Supporting Information for "Numerical Study on the Partitioning of the Molecular Polarizability into Fluctuating Charge and Induced Atomic Dipole Contributions"

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Coordinates of the molecules studied

acetic acid

C	-0.59072	1.79325	0.00000
H	-0.23404	2.29765	0.87365
H	-0.23404	2.29765	-0.87365
H	-1.66072	1.79326	0.00000
C	-0.07740	0.34132	0.00000
O	0.74457	-0.12385	1.07372
H	0.87981	0.58678	1.70484
O	-0.37880	-0.43718	-0.94163

adenine

N	0.27930	2.40684	-0.60575
C	-1.08486	2.44575	-0.55116
H	-1.65944	3.02303	-1.25609
N	-1.59771	1.71799	0.42875
C	-0.48973	1.17144	1.03019
C	-0.34614	0.29147	2.11723
N	-1.41871	-0.16778	2.81014
H	-1.23887	-0.95948	3.40476
H	-2.29187	-0.17882	2.30736
N	0.88576	-0.07008	2.49195
C	1.93523	0.40729	1.79680
H	2.90603	0.07884	2.14582
N	1.94098	1.22420	0.74022
C	0.69522	1.57799	0.40640
H	0.86101	2.82980	-1.31045

```
ala dipeptide
  N   -1.05923  -0.35001   0.19637
  H   -0.80988  -1.24854   0.59334
  C    0.05469   0.54552  -0.04213
  H   -0.04486   0.95423  -1.05597
  C    0.07581   1.72051   0.95605
  C    1.33633  -0.29795   0.05991
  H    0.18655   1.35011   1.98045
  H    0.90038   2.41109   0.74484
  H   -0.86587   2.26842   0.87285
  O    1.33705  -1.40269   0.59852
  C   -2.31973  -0.06559  -0.23442
  O   -2.60053   0.99066  -0.79508
  C   -3.36138  -1.14337   0.02785
  H   -2.96461  -2.02041   0.54824
  H   -4.17320  -0.71296   0.62228
  H   -3.79054  -1.45925  -0.92826
  N    2.44963   0.28357  -0.46109
  C    3.76380  -0.33479  -0.41123
  H    2.35526   1.18345  -0.91033
  H    3.65421  -1.29475   0.09441
  H    4.47255   0.28752   0.14740
  H    4.15796  -0.50362  -1.41989

ammonia
  N    0.00000   0.00000  -0.10000
```

```
  H    0.94281   0.00000   0.23333
  H   -0.47141  -0.81650   0.23333
  H   -0.47141   0.81650   0.23333

benzene
  C   -1.01655  -0.68558   0.00000
  C    0.37861  -0.68558   0.00000
  C    1.07615   0.52217   0.00000
  C    0.37850   1.73068  -0.00120
  C   -1.01633   1.73060  -0.00168
  C   -1.71393   0.52240  -0.00068
  H   -1.56631  -1.63790   0.00045
  H    0.92812  -1.63809   0.00131
  H    2.17583   0.52225   0.00063
  H    0.92870   2.68282  -0.00126
  H   -1.56645   2.68288  -0.00263
  H   -2.81353   0.52258  -0.00086

dodecahexene
  C    0.08069   6.73930   0.00000
  H   -0.99732   6.84420   0.00000
  H    0.66641   7.64727   0.00000
  C    0.65478   5.53717   0.00000
  H    1.73762   5.46023   0.00000
  C   -0.08069   4.28826   0.00000
  H   -1.16511   4.35574   0.00000
  C    0.50069   3.07896   0.00000
```

```
  H    1.58560   3.01696   0.00000
  C   -0.22441   1.83277   0.00000
  H   -1.30923   1.89309   0.00000
  C    0.36140   0.62294   0.00000
  H    1.44634   0.56362   0.00000
  C   -0.36140  -0.62294   0.00000
  H   -1.44634  -0.56362   0.00000
  C    0.22441  -1.83277   0.00000
  H    1.30923  -1.89309   0.00000
  C   -0.50069  -3.07896   0.00000
  H   -1.58560  -3.01696   0.00000
  C    0.08069  -4.28826   0.00000
  H    1.16511  -4.35574   0.00000
  C   -0.65478  -5.53717   0.00000
  H   -1.73762  -5.46023   0.00000
  C   -0.08069  -6.73930   0.00000
  H    0.99732  -6.84420   0.00000
  H   -0.66641  -7.64727   0.00000

ethanol
  C    1.22255  -0.22191   0.00005
  H    1.28862  -0.86063   0.88707
  H    2.07582   0.46577  -0.00005
  H    1.28861  -0.86083  -0.88683
  C   -0.08700   0.54899  -0.00004
  H   -0.13926   1.20115   0.88760
  H   -0.13915   1.20111  -0.88774
```

```
  O   -1.15023  -0.39997  -0.00010
  H   -1.98606   0.09077   0.00073

formamide
  C    0.00000   0.41961   0.00000
  H   -0.46875   1.43564   0.00000
  O    1.20062   0.23936   0.00000
  N   -0.93877  -0.56780   0.00000
  H   -0.63671  -1.53633   0.00000
  H   -1.92811  -0.35729   0.00000

formic acid
  C   -1.88890  -0.17969   0.00000
  O   -1.49328   1.07369   0.00000
  O   -1.17043  -1.16659   0.00000
  H   -2.97949  -0.25883   0.00000
  H   -0.49883   1.10719   0.00000

indole
  C   -1.37635   1.12840   0.00000
  C   -2.13978  -0.01192   0.00000
  C    0.00000   0.71306   0.00000
  H   -3.21430  -0.13222   0.00000
  N   -1.31754  -1.12107   0.00000
  C    0.00000  -0.71306   0.00000
  C    1.23486   1.38955   0.00000
  H   -1.63527  -2.07920   0.00000
```

```
  C    1.18380  -1.46147   0.00000
  C    2.41170   0.65004   0.00000
  H    1.26532   2.47657   0.00000
  H    1.16255  -2.54800   0.00000
  C    2.38621  -0.76221   0.00000
  H    3.36972   1.16332   0.00000
  H    3.32315  -1.31275   0.00000
  H   -1.74984   2.14345   0.00000

methanal
  C    0.00001   0.52896   0.00000
  H   -0.93793   1.12359   0.00000
  H    0.93785   1.12375   0.00000
  O    0.00001  -0.67764   0.00000

methane
  C    0.00000   0.00000   0.00000
  H    0.63134   0.63134   0.63134
  H   -0.63134  -0.63134   0.63134
  H   -0.63134   0.63134  -0.63134
  H    0.63134  -0.63134  -0.63134

methanol
  C    0.66233  -0.01954   0.00000
  H    1.07972   0.99103  -0.00000
  H    1.03696  -0.54366  -0.89315
  H    1.03696  -0.54366   0.89315
```

```
  O   -0.74917   0.12250   0.00000
  H   -1.13424  -0.76642   0.00000

methyl ether
  C    1.17104  -0.19524   0.00000
  H    2.02189   0.49141  -0.00009
  H    1.23255  -0.83979  -0.89289
  H    1.23263  -0.83967   0.89298
  O    0.00000   0.58988   0.00000
  C   -1.17104  -0.19524   0.00000
  H   -1.23259  -0.83973   0.89293
  H   -2.02189   0.49141   0.00000
  H   -1.23259  -0.83973  -0.89294

mNA
  C   -0.59193   0.12486  -0.00306
  C    0.40335  -0.84636  -0.00827
  C    1.74816  -0.44665  -0.00826
  C    2.03992   0.93127  -0.00078
  C    1.01858   1.87786   0.00499
  C   -0.32111   1.49091   0.00383
  H    0.12422  -1.89339  -0.01639
  H    3.07812   1.25483  -0.00481
  H    1.27157   2.93406   0.01209
  H   -1.13225   2.20666   0.00955
  N   -1.99725  -0.32050   0.00106
  N    2.76786  -1.39127  -0.07307
```

```
  O   -2.87212   0.54490   0.00052
  O   -2.21670  -1.53226   0.00573
  H    2.52506  -2.32099   0.24407
  H    3.66777  -1.09120   0.27878

neopentane
  C   -0.00003   0.00007   0.00000
  C    0.50985  -1.44168   0.00000
  C   -1.52955  -0.00025   0.00000
  C    0.50985   0.72093   1.24862
  C    0.50985   0.72093  -1.24862
  H    1.60098  -1.46812   0.00000
  H    0.15872  -1.97817   0.88328
  H    0.15872  -1.97817  -0.88328
  H   -1.91913   1.01932   0.00000
  H   -1.91877  -0.51017  -0.88318
  H   -1.91877  -0.51017   0.88318
  H    0.15752   0.22552   2.15514
  H    1.60103   0.73249   1.27267
  H    0.16067   1.75475   1.27126
  H    0.15752   0.22552  -2.15514
  H    0.16067   1.75475  -1.27126
  H    1.60103   0.73249  -1.27267

pNA
  C    1.36325   1.21464  -0.00496
  C    2.08197   0.00003  -0.00555
```

```
  C    1.36322  -1.21459  -0.00489
  C   -0.02194  -1.21561  -0.00384
  C   -0.71044   0.00004  -0.00267
  C   -0.02194   1.21567  -0.00383
  H    1.90469   2.15721  -0.00950
  H    1.90471  -2.15713  -0.00939
  H   -0.58336  -2.14191  -0.00129
  H   -0.58327   2.14202  -0.00124
  N    3.46137  -0.00004  -0.05562
  H    3.93557   0.84596   0.22896
  H    3.93548  -0.84613   0.22887
  N   -2.16615  -0.00001   0.00304
  O   -2.74416   1.09073   0.00541
  O   -2.74398  -1.09083   0.00535

thymine
  N    1.27546  -0.64790  -1.97791
  C    1.41305  -1.55368  -0.95507
  H    2.42588  -1.86708  -0.74688
  C    0.35760  -2.02395  -0.25306
  C    0.48213  -3.01795   0.85212
  H    0.17577  -2.57561   1.79863
  H   -0.16017  -3.87704   0.66395
  H    1.51124  -3.35728   0.95137
  C   -0.96847  -1.52981  -0.59398
  O   -2.00293  -1.83970  -0.01995
  N   -0.99569  -0.63839  -1.67204
```

```
  H   -1.90141  -0.25017  -1.89858
  C    0.06847  -0.11918  -2.37638
  O   -0.03979   0.72270  -3.25311
  H    2.08533  -0.27602  -2.44546

uracil
  N    2.01136  -1.21321  -0.09807
  C    2.02571  -0.69718  -1.36440
  H    2.29752  -1.39106  -2.14565
  C    1.71452   0.59197  -1.61249
  H    1.72729   0.99085  -2.61200
  C    1.30896   1.45753  -0.52059
  O    0.92059   2.61109  -0.62605
  N    1.37689   0.83975   0.73464
  H    1.05180   1.38622   1.52337
  C    1.64599  -0.48521   1.01873
  O    1.56111  -0.97181   2.12981
  H    2.12946  -2.20150   0.05681

val dipeptide
  N   -1.22317  -0.51401   0.24775
  H   -1.09878  -0.99629   1.12993
  C   -0.04006   0.12243  -0.31759
  H   -0.12777   0.07015  -1.40640
  C    0.06411   1.62900   0.07691
  C    1.16724  -0.69918   0.14273
  H   -0.91523   2.04452  -0.19314
```

```
  C    0.28075   1.84882   1.57899
  C    1.12716   2.35945  -0.75272
  O    1.19257  -1.22265   1.27156
  H    1.26933   1.49931   1.89925
  H    0.21511   2.91742   1.81335
  H   -0.47242   1.32958   2.18199
  H    0.97208   2.20813  -1.82785
  H    1.08363   3.43694  -0.55701
  H    2.13961   2.02094  -0.50374
  C   -2.44503  -0.45009  -0.32331
  O   -2.65278   0.15431  -1.39127
  C   -3.55635  -1.17596   0.40209
  H   -3.22607  -1.65336   1.32814
  H   -4.35755  -0.46504   0.62914
  H   -3.97282  -1.93840  -0.26504
  N    2.18225  -0.82006  -0.72894
  C    3.42119  -1.50186  -0.37474
  H    2.11962  -0.34997  -1.62302
  H    3.91655  -1.00982   0.46879
  H    4.08565  -1.48142  -1.23917
  H    3.22309  -2.54313  -0.10336

water
  O   -1.55101  -0.11452   0.00000
  H   -1.93426   0.76250   0.00000
  H   -0.59968   0.04071   0.00000
```

```
water dimer
  O  -1.551007  -0.114520   0.000000
  H  -1.934259   0.762503   0.000000
  H  -0.599677   0.040712   0.000000
  O   1.350625   0.111469   0.000000
  H   1.680398  -0.373741  -0.758561
  H   1.680398  -0.373741   0.758561


phenol dimer
  C    -2.0071056    0.7638459   -0.1083509
  O    -1.3885044    1.9298523   -0.4431206
  H    -0.5238121    1.9646519   -0.0064609
  C    -1.4630807   -0.1519120    0.7949930
  C    -2.1475789   -1.3295094    1.0883677
  C    -3.3743208   -1.6031427    0.4895864
  C    -3.9143727   -0.6838545   -0.4091028
  C    -3.2370496    0.4929609   -0.7096126
  H    -0.5106510    0.0566569    1.2642563
  H    -1.7151135   -2.0321452    1.7878417
  H    -3.9024664   -2.5173865    0.7197947
  H    -4.8670730   -0.8822939   -0.8811319
  H    -3.6431662    1.2134345   -1.4057590
  O     1.3531168    1.9382724    0.4723133
  C     2.0369747    0.7865043    0.1495491
  H     1.7842846    2.3487495    1.2297110
  C     1.5904026    0.0696860   -0.9574153
  C     2.2417367   -1.1069765   -1.3128110
```

