

Computational Study on the Conformational Preferences of Neutral, Protonated and Deprotonated Glycine Dimers

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Table S1. Cartesian coordinates (in Å) obtained with MP2/6-311++G(d,p) optimizations for the most significant structures described in this paper for diverse glycine dimers. See main text for nomenclature. All coordinates are collected in standard orientation with usual Gaussian format: Center number, Atomic number, Atomic type (0 always), $x/\text{Å}$, $y/\text{Å}$, $z/\text{Å}$.

| NN-G1 | | | | | |
|---------------|---------------|------------------------|--------------|--------------|--------------|
| Center Number | Atomic Number | Atomic Type (0 Always) | $x/\text{Å}$ | $y/\text{Å}$ | $z/\text{Å}$ |
| 1 | 6 | 0 | 1.904473 | 0.305780 | −0.015023 |
| 2 | 8 | 0 | 1.203294 | 1.429388 | 0.024629 |
| 3 | 8 | 0 | 1.414860 | −0.818018 | −0.066933 |
| 4 | 6 | 0 | 3.403103 | 0.555949 | −0.001970 |
| 5 | 7 | 0 | 4.243818 | −0.623255 | 0.047654 |
| 6 | 1 | 0 | 4.016176 | −1.239310 | −0.726306 |
| 7 | 1 | 0 | 3.619818 | 1.206567 | 0.850689 |
| 8 | 1 | 0 | 3.636575 | 1.141091 | −0.897769 |
| 9 | 1 | 0 | −3.619742 | −1.206653 | 0.850688 |
| 10 | 6 | 0 | −3.403081 | −0.556019 | −0.001972 |
| 11 | 7 | 0 | −4.243876 | 0.623130 | 0.047671 |
| 12 | 6 | 0 | −1.904468 | −0.305747 | −0.015047 |
| 13 | 1 | 0 | −3.636527 | −1.141173 | −0.897770 |
| 14 | 1 | 0 | −4.016211 | 1.239249 | −0.726232 |
| 15 | 8 | 0 | −1.414931 | 0.818084 | −0.066986 |
| 16 | 8 | 0 | −1.203198 | −1.429295 | 0.024609 |
| 17 | 1 | 0 | −4.048837 | 1.150790 | 0.892464 |
| 18 | 1 | 0 | 4.048693 | −1.150958 | 0.892400 |
| 19 | 1 | 0 | 0.237837 | 1.207242 | −0.011958 |
| 20 | 1 | 0 | −0.237754 | −1.207019 | −0.011955 |
| NN-W1 | | | | | |
| Center Number | Atomic Number | Atomic Type (0 Always) | $x/\text{Å}$ | $y/\text{Å}$ | $z/\text{Å}$ |
| 1 | 6 | 0 | 1.570198 | −0.716043 | −0.177706 |
| 2 | 8 | 0 | 2.070092 | −1.666324 | 0.628418 |
| 3 | 8 | 0 | 0.684062 | −0.915987 | −0.988102 |
| 4 | 6 | 0 | 2.253265 | 0.620271 | 0.060002 |
| 5 | 7 | 0 | 1.755519 | 1.730467 | −0.732505 |
| 6 | 1 | 0 | 0.760975 | 1.847917 | −0.560274 |
| 7 | 1 | 0 | 3.322512 | 0.472534 | −0.131322 |
| 8 | 1 | 0 | 2.152186 | 1.126243 | 1.126243 |
| 9 | 1 | 0 | −2.965874 | −0.768985 | 1.037962 |

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 10 | 6 | 0 | −2.095763 | −0.756199 | 0.371038 |
| 11 | 7 | 0 | −2.535396 | −0.722499 | −1.021499 |
| 12 | 6 | 0 | −1.323606 | 0.511514 | 0.709129 |
| 13 | 1 | 0 | −1.462437 | −1.609866 | 0.628695 |
| 14 | 1 | 0 | −3.469244 | −1.119889 | −1.120384 |
| 15 | 8 | 0 | −0.654070 | 0.648739 | 1.716168 |
| 16 | 8 | 0 | −1.457555 | 1.494855 | −0.185736 |
| 17 | 1 | 0 | −1.906695 | −1.261543 | −1.616223 |
| 18 | 1 | 0 | 1.850038 | 1.511672 | −1.725289 |
| 19 | 1 | 0 | −2.000874 | 1.097700 | −0.917732 |
| 20 | 1 | 0 | 1.613759 | −2.521000 | 0.415594 |

NZ-G1

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | 1.475881 | −0.271067 | −0.178714 |
| 2 | 8 | 0 | 0.873452 | −1.312086 | −0.686716 |
| 3 | 8 | 0 | 0.952831 | 0.824590 | 0.069421 |
| 4 | 6 | 0 | 2.945975 | −0.532671 | 0.118584 |
| 5 | 7 | 0 | 3.731979 | 0.608118 | 0.547958 |
| 6 | 1 | 0 | 3.296764 | 1.035751 | 1.359108 |
| 7 | 1 | 0 | 3.389195 | −0.976873 | −0.777398 |
| 8 | 1 | 0 | 2.974838 | −1.310671 | 0.888872 |
| 9 | 1 | 0 | −2.110469 | 1.253906 | 1.459605 |
| 10 | 6 | 0 | −2.397547 | 0.971810 | 0.447005 |
| 11 | 7 | 0 | −1.521459 | 1.691281 | −0.527395 |
| 12 | 6 | 0 | −2.167808 | −0.548470 | 0.206239 |
| 13 | 1 | 0 | −3.438890 | 1.241624 | 0.261963 |
| 14 | 1 | 0 | −0.519233 | 1.444810 | −0.305775 |
| 15 | 8 | 0 | −2.556199 | −1.315119 | 1.078333 |
| 16 | 8 | 0 | −1.576515 | −0.772606 | −0.913285 |
| 17 | 1 | 0 | −1.666070 | 2.698915 | −0.562637 |
| 18 | 1 | 0 | 3.734481 | 1.318126 | −0.177227 |
| 19 | 1 | 0 | −1.685213 | 1.240026 | −1.434878 |
| 20 | 1 | 0 | −0.136602 | −1.157260 | −0.796282 |

