.438925 | -0.592635 |
| 1 | 0.762129 | -2.293096 | 0.830686 |
| 8 | 1.403914 | -1.620980 | -0.984507 |
| 6 | 0.675196 | -1.560576 | 0.009770 |
| 6 | -0.628998 | -0.821379 | -0.037891 |
| 6 | -0.974254 | -0.141335 | -1.202952 |
| 6 | -1.489214 | -0.780699 | 1.058635 |
| 6 | -2.151501 | 0.595903 | -1.261172 |
| 1 | -0.300980 | -0.211051 | -2.049840 |
| 6 | -2.665353 | -0.047717 | 1.001679 |
| 1 | -1.220958 | -1.315687 | 1.965478 |
| 6 | -2.995947 | 0.649819 | -0.158579 |
| 1 | -2.415220 | 1.124348 | -2.171023 |
| 1 | -3.328944 | -0.018143 | 1.858977 |
| 1 | -3.915316 | 1.222961 | -0.203468 |

**TS-II-x**

E = -518.727331643 a.u.

| | | | |
|---|---|---|---|
| 6 | -3.532200 | 0.042740 | -0.516860 |
| 6 | -2.777112 | 1.202627 | -0.379775 |
| 6 | -1.488760 | 1.139970 | 0.134602 |
| 6 | -0.941194 | -0.085078 | 0.508060 |
| 6 | -1.704581 | -1.243328 | 0.377022 |
| 6 | -2.993873 | -1.181712 | -0.132763 |
| 1 | -4.539378 | 0.092376 | -0.915302 |
| 1 | -3.198627 | 2.159685 | -0.667579 |
| 1 | -0.889095 | 2.032875 | 0.271839 |
| 1 | -1.278982 | -2.198239 | 0.673179 |
| 1 | -3.582395 | -2.087373 | -0.230546 |
| 1 | 0.718703 | -1.097207 | 1.533096 |
| 6 | 0.449861 | -0.136328 | 1.058004 |
| 8 | 1.089721 | 0.891335 | 1.310304 |
| 6 | 1.418359 | -0.863425 | -0.878393 |
| 6 | 2.501826 | 1.213462 | -0.714490 |
| 1 | 1.589610 | -1.930522 | -0.927260 |
| 1 | 0.666818 | -0.446728 | -1.534656 |
| 1 | 3.357582 | 1.766821 | -0.364151 |
| 1 | 1.655615 | 1.710116 | -1.161823 |
| 7 | 2.525525 | -0.094037 | -0.680991 |
| 6 | 3.634465 | -0.728269 | 0.038129 |
| 1 | 3.381034 | -0.747537 | 1.099533 |

| | | | |
|---|---|---|---|
| 1 | 3.777563 | -1.739577 | -0.338180 |
| 1 | 4.544365 | -0.151065 | -0.114862 |

**CA-II-n**

E = -518.783450546 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.568207 | -0.157299 | 1.232866 |
| 6 | 2.652550 | 0.013818 | -0.718644 |
| 1 | 0.939683 | 0.365842 | 1.953667 |
| 1 | 2.217099 | -0.849753 | 1.777233 |
| 1 | 2.931973 | 0.646087 | -1.561974 |
| 1 | 3.447902 | -0.717733 | -0.524511 |
| 7 | 2.395311 | 0.774782 | 0.473278 |
| 6 | 1.727036 | 2.047749 | 0.208352 |
| 1 | 0.780319 | 1.951300 | -0.340098 |
| 1 | 1.524137 | 2.546797 | 1.157789 |
| 1 | 2.399292 | 2.690878 | -0.363705 |
| 1 | 0.781583 | -2.007874 | 0.364216 |
| 8 | 1.449579 | -0.680040 | -1.055287 |
| 6 | 0.749591 | -0.931479 | 0.151276 |
| 6 | -0.699957 | -0.507606 | 0.042339 |
| 6 | -1.203284 | 0.079514 | -1.113522 |
| 6 | -1.557576 | -0.717320 | 1.121922 |
| 6 | -2.537673 | 0.464741 | -1.183195 |
| 1 | -0.538535 | 0.227716 | -1.956174 |
| 6 | -2.889751 | -0.333184 | 1.054293 |
| 1 | -1.180660 | -1.188829 | 2.026498 |
| 6 | -3.384358 | 0.262964 | -0.100801 |
| 1 | -2.917286 | 0.922479 | -2.091144 |
| 1 | -3.544106 | -0.500919 | 1.903679 |
| 1 | -4.425323 | 0.563755 | -0.156810 |