C	3.3315674	-1.5665603	-0.5748636
C	3.7696838	-0.8396901	0.5286439
C	3.1224836	0.3383498	0.8960491
H	0.7445512	0.4367983	-1.5218583
H	1.8921463	-1.6649726	-2.1701843
H	3.8330227	-2.4811537	-0.8566666
H	4.6137632	-1.1850101	1.1092635
H	3.4598854	0.9030376	1.7569489

2-pyridoxine/2-aminopyridine

O	-1.3976213	-1.8858368	-0.3673061
N	-1.4642550	0.3641828	0.0192301
C	-4.1857398	0.3696669	0.0360960
C	-3.4832598	1.5783111	0.2500752
C	-2.1179502	1.5307048	0.2338383
C	-2.0773833	-0.8637492	-0.1899414
C	-3.5156032	-0.8051950	-0.1757585
H	-5.2678045	0.3707428	0.0411419
H	-3.9920334	2.5127560	0.4214414
H	-1.4929196	2.3984096	0.3885018
H	-4.0401226	-1.7348452	-0.3379269
H	-0.4265266	0.3612127	0.0073538
N	1.4327616	0.3639703	-0.0159508
C	2.1154200	-0.7803450	0.1681099
C	3.5237586	-0.8016096	0.1545027
C	4.2185897	0.3735783	-0.0525929
C	3.5099708	1.5615014	-0.2449763

```
  C     2.1280138    1.4953324   -0.2175374
  H     4.0459206   -1.7361356    0.3076883
  H     5.2999426    0.3666009   -0.0663349
  H     4.0110923    2.5024313   -0.4130052
  H     1.5339878    2.3893837   -0.3670565
  N     1.3883123   -1.9083038    0.4198149
  H     1.8694714   -2.7812773    0.2940385
  H     0.4089067   -1.9079942    0.1300860

hydrogen-bonded adenine/thymine complex
  N     0.9350155   -0.0279801   -0.3788916
  C     1.6739638   -0.0357766    0.7424316
  C     3.0747955   -0.0094480    0.5994562
  C     3.5646109    0.0195446   -0.7059872
  N     2.8531510    0.0258031   -1.8409596
  C     1.5490760    0.0012569   -1.5808009
  N     4.0885824   -0.0054429    1.5289786
  C     5.1829921    0.0253971    0.7872176
  N     4.9294871    0.0412404   -0.5567274
  N     1.0716177   -0.0765366    1.9391390
  H     0.8794435    0.0050260   -2.4315709
  H     6.1882591    0.0375542    1.1738824
  H     5.6035368    0.0648755   -1.3036811
  H     0.0586915   -0.0423765    2.0039181
  H     1.6443796   -0.0347395    2.7619159
  N    -3.9211729   -0.0009646   -1.5163659
  C    -4.6136833    0.0169051   -0.3336520
```

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  C    -3.9917387    0.0219348    0.8663338
  C    -2.5361367    0.0074651    0.8766724
  N    -1.9256484   -0.0110593   -0.3638948
  C    -2.5395897   -0.0149474   -1.5962357
  C    -4.7106131    0.0413373    2.1738637
  O    -1.8674730    0.0112093    1.9120833
  O    -1.9416783   -0.0291878   -2.6573783
  H    -4.4017172   -0.0036078   -2.4004924
  H    -0.8838255   -0.0216168   -0.3784269
  H    -5.6909220    0.0269347   -0.4227183
  H    -4.4439282   -0.8302573    2.7695655
  H    -4.4267056    0.9186178    2.7530256
  H    -5.7883971    0.0505530    2.0247280

adenine/thymine complex in stacking
  N     0.2793014    2.4068393   -0.6057517
  C    -1.0848570    2.4457461   -0.5511608
  H    -1.6594403    3.0230294   -1.2560905
  N    -1.5977117    1.7179877    0.4287543
  C    -0.4897255    1.1714358    1.0301910
  C    -0.3461366    0.2914710    2.1172343
  N    -1.4187090   -0.1677767    2.8101441
  H    -1.2388750   -0.9594802    3.4047578
  H    -2.2918734   -0.1788223    2.3073619
  N     0.8857630   -0.0700763    2.4919494
  C     1.9352348    0.4072878    1.7968022
  H     2.9060330    0.0788414    2.1458181
```

