Supplementary Materials
Benchmark Structures and Infrared Fingerprints of Vitamin-Relevant Motifs

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Contents

1 Cartesian Coordinates

1.1 PCS2 geometries

1.1.1 Cyclohexanone

```
17
Title
8 2.199119 0.000004 -0.340670
6 -1.844219 0.000002 0.079101
6 -1.062852 1.255328 -0.293038
6 -1.062856 -1.255326 -0.293031
6 0.310221 1.275005 0.387016
6 0.310223 -1.275011 0.387008
6 1.070775 -0.000003 0.101192
```

```
1 -2.038441 0.000011 1.155966
1 -2.814187 0.000002 -0.419411
1 -1.620000 2.151989 -0.021159
1 -0.923508 1.283352 -1.376927
1 -0.923527 -1.283357 -1.376919
1 -1.620000 -2.151983 -0.021152
1 0.168758 1.337436 1.470551
1 0.916338 2.120874 0.070278
1 0.916320 -2.120883 0.070253
1 0.168796 -1.337452 1.470540
```

1.1.2 cis-1,3,5-Hexatriene

```
14

 C 0.674650 0.761276 0.000000
 C -0.674650 0.761276 -0.000000
 C -1.532906 -0.410541 -0.000000
 C 1.532906 -0.410541 0.000000
 C -2.870547 -0.329402 -0.000000
 C 2.870547 -0.329402 0.000000
 H -3.489313 -1.214574 -0.000000
 H 3.489313 -1.214574 0.000000
 H -3.370475 0.630517 -0.000000
 H 3.370475 0.630517 0.000000
 H -1.067950 -1.388322 -0.000000
 H 1.067950 -1.388322 0.000000
 H -1.184627 1.718388 -0.000000
 H 1.184627 1.718388 0.000000
```

1.1.3 Isochroman

```
20
title
6 -2.329445 -0.615819 -0.366456
8 -2.318174 0.608790 0.345396
6 -1.224693 1.406944 -0.053570
6 0.093530 0.671679 -0.013085
6 1.290554 1.387384 -0.052423
6 2.511725 0.727423 -0.037536
6 2.542022 -0.664859 0.015310
6 1.351954 -1.378940 0.052874
6 0.119679 -0.722327 0.037646
6 -1.175793 -1.492407 0.085201
1 -2.258856 -0.417594 -1.443842
1 -3.290007 -1.084897 -0.164261
1 -1.201524 2.259597 0.623745
1 -1.398232 1.787869 -1.069638
1 1.262138 2.470162 -0.088928
1 3.433596 1.291899 -0.063231
1 3.488144 -1.188283 0.026553
1 1.372261 -2.461476 0.090889
1 -1.108412 -2.381130 -0.545822
1 -1.366162 -1.830478 1.106363
```

1.1.4 Nicotinic acid conformer 1

```
14
title
```

```
6 1.868391 1.220813 -0.000023
6 0.481311 1.230252 0.000061
6 -0.183140 0.007128 0.000097
6 0.569745 -1.167996 0.000073
7 1.902456 -1.188066 -0.000015
6 2.526595 -0.005148 -0.000077
6 -1.661489 -0.102822 0.000023
8 -2.273317 -1.140532 -0.000059
8 -2.271042 1.101613 -0.000022
1 2.433925 2.141173 -0.000068
1 -0.076959 2.154748 0.000081
1 0.060420 -2.122637 0.000105
1 3.608741 -0.042382 -0.000180
1 -3.218645 0.917588 -0.000288
```

1.1.5 Nicotinic acid conformer 2

```
14
title
6 1.906734 1.194101 0.000021
6 0.522716 1.246103 -0.000071
6 -0.182769 0.045763 -0.000098
6 0.529196 -1.153675 -0.000065
7 1.862749 -1.214842 0.000018
6 2.524581 -0.054349 0.000076
6 -1.664925 0.090499 -0.000024
8 -2.315563 1.105054 0.000054
8 -2.226012 -1.135024 0.000028
1 2.502230 2.095333 0.000071
1 -0.020000 2.180856 -0.000091
1 0.001914 -2.097659 -0.000095
1 3.604960 -0.127257 0.000180
1 -3.180367 -0.989986 0.000290
```

1.1.6 Benzoquinone

```
12
refined
O 2.655607 0.000000 0.000000
O -2.655607 0.000000 0.000000
C 1.436360 0.000000 0.000000
C -1.436360 0.000000 0.000000
C -0.670091 1.264773 0.000000
C 0.670091 1.264773 0.000000
C -0.670091 -1.264773 0.000000
C 0.670091 -1.264773 0.000000
H -1.253431 2.175303 0.000000
H -1.253431 -2.175303 0.000000
H 1.253431 2.175303 0.000000
H 1.253431 -2.175303 0.000000
```

1.2 DPCS3 geometries and final coordinate blocks

BDPCS3 geometries can be obtained from these DPCS3 structures with the PCS bond-correction web tool. For cyclohexanone and naphthoquinone, the final Gaussian principal-axis coordinate blocks are reported directly from the corresponding output files.