**CA-II-x**

E = -518.783555314 a.u.

| | | | |
|---|---|---|---|
| 6 | -3.576211 | 0.065845 | -0.342196 |
| 6 | -2.777477 | 1.201928 | -0.310696 |
| 6 | -1.423285 | 1.100267 | -0.011975 |
| 6 | -0.854758 | -0.139983 | 0.257292 |
| 6 | -1.662575 | -1.276279 | 0.232748 |
| 6 | -3.014362 | -1.176325 | -0.067228 |
| 1 | -4.633209 | 0.147015 | -0.573269 |
| 1 | -3.211048 | 2.175779 | -0.514557 |

| | | | |
|---|---|---|---|
| 1 | -0.798759 | 1.984906 | 0.034296 |
| 1 | -1.230706 | -2.249072 | 0.455321 |
| 1 | -3.632281 | -2.068366 | -0.081408 |
| 1 | 0.767242 | -0.918966 | 1.409840 |
| 6 | 0.623095 | -0.285008 | 0.526910 |
| 8 | 1.263428 | 0.955296 | 0.781707 |
| 6 | 1.398747 | -0.864162 | -0.695841 |
| 6 | 2.223643 | 1.165650 | -0.257763 |
| 1 | 1.561671 | -1.940415 | -0.628487 |
| 1 | 0.844657 | -0.656988 | -1.615927 |
| 1 | 3.043183 | 1.759415 | 0.148092 |
| 1 | 1.750372 | 1.703626 | -1.088991 |
| 7 | 2.658214 | -0.129156 | -0.710836 |
| 6 | 3.666321 | -0.721801 | 0.163454 |
| 1 | 3.350269 | -0.804462 | 1.214417 |
| 1 | 3.918190 | -1.718384 | -0.204211 |
| 1 | 4.575060 | -0.117693 | 0.125720 |

Cartesian coordinates of the stationary points involved in the 32CA reaction between AY **18** and MFB **21**.

MFB **21**

E = -573.384459008 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.239731 | -0.779842 | 0.035746 |
| 6 | 0.147001 | -0.773894 | 0.059013 |
| 6 | 0.858288 | 0.424553 | -0.016295 |
| 6 | 0.153552 | 1.639501 | -0.098151 |
| 6 | -1.240294 | 1.614157 | -0.115232 |
| 6 | -1.937026 | 0.418281 | -0.054814 |
| 1 | -1.774173 | -1.722245 | 0.087064 |
| 1 | 0.691752 | -1.706365 | 0.127489 |
| 1 | -1.761343 | 2.562920 | -0.172657 |
| 1 | -3.021492 | 0.420489 | -0.074217 |
| 6 | 0.792331 | 2.998700 | -0.114988 |
| 1 | 1.878934 | 3.043945 | 0.032166 |
| 8 | 0.145097 | 4.004333 | -0.266819 |
| 6 | 2.353484 | 0.370435 | -0.059210 |
| 8 | 3.074085 | 1.242662 | -0.472473 |
| 8 | 2.821499 | -0.794695 | 0.405630 |
| 6 | 4.238875 | -0.953203 | 0.357495 |
| 1 | 4.728672 | -0.189842 | 0.963031 |

| | | | |
|---|---|---|---|
| 1 | 4.434295 | -1.943953 | 0.760178 |
| 1 | 4.597754 | -0.877747 | -0.669692 |

**MC-III**

E = -746.572247408 a.u.