ZZ-G1

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | 1.332473 | 0.931088 | −0.050049 |
| 2 | 8 | 0 | 0.630848 | 0.852909 | −1.126897 |
| 3 | 8 | 0 | 1.335422 | 1.821120 | 0.800351 |
| 4 | 6 | 0 | 2.245039 | −0.299792 | 0.150357 |
| 5 | 7 | 0 | 1.537348 | −1.475036 | −0.434486 |
| 6 | 1 | 0 | 2.134615 | −2.286264 | −0.579386 |
| 7 | 1 | 0 | 2.417249 | −0.479162 | 1.210606 |
| 8 | 1 | 0 | 3.192960 | −0.148311 | −0.371914 |
| 9 | 1 | 0 | −1.108687 | 0.963065 | 1.478589 |
| 10 | 6 | 0 | −1.789368 | 0.506371 | 0.761811 |
| 11 | 7 | 0 | −1.781963 | 1.327356 | −0.485101 |
| 12 | 6 | 0 | −1.298343 | −0.892043 | 0.322578 |
| 13 | 1 | 0 | −2.804350 | 0.457487 | 1.163368 |
| 14 | 1 | 0 | −0.740094 | 1.322228 | −0.846567 |
| 15 | 8 | 0 | −1.686680 | −1.266876 | −0.798599 |
| 16 | 8 | 0 | −0.487934 | −1.469626 | 1.114943 |

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 17 | 1 | 0 | −2.135549 | 2.272394 | −0.351022 |
| 18 | 1 | 0 | 0.688692 | −1.705279 | 0.214577 |
| 19 | 1 | 0 | −2.328263 | 0.820516 | −1.187164 |
| 20 | 1 | 0 | 1.123683 | −1.156866 | −1.320539 |

ZZ-W1

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | −2.049306 | 0.505004 | 0.348083 |
| 2 | 8 | 0 | −1.336758 | 1.137380 | −0.486606 |
| 3 | 8 | 0 | −2.706560 | 0.974264 | 1.292829 |
| 4 | 6 | 0 | −2.135099 | −1.023745 | 0.171455 |
| 5 | 7 | 0 | −1.313315 | −1.500813 | −0.982707 |
| 6 | 1 | 0 | −1.460045 | −2.505054 | −1.155690 |
| 7 | 1 | 0 | −3.172965 | −1.315922 | 0.002364 |
| 8 | 1 | 0 | −1.774376 | −1.525083 | 1.071442 |
| 9 | 1 | 0 | 3.183366 | 1.303340 | −0.006729 |
| 10 | 6 | 0 | 2.144232 | 1.021379 | 0.172375 |
| 11 | 7 | 0 | 1.317103 | 1.506143 | −0.974797 |
| 12 | 6 | 0 | 2.046413 | −0.506615 | 0.348640 |
| 13 | 1 | 0 | 1.797432 | 1.526147 | 1.075762 |
| 14 | 1 | 0 | 1.462994 | 2.511578 | −1.141711 |
| 15 | 8 | 0 | 2.692247 | −0.980319 | 1.298825 |
| 16 | 8 | 0 | 1.337912 | −1.134258 | −0.493176 |
| 17 | 1 | 0 | 0.294173 | 1.345318 | −0.797686 |
| 18 | 1 | 0 | −0.289486 | −1.341426 | −0.808128 |
| 19 | 1 | 0 | 1.564736 | 1.000822 | −1.835987 |
| 20 | 1 | 0 | −1.564513 | −0.989705 | −1.839412 |

NA-G1

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | 1.597382 | −0.264875 | −0.046468 |
| 2 | 8 | 0 | 0.742476 | −1.094390 | 0.395015 |
| 3 | 8 | 0 | 1.371672 | 0.788696 | −0.675712 |
| 4 | 6 | 0 | 3.072654 | −0.649961 | 0.216296 |
| 5 | 7 | 0 | 4.067373 | 0.401621 | −0.033701 |
| 6 | 1 | 0 | 3.996370 | 1.090103 | 0.711171 |
| 7 | 1 | 0 | 3.292966 | −1.511299 | −0.425651 |
| 8 | 1 | 0 | 3.162766 | −1.008750 | 1.244799 |
| 9 | 1 | 0 | −1.265670 | 0.463521 | 1.525727 |
| 10 | 6 | 0 | −2.009275 | 0.809058 | 0.803034 |
| 11 | 7 | 0 | −1.385907 | 1.855020 | −0.015828 |
| 12 | 6 | 0 | −2.549802 | −0.385281 | 0.000585 |
| 13 | 1 | 0 | −2.859328 | 1.228343 | 1.347914 |
| 14 | 1 | 0 | −0.474840 | 1.541669 | −0.364079 |
| 15 | 8 | 0 | −3.735415 | −0.472449 | −0.277359 |
| 16 | 8 | 0 | −1.673131 | −1.285465 | −0.412866 |
| 17 | 1 | 0 | 3.751706 | 0.905683 | −0.861093 |
| 18 | 1 | 0 | −1.975039 | 2.069791 | −0.814424 |
| 19 | 1 | 0 | −0.709768 | −1.120324 | −0.090975 |

