

Insights into the carbonate effect on water oxidation over metal oxide photocatalysts/photoanodes

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Supplementary information

Table S1 Summary of the effect of carbonate on a photocatalyst and (photo)anode using TiO₂ and BiVO₄

| Semiconductor | TiO ₂ | BiVO ₄ |
|------------------------------------------------------------------------------------|------------------|-------------------|
| Photocatalytic activity for water splitting into H ₂ and O ₂ | Yes | No ^a |
| Improvement of photocurrent | Yes | Yes |
| H ₂ O ₂ production on photoanode | Yes ^b | Yes |
| H ₂ O ₂ production on anode in the dark | Yes | Yes |

^a BiVO₄ photocatalyst cannot evolve H₂ because of the positive conduction band.

^b Data in this work.

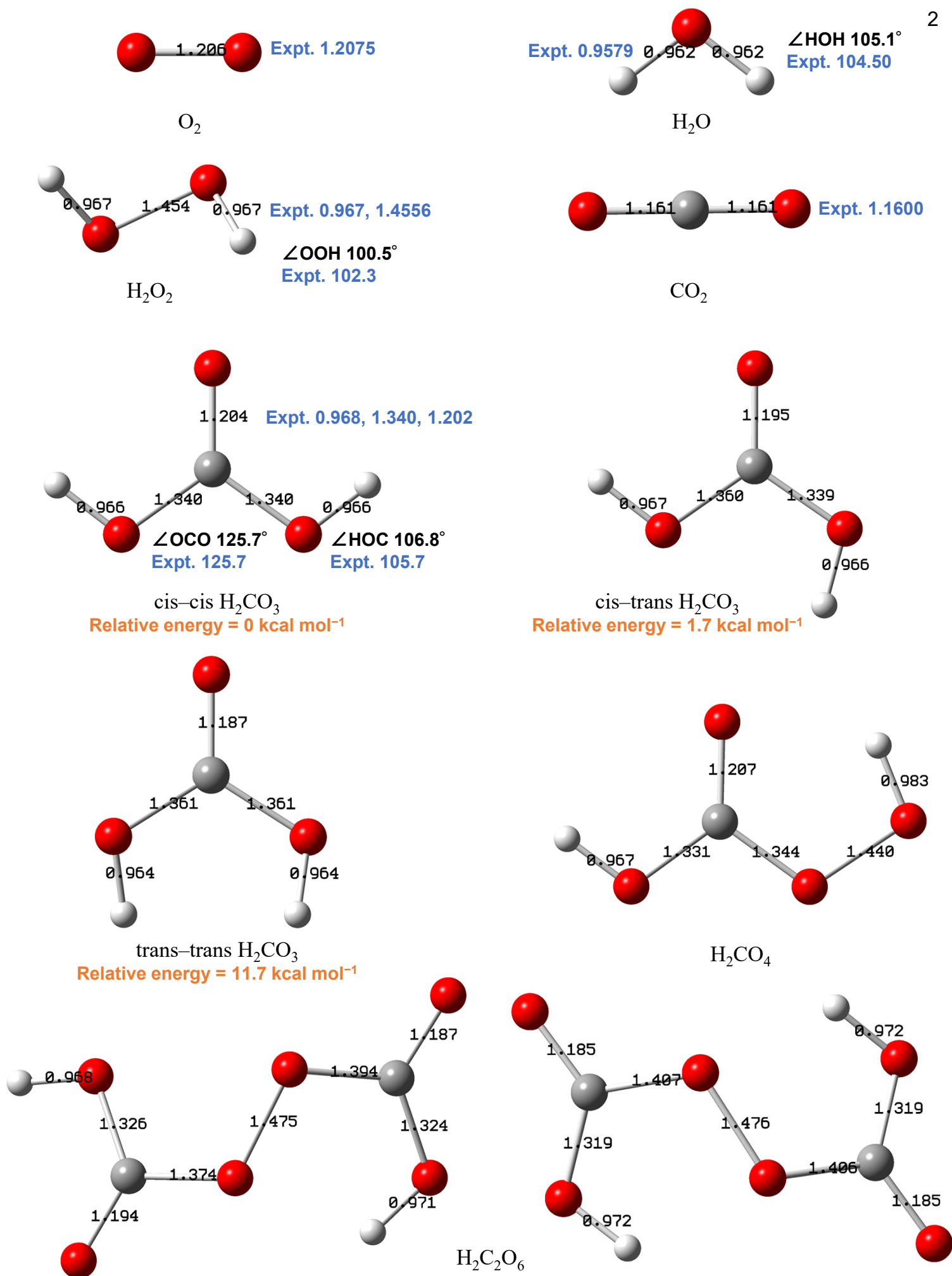


Fig. S1 Optimized geometries (in Å) of the isolated species.^{S1}

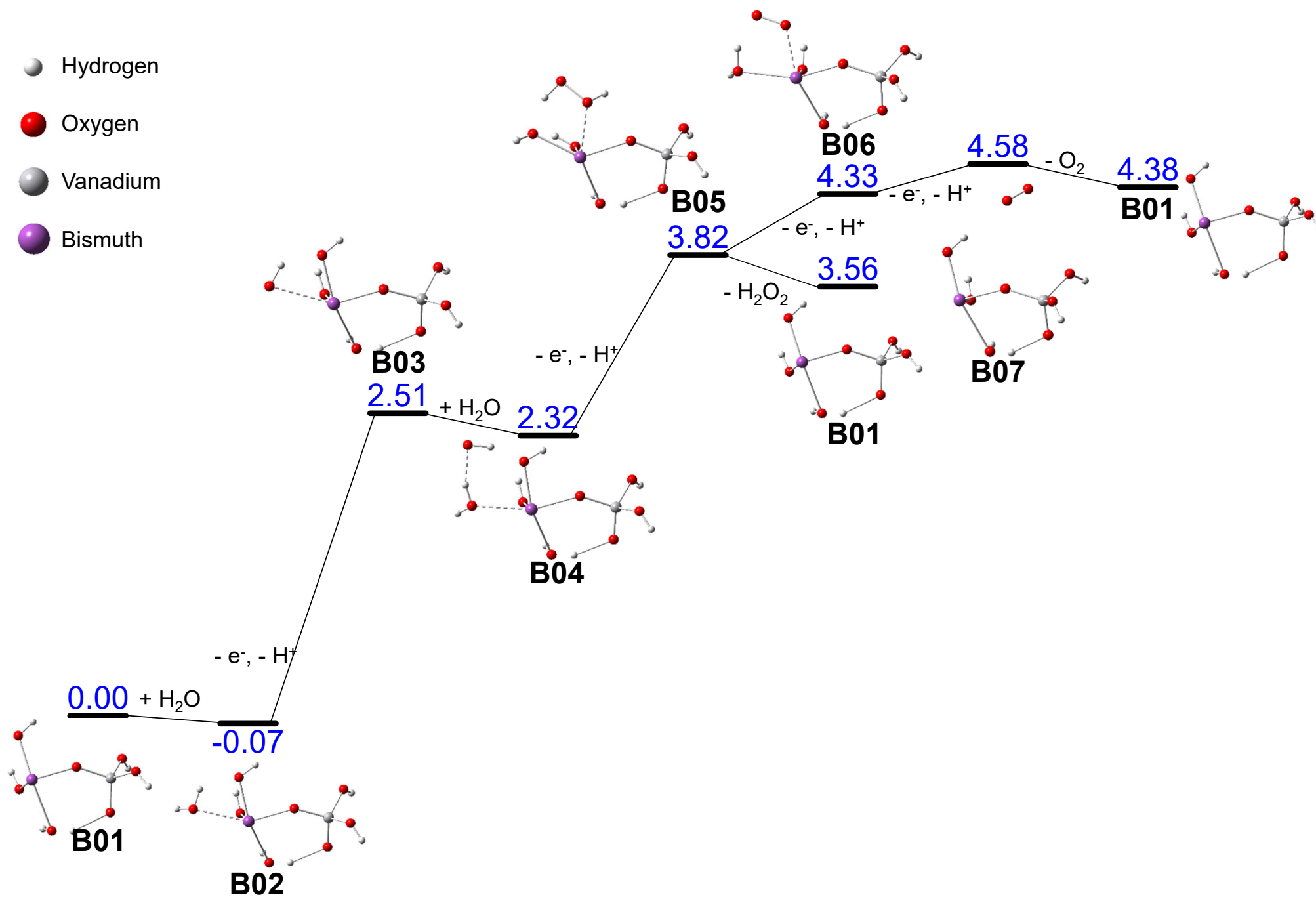


Fig. S2 Intermediate structures and free energies (in eV) of H_2O oxidation on BiVO_4 .