| | | | |
|---|---|---|---|
| 6 | 0.835840 | -2.238121 | 1.087363 |
| 6 | 2.941392 | -1.148405 | 1.336964 |
| 1 | -0.128154 | -2.364393 | 1.555918 |
| 1 | 1.283023 | -3.047885 | 0.529568 |
| 1 | 3.449321 | -0.286697 | 1.739406 |
| 1 | 3.434263 | -1.851781 | 0.685192 |
| 7 | 1.662415 | -1.315491 | 1.611608 |
| 6 | 1.051961 | -0.342381 | 2.532513 |
| 1 | -0.029451 | -0.379084 | 2.434286 |
| 1 | 1.346199 | -0.585500 | 3.553274 |
| 1 | 1.393270 | 0.658308 | 2.271257 |
| 1 | 0.188728 | -1.698428 | -1.534319 |
| 8 | 2.144747 | -1.213391 | -1.595651 |
| 6 | 0.988796 | -0.982666 | -1.313951 |
| 6 | 0.587340 | 0.337649 | -0.725924 |
| 6 | 1.578567 | 1.311199 | -0.627074 |
| 6 | -0.684705 | 0.609847 | -0.201438 |
| 6 | 1.310866 | 2.547923 | -0.053827 |
| 1 | 2.560920 | 1.069537 | -1.015110 |
| 6 | -0.941921 | 1.840264 | 0.396343 |
| 6 | 0.047077 | 2.814949 | 0.455783 |
| 1 | 2.090351 | 3.300890 | -0.001831 |
| 1 | -1.921017 | 2.032017 | 0.819413 |
| 1 | -0.170484 | 3.777199 | 0.906918 |
| 6 | -1.765279 | -0.420704 | -0.229057 |
| 8 | -2.029755 | -1.144600 | -1.151019 |
| 8 | -2.438395 | -0.442309 | 0.935405 |
| 6 | -3.508341 | -1.384283 | 1.004627 |
| 1 | -3.938225 | -1.266240 | 1.996383 |
| 1 | -4.253293 | -1.175760 | 0.235855 |
| 1 | -3.130963 | -2.398552 | 0.867268 |

**TS-III-n**

E = -746.595013107 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.213517 | -1.920265 | 0.816929 |
| 6 | 3.363039 | -0.966726 | 0.478706 |

| | | | |
|---|---|---|---|
| 1 | 0.350409 | -1.911754 | 1.463223 |
| 1 | 1.474180 | -2.804402 | 0.256990 |
| 1 | 4.021101 | -0.146170 | 0.709927 |
| 1 | 3.628283 | -1.731434 | -0.232305 |
| 7 | 2.190723 | -1.032336 | 1.077196 |
| 6 | 1.866060 | 0.007646 | 2.065697 |
| 1 | 0.853709 | 0.366038 | 1.884136 |
| 1 | 1.936222 | -0.422041 | 3.065331 |
| 1 | 2.560883 | 0.837423 | 1.962977 |
| 1 | 0.101819 | -1.689278 | -1.585902 |
| 8 | 1.934834 | -0.915247 | -1.968691 |
| 6 | 0.812196 | -0.864783 | -1.498546 |
| 6 | 0.309687 | 0.416949 | -0.885654 |
| 6 | 1.220983 | 1.473654 | -0.891393 |
| 6 | -0.956577 | 0.619973 | -0.298246 |
| 6 | 0.913341 | 2.698203 | -0.317479 |
| 1 | 2.179970 | 1.293386 | -1.361127 |
| 6 | -1.253827 | 1.857755 | 0.275910 |
| 6 | -0.327541 | 2.891321 | 0.273520 |
| 1 | 1.640739 | 3.502493 | -0.335547 |
| 1 | -2.225626 | 2.003392 | 0.727282 |
| 1 | -0.581710 | 3.844070 | 0.723348 |
| 6 | -1.989530 | -0.458589 | -0.247819 |
| 8 | -1.900177 | -1.554302 | -0.740882 |
| 8 | -3.081032 | -0.075830 | 0.436556 |
| 6 | -4.126019 | -1.043067 | 0.517309 |
| 1 | -4.920589 | -0.568145 | 1.088462 |
| 1 | -4.478565 | -1.311747 | -0.479832 |
| 1 | -3.776873 | -1.944880 | 1.023187 |