```
  N     1.9409775    1.2242019    0.7402202
  C     0.6952186    1.5779858    0.4063984
  H     0.8610073    2.8298045   -1.3104502
  N     1.2754606   -0.6478993   -1.9779104
  C     1.4130533   -1.5536850   -0.9550667
  H     2.4258769   -1.8670780   -0.7468778
  C     0.3575976   -2.0239499   -0.2530575
  C     0.4821292   -3.0179494    0.8521221
  H     0.1757705   -2.5756065    1.7986281
  H    -0.1601691   -3.8770412    0.6639498
  H     1.5112443   -3.3572767    0.9513659
  C    -0.9684711   -1.5298112   -0.5939792
  O    -2.0029280   -1.8396957   -0.0199453
  N    -0.9956916   -0.6383870   -1.6720420
  H    -1.9014057   -0.2501720   -1.8985760
  C     0.0684702   -0.1191762   -2.3763759
  O    -0.0397875    0.7227006   -3.2531083
  H     2.0853289   -0.2760176   -2.4454577

benzene/ammonia complex
  C    -0.7392810    0.5158785   -1.2071079
  C    -1.4261442    0.3965455    0.0000000
  C    -0.7392810    0.5158785    1.2071079
  C     0.6342269    0.7546398    1.2070735
  C     1.3210434    0.8737566    0.0000000
  C     0.6342269    0.7546398   -1.2070735
  H    -1.2719495    0.4206316   -2.1432894
```

```
  H    -2.4902205    0.2052381    0.0000000
  H    -1.2719495    0.4206316    2.1432894
  H     1.1668005    0.8474885    2.1436950
  H     2.3863585    1.0596312    0.0000000
  H     1.1668005    0.8474885   -2.1436950
  N     0.1803930   -2.9491231    0.0000000
  H     0.7595495   -3.1459477   -0.8060729
  H     0.7595495   -3.1459477    0.8060729
  H     0.0444167   -1.9449399    0.0000000

T-shaped benzene dimer
  C     0.0000000    0.0000000    1.0590353
  C     0.0000000   -1.2060084    1.7576742
  C     0.0000000   -1.2071767    3.1515905
  C     0.0000000    0.0000000    3.8485751
  C     0.0000000    1.2071767    3.1515905
  C     0.0000000    1.2060084    1.7576742
  H     0.0000000    0.0000000   -0.0215805
  H     0.0000000   -2.1416387    1.2144217
  H     0.0000000   -2.1435657    3.6929953
  H     0.0000000    0.0000000    4.9301499
  H     0.0000000    2.1435657    3.6929953
  H     0.0000000    2.1416387    1.2144217
  C    -1.3940633    0.0000000   -2.4541524
  C    -0.6970468    1.2072378   -2.4546277
  C     0.6970468    1.2072378   -2.4546277
  C     1.3940633    0.0000000   -2.4541524
```

```
  C     0.6970468   -1.2072378   -2.4546277
  C    -0.6970468   -1.2072378   -2.4546277
  H    -2.4753995    0.0000000   -2.4503221
  H    -1.2382321    2.1435655   -2.4536764
  H     1.2382321    2.1435655   -2.4536764
  H     2.4753995    0.0000000   -2.4503221
  H     1.2382321   -2.1435655   -2.4536764
  H    -1.2382321   -2.1435655   -2.4536764

benzene/HCN complex
  C    -0.7097741   -0.9904230    1.2077018
  C    -1.4065340   -0.9653529    0.0000000
  C    -0.7097741   -0.9904230   -1.2077018
  C     0.6839651   -1.0405105   -1.2078652
  C     1.3809779   -1.0655522    0.0000000
  C     0.6839651   -1.0405105    1.2078652
  H    -1.2499482   -0.9686280    2.1440507
  H    -2.4869197   -0.9237060    0.0000000
  H    -1.2499482   -0.9686280   -2.1440507
  H     1.2242882   -1.0580753   -2.1442563
  H     2.4615886   -1.1029818    0.0000000
  H     1.2242882   -1.0580753    2.1442563
  N    -0.0034118    3.5353926    0.0000000
  C     0.0751963    2.3707040    0.0000000
  H     0.1476295    1.3052847    0.0000000

benzene/methane complex
```

```
  C     1.3932178    0.0362913   -0.6332803
  C     0.7280364   -1.1884015   -0.6333017
  C    -0.6651797   -1.2247077   -0.6332803
  C    -1.3932041   -0.0362972   -0.6333017
  C    -0.7280381    1.1884163   -0.6332803
  C     0.6651677    1.2246987   -0.6333017
  H     2.4742737    0.0644484   -0.6317240
  H     1.2929588   -2.1105409   -0.6317401
  H    -1.1813229   -2.1750081   -0.6317240
  H    -2.4742614   -0.0644647   -0.6317401
  H    -1.2929508    2.1105596   -0.6317240
  H     1.1813026    2.1750056   -0.6317401
  C     0.0000000    0.0000000    3.0826195
  H     0.5868776    0.8381742    3.4463772
  H    -1.0193189    0.0891638    3.4463772
  H     0.0000000    0.0000000    1.9966697
  H     0.4324413   -0.9273380    3.4463772

benzene/water complex
  C     0.7806117   -0.6098875   -1.2075426
  C     0.4784039    0.7510406   -1.2079040
  C     0.3276592    1.4318573    0.0000000
  C     0.4784039    0.7510406    1.2079040
  C     0.7806117   -0.6098875    1.2075426
  C     0.9321510   -1.2899614    0.0000000
  H     0.8966688   -1.1376051   -2.1441482
  H     0.3573895    1.2782091   -2.1440546
```

```
  H     0.0918593    2.4871407    0.0000000
  H     0.3573895    1.2782091    2.1440546
  H     0.8966688   -1.1376051    2.1441482
  H     1.1690064   -2.3451668    0.0000000
  O    -2.7885270   -0.2744854    0.0000000
  H    -2.6229114   -1.2190831    0.0000000
  H    -1.9015103    0.0979110    0.0000000

benzene/indole complex in stacking
  C    -0.0210742    1.5318615   -1.3639345
  C    -1.2746794    0.9741030   -1.6074097
  C    -1.3783055   -0.2256981   -2.3084154
  C    -0.2289426   -0.8664053   -2.7687944
  C     1.0247882   -0.3035171   -2.5312410
  C     1.1289996    0.8966787   -1.8299830
  H     0.0600740    2.4565627   -0.8093957
  H    -2.1651002    1.4654521   -1.2405676
  H    -2.3509735   -0.6616122   -2.4926698
  H    -0.3103419   -1.7955762   -3.3172704
  H     1.9165847   -0.7940845   -2.8993942
  H     2.1000347    1.3326757   -1.6400420
  H    -2.9417647    0.8953834    2.2239054
  C    -2.0220674    0.4258540    1.9013549
  C    -0.8149418    1.0740453    2.1066982
  H    -0.7851529    2.0443812    2.5856086
  C     0.3704286    0.4492852    1.6847458
  C     1.7508619    0.8038935    1.7194004
```

```
  H     2.1870108    1.6998281    2.1275903
  C     2.4451359   -0.2310742    1.1353313
  N     1.5646462   -1.2137812    0.7555384
  C     0.2861214   -0.8269486    1.0618752
  C    -0.9284667   -1.4853121    0.8606937
  H    -0.9729200   -2.4554847    0.3834013
  C    -2.0792848   -0.8417668    1.2876443
  H    -3.0389974   -1.3203846    1.1468400
  H     1.8075741   -2.0366963    0.2333038
  H     3.5028794   -0.3485344    0.9695233
```

T-shaped benzene/indole complex

```
  C     2.5118997    1.6250148    0.0000000
  C     2.7130094    0.9578537   -1.2082918
  C     3.1177821   -0.3767436   -1.2083647
  C     3.3213848   -1.0437307    0.0000000
  C     3.1177821   -0.3767436    1.2083647
  C     2.7130094    0.9578537    1.2082918
  H     2.2024038    2.6611358    0.0000000
  H     2.5511760    1.4736908   -2.1445900
  H     3.2702999   -0.8951406   -2.1448379
  H     3.6368139   -2.0781521    0.0000000
  H     3.2702999   -0.8951406    2.1448379
  H     2.5511760    1.4736908    2.1445900
  H     0.8065245   -0.4358866    0.0000000
  N    -0.1442408   -0.7686927    0.0000000
  C    -0.5161122   -2.0893220    0.0000000
```

```
  C    -1.8898755   -2.1814495    0.0000000
  C    -2.3932317   -0.8470830    0.0000000
  C    -1.2640653    0.0195887    0.0000000
  C    -1.3896004    1.4117668    0.0000000
  C    -2.6726501    1.9366450    0.0000000
  C    -3.8054511    1.0974790    0.0000000
  C    -3.6798167   -0.2817209    0.0000000
  H     0.2310024   -2.8653173    0.0000000
  H    -2.4585759   -3.0956052    0.0000000
  H    -0.5188733    2.0539520    0.0000000
  H    -2.8077570    3.0097859    0.0000000
  H    -4.7905991    1.5439372    0.0000000
  H    -4.5580187   -0.9142916    0.0000000

water pentamer
  O    0.0000    0.0000    0.0000
  H    0.0090    1.0000   -0.0040
  H   -0.4750   -0.3250    0.8170
  O   -1.3140   -0.9010    2.2630
  H   -2.2540   -0.5590    2.2610
  H   -0.8400   -0.5690    3.0780
  O    0.0260    2.7680   -0.0110
  H   -0.4430    3.1020   -0.8290
  H    0.9710    3.0920   -0.0120
  O   -1.3140   -0.9190   -2.2560
  H   -2.2540   -0.5770   -2.2580
  H   -0.8400   -0.5870   -1.4410
```