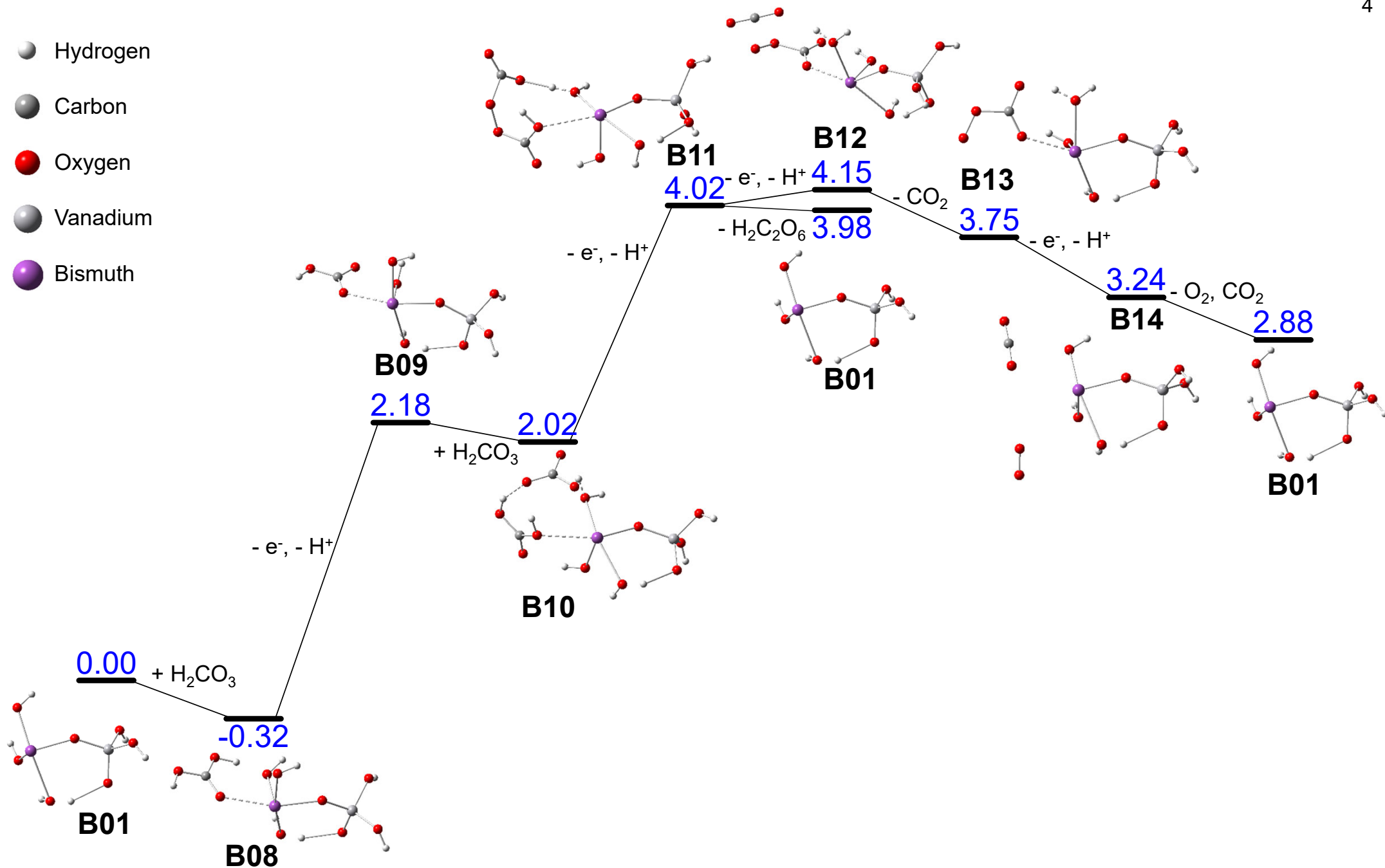
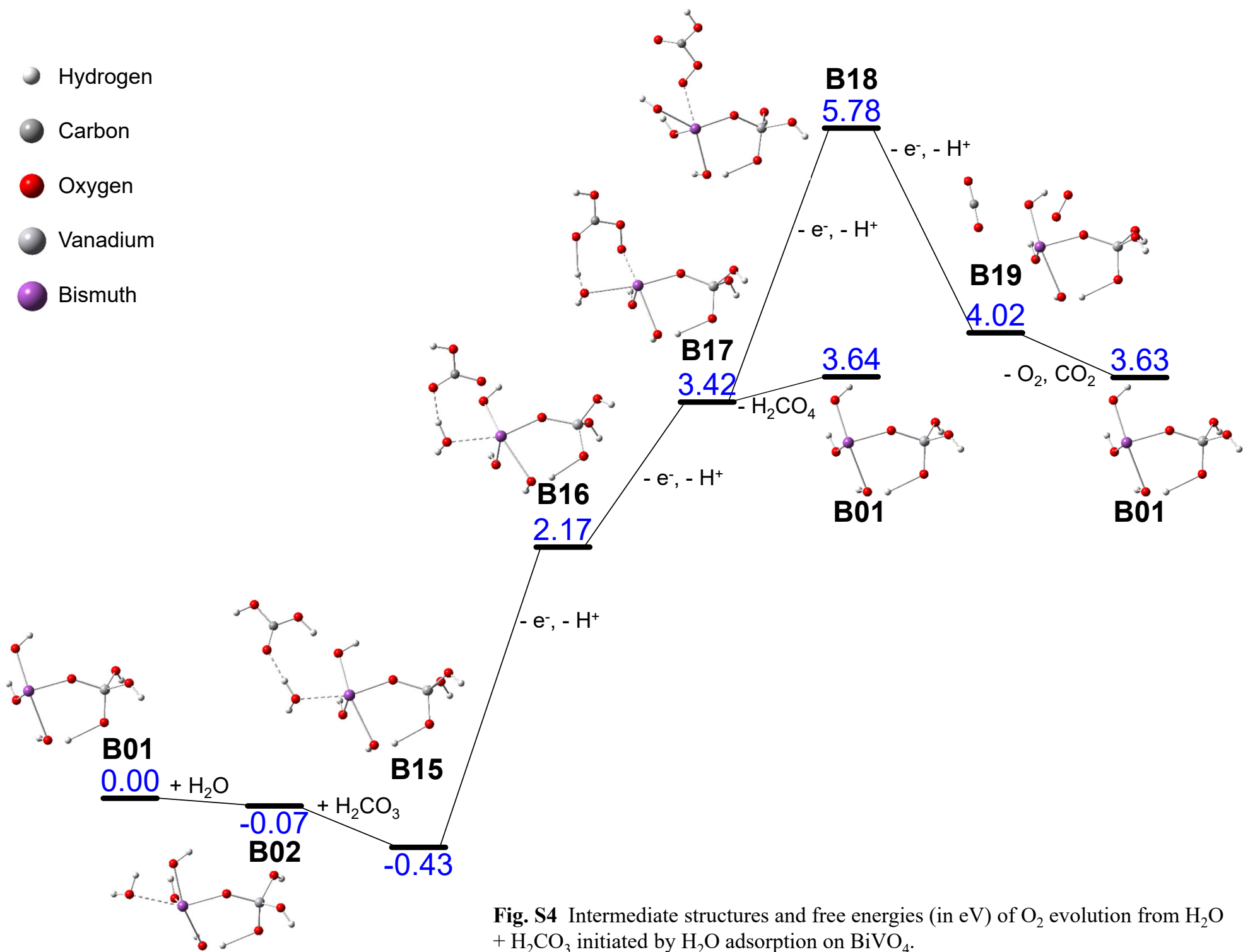


Fig. S3 Intermediate structures and free energies (in eV) of H_2CO_3 oxidation on BiVO_4 .



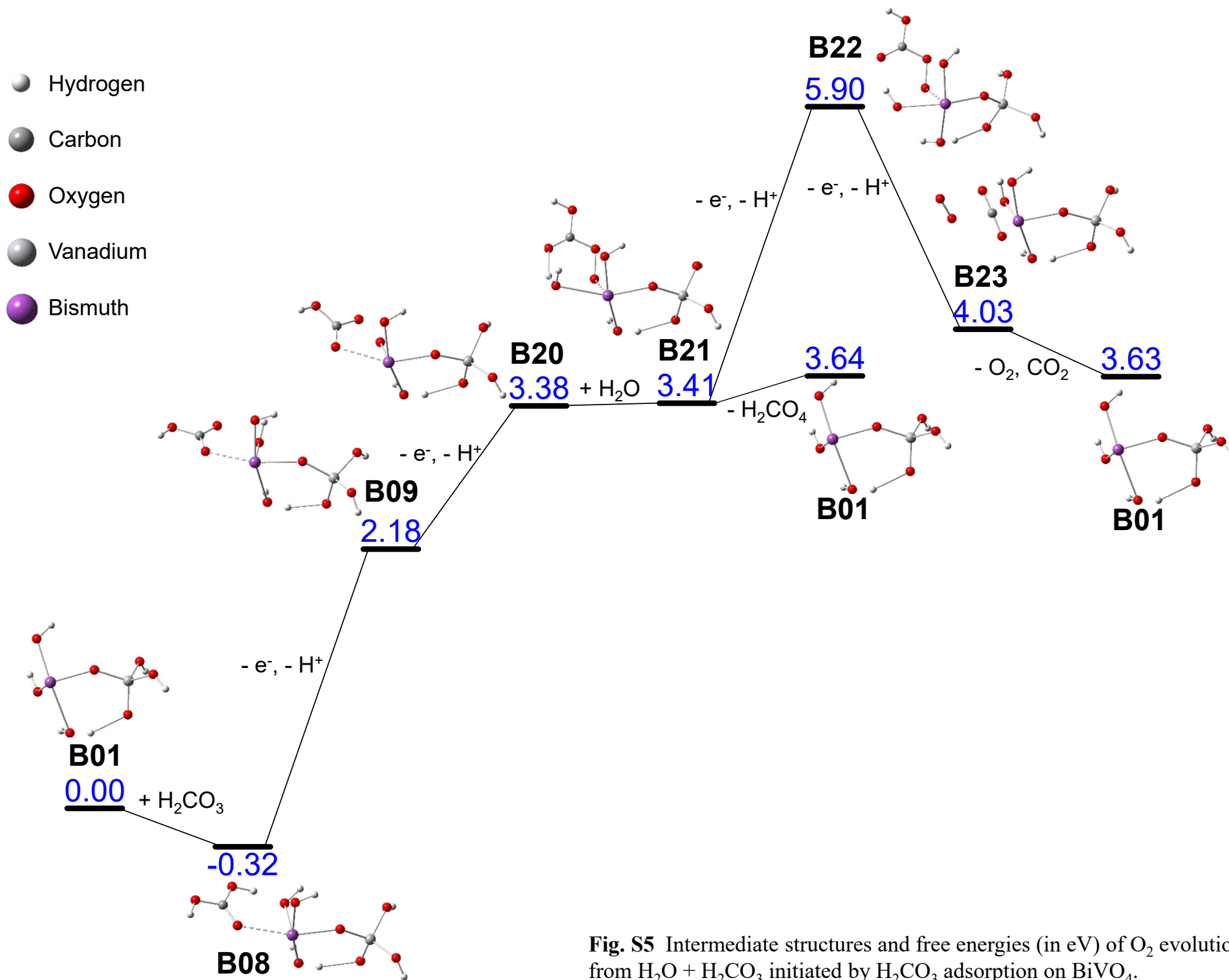
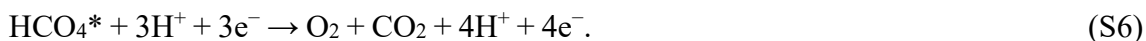
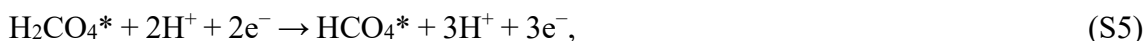
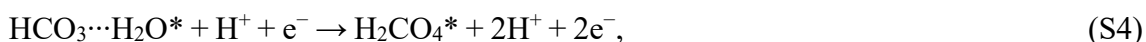


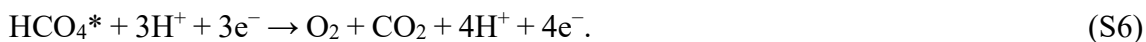
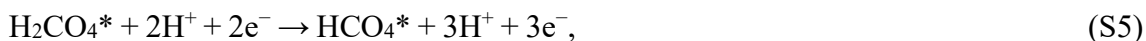
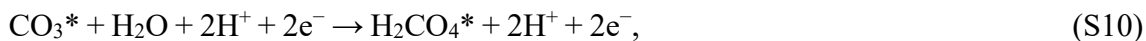
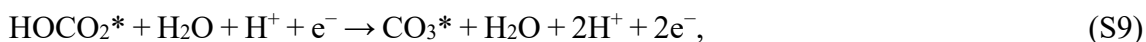
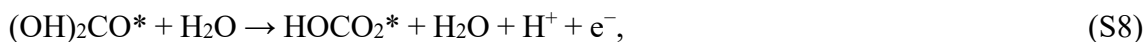
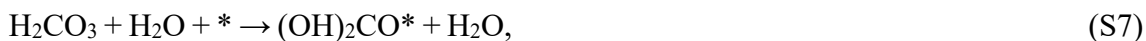
Fig. S5 Intermediate structures and free energies (in eV) of O₂ evolution from H₂O + H₂CO₃ initiated by H₂CO₃ adsorption on BiVO₄.