**TS-III-x**

E = -746.592998694 a.u.

| | | | |
|---|---|---|---|
| 6 | -1.980030 | 2.696373 | -0.536050 |
| 6 | -0.726464 | 3.142051 | -0.132904 |
| 6 | 0.196451 | 2.242565 | 0.373086 |
| 6 | -0.090800 | 0.879806 | 0.472618 |
| 6 | -1.364099 | 0.430929 | 0.069380 |
| 6 | -2.293434 | 1.352060 | -0.424614 |
| 1 | -2.712450 | 3.391913 | -0.928763 |
| 1 | -0.472712 | 4.194052 | -0.205216 |
| 1 | 1.170515 | 2.566501 | 0.719838 |

| | | | |
|---|---|---|---|
| 1 | -3.269458 | 0.996272 | -0.725492 |
| 1 | 0.744595 | -1.016283 | 1.276966 |
| 6 | 1.002053 | 0.022783 | 1.054534 |
| 8 | 2.031564 | 0.541057 | 1.485898 |
| 6 | 1.669296 | -0.775447 | -1.104773 |
| 6 | 3.626880 | 0.445815 | -0.610774 |
| 1 | 1.257912 | -1.763610 | -1.232460 |
| 1 | 1.260543 | 0.052901 | -1.664404 |
| 1 | 4.604132 | 0.434414 | -0.158481 |
| 1 | 3.189531 | 1.353420 | -0.996339 |
| 7 | 2.964327 | -0.680160 | -0.734515 |
| 6 | 3.535172 | -1.861110 | -0.075104 |
| 1 | 3.260583 | -1.816985 | 0.979815 |
| 1 | 3.135657 | -2.761223 | -0.537387 |
| 1 | 4.618448 | -1.844435 | -0.179806 |
| 6 | -1.750947 | -1.008546 | 0.123675 |
| 8 | -1.004334 | -1.943900 | 0.279578 |
| 8 | -3.073999 | -1.179170 | -0.038795 |
| 6 | -3.526095 | -2.530873 | -0.030677 |
| 1 | -3.284553 | -3.011058 | 0.919055 |
| 1 | -4.603833 | -2.479833 | -0.168794 |
| 1 | -3.062936 | -3.097245 | -0.840752 |

**TS-IV-n**

E = -746.582283929 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.438064 | 0.215566 | 1.470501 |
| 6 | 1.637286 | 2.312426 | 0.423456 |
| 1 | 0.930564 | -0.281788 | 2.287590 |
| 1 | 2.513854 | 0.089082 | 1.434741 |
| 1 | 1.148448 | 3.222244 | 0.110120 |
| 1 | 2.621038 | 2.046454 | 0.072761 |
| 7 | 1.014002 | 1.505333 | 1.231116 |
| 6 | -0.313594 | 1.889072 | 1.738617 |
| 1 | -0.831508 | 2.481005 | 0.984603 |
| 1 | -0.889052 | 0.986637 | 1.932815 |
| 1 | -0.187271 | 2.454225 | 2.662714 |
| 1 | -0.325947 | 0.927780 | -2.549603 |
| 8 | -1.185113 | 2.339804 | -1.400401 |
| 6 | -0.872335 | 1.194928 | -1.634320 |
| 6 | -1.305257 | 0.059474 | -0.752853 |
| 6 | -2.667395 | -0.029937 | -0.460936 |