NA-G2

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | −1.715355 | −0.243879 | −0.057195 |
| 2 | 8 | 0 | −0.974102 | −1.142097 | 0.458535 |

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 3 | 8 | 0 | −1.360088 | 0.699608 | −0.787048 |
| 4 | 6 | 0 | −3.222857 | −0.397496 | 0.259415 |
| 5 | 7 | 0 | −4.071909 | 0.747876 | −0.096051 |
| 6 | 1 | 0 | −3.694777 | 1.124629 | −0.964744 |
| 7 | 1 | 0 | −3.337579 | −0.629121 | 1.321469 |
| 8 | 1 | 0 | −3.570911 | −1.284248 | −0.283849 |
| 9 | 1 | 0 | 1.541926 | 0.625634 | 1.525323 |
| 10 | 6 | 0 | 1.753812 | 0.787460 | 0.460815 |
| 11 | 7 | 0 | 2.670987 | 1.919855 | 0.306853 |
| 12 | 6 | 0 | 2.297615 | −0.541975 | −0.081071 |
| 13 | 1 | 0 | 0.790740 | 1.004148 | −0.009012 |
| 14 | 1 | 0 | 2.556244 | 2.309936 | −0.623566 |
| 15 | 8 | 0 | 3.471564 | −0.663675 | −0.396551 |
| 16 | 8 | 0 | 1.446127 | −1.543489 | −0.141715 |
| 17 | 1 | 0 | 3.620728 | 1.554137 | 0.329547 |
| 18 | 1 | 0 | −3.906907 | 1.488329 | 0.580953 |
| 19 | 1 | 0 | 0.459690 | −1.294986 | 0.090713 |

NA-W1

| Center Number | Atomic Number | Atomic Type (0 Always) | $x/\text{\AA}$ | $y/\text{\AA}$ | $z/\text{\AA}$ |
|---------------|---------------|------------------------|----------------|----------------|----------------|
| 1 | 6 | 0 | 2.137921 | 0.098825 | 0.066351 |
| 2 | 8 | 0 | 1.162098 | −0.584816 | 0.629827 |
| 3 | 8 | 0 | 1.995391 | 1.170429 | −0.505631 |
| 4 | 6 | 0 | 3.489594 | −0.604426 | 0.204576 |
| 5 | 7 | 0 | 4.641354 | 0.070701 | −0.372921 |
| 6 | 1 | 0 | 4.762986 | 0.989121 | 0.054855 |
| 7 | 1 | 0 | 3.381785 | −1.598824 | −0.242670 |
| 8 | 1 | 0 | 3.658699 | −0.773786 | 1.273543 |
| 9 | 1 | 0 | −3.315606 | 1.649883 | −0.112553 |
| 10 | 6 | 0 | −3.460817 | 0.630434 | 0.261464 |
| 11 | 7 | 0 | −4.654542 | 0.057773 | −0.354905 |
| 12 | 6 | 0 | −2.124670 | −0.116080 | 0.069574 |
| 13 | 1 | 0 | −3.624363 | 0.728399 | 1.339990 |
| 14 | 1 | 0 | −4.507474 | −0.040629 | −1.359786 |
| 15 | 8 | 0 | −2.085053 | −1.165797 | −0.599622 |
| 16 | 8 | 0 | −1.124393 | 0.440575 | 0.644404 |
| 17 | 1 | 0 | 4.490034 | 0.237200 | −1.368198 |
| 18 | 1 | 0 | −4.799649 | −0.889997 | −0.005595 |
| 19 | 1 | 0 | 0.209392 | −0.136341 | 0.551576 |

NA-W2

| Center Number | Atomic Number | Atomic Type (0 Always) | $x/\text{\AA}$ | $y/\text{\AA}$ | $z/\text{\AA}$ |
|---------------|---------------|------------------------|----------------|----------------|----------------|
| 1 | 6 | 0 | −2.183356 | 0.553188 | −0.118522 |
| 2 | 8 | 0 | −1.304177 | −0.239375 | 0.355181 |
| 3 | 8 | 0 | −1.969521 | 1.712829 | −0.535104 |
| 4 | 6 | 0 | −3.639773 | 0.046486 | −0.174225 |
| 5 | 7 | 0 | −3.918318 | −1.329032 | 0.233554 |
| 6 | 1 | 0 | −3.565593 | −1.482174 | 1.178647 |
| 7 | 1 | 0 | −3.989573 | 0.193707 | −1.201312 |
| 8 | 1 | 0 | −4.232243 | 0.730080 | 0.444356 |
| 9 | 1 | 0 | 3.522795 | 0.255220 | 1.509719 |
| 10 | 6 | 0 | 3.417468 | 0.382373 | 0.426819 |
| 11 | 7 | 0 | 4.545184 | −0.238691 | −0.250304 |