The elementary steps of Eq. 3

For $\text{H}_2\text{O} \rightarrow \text{H}_2\text{CO}_3$:



For $\text{H}_2\text{CO}_3 \rightarrow \text{H}_2\text{O}$:



Geometry (atomic numbers followed by the Cartesian coordinates in Å) and energy of optimized structures from cluster models

T01

E = -2229.77807184 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -0.061327 | -0.701802 | 0.357136 |
| 8 | 2.541859 | 0.030213 | 1.634912 |
| 8 | 1.371079 | 1.493994 | -0.712161 |
| 8 | 2.522312 | -1.272369 | -1.003583 |
| 8 | -2.653888 | 0.145759 | 1.601574 |
| 8 | -2.688858 | -1.323680 | -0.989228 |
| 8 | -1.505493 | 1.393284 | -0.857071 |
| 1 | 3.318286 | -0.363397 | 2.039209 |
| 1 | 2.023452 | 2.165327 | -0.931585 |
| 1 | 2.362972 | -1.997229 | -1.611835 |
| 1 | 2.943807 | 0.894459 | 2.127260 |
| 1 | -0.610552 | 1.764255 | -0.967045 |
| 1 | -3.426236 | -1.917018 | -0.826947 |
| 22 | 1.622676 | -0.155905 | 0.088116 |
| 22 | -1.783160 | -0.135645 | 0.042787 |

T02

E = -2306.25607855 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.183380 | -0.587089 | -0.070137 |
| 8 | -2.351484 | 0.611538 | -1.492873 |
| 8 | -2.306264 | 0.212801 | 1.644058 |
| 8 | -2.391971 | -1.872886 | -0.174503 |
| 8 | 1.780521 | 1.707083 | 0.083877 |
| 8 | 2.814861 | -0.662900 | -1.493448 |
| 8 | 2.757889 | -0.809686 | 1.437381 |
| 1 | -2.924382 | 0.133886 | -2.101150 |
| 1 | -2.279435 | 1.127422 | 1.945905 |
| 1 | -2.983369 | -2.373281 | 0.393856 |
| 1 | 2.502205 | 2.331347 | 0.200272 |
| 1 | 2.498753 | -1.118223 | 2.308875 |
| 1 | 2.596390 | -0.897751 | -2.398214 |
| 22 | -1.654901 | -0.232001 | 0.002139 |
| 22 | 1.894028 | -0.159231 | -0.016133 |
| 8 | -0.920913 | 2.017525 | 0.133527 |
| 1 | 0.059058 | 2.110833 | 0.118701 |
| 1 | -1.258157 | 2.361790 | -0.703435 |

T03 (doublet)

E = -2305.55157657 a.u.

| | | | |
|---|-----------|-----------|-----------|
| 8 | 0.179963 | -0.832452 | -0.190083 |
| 8 | -2.192578 | 0.769906 | -1.393258 |
| 8 | -2.175124 | 0.066814 | 1.671173 |
| 8 | -2.528971 | -1.831304 | -0.336508 |
| 8 | 1.558220 | 1.722133 | -0.415899 |
| 8 | 2.861236 | -0.799305 | -1.436380 |
| 8 | 2.585737 | -0.365396 | 1.475515 |

| | | | |
|----|-----------|-----------|-----------|
| 1 | -2.842183 | 0.467824 | -2.036318 |
| 1 | -2.062527 | 0.898590 | 2.141329 |
| 1 | -3.173385 | -2.323332 | 0.178862 |
| 1 | 1.823489 | 2.405343 | 0.209249 |
| 1 | 2.320776 | -0.692845 | 2.338399 |
| 1 | 2.716125 | -1.313243 | -2.234474 |
| 22 | -1.605423 | -0.312065 | -0.018592 |
| 22 | 1.799949 | -0.127697 | -0.133775 |
| 8 | -0.589007 | 1.812037 | 0.371544 |
| 1 | -0.719148 | 2.245334 | -0.490787 |

T04 (doublet)

E = -2382.02603118 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.255873 | 0.288736 | -0.330747 |
| 8 | -2.592852 | -0.831556 | -0.911174 |
| 8 | -2.275853 | 1.434812 | 1.238139 |
| 8 | -1.239196 | -1.111201 | 1.588000 |
| 8 | 2.824737 | 0.993513 | 1.017280 |
| 8 | 2.832497 | -0.984293 | -1.203394 |
| 8 | 1.496165 | -1.657401 | 1.362769 |
| 1 | -2.825622 | -1.755306 | -0.775375 |
| 1 | -2.691115 | 2.247091 | 0.933503 |
| 1 | -1.763939 | -1.116371 | 2.395493 |
| 1 | 3.141859 | 1.186094 | 1.902406 |
| 1 | 0.573514 | -1.729143 | 1.679731 |
| 1 | 3.644346 | -0.747590 | -1.657318 |
| 22 | -1.505952 | 0.124932 | 0.226693 |
| 22 | 1.899871 | -0.341714 | 0.213533 |
| 8 | -1.974413 | 1.668519 | -1.390135 |
| 1 | -2.395357 | 1.175291 | -2.115402 |
| 8 | -0.154648 | 1.635205 | -2.662658 |
| 1 | 0.185332 | 1.129431 | -1.888139 |
| 1 | -0.044357 | 2.565177 | -2.429740 |

T05

E = -2381.39633008 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.175128 | 0.355660 | 0.109275 |
| 8 | -2.353356 | -0.232934 | -1.569242 |
| 8 | -2.419568 | -0.673873 | 1.493390 |
| 8 | -0.807011 | -2.277342 | -0.215961 |
| 8 | 2.756870 | 0.173170 | 1.597317 |
| 8 | 2.776406 | 1.001241 | -1.254939 |
| 8 | 1.972760 | -1.764962 | -0.536671 |
| 1 | -2.465011 | -0.849207 | -2.298917 |
| 1 | -3.010216 | -0.028708 | 1.893804 |
| 1 | -1.234303 | -3.056007 | 0.156143 |
| 1 | 3.144721 | -0.368959 | 2.287533 |
| 1 | 1.151418 | -2.289634 | -0.506420 |
| 1 | 3.460401 | 1.674661 | -1.235465 |
| 22 | -1.422265 | -0.549082 | -0.010135 |
| 22 | 1.969453 | -0.047022 | -0.014355 |

| | | | |
|---|-----------|----------|-----------|
| 8 | -2.206253 | 1.741406 | 0.083918 |
| 1 | -2.421209 | 1.891291 | -0.851412 |
| 8 | -1.177242 | 2.719594 | 0.356839 |
| 1 | -0.392896 | 2.129549 | 0.337596 |

T06 (doublet)

E = -2380.75378284 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.154137 | 0.472814 | 0.036746 |
| 8 | -2.377381 | -0.410650 | -1.510013 |
| 8 | -2.467447 | -0.583519 | 1.526866 |
| 8 | -0.693006 | -2.196920 | 0.019475 |
| 8 | 2.719575 | 0.391156 | 1.561202 |
| 8 | 2.764996 | 1.079912 | -1.324373 |
| 8 | 2.003456 | -1.662453 | -0.479310 |
| 1 | -2.418210 | -0.975490 | -2.286360 |
| 1 | -3.237662 | -0.093308 | 1.827832 |
| 1 | -1.091819 | -2.950490 | 0.467333 |
| 1 | 3.124104 | -0.111381 | 2.271617 |
| 1 | 1.190312 | -2.192579 | -0.363215 |
| 1 | 3.463218 | 1.738480 | -1.342994 |
| 22 | -1.445816 | -0.503659 | 0.034528 |
| 22 | 1.959200 | 0.076805 | -0.048283 |
| 8 | -2.167563 | 1.794905 | 0.173735 |
| 8 | -1.158152 | 2.639785 | 0.153697 |
| 1 | -0.362688 | 2.014456 | 0.085902 |

T07 (triplet)

E = -2380.14957768 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.050829 | 0.096041 | 0.665689 |
| 8 | -2.242278 | 1.329819 | -0.744946 |
| 8 | -2.676409 | 0.135443 | 1.912196 |
| 8 | -1.919882 | -1.642623 | -0.394636 |
| 8 | 2.370627 | -1.391662 | 1.852638 |
| 8 | 2.710089 | 0.030614 | -0.744999 |
| 8 | 0.878196 | -2.297002 | -0.572701 |
| 1 | -1.827122 | 1.930227 | -1.369844 |
| 1 | -3.307020 | 0.744604 | 2.302688 |
| 1 | -2.727769 | -2.117535 | -0.609433 |
| 1 | 2.477099 | -2.191336 | 2.372411 |
| 1 | -0.084153 | -2.421268 | -0.669378 |
| 1 | 3.582294 | 0.405516 | -0.600203 |
| 22 | -1.717369 | 0.025542 | 0.382368 |
| 22 | 1.559987 | -0.893625 | 0.315760 |
| 8 | 0.171457 | 2.968127 | -2.309487 |
| 8 | 1.116083 | 3.481109 | -1.764995 |

T08

E = -2494.89796053 a.u.

| | | | |
|---|-----------|-----------|-----------|
| 8 | -0.178351 | -0.402739 | 0.414778 |
| 8 | 2.506054 | 1.159161 | 0.926060 |
| 8 | 1.377590 | 0.687372 | -1.583356 |

| | | | |
|----|-----------|-----------|-----------|
| 8 | 2.455724 | -1.689030 | -0.635351 |
| 8 | -2.688488 | 1.135094 | 0.966584 |
| 8 | -2.856848 | -1.440313 | -0.523746 |
| 8 | -1.458815 | 0.882260 | -1.740238 |
| 1 | 2.612410 | 2.015684 | 0.502080 |
| 1 | 1.982179 | 0.560460 | -2.322545 |
| 1 | 2.677951 | -2.506040 | -0.180349 |
| 1 | -2.951079 | 2.057835 | 0.991405 |
| 1 | -0.521658 | 1.015350 | -1.981623 |
| 1 | -3.648037 | -1.811911 | -0.127045 |
| 22 | 1.562314 | -0.244083 | 0.011619 |
| 22 | -1.849597 | 0.037336 | -0.204493 |
| 8 | 1.989832 | -1.236672 | 2.011459 |
| 8 | 2.895170 | 0.396361 | 3.274706 |
| 8 | 2.449618 | -1.542117 | 4.181590 |
| 1 | 2.822730 | 0.885001 | 2.374738 |
| 1 | 2.060446 | -2.398562 | 3.957688 |
| 6 | 2.424064 | -0.792120 | 3.081712 |

T09 (doublet)