| | | | |
|---|---|---|---|
| 6 | -0.420998 | -0.883593 | -0.219359 |
| 6 | -3.157566 | -1.073629 | 0.308814 |
| 1 | -3.338824 | 0.723919 | -0.856711 |
| 6 | -0.921813 | -1.935155 | 0.545537 |
| 6 | -2.280593 | -2.035027 | 0.802811 |
| 1 | -4.218680 | -1.140916 | 0.519594 |
| 1 | -0.226085 | -2.660773 | 0.948098 |
| 1 | -2.657520 | -2.859259 | 1.398026 |
| 6 | 1.058410 | -0.666461 | -0.402228 |
| 8 | 1.466935 | 0.198970 | -1.189435 |
| 8 | 1.754345 | -1.841898 | -0.202748 |
| 6 | 3.095401 | -1.818612 | -0.646659 |
| 1 | 3.480345 | -2.826293 | -0.496055 |
| 1 | 3.157431 | -1.538799 | -1.700319 |
| 1 | 3.698197 | -1.110167 | -0.065795 |

**TS-IV-x**

E = -746.577104092 a.u.

| | | | |
|---|---|---|---|
| 6 | -2.616886 | -2.025882 | -0.622169 |
| 6 | -3.542404 | -0.989431 | -0.632974 |
| 6 | -3.140167 | 0.276109 | -0.244620 |
| 6 | -1.828337 | 0.528818 | 0.161461 |
| 6 | -0.888365 | -0.520318 | 0.166375 |
| 6 | -1.306970 | -1.791366 | -0.230476 |
| 1 | -2.914493 | -3.025831 | -0.918479 |
| 1 | -4.566579 | -1.168291 | -0.939182 |
| 1 | -3.833296 | 1.109224 | -0.239864 |
| 1 | -0.587772 | -2.598255 | -0.222286 |
| 1 | -0.511338 | 2.116729 | 0.956286 |
| 6 | -1.517694 | 1.938322 | 0.553574 |
| 8 | -2.321438 | 2.834636 | 0.444347 |
| 6 | 1.131319 | 0.426109 | -1.327335 |
| 6 | 2.686079 | 1.778015 | -0.193319 |
| 1 | 1.058429 | -0.337208 | -2.091821 |
| 1 | 0.442356 | 1.257791 | -1.406516 |
| 1 | 3.689441 | 1.896881 | 0.184632 |
| 1 | 1.914721 | 2.497385 | 0.027359 |
| 7 | 2.412649 | 0.774642 | -0.980042 |
| 6 | 3.458827 | -0.200274 | -1.309739 |
| 1 | 3.089391 | -1.192764 | -1.056633 |
| 1 | 3.670319 | -0.144188 | -2.377915 |

| | | | |
|---|---|---|---|
| 1 | 4.360961 | 0.018228 | -0.742018 |
| 6 | 0.554261 | -0.321787 | 0.581409 |
| 8 | 0.926552 | 0.560326 | 1.357874 |
| 8 | 1.242518 | -1.539365 | 0.574398 |
| 6 | 2.203341 | -1.680730 | 1.607676 |
| 1 | 1.745933 | -1.563597 | 2.593095 |
| 1 | 2.603492 | -2.689410 | 1.502798 |
| 1 | 3.010817 | -0.949480 | 1.518701 |