```
O     2.6000    -0.9470     0.0040
H     1.6600    -0.6050     0.0020
H     3.0740    -0.6150     0.8180
```

Correlation among all the charge definitions calculated at B3LYP/6-31G(d) level

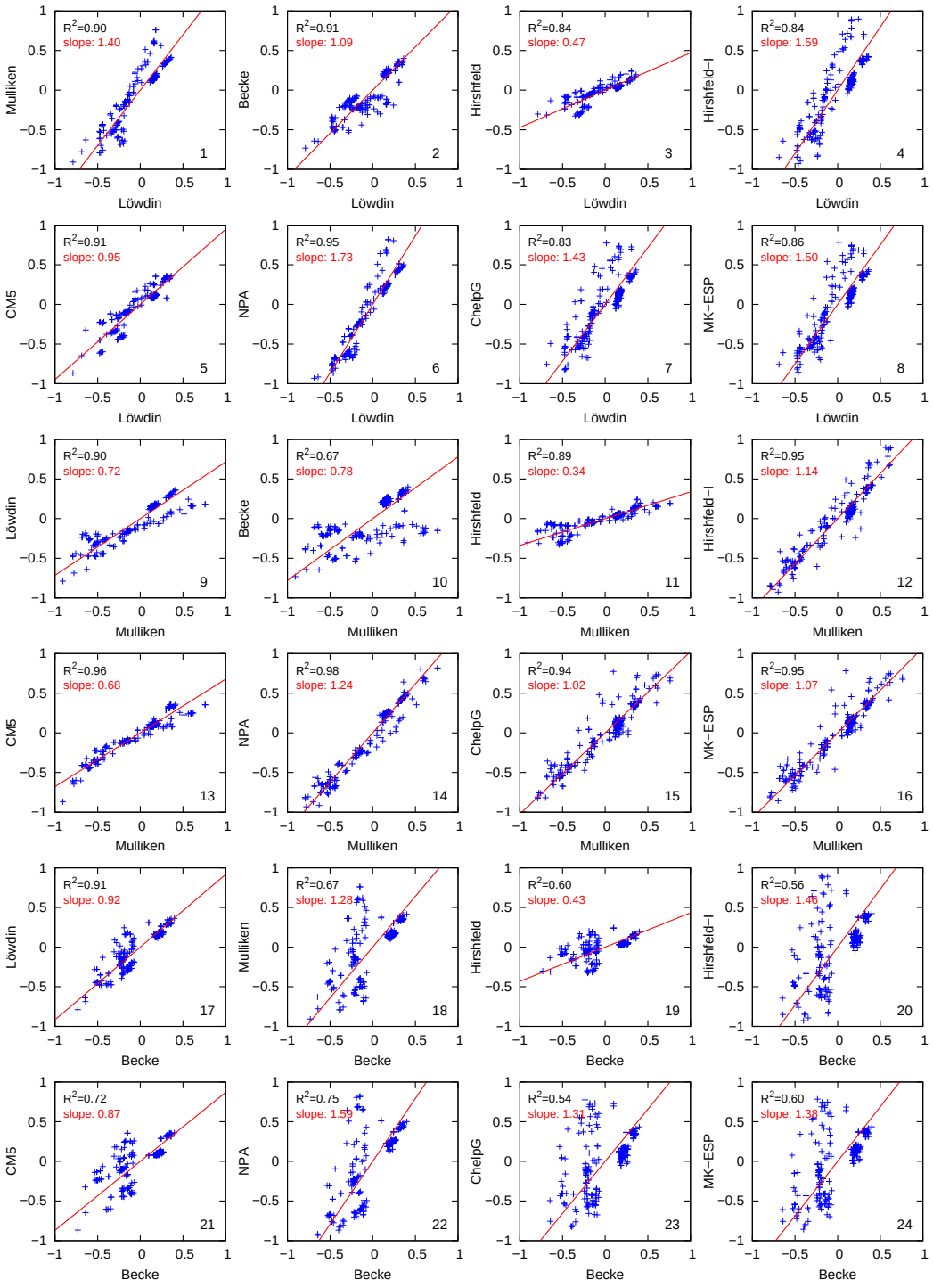
R2=0.90
slope: 1.40
Mulliken
Löwdin
1
R2=0.91
slope: 1.09
Becke
Löwdin
2
R2=0.84
slope: 0.47
Hirshfeld
Löwdin
3
R2=0.84
slope: 1.59
Hirshfeld−I
Löwdin
4
R2=0.91
slope: 0.95
CM5
Löwdin
5
R2=0.95
slope: 1.73
NPA
Löwdin
6
R2=0.83
slope: 1.43
ChelpG
Löwdin
7
R2=0.86
slope: 1.50
MK−ESP
Löwdin
8
R2=0.90
slope: 0.72
Löwdin
Mulliken
9
R2=0.67
slope: 0.78
Becke
Mulliken
10
R2=0.89
slope: 0.34
Hirshfeld
Mulliken
11
R2=0.95
slope: 1.14
Hirshfeld−I
Mulliken
12
R2=0.96
slope: 0.68
CM5
Mulliken
13
R2=0.98
slope: 1.24
NPA
Mulliken
14
R2=0.94
slope: 1.02
ChelpG
Mulliken
15
R2=0.95
slope: 1.07
MK−ESP
Mulliken
16
R2=0.91
slope: 0.92
Löwdin
Becke
17
R2=0.67
slope: 1.28
Mulliken
Becke
18
R2=0.60
slope: 0.43
Hirshfeld
Becke
19
R2=0.56
slope: 1.46
Hirshfeld−I
Becke
20
R2=0.72
slope: 0.87
CM5
Becke
21
R2=0.75
slope: 1.59
NPA
Becke
22
R2=0.54
slope: 1.31
ChelpG
Becke
23
R2=0.60
slope: 1.38
MK−ESP
Becke
24

Figure 1

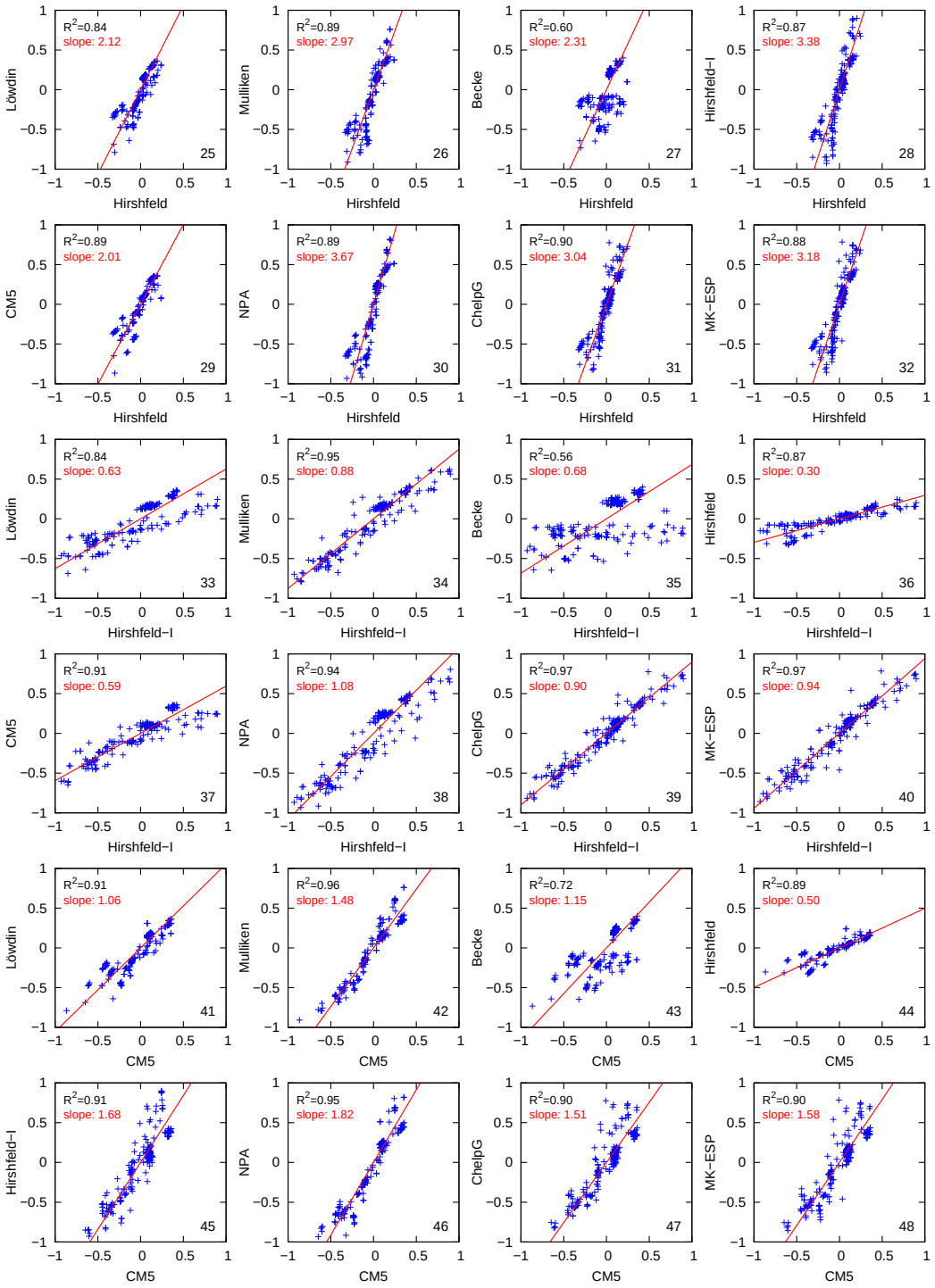

Figure 1: Continued

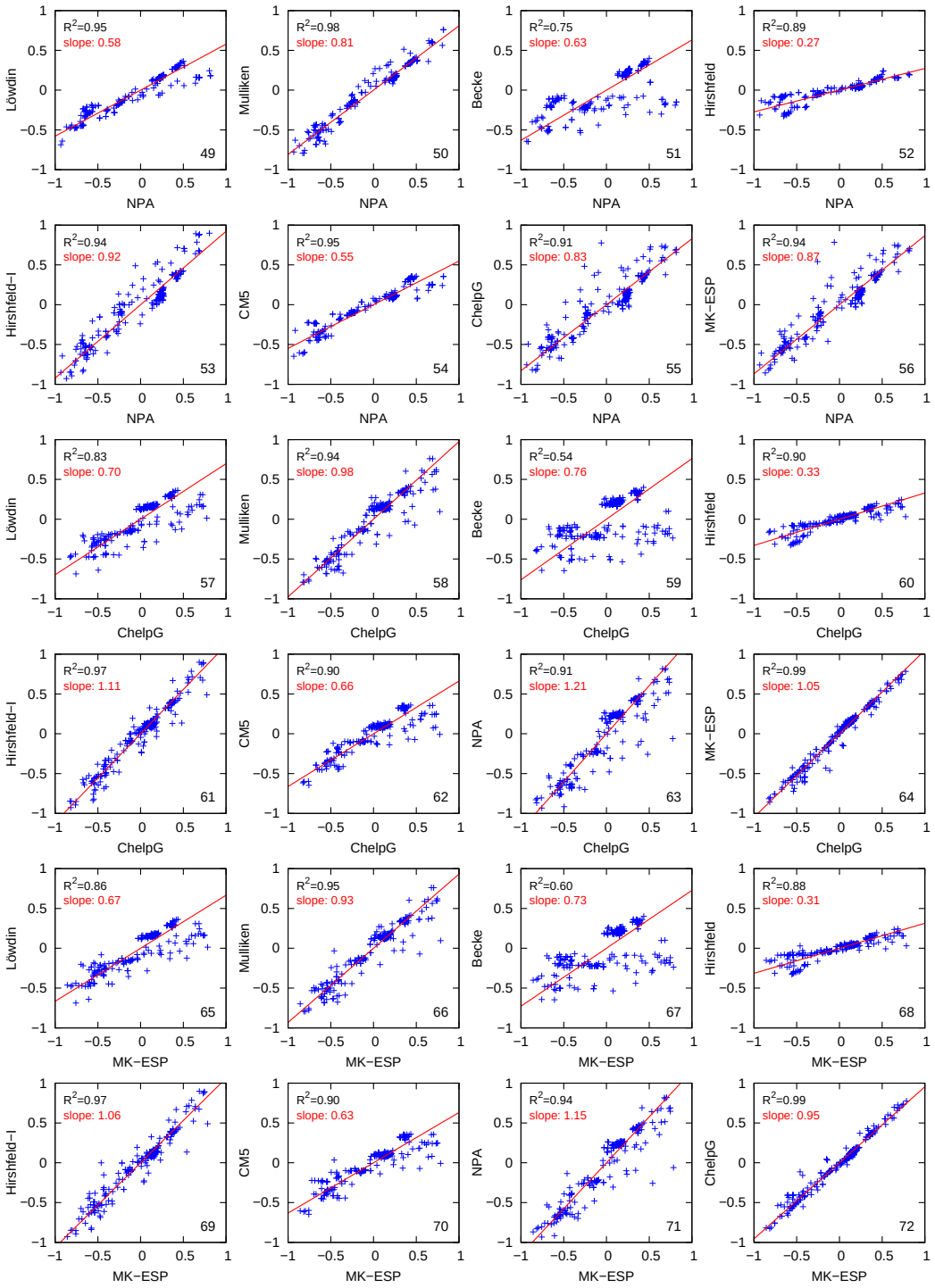

Figure 1: Continued

atomic polarizabilities under Hirshfeld-I scheme

acetic acid

atom C

v1	v2	v3
-1.0981283	0.4397581	0.2480772
0.2604062	-2.0007748	-0.0883950
0.1488067	0.1967390	-0.7432086

atom H

v1	v2	v3
-0.4473683	0.0190309	-0.0267187
-0.0250438	-0.5955736	-0.1389998
-0.0517041	-0.0676648	-0.5484241

atom H

v1	v2	v3
-0.4757272	0.0413473	0.0488627
0.0352478	-0.4340527	0.0647952
0.0435920	0.0084614	-0.4939985

atom H

v1	v2	v3
-0.5208675	-0.0492253	-0.0225022
-0.0013110	-0.4733387	0.0521591
0.0059445	0.0408179	-0.4102837

atom C

v1	v2	v3
-1.4440093	-0.6174179	1.2064980
-0.5733857	0.3313005	0.6418860
1.2439889	0.5731833	-0.0676071