E = -2494.20222649 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -0.604504 | -0.333961 | -0.343079 |
| 8 | 1.886797 | 1.138927 | 1.238683 |
| 8 | -0.371392 | 2.270993 | 0.437438 |
| 8 | 1.024771 | 1.684630 | -1.936468 |
| 8 | -2.625100 | -1.846232 | 1.272554 |
| 8 | -3.310578 | -1.044011 | -1.512579 |
| 8 | -2.899777 | 1.034003 | 0.558097 |
| 1 | 1.630917 | 1.022758 | 2.162684 |
| 1 | -0.077936 | 3.180961 | 0.552944 |
| 1 | 1.538529 | 1.307432 | -2.657249 |
| 1 | -2.934294 | -1.879403 | 2.180635 |
| 1 | -2.221510 | 1.732320 | 0.655705 |
| 1 | -3.750682 | -1.835472 | -1.831272 |
| 22 | 0.658450 | 0.917746 | -0.337306 |
| 22 | -2.405122 | -0.590734 | -0.009584 |
| 8 | 2.202423 | -0.464069 | -0.747452 |
| 8 | 3.104229 | -0.586233 | 1.317412 |
| 8 | 3.804179 | -1.942415 | -0.256645 |
| 1 | 3.596430 | -2.157549 | -1.176679 |
| 6 | 2.989594 | -0.942937 | 0.111935 |

T10 (doublet)

E = -2759.33630254 a.u.

| | | | |
|---|-----------|-----------|-----------|
| 8 | 0.232026 | 0.216960 | 1.105162 |
| 8 | -2.033599 | 1.866018 | -1.095232 |
| 8 | 0.645136 | 1.832132 | -0.518366 |
| 8 | -1.292750 | 2.876541 | 1.529999 |
| 8 | 2.368243 | 0.399682 | -1.793299 |
| 8 | 2.229135 | -1.450813 | 0.293638 |
| 8 | 3.251782 | 1.133339 | 0.955461 |

| | | | |
|----|-----------|-----------|-----------|
| 1 | -2.351638 | 1.276018 | -1.788369 |
| 1 | 0.702110 | 2.126608 | -1.433959 |
| 1 | -1.742970 | 3.724996 | 1.468179 |
| 1 | 2.864386 | -0.294141 | -2.239693 |
| 1 | 3.831643 | 1.869504 | 0.740891 |
| 1 | 1.680666 | -2.229308 | 0.105888 |
| 22 | -1.080617 | 1.524666 | 0.386245 |
| 22 | 1.972969 | 0.300155 | 0.002026 |
| 8 | -2.431374 | 0.200178 | 1.077325 |
| 8 | -2.252702 | -1.132133 | -0.710178 |
| 8 | -3.606637 | -1.691516 | 0.965828 |
| 1 | -3.865814 | -1.323783 | 1.821749 |
| 6 | -2.724040 | -0.853250 | 0.396755 |
| 8 | -0.025942 | -4.965321 | -1.579531 |
| 8 | 0.094550 | -3.324780 | -0.260505 |
| 8 | -1.672225 | -3.468853 | -1.684336 |
| 1 | 0.035202 | -0.508465 | 1.704966 |
| 1 | -1.960999 | -2.587413 | -1.284480 |
| 6 | -0.557102 | -3.888954 | -1.171851 |

T11

E = -2758.64830454 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.325439 | -0.226771 | 0.376563 |
| 8 | 1.299148 | 1.912042 | -2.028454 |
| 8 | 2.421038 | -0.345433 | -0.813414 |
| 8 | 2.404649 | 2.099483 | 0.728997 |
| 8 | 1.425656 | -2.665579 | -1.695560 |
| 8 | -0.175403 | -2.816258 | 0.661724 |
| 8 | 2.606319 | -2.512408 | 1.099765 |
| 1 | 0.751197 | 2.063670 | -2.803343 |
| 1 | 2.736029 | -0.523578 | -1.706986 |
| 1 | 3.029935 | 2.826393 | 0.651415 |
| 1 | 0.905358 | -3.402502 | -2.031970 |
| 1 | 3.551707 | -2.433886 | 0.938657 |
| 1 | -1.060964 | -2.491501 | 0.905989 |
| 22 | 1.344218 | 1.201342 | -0.393545 |
| 22 | 1.262258 | -2.000555 | 0.002881 |
| 8 | -0.364265 | 2.393003 | 0.185758 |
| 8 | -2.066068 | 1.239583 | -0.587016 |
| 8 | -2.391674 | 2.685159 | 1.098756 |
| 1 | -1.873779 | 3.263882 | 1.678284 |
| 6 | -1.570131 | 2.118693 | 0.247661 |
| 8 | -4.345824 | -0.951825 | 0.859372 |
| 8 | -2.083918 | -0.772462 | 1.041682 |
| 8 | -3.387448 | 0.715808 | -0.196733 |
| 1 | -0.642917 | -0.311423 | 0.658460 |
| 6 | -3.247411 | -0.501778 | 0.681097 |

T12 (doublet)

E = -2758.03472549 a.u.

| | | | |
|---|-----------|----------|-----------|
| 8 | -0.581266 | 0.046133 | -0.977563 |
|---|-----------|----------|-----------|

| | | | |
|----|-----------|-----------|-----------|
| 8 | -0.466719 | 2.826539 | 1.363398 |
| 8 | -2.141051 | 0.824850 | 0.560561 |
| 8 | -1.266296 | 2.977351 | -1.392459 |
| 8 | -2.324069 | -1.518359 | 1.671084 |
| 8 | -0.973584 | -2.596413 | -0.541106 |
| 8 | -3.462409 | -1.333267 | -1.084413 |
| 1 | 0.035081 | 2.788987 | 2.183016 |
| 1 | -2.454091 | 0.950539 | 1.462920 |
| 1 | -1.466664 | 3.918865 | -1.370453 |
| 1 | -2.189576 | -2.387113 | 2.063217 |
| 1 | -4.383314 | -1.133051 | -0.893634 |
| 1 | -0.033097 | -2.802685 | -0.489647 |
| 22 | -0.631736 | 1.872120 | -0.146129 |
| 22 | -1.971135 | -1.162641 | -0.093679 |
| 8 | 1.324482 | 1.820397 | -0.507332 |
| 8 | 1.657739 | 0.541446 | 1.285119 |
| 8 | 3.282864 | 0.680338 | -0.398563 |
| 6 | 2.214415 | 1.043437 | -0.030895 |
| 8 | 4.388857 | -2.560268 | -0.037322 |
| 8 | 2.149477 | -2.355197 | -0.612218 |
| 8 | 2.371541 | -0.400209 | 1.854635 |
| 1 | 0.068383 | -0.266422 | -1.614853 |
| 6 | 3.274171 | -2.440013 | -0.316496 |

T13 (doublet)

E = -2569.38279566 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -0.514774 | -0.576581 | -0.760259 |
| 8 | -0.788119 | 2.057843 | 1.575880 |
| 8 | -2.318552 | 0.013238 | 0.637522 |
| 8 | -1.793156 | 2.285237 | -1.182542 |
| 8 | -2.191832 | -2.388516 | 1.641816 |
| 8 | -0.882685 | -3.302737 | -0.658988 |
| 8 | -3.359166 | -2.051631 | -1.128845 |
| 1 | 0.008192 | 2.440725 | 1.970526 |
| 1 | -2.588638 | 0.040314 | 1.562946 |
| 1 | -2.141619 | 3.181678 | -1.165962 |
| 1 | -2.077114 | -3.281663 | 1.981237 |
| 1 | -4.227896 | -1.662083 | -0.988331 |
| 1 | -0.025240 | -3.727763 | -0.589593 |
| 22 | -0.927724 | 1.248479 | -0.015597 |
| 22 | -1.887106 | -1.913822 | -0.102255 |
| 8 | 0.946215 | 1.594832 | -0.480371 |
| 8 | 1.981656 | 2.631023 | 1.204715 |
| 8 | 3.137848 | 2.075707 | -0.745812 |
| 6 | 2.101639 | 2.050266 | -0.171689 |
| 8 | 3.101633 | 3.136433 | 1.674583 |
| 1 | 0.235308 | -0.756222 | -1.335664 |

T14 (triplet)

E = -2568.79932966 a.u.

| | | | |
|---|----------|-----------|-----------|
| 8 | 1.081732 | -0.654624 | -0.610350 |
|---|----------|-----------|-----------|

| | | | |
|----|-----------|-----------|-----------|
| 8 | -0.771674 | 1.637810 | -1.161566 |
| 8 | 0.212738 | 0.936529 | 1.557532 |
| 8 | -1.814816 | -0.777424 | 0.249448 |
| 8 | 2.905563 | -0.004753 | 1.424698 |
| 8 | 3.990363 | -0.485736 | -1.346347 |
| 8 | 3.048341 | -2.763164 | 0.228438 |
| 1 | -0.741524 | 2.597632 | -1.131786 |
| 1 | 1.147248 | 0.820032 | 1.815938 |
| 1 | -2.674404 | -0.901167 | -0.165263 |
| 1 | 3.666834 | 0.082158 | 2.005756 |
| 1 | 2.519070 | -3.496050 | 0.552172 |
| 1 | 4.043323 | 0.157601 | -2.056814 |
| 22 | -0.384446 | 0.297085 | -0.011263 |
| 22 | 2.761570 | -1.012121 | -0.127397 |
| 8 | -4.679422 | -1.510615 | -0.633629 |
| 8 | -0.471499 | 4.803438 | -0.237821 |
| 8 | -6.441685 | -2.771032 | 0.198597 |
| 6 | -5.560750 | -2.142690 | -0.214298 |
| 8 | -0.245898 | 5.159018 | 0.891375 |

T15

E = -2571.37924172 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.517831 | 0.526137 | -0.308514 |
| 8 | 1.582707 | 1.188796 | -0.930188 |
| 8 | 0.070637 | 2.366390 | 1.674341 |
| 8 | -0.393582 | 3.079419 | -0.892854 |
| 8 | -1.426877 | -1.980387 | 0.898440 |
| 8 | -2.855767 | -1.737550 | -1.752848 |
| 8 | -4.114886 | -0.631352 | 0.648833 |
| 1 | 1.752743 | 1.859797 | -1.602804 |
| 1 | 0.339952 | 1.829797 | 2.428624 |
| 1 | -0.474582 | 3.991124 | -0.599509 |
| 1 | -1.593451 | -2.852548 | 1.266326 |
| 1 | -4.472683 | 0.008886 | 1.268440 |
| 1 | -2.428464 | -1.796227 | -2.610578 |
| 22 | -0.019565 | 1.570674 | 0.037514 |
| 22 | -2.528959 | -0.924146 | -0.170343 |
| 8 | 0.654704 | -0.220205 | 1.193802 |
| 1 | 0.031477 | -0.979064 | 1.195500 |
| 1 | 1.570253 | -0.576438 | 1.114673 |
| 8 | 3.137665 | -1.247204 | 0.919572 |
| 8 | 3.638994 | -0.360782 | -1.101435 |
| 8 | 4.982736 | -1.830437 | -0.219345 |
| 1 | 2.802018 | 0.197831 | -0.978554 |
| 1 | 5.076220 | -2.381782 | 0.568685 |
| 6 | 3.847434 | -1.132650 | -0.072542 |

T16 (doublet)

E = -2570.67659787 a.u.

| | | | |
|---|-----------|----------|----------|
| 8 | 1.254498 | 0.433927 | 0.371429 |
| 8 | -1.850352 | 1.396299 | 0.328234 |