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 12 | 6 | 0 | 2.023983 | −0.120688 | 0.047202 |
| 13 | 1 | 0 | 3.429105 | 1.463361 | 0.248864 |
| 14 | 1 | 0 | 1.828116 | −0.991536 | −0.787976 |
| 15 | 8 | 0 | 1.073939 | 0.494588 | 0.724017 |
| 16 | 8 | 0 | 4.446389 | −0.141030 | −1.261266 |
| 17 | 1 | 0 | −3.395076 | −1.973701 | −0.359748 |
| 18 | 1 | 0 | 0.098410 | 0.189638 | 0.482055 |
| 19 | 1 | 0 | 4.560950 | −1.241247 | −0.060658 |

ZA-G1

| Center Number | Atomic Number | Atomic Type (0 Always) | $x/\text{\AA}$ | $y/\text{\AA}$ | $z/\text{\AA}$ |
|---------------|---------------|------------------------|----------------|----------------|----------------|
| 1 | 6 | 0 | −3.399001 | −0.087864 | −0.016033 |
| 2 | 8 | 0 | −4.391892 | −0.011802 | −0.752619 |
| 3 | 8 | 0 | −3.303740 | −0.303208 | 1.222195 |
| 4 | 6 | 0 | −2.015326 | 0.120703 | −0.732497 |
| 5 | 7 | 0 | −0.933299 | −0.029056 | 0.283071 |
| 6 | 1 | 0 | −0.258138 | 0.770898 | 0.361005 |
| 7 | 1 | 0 | −1.974345 | 1.116972 | −1.171853 |
| 8 | 1 | 0 | −1.891660 | −0.615366 | −1.525867 |
| 9 | 1 | 0 | 3.968860 | 1.157176 | 0.665450 |
| 10 | 6 | 0 | 3.625193 | 0.482346 | −0.122579 |
| 11 | 7 | 0 | 4.457754 | −0.726481 | −0.140617 |
| 12 | 6 | 0 | 2.103547 | 0.266574 | 0.047063 |
| 13 | 1 | 0 | 3.761398 | 1.025054 | −1.065676 |
| 14 | 1 | 0 | 1.422495 | 1.304255 | 0.287060 |
| 15 | 8 | 0 | 1.665422 | −0.906791 | −0.095852 |
| 16 | 8 | 0 | 3.940267 | −1.430671 | −0.663710 |
| 17 | 1 | 0 | −0.256908 | −0.790278 | 0.101365 |
| 18 | 1 | 0 | 4.497177 | −1.102450 | 0.803105 |
| 19 | 1 | 0 | −1.482578 | −0.192768 | 1.157009 |

ZA-G2

| Center Number | Atomic Number | Atomic Type (0 Always) | $x/\text{\AA}$ | $y/\text{\AA}$ | $z/\text{\AA}$ |
|---------------|---------------|------------------------|----------------|----------------|----------------|
| 1 | 6 | 0 | −3.397741 | −0.089292 | −0.015407 |
| 2 | 8 | 0 | −3.302511 | −0.294880 | 1.224509 |
| 3 | 8 | 0 | −4.390603 | −0.019898 | −0.752690 |
| 4 | 6 | 0 | −2.014115 | 0.113960 | −0.733387 |
| 5 | 7 | 0 | −0.932454 | −0.022333 | 0.284390 |
| 6 | 1 | 0 | −0.249581 | −0.779995 | 0.108596 |
| 7 | 1 | 0 | −1.974750 | 1.104877 | −1.184759 |
| 8 | 1 | 0 | −1.888836 | −0.631428 | −1.517849 |
| 9 | 1 | 0 | 3.972103 | 1.158488 | 0.654806 |
| 10 | 6 | 0 | 3.625633 | 0.477938 | −0.127049 |
| 11 | 7 | 0 | 4.453403 | −0.734368 | −0.134264 |
| 12 | 6 | 0 | 2.103150 | 0.269678 | 0.044629 |
| 13 | 1 | 0 | 3.763793 | 1.011409 | −1.075125 |
| 14 | 1 | 0 | 4.491472 | −1.101886 | 0.812833 |
| 15 | 8 | 0 | 1.660844 | −0.903465 | −0.090183 |
| 16 | 8 | 0 | 1.426001 | 1.311134 | 0.277438 |
| 17 | 1 | 0 | −1.481798 | −0.182506 | 1.158996 |
| 18 | 1 | 0 | 3.933093 | −1.441083 | −0.651088 |
| 19 | 1 | 0 | −0.263537 | 0.782192 | 0.357406 |

ZA-W1

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | 3.144312 | −0.076919 | −0.118278 |
| 2 | 8 | 0 | 3.260506 | −0.061511 | 1.134145 |
| 3 | 8 | 0 | 4.046550 | 0.032561 | −0.978072 |
| 4 | 6 | 0 | 1.710004 | −0.249898 | −0.675783 |
| 5 | 7 | 0 | 0.719781 | −0.343314 | 0.434091 |
| 6 | 1 | 0 | 0.170395 | −1.207852 | 0.428815 |
| 7 | 1 | 0 | 1.663189 | −1.150077 | −1.289737 |
| 8 | 1 | 0 | 1.463696 | 0.607513 | −1.305255 |
| 9 | 1 | 0 | −3.378044 | 1.655695 | −0.187289 |
| 10 | 6 | 0 | −2.477701 | 1.051923 | −0.353259 |
| 11 | 7 | 0 | −1.313501 | 1.552562 | 0.400578 |
| 12 | 6 | 0 | −2.841589 | −0.419749 | −0.053223 |
| 13 | 1 | 0 | −2.250014 | 1.116677 | −1.422335 |
| 14 | 1 | 0 | −1.069651 | 2.490879 | 0.075030 |
| 15 | 8 | 0 | −3.900281 | −0.829294 | −0.599687 |
| 16 | 8 | 0 | −2.074741 | −1.091905 | 0.686091 |
| 17 | 1 | 0 | −0.016827 | 0.442124 | 0.420138 |
| 18 | 1 | 0 | −1.556294 | 1.647498 | 1.389632 |
| 19 | 1 | 0 | 1.263167 | −0.298145 | 1.311755 |