```
atom O
      v1          v2          v3
  -2.1329143  -0.2435839   0.0628035
   0.2662727  -0.8721674   1.2549639
   0.3584075   0.4025172  -1.4312196
atom H
      v1          v2          v3
  -0.2451283   0.0079157  -0.0005705
  -0.0501856  -0.0564050   0.0280412
  -0.0353579   0.1196117  -0.2260767
atom O
      v1          v2          v3
  -2.3629372   0.0809285   0.3715817
  -0.0729440  -1.6562036   0.3923361
   0.2883497   0.6570099  -1.7317090


adenine
atom N
      v1          v2          v3
  -0.5282288   0.0552556  -0.3521580
   0.1990152  -1.8760879  -1.0560684
  -0.6123398  -1.1900926  -0.9292477
atom C
      v1          v2          v3
  -0.1799019  -0.1584020   0.0623110
  -0.2150092  -1.7072758  -1.7224391
   0.0535436  -1.7512806  -0.7867852
```

```
atom H
      v1          v2          v3
  -0.5926845   0.1008926  -0.1259750
   0.0267506  -0.6777004   0.1104958
  -0.0336592   0.0986856  -0.7232681
atom N
      v1          v2          v3
  -1.8006195   0.2818652  -0.3830178
   0.1633401  -2.2856720  -0.9728153
  -0.2988962  -0.9606830  -1.7010827
atom C
      v1          v2          v3
  -0.0215314  -0.3649564   0.0931245
  -0.4997426  -2.1094124  -1.2835855
   0.4159896  -1.3971573  -1.5767819
atom C
      v1          v2          v3
   0.6159546  -0.1484788  -0.1990884
   0.1720821  -1.1618972  -1.2985171
  -0.2698899  -1.1214093  -0.5524282
atom N
      v1          v2          v3
  -1.2550040  -0.4242796   1.0664342
   0.4521228  -1.0154490  -1.6202020
   1.6127305  -0.3464852  -2.2224144
atom H
      v1          v2          v3
```

```
  -0.2241375  -0.0067872   0.0311660
  -0.0624329  -0.2527946   0.0751543
   0.0504834  -0.0531544  -0.2834362
atom H
      v1          v2          v3
  -0.2506539   0.0139513   0.1089560
  -0.0737009  -0.2467215  -0.0127159
   0.0288479  -0.0251582  -0.2005664
atom N
      v1          v2          v3
  -1.3992554   0.0376533  -0.1294183
   0.0321549  -2.8101610  -0.5681892
  -0.2341932  -0.4833079  -2.4121083
atom C
      v1          v2          v3
   0.4792664  -0.1441348  -0.0587023
  -0.1760522  -1.6066877  -1.5190336
  -0.0410382  -1.5153938  -0.7881038
atom H
      v1          v2          v3
  -0.8273595   0.1287055  -0.1531101
   0.0915286  -0.6270655  -0.0131855
  -0.0978679  -0.0102846  -0.6027647
atom N
      v1          v2          v3
  -1.9146946  -0.1414992   0.0797773
  -0.0704892  -2.4548009  -0.9051994
```