1.2.1 Cyclohexanone

```
             Principal axis orientation:
---------------------------------------------------------------------
Center Atomic Coordinates (Angstroms)
Number Number X Y Z
---------------------------------------------------------------------
     1 8 2.202649 -0.000000 -0.344935
     2 6 -1.848561 0.000000 0.074951
     3 6 -1.064341 1.258591 -0.292535
     4 6 -1.064341 -1.258591 -0.292535
     5 6 0.311246 1.277181 0.390368
     6 6 0.311246 -1.277181 0.390368
     7 6 1.073568 -0.000000 0.102687
     8 1 -2.053421 0.000000 1.152522
     9 1 -2.817460 0.000000 -0.431864
    10 1 -1.623136 2.156447 -0.016329
    11 1 -0.925115 1.293595 -1.378859
    12 1 -0.925115 -1.293595 -1.378859
    13 1 -1.623137 -2.156446 -0.016329
    14 1 0.168828 1.342668 1.476304
    15 1 0.916869 2.126809 0.073308
    16 1 0.916869 -2.126809 0.073307
    17 1 0.168828 -1.342668 1.476304
---------------------------------------------------------------------
Rotational constants (MHZ):
  4203.2686447 2519.8404958 1769.2142708
Nuclear quadrupole coupling constants [Chi] (MHz):
Dipole moment (Debye):
    -3.1644899 0.0000000 0.9685937 Tot= 3.3094063
```

1.2.2 Nicotinic acid conformer 1

```
14
 Conformer 1 nicotinic acid DPCS3
 6 1.872540 1.221066 -0.0000
 6 0.483869 1.230520 0.0000
 6 -0.183820 0.006498 0.0000
 6 0.571179 -1.169387 0.0000
 7 1.904621 -1.188443 -0.0000
 6 2.531358 -0.005878 -0.0000
 6 -1.664459 -0.103148 0.0000
 8 -2.279846 -1.142236 -0.0000
 8 -2.274135 1.105059 -0.0000
 1 2.438689 2.144016 -0.0000
 1 -0.073274 2.158321 0.0000
 1 0.062919 -2.127116 0.0000
 1 3.616070 -0.044459 -0.0000
 1 -3.224499 0.925763 0.0000
```

1.2.3 Nicotinic acid conformer 2

```
14
Nicotinic acid conformer 2 DPCS3
 6 1.910613 1.194705 0.0000
 6 0.524942 1.246457 0.0000
 6 -0.183458 0.045247 0.0000
 6 0.530884 -1.154970 0.0000
 7 1.865152 -1.214832 0.0000
 6 2.529333 -0.054577 0.0000
 6 -1.667835 0.091290 0.0000
```

```
 8 -2.320945 1.107874 0.0000
 8 -2.230141 -1.137306 0.0000
 1 2.506542 2.098686 0.0000
 1 -0.016839 2.184322 0.0000
 1 0.004734 -2.102169 0.0000
 1 3.612251 -0.128614 0.0000
 1 -3.186921 -0.996167 0.0000
```

1.2.4 cis-1,3,5-Hexatriene

```
14
cis-hexatriene DPCS3
6 -0.000000 0.675257 0.765565
6 -0.000000 -0.675257 0.765565
6 0.000000 -1.537509 -0.404435
6 0.000000 1.537509 -0.404435
6 0.000000 -2.875898 -0.322747
6 0.000000 2.875898 -0.322747
1 0.000000 -3.496860 -1.209562
1 0.000000 3.496860 -1.209562
1 0.000000 -3.378683 0.638616
1 0.000000 3.378683 0.638616
1 0.000000 -1.073823 -1.385367
1 0.000000 1.073823 -1.385367
1 0.000000 -1.184151 1.726015
1 0.000000 1.184151 1.726015
```

1.2.5 Isochroman

```
20
 isochroman twisted DPCS3
  6 -2.334138 -0.619448 -0.366755
  8 -2.324072 0.611152 0.341117
  6 -1.224937 1.410294 -0.051322
  6 0.094345 0.673032 -0.012159
  6 1.293226 1.388534 -0.052126
  6 2.515728 0.727679 -0.038141
  6 2.545729 -0.666011 0.014354
  6 1.353957 -1.380286 0.052314
  6 0.120238 -0.723116 0.038268
  6 -1.176827 -1.494054 0.087624
  1 -2.267785 -0.426518 -1.447548
  1 -3.296182 -1.088566 -0.159084
  1 -1.204268 2.260688 0.632511
  1 -1.396009 1.799764 -1.067146
  1 1.265726 2.473626 -0.089048
  1 3.439751 1.293336 -0.064444
  1 3.493797 -1.190999 0.024919
  1 1.374697 -2.465124 0.090453
  1 -1.109619 -2.387154 -0.541468
  1 -1.366273 -1.831615 1.111849
```