ZA-W2

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | 3.203506 | 0.146069 | 0.026282 |
| 2 | 8 | 0 | 3.949625 | 1.029451 | −0.458622 |
| 3 | 8 | 0 | 3.460837 | −0.649328 | 0.964898 |
| 4 | 6 | 0 | 1.792141 | 0.060709 | −0.592706 |
| 5 | 7 | 0 | 1.058615 | −1.161252 | −0.154480 |
| 6 | 1 | 0 | 1.290906 | −1.973945 | −0.742967 |
| 7 | 1 | 0 | 1.849411 | 0.066777 | −1.681407 |
| 8 | 1 | 0 | 1.199505 | 0.920239 | −0.272695 |
| 9 | 1 | 0 | −3.699732 | 1.450688 | −0.546083 |
| 10 | 6 | 0 | −3.507034 | 0.629576 | 0.153193 |
| 11 | 7 | 0 | −4.413749 | −0.477212 | −0.145324 |
| 12 | 6 | 0 | −1.985793 | 0.366813 | 0.124349 |
| 13 | 1 | 0 | −3.741424 | 1.024038 | 1.147785 |
| 14 | 1 | 0 | −4.192568 | −0.861719 | −1.064144 |
| 15 | 8 | 0 | −1.238746 | 1.331226 | 0.410844 |
| 16 | 8 | 0 | −1.589383 | −0.802240 | −0.186789 |
| 17 | 1 | 0 | −4.251113 | −1.238666 | 0.514122 |
| 18 | 1 | 0 | −0.007425 | −1.011693 | −0.167615 |
| 19 | 1 | 0 | 1.362789 | −1.398345 | 0.802268 |

NC-G1

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | −1.982099 | −0.472090 | 0.152869 |
| 2 | 8 | 0 | −2.903092 | −1.389741 | −0.138178 |
| 3 | 8 | 0 | −1.369535 | −0.414199 | 1.203064 |
| 4 | 6 | 0 | −1.767097 | 0.475162 | −1.011697 |
| 5 | 7 | 0 | −1.026912 | 1.666253 | −0.564948 |
| 6 | 1 | 0 | −1.682189 | 2.349560 | −0.187488 |
| 7 | 1 | 0 | −2.732444 | 0.704241 | −1.472090 |
| 8 | 1 | 0 | −1.168791 | −0.056954 | −1.758093 |

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 9 | 1 | 0 | 2.565061 | −0.146544 | 1.722899 |
| 10 | 6 | 0 | 1.667466 | −0.127793 | 1.101617 |
| 11 | 7 | 0 | 0.955978 | 1.167148 | 1.259667 |
| 12 | 6 | 0 | 2.025474 | −0.313198 | −0.361604 |
| 13 | 1 | 0 | 0.997291 | −0.926527 | 1.421367 |
| 14 | 1 | 0 | 0.501691 | 1.202311 | 2.174263 |
| 15 | 8 | 0 | 1.675671 | 0.450354 | −1.234464 |
| 16 | 8 | 0 | 2.746733 | −1.420976 | −0.521560 |
| 17 | 1 | 0 | −0.595177 | 2.104585 | −1.376590 |
| 18 | 1 | 0 | −2.980807 | −1.991494 | 0.619314 |
| 19 | 1 | 0 | 1.606125 | 1.952563 | 1.188567 |
| 20 | 1 | 0 | 0.166635 | 1.313924 | 0.511343 |
| 21 | 1 | 0 | 2.958470 | −1.515455 | −1.464524 |

NC-G2

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | −2.434238 | −0.567273 | −0.183834 |
| 2 | 8 | 0 | −3.320893 | −1.338706 | 0.437432 |
| 3 | 8 | 0 | −1.671005 | −0.895291 | −1.063776 |
| 4 | 6 | 0 | −2.500815 | 0.858036 | 0.341717 |
| 5 | 7 | 0 | −1.325608 | 1.580994 | −0.213463 |
| 6 | 1 | 0 | −1.414353 | 2.592882 | −0.109184 |
| 7 | 1 | 0 | −2.451839 | 0.878748 | 1.431215 |
| 8 | 1 | 0 | −3.427111 | 1.332497 | 0.010860 |
| 9 | 1 | 0 | 2.512679 | −1.560932 | 1.041684 |
| 10 | 6 | 0 | 2.884418 | −0.578256 | 0.739119 |
| 11 | 7 | 0 | 3.823409 | −0.645843 | −0.382020 |
| 12 | 6 | 0 | 1.681694 | 0.251665 | 0.308407 |
| 13 | 1 | 0 | 3.310751 | −0.104016 | 1.627180 |
| 14 | 1 | 0 | 0.727295 | 0.491970 | 1.043554 |
| 15 | 8 | 0 | 1.739684 | 0.699393 | −0.929407 |
| 16 | 8 | 0 | 4.721122 | −0.232484 | −0.155109 |
| 17 | 1 | 0 | −1.212627 | 1.348783 | −1.205933 |
| 18 | 1 | 0 | −3.278873 | −2.227731 | 0.049128 |
| 19 | 1 | 0 | 3.991922 | −1.598899 | −0.684261 |
| 20 | 1 | 0 | 2.616977 | 0.342041 | −1.253293 |
| 21 | 1 | 0 | −0.440262 | 1.239084 | 0.281214 |