```
  -0.0132962  -0.8779438  -2.0178444
atom C
      v1          v2          v3
   0.4640993  -0.2168652  -0.0425965
  -0.4040859  -1.4409043  -1.0719775
   0.2583050  -1.1389810  -0.9477678
atom H
      v1          v2          v3
  -0.2300059  -0.0244916   0.0135459
   0.0129370  -0.2631772  -0.0081264
  -0.0167097   0.0143539  -0.2538461

ala dipeptide
atom N
      v1          v2          v3
  -1.1531950   0.0220898   0.3371764
  -0.0019581  -0.5150832  -0.7865190
   0.1589676  -0.7189022  -2.0189099
atom H
      v1          v2          v3
   0.0006852  -0.0773141   0.0330352
  -0.1357477  -0.2176533  -0.0144256
   0.0506399  -0.0304932  -0.2896917
atom C
      v1          v2          v3
  -0.6042111   0.1069474  -0.0039184
   0.0570377  -0.6075051  -0.3320856
```

```
  -0.0209214  -0.3938667  -0.1581357
atom H
      v1          v2          v3
  -0.3220746   0.0013388  -0.0021227
  -0.1144612  -0.6401151  -0.0999477
   0.0863740   0.0033412  -0.6793350
atom C
      v1          v2          v3
  -0.4536674   0.0897990  -0.0071760
   0.0801299  -0.8476843  -0.4720626
   0.0512340  -0.3104603  -0.8309582
atom C
      v1          v2          v3
   0.2834490  -0.2436776  -0.6037400
  -0.0314713   0.0881364  -1.0548356
  -0.5417489  -1.1697614  -1.5915429
atom H
      v1          v2          v3
  -0.3987843   0.0078585  -0.0364021
   0.0107230  -0.4658779  -0.0190014
  -0.0240999   0.0143172  -0.6990261
atom H
      v1          v2          v3
  -0.5569819  -0.1587796   0.0358683
  -0.2447128  -0.6471812   0.0043174
  -0.0141103  -0.0449514  -0.4973665
atom H
```

```
      v1          v2          v3
  -0.4326415   0.1024527   0.0383470
   0.1449531  -0.5310790  -0.0075534
   0.1151891  -0.0511894  -0.4246429
atom O
      v1          v2          v3
  -2.2625743   0.1115846  -0.1253914
  -0.2553425  -1.5273790  -0.3933502
   0.0943755  -0.4038597  -2.0618113
atom C
      v1          v2          v3
   0.3352161   0.2251102   0.4160930
  -0.1368445   0.1199509  -0.9943680
   0.5643992  -0.9221643  -1.3719280
atom O
      v1          v2          v3
  -2.2419182  -0.1668771   0.1032242
   0.0925507  -1.4562477  -0.4097719
  -0.0736943  -0.4706600  -2.1757068
atom C
      v1          v2          v3
  -1.1857018  -0.7207689   0.2961760
  -0.6439363  -1.2642684  -0.0252967
   0.2519086  -0.0288822  -0.9068514
atom H
      v1          v2          v3
  -0.5141719  -0.0726246   0.0125435
```

```
   0.0079653  -0.6548859   0.1165582
  -0.0272364   0.0984399  -0.4776816
atom H
      v1          v2          v3
  -0.6417544   0.0229630   0.0629820
  -0.0331326  -0.5067033  -0.0713533
   0.0868141  -0.0808375  -0.4738614
atom H
      v1          v2          v3
  -0.5708866  -0.0632552  -0.0538379
  -0.1092879  -0.4390476  -0.0561805
  -0.0386424  -0.0211443  -0.6089231
atom N
      v1          v2          v3
  -1.0413045  -0.5721377   0.1179162
  -0.0306738  -0.5128480  -0.8342259
  -0.1554238  -0.7618090  -1.7645766
atom C
      v1          v2          v3
  -0.9003596   0.5114560  -0.1437038
   0.3034753  -0.5019190   0.0914436
  -0.0016961   0.0356015  -0.2501868
atom H
      v1          v2          v3
  -0.2747624  -0.0030224  -0.0009013
  -0.1634373  -0.1869744   0.0028461
   0.0627569  -0.0202253  -0.2579971
```

```
atom H
      v1          v2          v3
  -0.3589386   0.1011523  -0.0666592
   0.1152436  -0.5061890   0.0025768
  -0.0725846   0.0076470  -0.4413413
atom H
      v1          v2          v3
  -0.7506754  -0.0990219  -0.0577206
  -0.0563135  -0.5448489  -0.0869139
  -0.0477228  -0.1147085  -0.5610445
atom H
      v1          v2          v3
  -0.6757912   0.0169387   0.1128688
   0.0254974  -0.4592872  -0.0763609
   0.0821736  -0.0377088  -0.7146431


ammonia
atom N
      v1          v2          v3
  -0.7504792   0.0000000   0.0000431
   0.0000000  -0.7505049   0.0000000
   0.0000127   0.0000000  -1.5903887
atom H
      v1          v2          v3
  -0.2798696   0.0000000   0.0785364
   0.0000000  -0.2329101   0.0000000
  -0.1103384   0.0000000  -0.2683532
```

```
atom H
      v1          v2          v3
  -0.2446459  -0.0203305  -0.0392690
  -0.0203255  -0.2681237  -0.0680134
   0.0551633   0.0955468  -0.2683556
atom H
      v1          v2          v3
  -0.2446459   0.0203305  -0.0392690
   0.0203255  -0.2681237   0.0680134
   0.0551633  -0.0955468  -0.2683556


benzene
atom C
      v1          v2          v3
  -0.3261430   0.4555814  -0.0019792
   0.4559179   0.2010876  -0.0011781
   0.0001256  -0.0017521  -3.0017797
atom C
      v1          v2          v3
  -0.3264592  -0.4551742   0.0020575
  -0.4553424   0.2010556  -0.0026387
   0.0026186  -0.0046214  -3.0017864
atom C
      v1          v2          v3
   0.4635420  -0.0003394   0.0026814
   0.0005126  -0.5891846   0.0005223
   0.0015990  -0.0013427  -3.0023840
```

```
atom C
      v1          v2          v3
  -0.3251637   0.4565333   0.0003192
   0.4558382   0.1999260  -0.0012028
   0.0014274  -0.0006969  -3.0023618
atom C
      v1          v2          v3
  -0.3251329  -0.4562768   0.0010616
  -0.4560689   0.1997107  -0.0030459
   0.0009428  -0.0023447  -3.0020614
atom C
      v1          v2          v3
   0.4635867  -0.0003156   0.0003713
  -0.0008583  -0.5891170  -0.0004149
   0.0012617  -0.0016237  -3.0019962
atom H
      v1          v2          v3
  -0.6191717  -0.2068781   0.0000351
  -0.2066217  -0.8579175   0.0001467
   0.0001695   0.0000713  -0.4959319
atom H
      v1          v2          v3
  -0.6190983   0.2069075  -0.0000894
   0.2066412  -0.8579831   0.0001644
  -0.0003793   0.0006461  -0.4958685
atom H
      v1          v2          v3
```

```
  -0.9773720   0.0000894  -0.0002649
   0.0001913  -0.4998390   0.0000046
  -0.0001897  -0.0000494  -0.4957808
atom H
      v1          v2          v3
  -0.6191573  -0.2065949   0.0000617
  -0.2068128  -0.8579491   0.0000345
  -0.0000319  -0.0000176  -0.4957521
atom H
      v1          v2          v3
  -0.6192783   0.2066736  -0.0001551
   0.2069993  -0.8580236   0.0001926
  -0.0001564   0.0004000  -0.4958078
atom H
      v1          v2          v3
  -0.9773471   0.0001444  -0.0000024
  -0.0001095  -0.4997644  -0.0000316
  -0.0001538   0.0000131  -0.4958867


dodecahexene
atom C
      v1          v2          v3
  -0.0592488  -0.7985771  -0.0000001
   0.6293679   0.1199170   0.0000000
   0.0000000   0.0000000  -3.4837955
atom H
      v1          v2          v3
```

```
  -0.7051483   0.8156963   0.0000000
   0.0551868  -0.8436946   0.0000000
   0.0000000   0.0000000  -0.3994628
atom H
      v1          v2          v3
  -0.5865379  -0.4540568   0.0000000
  -0.0489167  -1.3181695   0.0000000
   0.0000000   0.0000000  -0.4235359
atom C
      v1          v2          v3
   0.1326120  -0.8233325  -0.0000001
  -0.2653269  -0.1553052  -0.0000001
   0.0000000   0.0000000  -2.8967208
atom H
      v1          v2          v3
  -0.7455702  -0.1909998   0.0000000
  -0.0403430  -0.4749396   0.0000000
   0.0000000   0.0000000  -0.4583720
atom C
      v1          v2          v3
   0.0342760  -2.2757167  -0.0000001
   0.0658486   0.0755267   0.0000001
   0.0000000   0.0000000  -3.0201516
atom H
      v1          v2          v3
  -0.7120615   0.8377642   0.0000000
  -0.0054014  -0.4594068   0.0000000
```