1.2.6 2-Decalone trans

```
 27
 Trans DPCS3
    6 2.732250 -0.979386 -0.310975
    6 2.947920 0.468959 0.125651
    6 1.763656 1.344951 -0.280207
```

```
 6 0.441833 0.805848 0.267575
 6 0.229250 -0.650006 -0.165646
 6 1.415318 -1.525451 0.238031
 6 -1.087513 -1.203164 0.397284
 6 -2.258022 -0.311954 0.042664
 6 -2.071578 1.148463 0.395288
 6 -0.740844 1.672818 -0.160522
 1 3.065451 0.503390 1.215676
 1 3.873693 0.862540 -0.303837
 1 3.566667 -1.605271 0.018267
 1 2.713987 -1.027421 -1.406511
 1 1.913137 2.373666 0.063970
 1 1.700335 1.385263 -1.375522
 1 1.465718 -1.564529 1.334254
 1 1.251678 -2.551649 -0.106628
 1 -0.587051 2.706270 0.164620
 1 -0.789047 1.690936 -1.256081
 1 0.158605 -0.657901 -1.264054
 1 -2.058779 1.228946 1.489327
 1 -2.925828 1.713724 0.021011
 1 -1.009428 -1.241645 1.492031
 1 -1.288380 -2.212766 0.034029
 1 0.497689 0.817820 1.367817
 8 -3.257664 -0.731062 -0.505769
```

1.2.7 2-Decalone cis-S

```
27
cis-S DPCS3
 6 0.256314 1.512810 -0.488433
 6 -0.556817 0.902390 0.658074
 6 -0.210899 -0.582981 0.871168
 6 1.301157 -0.773978 1.073711
 6 2.094023 -0.128625 -0.042261
 6 1.765894 1.329588 -0.280029
 6 -0.741606 -1.453691 -0.271828
 6 -2.249045 -1.274169 -0.450027
 6 -2.610536 0.193398 -0.677000
 6 -2.066956 1.072742 0.450959
 1 -2.607730 -1.888095 -1.281115
 1 -2.759928 -1.633751 0.451928
 1 -3.696242 0.309336 -0.742832
 1 -2.205852 0.523311 -1.639780
 1 -0.226381 -1.205381 -1.207222
 1 -0.505385 -2.502179 -0.064303
 1 -2.580191 0.804718 1.382271
 1 -2.296671 2.125854 0.257679
 1 -0.025736 1.059129 -1.442414
 1 0.024101 2.578889 -0.571899
 1 -0.714853 -0.910730 1.789729
 1 1.600226 -0.289234 2.011400
 1 2.075541 1.890846 0.610243
 1 2.344563 1.689749 -1.131421
 1 1.567808 -1.830879 1.133657
 1 -0.276454 1.441280 1.573814
 8 2.912507 -0.734584 -0.704634
```

1.2.8 2-Decalone cis-NS

```
27
decalon_NS DPCS3
 6 -0.701266 -1.147888 -0.328354
 6 0.253832 -0.627484 0.762151
 6 0.443627 0.896550 0.669033
 6 -0.909831 1.612355 0.703607
 6 -1.877292 1.111682 -0.379686
 6 -2.012673 -0.394042 -0.312317
 6 1.297298 1.287684 -0.541891
 6 2.646766 0.569093 -0.524894
 6 2.461617 -0.946999 -0.471028
 6 1.604907 -1.351434 0.729560
 1 3.236947 0.850124 -1.401933
 1 3.214444 0.893461 0.355956
 1 3.433304 -1.445899 -0.414030
 1 1.993986 -1.289632 -1.400830
 1 0.776093 1.047149 -1.475220
 1 1.444452 2.372888 -0.541552
 1 2.151427 -1.106559 1.648137
 1 1.444411 -2.434417 0.738273
 1 -0.251606 -1.011950 -1.318114
 1 -0.904996 -2.211933 -0.194042
 1 1.002779 1.204729 1.562813
 1 -1.372059 1.450259 1.683658
 1 -1.490464 1.371789 -1.371482
 1 -2.866176 1.559294 -0.274753
 1 -0.766320 2.692103 0.597437
 1 -0.222055 -0.842123 1.727798
 8 -3.088025 -0.952662 -0.224801
```