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.348888 | 2.497094 | -1.766787 |
| 8 | 0.266539 | 3.053757 | 0.899823 |
| 8 | 1.300737 | -1.839720 | -1.247745 |
| 8 | 2.094667 | -2.142129 | 1.651709 |
| 8 | 3.930604 | -0.806554 | -0.196897 |
| 1 | -2.169643 | 1.860529 | 1.110681 |
| 1 | 0.074405 | 2.082568 | -2.593040 |
| 1 | 0.367588 | 3.994278 | 0.730172 |
| 1 | 1.514505 | -2.646467 | -1.724697 |
| 1 | 4.457157 | -0.116492 | -0.607519 |
| 1 | 1.471179 | -2.282955 | 2.368470 |
| 22 | -0.023600 | 1.647176 | -0.201791 |
| 22 | 2.186369 | -1.068657 | 0.199028 |
| 8 | -0.696900 | 0.023167 | -1.582862 |
| 1 | -0.075637 | -0.735237 | -1.635048 |
| 1 | -1.580178 | -0.345820 | -1.346350 |
| 8 | -2.996649 | -1.151464 | -0.761503 |
| 8 | -2.800243 | -0.340207 | 1.336750 |
| 8 | -4.216266 | -1.946035 | 0.960158 |
| 1 | -4.502168 | -2.542058 | 0.252996 |
| 6 | -3.295813 | -1.120664 | 0.422614 |

T17

E = -2570.03452499 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.951114 | 0.134321 | 0.432327 |
| 8 | -2.137023 | 1.292106 | -0.159428 |
| 8 | 0.365000 | 2.729565 | -1.211169 |
| 8 | -0.186423 | 2.446017 | 1.513005 |
| 8 | 1.547615 | -1.630866 | -1.644599 |
| 8 | 1.993758 | -2.573912 | 1.194599 |
| 8 | 3.826844 | -0.605716 | 0.034511 |
| 1 | 0.377924 | 2.457870 | -2.137844 |
| 1 | -0.761935 | 3.100200 | 1.918032 |
| 1 | 1.932004 | -2.274664 | -2.246222 |
| 1 | 4.294978 | 0.220388 | -0.108733 |
| 1 | 1.377278 | -2.931773 | 1.837104 |
| 22 | -0.224373 | 1.499390 | -0.016663 |
| 22 | 2.108450 | -1.162492 | 0.070565 |
| 8 | -0.470416 | 0.216381 | -1.938347 |
| 1 | 0.179910 | -0.513004 | -2.032198 |
| 1 | -1.355325 | -0.188202 | -1.889150 |
| 8 | -2.848469 | -1.079507 | -0.977887 |
| 8 | -2.681630 | 0.365890 | 0.788928 |
| 8 | -3.746143 | -1.491244 | 1.060092 |
| 1 | -3.991933 | -2.318117 | 0.623225 |
| 6 | -3.071358 | -0.761500 | 0.163541 |

T18 (doublet)

E = -2569.38488142 a.u.

| | | | |
|---|-----------|-----------|-----------|
| 8 | -1.542202 | -0.133760 | 0.029775 |
| 8 | 4.847732 | 1.408759 | -0.464362 |

| | | | |
|----|-----------|-----------|-----------|
| 8 | -2.587193 | 2.232015 | 1.547685 |
| 8 | -2.576545 | 2.255761 | -1.417208 |
| 8 | -2.223690 | -2.902111 | 0.746522 |
| 8 | 0.601822 | -2.018740 | 0.916525 |
| 8 | -0.713968 | -2.291952 | -1.750864 |
| 1 | -2.339346 | 2.678401 | 2.360962 |
| 1 | -2.375061 | 2.843885 | -2.148877 |
| 1 | -2.822022 | -3.626160 | 0.548957 |
| 1 | -0.816984 | -1.926352 | -2.632878 |
| 1 | 0.615074 | -2.535494 | 1.730100 |
| 22 | -1.686404 | 1.711241 | 0.064937 |
| 22 | -1.018696 | -1.825917 | -0.042898 |
| 8 | -0.034545 | 2.355441 | 0.080280 |
| 1 | 0.863921 | 1.991616 | 0.015264 |
| 8 | 2.333334 | 0.823880 | -0.126387 |
| 8 | 4.553673 | 0.180220 | -0.083734 |
| 8 | 3.014451 | -1.268542 | 0.440807 |
| 1 | 2.039417 | -1.520471 | 0.594632 |
| 6 | 3.142755 | -0.033028 | 0.073069 |

T19 (triplet)

E = -2568.80016937 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.718613 | 0.004997 | -0.033033 |
| 8 | 7.058296 | -0.399610 | -0.034209 |
| 8 | -2.396899 | -2.457990 | -1.536969 |
| 8 | -2.755338 | -2.389297 | 1.401724 |
| 8 | -2.178842 | 2.595187 | -1.436220 |
| 8 | 0.378705 | 2.038736 | -0.021745 |
| 8 | -2.153056 | 2.500799 | 1.490219 |
| 1 | -2.085464 | -3.004002 | -2.262187 |
| 1 | -3.586756 | -2.867668 | 1.445692 |
| 1 | -2.916427 | 3.191258 | -1.583672 |
| 1 | -2.566671 | 2.226103 | 2.311191 |
| 22 | -1.729124 | -1.818637 | 0.015828 |
| 22 | -1.436860 | 1.779896 | 0.000216 |
| 8 | -0.038505 | -2.377501 | 0.258278 |
| 1 | 0.817395 | -1.940973 | 0.177699 |
| 8 | 2.369242 | -0.529711 | -0.054411 |
| 8 | 5.949930 | -0.873851 | -0.042063 |
| 8 | 3.364245 | 1.566425 | -0.042566 |
| 1 | 0.864817 | 2.867337 | -0.069466 |
| 6 | 2.845538 | 0.530229 | -0.047281 |

T20

E = -2493.56489772 a.u.

| | | | |
|---|-----------|-----------|-----------|
| 8 | 0.693336 | -0.344595 | 0.544477 |
| 8 | -2.023551 | 0.689886 | -1.150649 |
| 8 | 0.094289 | 2.025142 | -0.675481 |
| 8 | -1.218538 | 1.586678 | 1.875784 |
| 8 | 2.674337 | -1.932225 | -1.047893 |
| 8 | 3.551982 | -0.640749 | 1.493323 |

| | | | |
|----|-----------|-----------|-----------|
| 8 | 2.737971 | 1.043022 | -0.804180 |
| 1 | -0.381745 | 2.689916 | -1.184976 |
| 1 | -0.767828 | 2.142278 | 2.516744 |
| 1 | 2.859870 | -2.070990 | -1.979381 |
| 1 | 1.974924 | 1.629973 | -0.977373 |
| 1 | 4.078597 | -1.347712 | 1.873659 |
| 22 | -0.724969 | 0.727755 | 0.363446 |
| 22 | 2.459628 | -0.508503 | 0.049345 |
| 8 | -2.117886 | -0.863491 | 0.792990 |
| 8 | -3.157147 | -0.199276 | -1.069373 |
| 8 | -4.040962 | -1.821475 | 0.092684 |
| 1 | -3.904953 | -2.336086 | 0.901214 |
| 6 | -3.047292 | -0.956356 | -0.010288 |

T21

E = -2570.02968911 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 1.228343 | 0.370676 | -0.339821 |
| 8 | -1.678972 | -0.705204 | -0.737192 |
| 8 | -0.957012 | 1.939347 | -1.291276 |
| 8 | -0.910628 | 1.677660 | 1.452835 |
| 8 | 3.239195 | -1.526625 | -1.303868 |
| 8 | 3.400388 | -0.543181 | 1.482368 |
| 8 | 4.024329 | 1.288471 | -0.712867 |
| 1 | -1.566624 | 1.964806 | -2.032770 |
| 1 | -1.123696 | 2.613215 | 1.371680 |
| 1 | 3.844930 | -1.799091 | -1.996140 |
| 1 | 3.925807 | 2.098203 | -1.218880 |
| 1 | 3.312580 | -1.376058 | 1.953669 |
| 22 | -0.521522 | 0.687631 | -0.055161 |
| 22 | 2.978900 | -0.100079 | -0.226200 |
| 8 | -3.108452 | -1.702403 | 1.218052 |
| 8 | -3.077521 | -0.402889 | -0.664920 |
| 8 | -4.977499 | -0.897183 | 0.228259 |
| 1 | -5.389889 | -1.335363 | 0.985198 |
| 6 | -3.656647 | -1.071950 | 0.346433 |
| 8 | -0.441804 | -0.892672 | 1.611903 |
| 1 | -0.450934 | -0.412828 | 2.449469 |
| 1 | -1.282518 | -1.389083 | 1.559298 |

T22 (doublet)

E = -2569.36414462 a.u.

| | | | |
|---|-----------|-----------|-----------|
| 8 | 1.428286 | 0.026750 | 0.383450 |
| 8 | -3.251008 | 1.326123 | -1.757874 |
| 8 | -0.654954 | 1.972437 | -0.237056 |
| 8 | -0.647861 | 0.681452 | 2.436722 |
| 8 | 3.235002 | -1.779352 | -1.019779 |
| 8 | 4.087991 | -0.610874 | 1.571957 |
| 8 | 3.932983 | 1.107536 | -0.787819 |
| 1 | -1.388144 | 2.269743 | -0.787368 |
| 1 | -0.741816 | 1.433943 | 3.025325 |
| 1 | 3.733797 | -2.053019 | -1.792805 |

| | | | |
|----|-----------|-----------|-----------|
| 1 | 3.634333 | 1.891105 | -1.255378 |
| 1 | 4.233575 | -1.379789 | 2.128145 |
| 22 | -0.306747 | 0.453870 | 0.673696 |
| 22 | 3.175264 | -0.307780 | 0.036003 |
| 8 | -4.054112 | -1.173373 | -1.592262 |
| 8 | -3.822370 | 0.933145 | -0.637855 |
| 8 | -4.714505 | -0.666518 | 0.529581 |
| 1 | -4.929940 | -1.607553 | 0.597738 |
| 6 | -4.190374 | -0.449801 | -0.666224 |
| 8 | -1.390037 | -0.884991 | 0.069342 |
| 1 | -1.230745 | -1.503855 | -0.650522 |

T23 (triplet)

E = -2568.80066092 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 1.092625 | -0.386279 | -0.057233 |
| 8 | -3.511233 | -2.691111 | 2.684630 |
| 8 | -0.480183 | -2.422389 | 1.385944 |
| 8 | 0.350858 | -2.944039 | -1.415042 |
| 8 | 1.094491 | 2.490636 | -0.346497 |
| 8 | 3.483447 | 0.955174 | -1.256082 |
| 8 | 2.987438 | 1.234482 | 1.594612 |
| 1 | -1.251567 | -2.587326 | 1.934605 |
| 1 | 0.695241 | -3.835407 | -1.320525 |
| 1 | 1.354701 | 3.412281 | -0.437685 |
| 1 | 2.789618 | 1.037948 | 2.512932 |
| 1 | 3.581287 | 0.600312 | -2.142663 |
| 22 | -0.188876 | -1.676950 | -0.234572 |
| 22 | 2.175238 | 1.044173 | -0.010317 |
| 8 | -1.258639 | 4.260536 | -1.021411 |
| 8 | -4.524894 | -2.331341 | 2.141042 |
| 8 | -2.100811 | 2.111519 | -0.783214 |
| 6 | -1.655040 | 3.178866 | -0.898749 |
| 8 | -1.689664 | -0.907810 | -0.856592 |
| 1 | -1.987993 | 0.008912 | -0.883260 |