```
   0.0000000   0.0000000  -0.4358105
atom C
      v1          v2          v3
   0.0025648  -1.6151966  -0.0000001
   0.0082422   0.0526797   0.0000001
   0.0000000   0.0000000  -2.9738626
atom H
      v1          v2          v3
  -0.7121530   0.1538071   0.0000000
  -0.0039680  -0.3753197   0.0000000
   0.0000000   0.0000000  -0.4380521
atom C
      v1          v2          v3
  -0.0152142  -2.1459873  -0.0000001
   0.0175463  -0.0065948   0.0000000
   0.0000000   0.0000000  -2.9744237
atom H
      v1          v2          v3
  -0.6968752   0.6180483   0.0000000
  -0.0011210  -0.4119762   0.0000000
   0.0000000   0.0000000  -0.4367485
atom C
      v1          v2          v3
  -0.0182066  -1.9267068   0.0000000
   0.0149777   0.0090277   0.0000001
   0.0000000   0.0000000  -2.9701222
atom H
```

```
      v1          v2          v3
  -0.6995008   0.3922661   0.0000000
  -0.0016579  -0.3859908   0.0000000
   0.0000000   0.0000000  -0.4360730
atom C
      v1          v2          v3
  -0.0182066  -1.9267068   0.0000000
   0.0149777   0.0090278  -0.0000001
   0.0000000   0.0000000  -2.9701222
atom H
      v1          v2          v3
  -0.6995008   0.3922661   0.0000000
  -0.0016579  -0.3859908   0.0000000
   0.0000000   0.0000000  -0.4360730
atom C
      v1          v2          v3
  -0.0152143  -2.1459875   0.0000001
   0.0175463  -0.0065948   0.0000000
   0.0000000   0.0000000  -2.9744237
atom H
      v1          v2          v3
  -0.6968752   0.6180484   0.0000000
  -0.0011210  -0.4119762   0.0000000
   0.0000000   0.0000000  -0.4367485
atom C
      v1          v2          v3
   0.0025648  -1.6151967   0.0000001
```

```
   0.0082423   0.0526799  -0.0000001
   0.0000000   0.0000000  -2.9738626
atom H
      v1          v2          v3
  -0.7121529   0.1538071   0.0000000
  -0.0039680  -0.3753197   0.0000000
   0.0000000   0.0000000  -0.4380521
atom C
      v1          v2          v3
   0.0342760  -2.2757169   0.0000001
   0.0658487   0.0755268  -0.0000001
   0.0000000   0.0000000  -3.0201516
atom H
      v1          v2          v3
  -0.7120614   0.8377642   0.0000000
  -0.0054014  -0.4594068   0.0000000
   0.0000000   0.0000000  -0.4358105
atom C
      v1          v2          v3
   0.1326120  -0.8233326   0.0000001
  -0.2653269  -0.1553052   0.0000001
   0.0000000   0.0000000  -2.8967208
atom H
      v1          v2          v3
  -0.7455702  -0.1909998   0.0000000
  -0.0403430  -0.4749396   0.0000000
   0.0000000   0.0000000  -0.4583720
```

```
atom C
      v1          v2          v3
  -0.0592488  -0.7985772   0.0000001
   0.6293679   0.1199170   0.0000000
   0.0000000   0.0000000  -3.4837955
atom H
      v1          v2          v3
  -0.7051483   0.8156963   0.0000000
   0.0551868  -0.8436946   0.0000000
   0.0000000   0.0000000  -0.3994628
atom H
      v1          v2          v3
  -0.5865379  -0.4540568   0.0000000
  -0.0489167  -1.3181695   0.0000000
   0.0000000   0.0000000  -0.4235359


ethanol
atom C
      v1          v2          v3
  -0.9934320   0.5964475  -0.0000262
   0.3106359  -0.6803925   0.0000336
  -0.0001060  -0.0000041  -0.4901134
atom H
      v1          v2          v3
  -0.4885565   0.1141941  -0.0429643
   0.0583684  -0.5520594   0.1639591
   0.0181959   0.1189422  -0.6377811
```

```
atom H
      v1          v2          v3
  -0.6824808  -0.1666219   0.0000232
  -0.0914902  -0.6335277   0.0000271
   0.0000089   0.0000383  -0.4497592
atom H
      v1          v2          v3
  -0.4885325   0.1142153   0.0429717
   0.0583607  -0.5520980  -0.1639482
  -0.0182366  -0.1189430  -0.6377009
atom C
      v1          v2          v3
  -0.6878984   0.2704365  -0.0000459
  -0.0305659   0.0569857   0.0000915
  -0.0002806   0.0000101   0.1610352
atom H
      v1          v2          v3
  -0.6160479   0.1167121   0.0605116
  -0.0026099  -0.7254584  -0.2068020
  -0.0189487  -0.1554415  -0.8020646
atom H
      v1          v2          v3
  -0.6161811   0.1167550  -0.0605429
  -0.0027142  -0.7255049   0.2068525
   0.0190068   0.1555165  -0.8021036
atom O
      v1          v2          v3
```

```
  -0.5978902  -0.6736576  -0.0009457
  -0.9713786  -1.4387588   0.0008958
  -0.0015286   0.0005904  -1.7901578
atom H
      v1          v2          v3
  -0.1785046  -0.1366415  -0.0000957
  -0.0577066  -0.2175625   0.0000886
  -0.0001617   0.0001507  -0.2111119

formamide
atom C
      v1          v2          v3
   0.7625248  -0.3156267   0.0000000
  -0.3238891   0.4282926   0.0000000
   0.0000000   0.0000000  -2.7764171
atom H
      v1          v2          v3
  -0.7870110  -0.0687880   0.0000000
   0.1385660  -0.5328235   0.0000000
   0.0000000   0.0000000  -0.7064032
atom O
      v1          v2          v3
  -1.3219010   0.1298099   0.0000000
  -0.2274134  -1.9580411   0.0000000
   0.0000000   0.0000000  -2.6391493
atom N
      v1          v2          v3
```

```
  -0.4448007  -0.6931846   0.0000000
  -0.8521426  -0.4947278   0.0000000
   0.0000000   0.0000000  -3.0723831
atom H
      v1          v2          v3
  -0.2422073  -0.0352536   0.0000000
   0.0047786  -0.2761542   0.0000000
   0.0000000   0.0000000  -0.2369366
atom H
      v1          v2          v3
  -0.2686623   0.0157427   0.0000000
  -0.0179312  -0.2704416   0.0000000
   0.0000000   0.0000000  -0.2413642

formic acid
atom C
      v1          v2          v3
   0.7057304  -0.1864738   0.0000001
  -0.4190412   0.4879185   0.0000000
   0.0000000   0.0000000  -3.0199824
atom O
      v1          v2          v3
  -0.0719276   0.3291280  -0.0000001
  -0.2313009  -1.8905272   0.0000002
   0.0000000   0.0000000  -2.2790971
atom O
      v1          v2          v3
```

```
  -1.8683403  -0.4413852   0.0000001
  -0.1971065  -1.3787412  -0.0000001
   0.0000000   0.0000000  -2.6110372
atom H
      v1          v2          v3
  -0.5975976   0.1461551  -0.0000001
   0.0324567  -0.6199021   0.0000000
   0.0000000   0.0000000  -0.6959858
atom H
      v1          v2          v3
  -0.1347217  -0.1323269   0.0000000
   0.0164738  -0.1810925   0.0000000
   0.0000000   0.0000000  -0.2335619

indole
atom C
      v1          v2          v3
  -1.0757244  -0.4002163   0.0000001
  -0.3093439   0.3344652  -0.0000001
   0.0000000   0.0000000  -3.4182537
atom C
      v1          v2          v3
   0.4476992   0.1726081   0.0000000
   0.6805337  -0.3444066  -0.0000002
   0.0000000   0.0000000  -3.0984392
atom C
      v1          v2          v3
```

```
   0.0098750   0.0919420   0.0000000
  -0.0732785  -0.3196276  -0.0000002
   0.0000000   0.0000000  -2.5930876
atom H
      v1          v2          v3
  -0.9919264  -0.0508218   0.0000000
  -0.0073660  -0.5497747   0.0000000
   0.0000000   0.0000000  -0.5318904
atom N
      v1          v2          v3
  -0.5411446   0.2762591   0.0000000
   0.0868033   0.0509203   0.0000000
   0.0000000   0.0000000  -2.4558887
atom C
      v1          v2          v3
   0.0332782  -0.1042581   0.0000000
   0.1044595  -0.3067755  -0.0000001
   0.0000000   0.0000000  -2.5146189
atom C
      v1          v2          v3
  -0.5772248  -0.2270594   0.0000000
   0.0648678   0.5325647  -0.0000001
   0.0000000   0.0000000  -3.0375586
atom H
      v1          v2          v3
  -0.2720134   0.0096547   0.0000000
  -0.0389826  -0.2414816   0.0000000
```