NC-W1

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | −2.140858 | −0.110195 | −0.190371 |
| 2 | 8 | 0 | −2.902380 | −1.178180 | −0.452799 |
| 3 | 8 | 0 | −1.936001 | 0.798433 | −0.972558 |
| 4 | 6 | 0 | −1.575674 | −0.176538 | 1.212011 |
| 5 | 7 | 0 | −0.666480 | 0.947387 | 1.452978 |
| 6 | 1 | 0 | −0.132066 | 0.761746 | 2.308117 |
| 7 | 1 | 0 | −1.029595 | −1.119271 | 1.312244 |
| 8 | 1 | 0 | −2.420934 | −0.212324 | 1.911764 |
| 9 | 1 | 0 | 3.001013 | 1.003291 | −1.115522 |
| 10 | 6 | 0 | 2.283060 | 0.858302 | −0.301841 |
| 11 | 7 | 0 | 0.997891 | 1.506101 | −0.650141 |
| 12 | 6 | 0 | 2.122374 | −0.631160 | −0.067233 |
| 13 | 1 | 0 | 2.676761 | 1.320756 | 0.605848 |

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 14 | 1 | 0 | 2.943537 | −1.286369 | 0.536143 |
| 15 | 8 | 0 | 1.009941 | −1.106847 | −0.634376 |
| 16 | 8 | 0 | 0.278746 | 1.314938 | 0.135924 |
| 17 | 1 | 0 | −1.209320 | 1.797079 | 1.641110 |
| 18 | 1 | 0 | −3.260678 | −1.080286 | −1.373745 |
| 19 | 1 | 0 | 0.624942 | 1.148732 | −1.538966 |
| 20 | 1 | 0 | 0.974742 | −2.092129 | −0.482060 |
| 21 | 1 | 0 | 1.122317 | 2.524301 | −0.751253 |

NC-W2

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | 2.889724 | −0.168166 | 0.091398 |
| 2 | 8 | 0 | 3.714225 | −0.408979 | −0.936021 |
| 3 | 8 | 0 | 3.162040 | −0.375025 | 1.257195 |
| 4 | 6 | 0 | 1.566442 | 0.390053 | −0.398261 |
| 5 | 7 | 0 | 0.655181 | 0.796405 | 0.668752 |
| 6 | 1 | 0 | 1.098846 | 1.522707 | 1.241434 |
| 7 | 1 | 0 | 1.089124 | −0.380687 | −1.012892 |
| 8 | 1 | 0 | 1.775160 | 1.243645 | −1.051856 |
| 9 | 1 | 0 | −2.795158 | 0.990305 | 1.302009 |
| 10 | 6 | 0 | −2.780494 | 0.793141 | 0.227275 |
| 11 | 7 | 0 | −1.715338 | 1.617340 | −0.390886 |
| 12 | 6 | 0 | −2.570254 | −0.693221 | 0.007332 |
| 13 | 1 | 0 | −3.751477 | 1.069888 | −0.194714 |
| 14 | 1 | 0 | −0.745342 | 1.333330 | 0.019292 |
| 15 | 8 | 0 | −3.218236 | −1.527101 | 0.600921 |
| 16 | 8 | 0 | −1.632639 | −0.939539 | −0.909811 |
| 17 | 1 | 0 | 0.501031 | 0.003831 | 1.301918 |
| 18 | 1 | 0 | −1.699494 | 1.501300 | −1.413955 |
| 19 | 1 | 0 | 4.553122 | −0.795928 | −0.572372 |
| 20 | 1 | 0 | −1.561452 | −1.926917 | −1.031182 |
| 21 | 1 | 0 | −1.878885 | 2.616620 | −0.197479 |

NC-W3

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | 2.239264 | 0.565511 | 0.168317 |
| 2 | 8 | 0 | 2.972679 | 1.516970 | −0.397134 |
| 3 | 8 | 0 | 1.480511 | 0.703778 | 1.106421 |
| 4 | 6 | 0 | 2.458126 | −0.761302 | −0.529457 |
| 5 | 7 | 0 | 1.631560 | −1.801855 | 0.124461 |
| 6 | 1 | 0 | 1.763024 | −2.718362 | −0.342295 |
| 7 | 1 | 0 | 3.511426 | −1.048772 | −0.474862 |
| 8 | 1 | 0 | 2.162547 | −0.686796 | −1.580098 |
| 9 | 1 | 0 | −1.373795 | 0.960337 | −1.395741 |
| 10 | 6 | 0 | −1.663551 | 0.911912 | −0.338346 |
| 11 | 7 | 0 | −2.688562 | 1.904116 | −0.068540 |
| 12 | 6 | 0 | −1.985713 | −0.549615 | −0.076028 |
| 13 | 1 | 0 | −0.764633 | 1.132654 | 0.242286 |
| 14 | 1 | 0 | −1.129924 | −1.427886 | −0.068007 |
| 15 | 8 | 0 | −3.276634 | −0.797020 | 0.105916 |
| 16 | 8 | 0 | −2.961240 | 1.866040 | 0.914570 |
| 17 | 1 | 0 | 0.621587 | −1.564688 | 0.081969 |
| 18 | 1 | 0 | 2.799747 | 2.373787 | 0.081488 |