B01

E = -1480.02827234 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.714540 | -0.057648 | -0.453586 |
| 8 | 3.205837 | -0.619224 | 0.852530 |
| 8 | 2.121792 | 1.914688 | 0.738243 |
| 8 | 3.138066 | 0.925340 | -1.625657 |
| 8 | -1.592446 | -0.131753 | 1.822234 |
| 8 | -0.644381 | 2.282024 | 1.179098 |
| 1 | 3.584011 | -0.414148 | 1.713928 |
| 1 | 0.319704 | 2.425993 | 1.159499 |
| 1 | 3.531131 | 1.784882 | -1.809581 |
| 1 | -0.829147 | 1.840454 | 2.023013 |
| 1 | -1.742858 | -1.062892 | 2.025382 |
| 23 | 2.278481 | 0.568700 | -0.102329 |
| 83 | -1.408743 | 0.202258 | -0.253847 |
| 8 | -1.733187 | -1.835716 | -0.708332 |

1 -0.937540 -2.376685 -0.767532

B02

E = -1556.50748680 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.834757 | -0.639175 | -0.033437 |
| 8 | 3.140558 | -0.606010 | 1.663053 |
| 8 | 2.548502 | 1.439265 | -0.102865 |
| 8 | 3.412566 | -0.928974 | -1.236378 |
| 8 | -1.830509 | -1.857734 | 0.507565 |
| 8 | -1.525479 | 1.013468 | 1.478212 |
| 8 | -0.086377 | 2.390109 | -0.324599 |
| 1 | 3.558831 | 0.036555 | 2.245074 |
| 1 | 0.888090 | 2.324554 | -0.305932 |
| 1 | 3.978563 | -0.421738 | -1.827220 |
| 1 | -1.108962 | -2.447464 | 0.750191 |
| 1 | -1.758571 | 0.396313 | 2.181718 |
| 1 | -0.354240 | 2.571724 | 0.589640 |
| 23 | 2.468802 | -0.148447 | 0.069049 |
| 83 | -1.232130 | 0.012906 | -0.357220 |
| 8 | -3.854264 | -0.573050 | -0.439911 |
| 1 | -3.617946 | -1.395184 | 0.031973 |
| 1 | -4.568229 | -0.152636 | 0.050045 |

B03 (doublet)

E = -1555.80796978 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.973839 | -0.645795 | -0.032600 |
| 8 | 3.344609 | -0.704982 | 1.575297 |
| 8 | 2.751719 | 1.376727 | -0.143116 |
| 8 | 3.499786 | -1.001854 | -1.329866 |
| 8 | -1.709406 | -1.792465 | 0.606380 |
| 8 | -1.249453 | 1.056776 | 1.604181 |
| 8 | 0.138781 | 2.387513 | -0.261013 |
| 1 | 3.788930 | -0.085577 | 2.163370 |
| 1 | 1.112282 | 2.304418 | -0.276795 |
| 1 | 4.052150 | -0.511312 | -1.947361 |
| 1 | -1.018716 | -2.404339 | 0.883012 |
| 1 | -0.092647 | 2.614237 | 0.653109 |
| 1 | -1.553062 | 0.467454 | 2.304646 |
| 23 | 2.631462 | -0.208399 | 0.015120 |
| 83 | -1.062773 | 0.077417 | -0.250438 |
| 8 | -3.841085 | -0.616241 | -0.181062 |
| 1 | -3.418183 | -1.384788 | 0.286820 |

B04 (doublet)

E = -1632.29170104 a.u.

| | | | |
|---|-----------|-----------|-----------|
| 8 | 0.997971 | -0.531663 | -0.075813 |
| 8 | 3.308437 | -0.924654 | 1.565978 |
| 8 | 2.996934 | 1.272850 | -0.088102 |
| 8 | 3.483129 | -1.139717 | -1.350209 |
| 8 | -1.752018 | -1.404794 | 0.377633 |
| 8 | -1.030820 | 1.336339 | 1.597333 |

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.547629 | 2.621357 | -0.146436 |
| 1 | 3.827597 | -0.383928 | 2.169890 |
| 1 | 1.500211 | 2.401314 | -0.177225 |
| 1 | 4.113151 | -0.696773 | -1.927855 |
| 1 | -1.051625 | -2.041032 | 0.565503 |
| 1 | 0.345796 | 2.776410 | 0.789480 |
| 1 | -1.374646 | 0.723469 | 2.257409 |
| 23 | 2.687868 | -0.293973 | 0.011581 |
| 83 | -0.940612 | 0.478992 | -0.326047 |
| 8 | -4.346453 | -1.614916 | 0.435009 |
| 1 | -3.344975 | -1.740846 | 0.466993 |
| 8 | -3.539766 | 0.847226 | -0.444405 |
| 1 | -3.975313 | 1.608487 | -0.046596 |
| 1 | -4.038748 | 0.043955 | -0.159852 |

B05

E = -1631.64226927 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.814794 | -0.587696 | -0.125467 |
| 8 | 3.070179 | -1.312495 | 1.472661 |
| 8 | 2.900183 | 1.093712 | 0.092547 |
| 8 | 3.270829 | -1.186028 | -1.443536 |
| 8 | -1.565744 | -1.665918 | -0.220990 |
| 8 | -0.972376 | 1.024137 | 1.755838 |
| 8 | 0.624894 | 2.618242 | 0.220833 |
| 1 | 3.563631 | -0.874213 | 2.173238 |
| 1 | 1.552119 | 2.298589 | 0.142704 |
| 1 | 3.960622 | -0.730971 | -1.937433 |
| 1 | -0.895309 | -2.091652 | 0.338817 |
| 1 | 0.443151 | 2.654023 | 1.172943 |
| 1 | -1.880462 | 0.957927 | 2.082646 |
| 23 | 2.507928 | -0.460914 | 0.004553 |
| 83 | -1.011847 | 0.735044 | -0.310735 |
| 8 | -2.828342 | -2.011481 | 0.407504 |
| 8 | -3.202865 | 0.527254 | 0.144738 |
| 1 | -3.878295 | 0.831848 | -0.469225 |
| 1 | -3.236928 | -1.090658 | 0.402802 |

B06 (doublet)

E = -1631.01879319 a.u.

| | | | |
|---|-----------|-----------|-----------|
| 8 | 1.158247 | -0.767860 | -0.077369 |
| 8 | 3.481607 | -0.838747 | 1.600272 |
| 8 | 2.806435 | 1.351583 | 0.056122 |
| 8 | 3.735282 | -0.859839 | -1.315402 |
| 8 | -1.440153 | -2.207650 | 0.270331 |
| 8 | -1.127362 | 0.562967 | 1.680142 |
| 8 | 0.186768 | 2.259571 | 0.060115 |
| 1 | 3.890235 | -0.252882 | 2.245662 |
| 1 | 1.164999 | 2.195067 | 0.015839 |
| 1 | 4.284693 | -0.283914 | -1.857088 |
| 1 | -0.026345 | 2.321298 | 1.004579 |
| 1 | -1.206462 | -0.171354 | 2.300251 |

| | | | |
|----|-----------|-----------|-----------|
| 23 | 2.782037 | -0.250343 | 0.067127 |
| 83 | -0.882277 | -0.039341 | -0.321041 |
| 8 | -2.715381 | -2.516183 | 0.328140 |
| 8 | -3.447275 | -0.124118 | -0.361357 |
| 1 | -3.953969 | 0.391224 | 0.276277 |
| 1 | -3.508427 | -1.080603 | -0.082526 |

B07 (triplet)

E = -1630.39962992 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -0.343105 | -0.046821 | -0.390359 |
| 8 | -2.251369 | 1.646870 | 0.912009 |
| 8 | -2.844878 | -0.928803 | 0.115165 |
| 8 | -2.573194 | 0.930235 | -1.902323 |
| 8 | 1.116174 | 3.835446 | 1.079715 |
| 8 | 1.032976 | -1.857003 | 1.927259 |
| 8 | -0.957509 | -2.991402 | 0.551592 |
| 1 | -2.862364 | 1.554777 | 1.650457 |
| 1 | -1.797303 | -2.508538 | 0.442922 |
| 1 | -3.338471 | 0.549986 | -2.346014 |
| 1 | -0.742650 | -2.938956 | 1.496204 |
| 1 | 1.633727 | -1.270888 | 2.403353 |
| 23 | -2.011015 | 0.363726 | -0.305343 |
| 83 | 1.153138 | -1.571681 | -0.160822 |
| 8 | 1.525080 | 3.149540 | 0.176961 |
| 8 | 2.657072 | -0.102687 | 0.036289 |
| 1 | 2.340301 | 0.807398 | 0.075656 |

B08

E = -1745.15562677 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.990420 | -0.629602 | 0.021672 |
| 8 | 3.061779 | -0.512225 | 1.978242 |
| 8 | 2.881799 | 1.288425 | -0.111550 |
| 8 | 3.656922 | -1.273522 | -0.796328 |
| 8 | -1.757617 | -1.784831 | -0.092183 |
| 8 | -1.292385 | 0.995654 | 1.266792 |
| 8 | 0.372635 | 2.453288 | -0.618638 |
| 1 | 3.549675 | 0.141800 | 2.489186 |
| 1 | 1.332872 | 2.297854 | -0.529489 |
| 1 | 4.328581 | -0.902684 | -1.377871 |
| 1 | -1.097168 | -2.362302 | 0.308744 |
| 1 | -0.857036 | 0.495036 | 1.967642 |
| 1 | 0.084925 | 2.765908 | 0.248769 |
| 23 | 2.638550 | -0.248628 | 0.258148 |
| 83 | -0.970542 | 0.079970 | -0.678622 |
| 8 | -3.399607 | 0.805509 | -0.749046 |
| 8 | -3.792053 | 1.367789 | 1.402281 |
| 8 | -5.466802 | 1.221699 | 0.009448 |
| 1 | -2.773660 | 1.238563 | 1.471375 |
| 1 | -5.653278 | 1.000963 | -0.913287 |
| 6 | -4.151514 | 1.111241 | 0.186568 |

B09 (doublet)