**CA-III-n**

E = -746.649796771 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.133362 | -1.432049 | 0.287004 |
| 6 | 3.052996 | -1.133829 | -0.834067 |
| 1 | 0.585090 | -1.140585 | 1.181715 |
| 1 | 0.847476 | -2.454056 | 0.034496 |
| 1 | 4.051839 | -0.696606 | -0.855740 |
| 1 | 3.052107 | -2.083518 | -1.385572 |
| 7 | 2.576022 | -1.354547 | 0.502782 |
| 6 | 2.958036 | -0.292872 | 1.429304 |
| 1 | 2.617575 | 0.708596 | 1.130092 |
| 1 | 2.543009 | -0.514313 | 2.414519 |
| 1 | 4.045865 | -0.275526 | 1.527676 |
| 1 | 0.277029 | -1.040080 | -1.685867 |
| 8 | 2.151481 | -0.223807 | -1.461702 |
| 6 | 0.859137 | -0.496333 | -0.938518 |
| 6 | 0.150158 | 0.802054 | -0.599002 |
| 6 | 0.867625 | 1.995547 | -0.656488 |
| 6 | -1.209026 | 0.862214 | -0.235322 |
| 6 | 0.279541 | 3.211104 | -0.341236 |
| 1 | 1.903754 | 1.951448 | -0.965342 |
| 6 | -1.793117 | 2.094031 | 0.077879 |
| 6 | -1.056523 | 3.264635 | 0.033707 |
| 1 | 0.868759 | 4.121027 | -0.393793 |
| 1 | -2.838730 | 2.121811 | 0.354772 |
| 1 | -1.524024 | 4.211160 | 0.281915 |
| 6 | -2.050791 | -0.366146 | -0.190345 |
| 8 | -1.657610 | -1.494640 | -0.362215 |
| 8 | -3.339083 | -0.094293 | 0.066000 |
| 6 | -4.206815 | -1.222663 | 0.129451 |
| 1 | -5.193292 | -0.819662 | 0.346224 |
| 1 | -4.212392 | -1.756482 | -0.821786 |

| | | | |
|---|---|---|---|
| 1 | -3.890966 | -1.906768 | 0.918356 |

**CA-III-x**

E = -746.649589615 a.u.

| | | | |
|---|---|---|---|
| 6 | -2.080517 | 2.873125 | -0.438814 |
| 6 | -0.805269 | 3.295863 | -0.088585 |
| 6 | 0.141945 | 2.375514 | 0.334222 |
| 6 | -0.145295 | 1.013691 | 0.409506 |
| 6 | -1.442968 | 0.589612 | 0.063044 |
| 6 | -2.393320 | 1.527802 | -0.353956 |
| 1 | -2.828836 | 3.585651 | -0.768007 |
| 1 | -0.545772 | 4.348514 | -0.137732 |
| 1 | 1.126240 | 2.707726 | 0.637639 |
| 1 | -3.387322 | 1.186399 | -0.610822 |
| 1 | 0.594574 | -0.625540 | 1.588542 |
| 6 | 0.963943 | 0.069070 | 0.833770 |
| 8 | 2.063950 | 0.774373 | 1.397260 |
| 6 | 1.590630 | -0.708716 | -0.365940 |
| 6 | 3.180535 | 0.592539 | 0.523138 |
| 1 | 1.203850 | -1.721210 | -0.442990 |
| 1 | 1.382637 | -0.182262 | -1.302661 |
| 1 | 4.092776 | 0.658432 | 1.116931 |
| 1 | 3.178878 | 1.379101 | -0.243680 |
| 7 | 3.026247 | -0.689435 | -0.106980 |
| 6 | 3.451948 | -1.791247 | 0.751887 |
| 1 | 2.941152 | -1.816059 | 1.726069 |
| 1 | 3.265966 | -2.736518 | 0.239054 |
| 1 | 4.527205 | -1.715832 | 0.927946 |
| 6 | -1.840333 | -0.844536 | 0.145915 |
| 8 | -1.105920 | -1.766974 | 0.405163 |
| 8 | -3.146386 | -1.026560 | -0.100218 |
| 6 | -3.602729 | -2.375084 | -0.045279 |
| 1 | -3.439163 | -2.795540 | 0.947854 |
| 1 | -4.665702 | -2.332239 | -0.270663 |
| 1 | -3.080063 | -2.988200 | -0.780848 |

**CA-IV-n**

E = -746.612829183 a.u.