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 19 | 1 | 0 | −3.527190 | 1.700240 | −0.613099 |
| 20 | 1 | 0 | −3.383952 | −1.776193 | 0.248718 |
| 21 | 1 | 0 | 1.889686 | −1.919856 | 1.121139 |

ZC-G1

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | 2.896770 | −0.315089 | 0.083536 |
| 2 | 8 | 0 | 3.522204 | −1.280237 | −0.588964 |
| 3 | 8 | 0 | 3.209721 | 0.124178 | 1.167600 |
| 4 | 6 | 0 | 1.673915 | 0.170057 | −0.673508 |
| 5 | 7 | 0 | 1.152642 | 1.385259 | 0.002098 |
| 6 | 1 | 0 | 1.584218 | 2.234710 | −0.364010 |
| 7 | 1 | 0 | 0.894360 | −0.595525 | −0.629601 |
| 8 | 1 | 0 | 1.909277 | 0.386272 | −1.715882 |
| 9 | 1 | 0 | −3.860797 | 0.554241 | −1.006800 |
| 10 | 6 | 0 | −3.455581 | 0.241686 | −0.045102 |
| 11 | 7 | 0 | −3.760240 | −1.205979 | 0.204790 |
| 12 | 6 | 0 | −1.910446 | 0.320633 | −0.044195 |
| 13 | 1 | 0 | −3.876070 | 0.859381 | 0.747569 |
| 14 | 1 | 0 | −4.258299 | −1.657575 | −0.562187 |
| 15 | 8 | 0 | −1.417935 | 1.456947 | −0.238964 |
| 16 | 8 | 0 | −1.323297 | −0.773877 | 0.155811 |
| 17 | 1 | 0 | 1.410645 | 1.330068 | 0.994552 |
| 18 | 1 | 0 | −2.760228 | −1.579958 | 0.281187 |
| 19 | 1 | 0 | 4.270724 | −1.584794 | −0.051087 |
| 20 | 1 | 0 | −4.274662 | −1.371929 | 1.069757 |
| 21 | 1 | 0 | 0.060524 | 1.450330 | −0.099970 |

ZC-G2

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----------|-----------|-----------|
| 1 | 6 | 0 | 2.434676 | −0.554128 | −0.152404 |
| 2 | 8 | 0 | 3.425151 | −1.187434 | 0.477102 |
| 3 | 8 | 0 | 1.632586 | −1.046976 | −0.912328 |
| 4 | 6 | 0 | 2.446898 | 0.926447 | 0.185254 |
| 5 | 7 | 0 | 1.179596 | 1.509587 | −0.311475 |
| 6 | 1 | 0 | 1.216467 | 2.528518 | −0.340597 |
| 7 | 1 | 0 | 0.965792 | 1.156701 | −1.249371 |
| 8 | 1 | 0 | 3.307353 | 1.398714 | −0.294819 |
| 9 | 1 | 0 | 2.514278 | 1.075767 | 1.263940 |
| 10 | 6 | 0 | −3.354228 | 0.031172 | 1.591651 |
| 11 | 7 | 0 | −2.836776 | −0.510896 | 0.800902 |
| 12 | 6 | 0 | −3.728198 | −0.674705 | −0.393793 |
| 13 | 1 | 0 | −1.631739 | 0.299625 | 0.268449 |
| 14 | 1 | 0 | −2.516349 | −1.483954 | 1.171456 |
| 15 | 8 | 0 | −4.638742 | −0.227496 | −0.289191 |
| 16 | 8 | 0 | −3.130496 | −0.156405 | −1.119436 |
| 17 | 1 | 0 | −1.686746 | 0.595454 | −0.950272 |
| 18 | 1 | 0 | −0.730448 | 0.570754 | 1.101869 |
| 19 | 1 | 0 | −3.870605 | −1.646464 | −0.668272 |
| 20 | 1 | 0 | 0.332854 | 1.176037 | 0.327029 |
| 21 | 1 | 0 | 3.411201 | −2.117434 | 0.200312 |

ZC-W1

| Center Number | Atomic Number | Atomic Type (0 Always) | x/Å | y/Å | z/Å |
|---------------|---------------|------------------------|-----|-----|-----|
|---------------|---------------|------------------------|-----|-----|-----|