E = -1744.46075242 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 1.552544 | -0.565547 | 0.387475 |
| 8 | 3.609790 | 0.850402 | 1.779422 |
| 8 | 2.974101 | 1.343885 | -0.869031 |
| 8 | 4.269257 | -1.045952 | -0.357294 |
| 8 | -1.000048 | -1.763619 | 1.349843 |
| 8 | -0.928225 | 1.220925 | 0.854463 |
| 8 | 0.300234 | 1.604650 | -1.613249 |
| 1 | 3.895332 | 1.764965 | 1.873098 |
| 1 | 1.274014 | 1.676668 | -1.537506 |
| 1 | 4.839754 | -0.887997 | -1.116535 |
| 1 | -0.210505 | -2.019942 | 1.842132 |
| 1 | -0.988080 | 1.005339 | 1.798177 |
| 1 | -0.049001 | 2.333702 | -1.084463 |
| 23 | 3.084701 | 0.167785 | 0.211866 |
| 83 | -0.532233 | -0.602026 | -0.345833 |
| 8 | -2.938148 | -0.235803 | -0.526771 |
| 8 | -3.059330 | 1.406564 | 1.020931 |
| 8 | -4.899768 | 0.586233 | 0.178911 |
| 1 | -5.182806 | -0.102090 | -0.439612 |
| 6 | -3.559015 | 0.561024 | 0.207497 |

B10 (doublet)

E = -2009.58391896 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 1.357192 | -0.239476 | 0.464543 |
| 8 | 3.668965 | 0.808373 | 1.795285 |
| 8 | 3.259573 | 1.044124 | -0.933257 |
| 8 | 3.902434 | -1.473278 | 0.012501 |
| 8 | -1.109072 | -0.764677 | 1.705149 |
| 8 | -0.674552 | 2.111375 | 0.422252 |
| 8 | 0.757861 | 1.739170 | -1.820406 |
| 1 | 4.059210 | 1.687888 | 1.838667 |
| 1 | 1.729991 | 1.619944 | -1.733669 |
| 1 | 4.479167 | -1.632199 | -0.742420 |
| 1 | -0.299213 | -0.831350 | 2.229914 |
| 1 | -1.542259 | 2.341448 | 0.800755 |
| 1 | 0.538845 | 2.558465 | -1.343772 |
| 23 | 3.049090 | 0.058562 | 0.307865 |
| 83 | -0.561004 | 0.214709 | -0.426454 |
| 8 | -3.293535 | 0.541602 | -0.314534 |
| 8 | -3.486093 | 2.159522 | 1.211146 |
| 8 | -4.891148 | 0.425180 | 1.310116 |
| 1 | -4.948952 | -0.481806 | 0.941064 |
| 6 | -3.885476 | 1.112755 | 0.783326 |
| 8 | -2.136070 | -2.267155 | -0.785281 |
| 8 | -2.706761 | -2.926235 | 1.159590 |
| 8 | -4.228294 | -1.892703 | -0.117313 |
| 1 | -1.578093 | -1.632567 | 1.734699 |
| 1 | -3.736997 | -0.317789 | -0.546757 |
| 6 | -3.082624 | -2.376702 | 0.066612 |

B11

E = -2008.91006596 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 2.025984 | -0.412982 | 0.285631 |
| 8 | 4.171521 | 0.209494 | 2.089173 |
| 8 | 4.108671 | 1.077514 | -0.533310 |
| 8 | 4.595036 | -1.610493 | -0.133114 |
| 8 | -0.642300 | -1.161796 | 0.923563 |
| 8 | 0.053533 | 1.994249 | 0.544417 |
| 8 | 1.733572 | 2.028012 | -1.547706 |
| 1 | 4.556341 | 1.040326 | 2.388654 |
| 1 | 2.687639 | 1.865583 | -1.379644 |
| 1 | 5.273787 | -1.613573 | -0.816760 |
| 1 | -0.064212 | -1.515663 | 1.609630 |
| 1 | -0.834407 | 2.107235 | 0.932212 |
| 1 | 1.474740 | 2.761002 | -0.964326 |
| 23 | 3.732070 | -0.155265 | 0.409592 |
| 83 | 0.237014 | 0.302204 | -0.637182 |
| 8 | -2.593461 | 0.532396 | -0.717578 |
| 8 | -2.735522 | 1.802209 | 1.133647 |
| 8 | -4.282478 | 0.244684 | 0.773941 |
| 6 | -3.176167 | 0.921833 | 0.446889 |
| 8 | -4.316061 | -3.091696 | -0.334993 |
| 8 | -2.980083 | -2.029328 | 1.182792 |
| 8 | -4.535544 | -0.856620 | -0.151623 |
| 1 | -1.604448 | -1.511454 | 1.033881 |
| 1 | -3.209960 | -0.142573 | -1.095660 |
| 6 | -3.843702 | -2.211645 | 0.319663 |

B12 (doublet)

E = -2008.29632626 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.795833 | 0.702544 | 0.200946 |
| 8 | -3.985371 | 0.869715 | 2.036987 |
| 8 | -4.051787 | -0.683077 | -0.261361 |
| 8 | -4.166114 | 2.063822 | -0.616648 |
| 8 | 0.740461 | 1.508512 | 0.455838 |
| 8 | -0.184323 | -1.732070 | 1.169307 |
| 8 | -1.878117 | -2.235035 | -0.887611 |
| 1 | -4.491003 | 0.204815 | 2.515869 |
| 1 | -2.786396 | -1.868341 | -0.801383 |
| 1 | -4.876321 | 1.955025 | -1.257817 |
| 1 | 0.105425 | 2.009419 | 0.983017 |
| 1 | 0.708782 | -1.966477 | 1.492623 |
| 1 | -1.719405 | -2.743393 | -0.075181 |
| 23 | -3.503352 | 0.701360 | 0.328967 |
| 83 | -0.102625 | -0.523960 | -0.514668 |
| 8 | 2.287732 | -0.691894 | -0.331739 |
| 8 | 2.602300 | -2.094500 | 1.419986 |
| 8 | 4.405686 | -1.229357 | 0.420513 |
| 6 | 2.933921 | -1.355241 | 0.518274 |
| 8 | 5.338696 | 2.789259 | -0.524984 |

| | | | |
|---|----------|-----------|-----------|
| 8 | 3.508934 | 2.333476 | 0.827778 |
| 8 | 4.836047 | -0.301278 | -0.405338 |
| 1 | 1.654382 | 1.706374 | 0.715046 |
| 6 | 4.428962 | 2.543039 | 0.141683 |

B13 (doublet)

E = -1819.65095204 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.867457 | 0.756444 | 0.212984 |
| 8 | -4.151582 | 0.937040 | 1.930040 |
| 8 | -4.130555 | -0.551590 | -0.407383 |
| 8 | -4.155986 | 2.201279 | -0.698840 |
| 8 | 0.794147 | 1.342185 | 0.738685 |
| 8 | -0.352080 | -1.733945 | 1.212843 |
| 8 | -1.946605 | -2.119225 | -0.963149 |
| 1 | -4.720639 | 0.285020 | 2.352079 |
| 1 | -2.851666 | -1.738789 | -0.908664 |
| 1 | -4.824948 | 2.127654 | -1.387639 |
| 1 | 0.245963 | 1.810415 | 1.378957 |
| 1 | 0.497910 | -1.970265 | 1.603367 |
| 1 | -1.854110 | -2.695363 | -0.188490 |
| 23 | -3.579787 | 0.802442 | 0.247126 |
| 83 | -0.155404 | -0.451106 | -0.426743 |
| 8 | 2.206744 | -1.013440 | -0.159700 |
| 8 | 3.179934 | 0.549672 | 1.150838 |
| 8 | 4.445622 | -1.103121 | 0.375990 |
| 6 | 3.142613 | -0.464361 | 0.456950 |
| 8 | 4.475219 | -2.204727 | -0.348675 |
| 1 | 1.745247 | 1.192323 | 1.058273 |

B14 (triplet)

E = -1819.05354668 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 1.521548 | -0.798058 | 0.049582 |
| 8 | 3.956257 | -0.724440 | 1.560815 |
| 8 | 3.299602 | 1.199569 | -0.306740 |
| 8 | 3.997298 | -1.273644 | -1.309951 |
| 8 | -1.143593 | -1.891457 | 0.895766 |
| 8 | -0.658482 | 1.031727 | 1.606944 |
| 8 | 0.662217 | 2.193989 | -0.407425 |
| 1 | 4.420318 | -0.057328 | 2.077128 |
| 1 | 1.634007 | 2.123426 | -0.455814 |
| 1 | 4.520481 | -0.840912 | -1.992664 |
| 1 | -0.426068 | -2.419621 | 1.263136 |
| 1 | -0.922318 | 0.509447 | 2.373810 |
| 1 | 0.461543 | 2.469226 | 0.500895 |
| 23 | 3.182624 | -0.363368 | -0.006951 |
| 83 | -0.523818 | -0.142000 | -0.140633 |
| 8 | -3.516141 | -1.039198 | -0.317677 |
| 8 | -4.074915 | -2.971287 | 0.842251 |
| 8 | -2.868798 | 2.574535 | -1.063112 |
| 6 | -3.765299 | -2.012859 | 0.275466 |
| 8 | -2.862578 | 3.723295 | -0.698830 |

B15

E = -1821.63640703 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 1.144153 | -0.632834 | 0.131515 |
| 8 | 3.565402 | -0.247438 | 1.603777 |
| 8 | 2.728608 | 1.479975 | -0.392721 |
| 8 | 3.629942 | -0.998612 | -1.228724 |
| 8 | -1.302010 | -1.930975 | 0.894187 |
| 8 | -1.124621 | 1.074244 | 1.621201 |
| 8 | 0.069373 | 2.323324 | -0.451295 |
| 1 | 4.009185 | 0.486963 | 2.040021 |
| 1 | 1.043252 | 2.274998 | -0.537023 |
| 1 | 4.130377 | -0.566895 | -1.928699 |
| 1 | -0.443957 | -2.333262 | 1.083042 |
| 1 | -1.158884 | 0.512043 | 2.403999 |
| 1 | -0.096601 | 2.598447 | 0.463657 |
| 23 | 2.750817 | -0.066511 | 0.021070 |
| 83 | -0.972108 | -0.052781 | -0.156180 |
| 8 | -3.495663 | 0.019879 | 0.073515 |
| 1 | -3.968508 | -0.836330 | 0.236273 |
| 1 | -3.753861 | 0.621182 | 0.781740 |
| 8 | -4.711169 | -2.305407 | 0.548114 |
| 8 | -3.088354 | -3.682925 | 1.325498 |
| 8 | -5.147492 | -4.384316 | 1.263427 |
| 1 | -2.421039 | -2.928287 | 1.130903 |
| 1 | -6.030987 | -4.086357 | 1.009776 |
| 6 | -4.307453 | -3.368679 | 1.013711 |

B16 (doublet)