| | | | |
|---|---|---|---|
| 6 | 1.370182 | 0.058392 | 1.506166 |
| 6 | 1.894498 | 1.664679 | 0.021539 |
| 1 | 0.645942 | -0.223406 | 2.268800 |

| | | | |
|---|---|---|---|
| 1 | 2.337017 | -0.371199 | 1.783626 |
| 1 | 1.600485 | 2.628791 | -0.393181 |
| 1 | 2.978060 | 1.528422 | -0.069308 |
| 7 | 1.477485 | 1.503491 | 1.383546 |
| 6 | 0.247000 | 2.222489 | 1.716492 |
| 1 | 0.431194 | 3.295375 | 1.636499 |
| 1 | -0.611348 | 1.974909 | 1.080005 |
| 1 | -0.012750 | 2.010239 | 2.755050 |
| 1 | -0.445057 | 0.908193 | -2.464816 |
| 8 | -1.449796 | 2.256785 | -1.366589 |
| 6 | -1.043264 | 1.140208 | -1.568120 |
| 6 | -1.424721 | -0.030875 | -0.705461 |
| 6 | -2.785872 | -0.335133 | -0.639997 |
| 6 | -0.508293 | -0.819777 | -0.009005 |
| 6 | -3.232631 | -1.440166 | 0.067239 |
| 1 | -3.492067 | 0.302144 | -1.161992 |
| 6 | -0.966040 | -1.931036 | 0.696175 |
| 6 | -2.315159 | -2.248351 | 0.728781 |
| 1 | -4.292075 | -1.670123 | 0.102255 |
| 1 | -0.248805 | -2.550353 | 1.224272 |
| 1 | -2.652000 | -3.120094 | 1.279682 |
| 6 | 0.964451 | -0.457787 | 0.085660 |
| 8 | 1.247593 | 0.636486 | -0.753391 |
| 8 | 1.668375 | -1.611807 | -0.296163 |
| 6 | 3.034722 | -1.440920 | -0.602211 |
| 1 | 3.403739 | -2.424779 | -0.887688 |
| 1 | 3.167015 | -0.746932 | -1.436194 |
| 1 | 3.618566 | -1.084743 | 0.255640 |

**CA-IV-x**

E = -746.618934159 a.u.

| | | | |
|---|---|---|---|
| 6 | -2.556137 | -2.095964 | -0.352681 |
| 6 | -3.486798 | -1.092048 | -0.118350 |
| 6 | -3.043254 | 0.197085 | 0.118940 |
| 6 | -1.680657 | 0.505977 | 0.125509 |
| 6 | -0.736104 | -0.515511 | -0.072113 |
| 6 | -1.199364 | -1.806678 | -0.324179 |
| 1 | -2.883644 | -3.111128 | -0.551457 |
| 1 | -4.548955 | -1.311177 | -0.127912 |
| 1 | -3.745053 | 1.004420 | 0.294994 |
| 1 | -0.474559 | -2.595295 | -0.485147 |

| | | | |
|---|---|---|---|
| 1 | -0.345481 | 2.278904 | -0.010189 |
| 6 | -1.346195 | 1.951243 | 0.305884 |
| 8 | -2.136519 | 2.759213 | 0.724290 |
| 6 | 1.359291 | 0.184367 | -1.402922 |
| 6 | 2.189435 | 1.506636 | 0.240854 |
| 1 | 1.576946 | -0.643023 | -2.076496 |
| 1 | 0.648947 | 0.861711 | -1.888659 |
| 1 | 3.036340 | 1.561142 | 0.927663 |
| 1 | 1.775635 | 2.511096 | 0.094978 |
| 7 | 2.559815 | 0.908879 | -1.013931 |
| 6 | 3.776555 | 0.102177 | -0.961455 |
| 1 | 3.742465 | -0.701919 | -0.217041 |
| 1 | 3.946041 | -0.342945 | -1.943567 |
| 1 | 4.626065 | 0.755372 | -0.750629 |
| 6 | 0.777014 | -0.304913 | -0.063426 |
| 8 | 1.144766 | 0.707635 | 0.836253 |
| 8 | 1.450240 | -1.507032 | 0.241218 |
| 6 | 1.385071 | -1.901900 | 1.599419 |
| 1 | 0.349528 | -2.019622 | 1.937317 |
| 1 | 1.894396 | -2.862890 | 1.660557 |
| 1 | 1.885819 | -1.176301 | 2.244196 |