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 1 | 6 | 0 | 1.937460 | −0.818709 | 0.122903 |
| 2 | 8 | 0 | 1.704178 | −0.413905 | 1.373314 |
| 3 | 8 | 0 | 2.024601 | −1.971930 | −0.239992 |
| 4 | 6 | 0 | 2.172839 | 0.343876 | −0.817359 |
| 5 | 7 | 0 | 1.724608 | 1.637337 | −0.251732 |
| 6 | 1 | 0 | 2.238010 | 1.865411 | 0.614853 |
| 7 | 1 | 0 | 1.904369 | 2.401624 | −0.924351 |
| 8 | 1 | 0 | 1.625391 | 0.156507 | −1.740495 |
| 9 | 1 | 0 | 3.244552 | 0.400792 | −1.033266 |
| 10 | 6 | 0 | −3.440987 | 1.110166 | 0.065025 |
| 11 | 7 | 0 | −2.804864 | 0.281536 | 0.381347 |
| 12 | 6 | 0 | −3.317646 | −0.968325 | −0.246848 |
| 13 | 1 | 0 | −1.346869 | 0.512588 | −0.033462 |
| 14 | 1 | 0 | −2.872739 | 0.165100 | 1.465774 |
| 15 | 8 | 0 | −4.258803 | −1.214257 | 0.096220 |
| 16 | 8 | 0 | −3.366006 | −0.875430 | −1.272466 |
| 17 | 1 | 0 | −0.862767 | 1.625593 | 0.335790 |
| 18 | 1 | 0 | −0.771283 | −0.398095 | −0.664990 |
| 19 | 1 | 0 | −2.679188 | −1.754135 | −0.053482 |
| 20 | 1 | 0 | 0.673065 | 1.630224 | −0.024857 |
| 21 | 1 | 0 | 1.574371 | −1.218139 | 1.943548 |

ZC-W2

| Center Number | Atomic Number | Atomic Type (0 Always) | $x/\text{\AA}$ | $y/\text{\AA}$ | $z/\text{\AA}$ |
|---------------|---------------|------------------------|----------------|----------------|----------------|
| 1 | 6 | 0 | −1.917383 | −0.826207 | 0.116913 |
| 2 | 8 | 0 | −1.649185 | −0.457895 | 1.370933 |
| 3 | 8 | 0 | −2.007068 | −1.968915 | −0.277476 |
| 4 | 6 | 0 | −2.187383 | 0.359072 | −0.784953 |
| 5 | 7 | 0 | −1.733641 | 1.641623 | −0.199215 |
| 6 | 1 | 0 | −1.938442 | 2.421856 | −0.846453 |
| 7 | 1 | 0 | −2.224801 | 1.842913 | 0.686399 |
| 8 | 1 | 0 | 2.971586 | 0.358765 | 1.384908 |
| 9 | 1 | 0 | 2.832887 | 0.315743 | 0.303441 |
| 10 | 6 | 0 | 3.237692 | −1.033345 | −0.192221 |
| 11 | 7 | 0 | 1.354084 | 0.543139 | −0.053936 |
| 12 | 6 | 0 | 3.455165 | 1.075759 | −0.172106 |
| 13 | 1 | 0 | 3.514733 | −1.670271 | 0.568250 |
| 14 | 1 | 0 | 2.398359 | −1.425736 | −0.662613 |
| 15 | 8 | 0 | 0.765413 | −0.375277 | −0.668579 |
| 16 | 8 | 0 | 0.876778 | 1.653379 | 0.318879 |
| 17 | 1 | 0 | 4.013077 | −0.994966 | −0.868891 |
| 18 | 1 | 0 | −0.679874 | 1.638625 | −0.000538 |
| 19 | 1 | 0 | −1.663426 | 0.199392 | −1.726941 |
| 20 | 1 | 0 | −3.264852 | 0.413723 | −0.971195 |
| 21 | 1 | 0 | −1.490610 | −1.278821 | 1.910384 |

ZC-W3

| Center Number | Atomic Number | Atomic Type (0 Always) | $x/\text{\AA}$ | $y/\text{\AA}$ | $z/\text{\AA}$ |
|---------------|---------------|------------------------|----------------|----------------|----------------|
| 1 | 6 | 0 | 2.244448 | 0.589173 | 0.103702 |
| 2 | 8 | 0 | 3.056458 | 1.382346 | −0.585943 |
| 3 | 8 | 0 | 1.440533 | 0.944289 | 0.942963 |
| 4 | 6 | 0 | 2.453745 | −0.857798 | −0.289448 |
| 5 | 7 | 0 | 1.491031 | −1.714162 | 0.433904 |

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 6 | 1 | 0 | 1.680280 | −2.713174 | 0.239828 |
| 7 | 1 | 0 | 3.474900 | −1.159893 | −0.039681 |
| 8 | 1 | 0 | 2.300695 | −0.982912 | −1.364973 |
| 9 | 1 | 0 | −1.581362 | 1.055127 | −1.421871 |
| 10 | 6 | 0 | −1.684988 | 0.821636 | −0.358616 |
| 11 | 7 | 0 | −2.808489 | 1.639883 | 0.176607 |
| 12 | 6 | 0 | −2.001414 | −0.672708 | −0.193607 |
| 13 | 1 | 0 | −0.770079 | 1.098673 | 0.162792 |
| 14 | 1 | 0 | −1.021657 | −1.450018 | −0.399742 |
| 15 | 8 | 0 | −3.179094 | −0.974706 | 0.084303 |
| 16 | 8 | 0 | −2.867076 | 1.567377 | 1.203481 |
| 17 | 1 | 0 | 0.495159 | −1.513786 | 0.139130 |
| 18 | 1 | 0 | 2.902241 | 2.322033 | −0.293099 |
| 19 | 1 | 0 | −3.704151 | 1.289982 | −0.195225 |
| 20 | 1 | 0 | 1.563416 | −1.578325 | 1.456933 |
| 21 | 1 | 0 | −2.712478 | 2.637744 | −0.065717 |