E = -1820.93872419 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.036504 | 0.851491 | 0.256178 |
| 8 | -3.461883 | 1.689202 | 1.516368 |
| 8 | -3.391601 | -0.202782 | -0.506009 |
| 8 | -2.891217 | 2.411771 | -1.262207 |
| 8 | 1.596236 | 0.705409 | 1.452779 |
| 8 | -0.104955 | -1.770995 | 1.851973 |
| 8 | -1.515776 | -2.242081 | -0.386568 |
| 1 | -4.246526 | 1.263283 | 1.876325 |
| 1 | -2.324140 | -1.710793 | -0.547484 |
| 1 | -3.450462 | 2.287745 | -2.035937 |
| 1 | 1.175380 | 1.578303 | 1.385034 |
| 1 | 0.105740 | -1.323835 | 2.678860 |
| 1 | -1.604251 | -2.586076 | 0.516587 |
| 23 | -2.696686 | 1.152569 | -0.008764 |
| 83 | 0.496108 | -0.735049 | 0.110697 |
| 8 | 2.703646 | -1.891097 | 0.568972 |
| 1 | 3.424298 | -1.207635 | 0.520939 |
| 1 | 2.773308 | -2.340837 | 1.418067 |
| 8 | 4.322411 | 0.158206 | 0.121525 |
| 8 | 2.411646 | 1.202049 | -0.504680 |
| 8 | 4.336535 | 1.974568 | -1.200327 |
| 1 | 5.275280 | 1.739901 | -1.194884 |

| | | | |
|---|----------|----------|-----------|
| 6 | 3.698253 | 1.039513 | -0.465730 |
|---|----------|----------|-----------|

B17

E = -1820.29339127 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.335446 | 0.778781 | 0.126212 |
| 8 | -3.772999 | 1.005359 | 1.616573 |
| 8 | -3.537327 | -0.542377 | -0.664603 |
| 8 | -3.520120 | 2.196858 | -1.048275 |
| 8 | 1.686115 | 0.552258 | 1.149355 |
| 8 | 0.120514 | -1.824073 | 1.234154 |
| 8 | -1.360024 | -2.222587 | -0.978002 |
| 1 | -4.432065 | 0.390501 | 1.954331 |
| 1 | -2.248461 | -1.805844 | -1.007734 |
| 1 | -4.137290 | 2.085568 | -1.778707 |
| 1 | 0.378984 | -1.450332 | 2.086052 |
| 1 | -1.335297 | -2.717079 | -0.144276 |
| 23 | -3.035819 | 0.829046 | -0.001821 |
| 83 | 0.405731 | -0.471547 | -0.345097 |
| 8 | 2.675688 | -1.786319 | -0.509012 |
| 1 | 3.317104 | -1.107629 | -0.211107 |
| 1 | 2.697352 | -2.490617 | 0.149355 |
| 8 | 4.088060 | 0.542858 | 0.052396 |
| 8 | 2.263951 | 1.781491 | 0.667599 |
| 8 | 4.067246 | 2.801715 | 0.065645 |
| 1 | 4.956021 | 2.658323 | -0.287026 |
| 6 | 3.521491 | 1.594533 | 0.255172 |

B18 (doublet)

E = -1819.60181600 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.094199 | 0.536690 | -0.123782 |
| 8 | -3.169322 | 1.558715 | 1.565419 |
| 8 | -3.568281 | -0.498570 | -0.246456 |
| 8 | -3.212723 | 2.027541 | -1.323984 |
| 8 | 1.836478 | 0.259348 | 0.641203 |
| 8 | 0.062514 | -2.003979 | 1.428797 |
| 8 | -1.775363 | -2.562512 | -0.423413 |
| 1 | -3.828113 | 1.164858 | 2.146268 |
| 1 | -2.579684 | -1.994483 | -0.424537 |
| 1 | -3.956529 | 1.869320 | -1.914387 |
| 1 | 0.714464 | -1.739187 | 2.087721 |
| 1 | -1.699817 | -2.909492 | 0.479091 |
| 23 | -2.762197 | 0.873865 | -0.033783 |
| 83 | 0.305785 | -1.137261 | -0.462612 |
| 8 | 2.626069 | -1.511884 | -0.473799 |
| 1 | 3.239484 | -1.577307 | 0.271171 |
| 8 | 4.250572 | 1.173369 | 0.879893 |
| 8 | 2.182262 | 1.381615 | -0.098608 |
| 8 | 3.695529 | 2.849306 | -0.553423 |
| 1 | 4.608478 | 3.124128 | -0.392117 |
| 6 | 3.484066 | 1.741504 | 0.165709 |

B19 (triplet)

E = -1819.05411427 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.091192 | 0.451874 | 0.426741 |
| 8 | -3.550236 | 0.536272 | 1.899009 |
| 8 | -3.336420 | -0.653735 | -0.583707 |
| 8 | -3.214793 | 2.102226 | -0.548307 |
| 8 | 0.879727 | 2.561726 | -1.594403 |
| 8 | 0.378596 | -2.364684 | 1.028264 |
| 8 | -1.096871 | -2.252098 | -1.202835 |
| 1 | -4.220468 | -0.109614 | 2.145198 |
| 1 | -2.005029 | -1.898487 | -1.160799 |
| 1 | -3.795275 | 2.127456 | -1.316118 |
| 1 | 0.745782 | -2.280871 | 1.916069 |
| 1 | -1.031639 | -2.903704 | -0.487225 |
| 23 | -2.798034 | 0.574827 | 0.280541 |
| 83 | 0.683955 | -0.635659 | -0.138293 |
| 8 | 1.739472 | 0.341189 | 1.427195 |
| 1 | 1.190185 | 0.851970 | 2.032046 |
| 8 | 4.865881 | 0.402264 | 1.567725 |
| 8 | 0.724236 | 3.631498 | -1.062083 |
| 8 | 3.789594 | -0.684682 | -0.178916 |
| 6 | 4.301214 | -0.130403 | 0.711752 |

B20

E = -1743.82017670 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | 1.404659 | -0.516592 | 0.201360 |
| 8 | 3.212814 | 0.893233 | 1.921466 |
| 8 | 2.950394 | 1.458902 | -0.772265 |
| 8 | 4.216490 | -0.915732 | -0.141246 |
| 8 | -1.214070 | -1.595825 | 1.077635 |
| 8 | -1.210557 | 1.379340 | 0.081982 |
| 8 | 0.433640 | 1.471596 | -1.966871 |
| 1 | 3.357711 | 1.828142 | 2.099851 |
| 1 | 1.365774 | 1.641762 | -1.722347 |
| 1 | 4.877863 | -0.733368 | -0.816760 |
| 1 | -0.519910 | -1.630110 | 1.746929 |
| 1 | -0.073036 | 2.216173 | -1.614213 |
| 23 | 2.932986 | 0.254478 | 0.278604 |
| 83 | -0.584730 | -0.608277 | -0.670913 |
| 8 | -3.126911 | -0.228215 | -0.610495 |
| 8 | -2.427280 | 1.360867 | 0.843644 |
| 8 | -4.478732 | 0.675380 | 0.961287 |
| 1 | -5.079403 | -0.004442 | 0.625449 |
| 6 | -3.325908 | 0.540708 | 0.318565 |

B21

E = -1820.29530816 a.u.

| | | | |
|---|----------|-----------|-----------|
| 8 | 1.530485 | -0.282229 | 0.544131 |
| 8 | 2.882181 | 2.093322 | 1.404276 |
| 8 | 3.097426 | 1.088432 | -1.164415 |
| 8 | 4.374289 | -0.352599 | 0.819646 |

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.085176 | -1.427871 | 1.381711 |
| 8 | -1.193138 | 0.733589 | -0.936464 |
| 8 | 0.865208 | 0.185858 | -2.582205 |
| 1 | 2.943413 | 2.988311 | 1.055133 |
| 1 | 1.729650 | 0.558676 | -2.313965 |
| 1 | 5.143221 | -0.439326 | 0.246806 |
| 1 | -0.571936 | -1.063273 | 2.112370 |
| 1 | 0.271365 | 0.947434 | -2.638497 |
| 23 | 2.959574 | 0.642789 | 0.365816 |
| 83 | -0.174710 | -1.164821 | -0.507415 |
| 8 | -3.764033 | 0.396511 | -0.393603 |
| 8 | -1.783658 | 1.394677 | 0.185160 |
| 8 | -3.584197 | 1.985017 | 1.204388 |
| 1 | -4.526622 | 1.788766 | 1.293274 |
| 6 | -3.103655 | 1.172629 | 0.256191 |
| 8 | -2.570801 | -2.062914 | -0.824655 |
| 1 | -3.114767 | -1.253995 | -0.917796 |
| 1 | -2.737090 | -2.347651 | 0.086420 |

B22 (doublet)

E = -1819.59904923 a.u.

| | | | |
|----|-----------|-----------|-----------|
| 8 | -1.488654 | -0.093228 | -0.873835 |
| 8 | -2.706145 | 2.468560 | -0.460998 |
| 8 | -2.670403 | 0.491462 | 1.473531 |
| 8 | -4.338309 | 0.056846 | -0.690575 |
| 8 | 1.289560 | -0.487205 | -2.187823 |
| 8 | 1.037128 | 0.607316 | 0.696802 |
| 8 | -0.564104 | -1.228979 | 1.974853 |
| 1 | -2.606296 | 3.132792 | 0.228625 |
| 1 | -1.314771 | -0.604396 | 2.063348 |
| 1 | -5.024267 | -0.251668 | -0.089574 |
| 1 | 0.861043 | 0.283656 | -2.578435 |
| 1 | 0.122973 | -0.934716 | 2.585614 |
| 23 | -2.785393 | 0.720611 | -0.106255 |
| 83 | 0.329296 | -1.246047 | -0.479032 |
| 8 | 3.611419 | 1.171479 | 0.409357 |
| 8 | 1.447306 | 1.637288 | -0.181120 |
| 8 | 3.012893 | 2.954056 | -0.853252 |
| 1 | 3.971590 | 3.075703 | -0.893173 |
| 6 | 2.783965 | 1.849193 | -0.140886 |
| 8 | 2.303375 | -1.261764 | 0.853059 |
| 1 | 3.023676 | -0.607336 | 0.739998 |

B23 (triplet)

E = -1819.05326386 a.u.

| | | | |
|---|-----------|-----------|-----------|
| 8 | -1.388299 | -0.112421 | 0.196039 |
| 8 | -3.329079 | 1.046827 | -1.569311 |
| 8 | -2.245578 | 2.417633 | 0.568301 |
| 8 | -4.022276 | 0.402899 | 1.194242 |
| 8 | 0.670612 | -2.269325 | -0.268429 |
| 8 | 3.869821 | -3.244481 | 0.972613 |

| | | | |
|----|-----------|-----------|-----------|
| 8 | 0.498812 | 2.204767 | 1.125923 |
| 1 | -3.397265 | 1.872199 | -2.060295 |
| 1 | -0.415751 | 2.530093 | 1.021602 |
| 1 | -4.421980 | 0.971862 | 1.860292 |
| 1 | -0.154632 | -2.490439 | -0.714700 |
| 1 | 1.032078 | 2.693212 | 0.481326 |
| 23 | -2.722826 | 0.966297 | 0.106948 |
| 83 | 0.690589 | -0.379571 | 0.684821 |
| 8 | 3.011486 | 2.334181 | -2.900228 |
| 8 | 3.485632 | -2.205487 | 1.445650 |
| 8 | 2.229411 | 3.417017 | -1.002083 |
| 6 | 2.607782 | 2.842321 | -1.942306 |
| 8 | 1.566660 | 0.509276 | -1.016116 |
| 1 | 1.668531 | -0.166805 | -1.699213 |

References

S1 Chapter 16.2, Handbook of Chemistry: Pure Chemistry, 6th ed. Maruzen Publishing, Tokyo, Japan, 2021.