1.2.9 Ascorbic acid conformer 1

```
20
 conformer 1 DPCS3
  6 0.361553 -0.374782 -0.480372
  8 -0.659871 -1.385272 -0.421275
  6 -1.842017 -0.793483 -0.061269
  6 -1.635212 0.646182 0.068820
  6 -0.349278 0.920069 -0.204284
  8 -2.870141 -1.400832 0.094768
  8 -2.652720 1.475715 0.374702
  8 0.249636 2.116350 -0.272026
  6 1.450597 -0.773464 0.521105
  6 2.434581 0.343503 0.810716
  8 2.812302 1.060943 -0.368013
  8 2.197932 -1.864530 0.002534
  1 0.785392 -0.389676 -1.488534
  1 -3.440321 0.922976 0.469819
  1 1.179961 1.987416 -0.527804
  1 0.955514 -1.051621 1.460013
  1 1.589403 -2.587839 -0.180827
  1 3.283137 0.459173 -0.952888
  1 1.978087 1.080267 1.470573
  1 3.311777 -0.077645 1.306850
```

1.2.10 Ascorbic acid conformer 2

```
 20
 conformer 2 DPCS3
```

```
 6 0.209049 -0.011450 -1.031037
 8 -0.621378 -1.173063 -0.957607
 6 -1.728804 -0.873309 -0.206892
 6 -1.629946 0.504469 0.268000
 6 -0.479137 1.024724 -0.184620
 8 -2.613243 -1.659799 0.015650
 8 -2.586005 1.047604 1.049446
 8 0.035791 2.245045 0.018108
 6 1.624508 -0.338690 -0.570301
 6 1.705894 -0.804554 0.869259
 8 3.101133 -0.940891 1.135938
 8 2.349948 0.881034 -0.739754
 1 0.258195 0.314487 -2.074975
 1 -3.267626 0.370971 1.160657
 1 0.965498 2.213149 -0.260468
 1 2.043806 -1.116106 -1.218187
 1 3.190825 0.765914 -0.281092
 1 3.225163 -1.139298 2.066541
 1 1.253684 -0.060036 1.532473
 1 1.180780 -1.757034 0.981391
```

1.2.11 Ascorbic acid conformer 3

```
20
 conformer 3 DPCS3
 6 -0.353519 -0.455254 -0.795411
 8 -0.187169 0.973222 -0.674403
 6 1.050054 1.243865 -0.151032
 6 1.756911 -0.015612 0.041885
 6 0.953247 -1.016298 -0.336274
 8 1.443479 2.355906 0.088475
 8 3.012415 -0.082443 0.539720
 8 1.128011 -2.347770 -0.340589
 6 -1.551265 -0.920426 0.039779
 6 -2.837347 -0.192063 -0.356412
 8 -2.889498 1.108738 0.209415
 8 -1.303827 -0.764983 1.417512
 1 -0.538968 -0.679485 -1.851147
 1 3.293438 0.822605 0.727881
 1 1.987448 -2.555694 0.044156
 1 -1.669636 -1.990549 -0.160574
 1 -1.679392 0.090364 1.663762
 1 -2.169371 1.625716 -0.169457
 1 -2.939196 -0.162920 -1.447334
 1 -3.691792 -0.728958 0.055424
```

1.2.12 1,4-Naphthoquinone

```
Principal axis orientation:
---------------------------------------------------------------------
Center Atomic Coordinates (Angstroms)
Number Number X Y Z
---------------------------------------------------------------------
     1 6 -0.283426 0.701127 0.000000
     2 6 -0.283426 -0.701127 -0.000000
     3 6 0.999224 -1.457009 -0.000000
     4 6 2.254097 -0.670823 -0.000000
     5 6 2.254097 0.670823 0.000000
     6 6 0.999224 1.457009 0.000000
```

```
     7 1 3.171308 -1.248976 -0.000000
     8 1 3.171308 1.248976 0.000000
     9 8 1.034343 2.678015 0.000000
    10 8 1.034343 -2.678015 -0.000000
    11 6 -1.492855 1.397960 0.000000
    12 6 -2.693558 0.698699 0.000000
    13 6 -2.693558 -0.698699 -0.000000
    14 6 -1.492855 -1.397960 -0.000000
    15 1 -3.632944 -1.238784 -0.000000
    16 1 -1.469269 -2.480708 -0.000000
    17 1 -1.469269 2.480708 0.000000
    18 1 -3.632944 1.238784 0.000000
---------------------------------------------------------------------
Rotational constants (MHZ):
  1329.1352724 1096.5106128 600.8341699
Dipole moment (Debye):
    -1.3146377 -0.0000000 0.0000000 Tot= 1.3146377
```