```
   0.0000000   0.0000000  -0.2843844
atom C
      v1          v2          v3
  -0.5882442   0.2625779   0.0000000
   0.1241939   0.3448471   0.0000000
   0.0000000   0.0000000  -3.2416983
atom C
      v1          v2          v3
   0.1343727   0.4013176   0.0000001
   0.3686318  -0.4852394  -0.0000001
   0.0000000   0.0000000  -3.0194334
atom H
      v1          v2          v3
  -0.5188008  -0.0752729   0.0000000
  -0.1137913  -0.9802395   0.0000000
   0.0000000   0.0000000  -0.4899280
atom H
      v1          v2          v3
  -0.4957600   0.0223145   0.0000000
   0.0594563  -0.9705218   0.0000000
   0.0000000   0.0000000  -0.4730490
atom C
      v1          v2          v3
   0.1766096  -0.4029834   0.0000000
  -0.4332830  -0.3619180   0.0000000
   0.0000000   0.0000000  -2.9303153
atom H
```

```
      v1          v2          v3
  -0.9089179  -0.1631086   0.0000000
  -0.2536778  -0.5732046   0.0000000
   0.0000000   0.0000000  -0.4892152
atom H
      v1          v2          v3
  -0.9221709   0.1751435   0.0000000
   0.2791429  -0.5995877   0.0000000
   0.0000000   0.0000000  -0.4968527
atom H
      v1          v2          v3
  -0.6436717   0.1869761   0.0000000
   0.1377775  -0.7804097   0.0000000
   0.0000000   0.0000000  -0.4676665

methanal
atom C
      v1          v2          v3
   0.6868329   0.0001863   0.0000000
   0.0001527   0.5005146   0.0000001
   0.0000000   0.0000000  -3.2878282
atom H
      v1          v2          v3
  -1.0091540   0.3069968   0.0000000
   0.1365780  -0.7980365   0.0000000
   0.0000000   0.0000000  -0.5094599
atom H
```

```
      v1          v2          v3
  -1.0091804  -0.3070228   0.0000000
  -0.1365972  -0.7981388   0.0000000
   0.0000000   0.0000000  -0.5094465
atom O
      v1          v2          v3
  -1.7561311  -0.0000191   0.0000000
   0.0000324  -1.0456250   0.0000001
   0.0000000   0.0000000  -2.4558877

methane
atom C
      v1          v2          v3
  -0.7606964   0.0000000   0.0000000
   0.0000000  -0.7606964   0.0000000
   0.0000000   0.0000000  -0.7606964
atom H
      v1          v2          v3
  -0.5296715  -0.1194060  -0.1194060
  -0.1194060  -0.5296715  -0.1194060
  -0.1194060  -0.1194060  -0.5296715
atom H
      v1          v2          v3
  -0.5296715  -0.1194060   0.1194060
  -0.1194060  -0.5296715   0.1194060
   0.1194060   0.1194060  -0.5296715
atom H
```

```
      v1          v2          v3
  -0.5296715   0.1194060  -0.1194060
   0.1194060  -0.5296715   0.1194060
  -0.1194060   0.1194060  -0.5296715
atom H
      v1          v2          v3
  -0.5296715   0.1194060   0.1194060
   0.1194060  -0.5296715  -0.1194060
   0.1194060  -0.1194060  -0.5296715

methanol
atom C
      v1          v2          v3
  -0.3939812  -0.2551662  -0.0000001
   0.0213391  -0.0759758  -0.0000015
  -0.0000006  -0.0000016  -0.1489313
atom H
      v1          v2          v3
  -0.4598367  -0.1405109  -0.0000001
  -0.0775538  -0.7113364   0.0000000
  -0.0000004   0.0000000  -0.5005198
atom H
      v1          v2          v3
  -0.5397625   0.0662841   0.1053318
   0.1020467  -0.6066487  -0.1451177
   0.1051514  -0.1760383  -0.8147127
atom H
```

```
      v1          v2          v3
  -0.5397628   0.0662839  -0.1053320
   0.1020461  -0.6066489   0.1451174
  -0.1051514   0.1760379  -0.8147128
atom O
      v1          v2          v3
  -1.7785099   0.3126090   0.0000007
   0.7819634  -0.3229474  -0.0000006
  -0.0000001  -0.0000002  -1.8734590
atom H
      v1          v2          v3
  -0.3108370   0.0440295   0.0000001
   0.0342318  -0.0756808  -0.0000001
   0.0000000   0.0000000  -0.2099355

methyl ether
atom C
      v1          v2          v3
  -0.4397525   0.1175586  -0.0000021
   0.0951992  -0.1379864  -0.0000233
   0.0000094  -0.0000136  -0.1748961
atom H
      v1          v2          v3
  -0.6097519  -0.2009660   0.0000173
  -0.1352294  -0.5687755   0.0000177
   0.0000106   0.0000194  -0.4912609
atom H
```

```
      v1          v2          v3
  -0.4944155  -0.0209379   0.0053370
   0.0941765  -0.6297882  -0.1968057
   0.0710159  -0.2087855  -0.8091984
atom H
      v1          v2          v3
  -0.4944466  -0.0209349  -0.0053657
   0.0941728  -0.6297402   0.1967846
  -0.0710584   0.2087645  -0.8092516
atom O
      v1          v2          v3
  -1.5138264   0.0000005  -0.0000105
   0.0000000  -1.3095459  -0.0000083
   0.0000054  -0.0000164  -1.4919609
atom C
      v1          v2          v3
  -0.4397530  -0.1175585  -0.0000150
  -0.0951998  -0.1379881   0.0000060
  -0.0000036   0.0000030  -0.1748959
atom H
      v1          v2          v3
  -0.4944284   0.0209331   0.0053532
  -0.0941779  -0.6297630   0.1967946
   0.0710376   0.2087764  -0.8092251
atom H
      v1          v2          v3
  -0.6097520   0.2009660   0.0000011
```

```
   0.1352296  -0.5687754   0.0000008
  -0.0000013   0.0000001  -0.4912607
atom H
      v1          v2          v3
  -0.4944333   0.0209398  -0.0053493
  -0.0941715  -0.6297649  -0.1967950
  -0.0710364  -0.2087728  -0.8092238

mNA
atom C
      v1          v2          v3
  -0.5878961  -0.3427614   0.0070704
  -0.1579832   0.2623399   0.0505274
  -0.0110286   0.0162238  -2.7608197
atom C
      v1          v2          v3
  -0.4209692   0.7987657   0.0642919
  -0.0108582   0.0385690   0.1031180
  -0.0248588   0.0403339  -3.3081118
atom C
      v1          v2          v3
   0.1779713  -0.4656779  -0.1807375
  -0.3812486   0.1749158   0.1839345
   0.0454072  -0.0303533  -2.1959685
atom C
      v1          v2          v3
   0.3301796   0.3646035  -0.0833635
```

```
   0.3038803  -0.7271160  -0.0590351
  -0.0422163   0.0150575  -3.2487574
atom C
      v1          v2          v3
  -0.4564423   0.2816834  -0.0212418
   0.1952750   0.3506259   0.0144604
  -0.0057136   0.0243885  -2.8172292
atom C
      v1          v2          v3
  -0.0304223  -0.8211261  -0.0085671
  -0.0511432  -0.5275009   0.0152405
   0.0019383   0.0096024  -3.1169637
atom H
      v1          v2          v3
  -0.2037651   0.0609877  -0.0024582
   0.0055942  -0.6738360  -0.0106483
  -0.0002805  -0.0002713  -0.4308453
atom H
      v1          v2          v3
  -0.8840038  -0.1971469   0.0086578
  -0.1736455  -0.5333334   0.0080967
  -0.0015436  -0.0014661  -0.4542345
atom H
      v1          v2          v3
  -0.4922306  -0.0961057  -0.0037352
  -0.1040098  -0.8591020  -0.0002533
  -0.0003995  -0.0038927  -0.4966031
```

```
atom H
      v1          v2          v3
  -0.3376810   0.1999207  -0.0071985
   0.2061159  -0.6413286  -0.0094600
   0.0005429  -0.0009547  -0.4596046
atom N
      v1          v2          v3
   0.4120033  -0.0948033  -0.0589240
  -0.1163000   0.9206591   0.1032047
  -0.0079677  -0.0079536  -1.8344499
atom N
      v1          v2          v3
  -1.2289820   1.0594192   0.3334494
   1.0924286  -0.9501268  -0.2546589
   1.7578688  -1.3812122  -2.1879669
atom O
      v1          v2          v3
  -1.8640577   0.2208319  -0.0983103
  -0.4386099  -1.4860105   0.0821401
  -0.0002315  -0.0006195  -2.1702387
atom O
      v1          v2          v3
  -1.8961303  -0.3018103   0.0079881
   0.1079258  -1.1240404   0.0330689
  -0.0006778  -0.0026196  -2.1660386
atom H
      v1          v2          v3
```

```
  -0.2760541   0.0646931  -0.0166808
   0.0641427  -0.2760450  -0.0813988
  -0.0104652   0.0424623  -0.2563581
atom H
      v1          v2          v3
  -0.3004540   0.0535138   0.0807618
   0.0688060  -0.2516556   0.0205667
  -0.0456990   0.0096654  -0.2585732

neopentane
atom C
      v1          v2          v3
  -0.3685463   0.0000021   0.0000000
  -0.0000782  -0.3683128   0.0000000
   0.0000000   0.0000000  -0.3686156
atom C
      v1          v2          v3
  -0.4850946   0.2208019   0.0000000
   0.2214692  -1.0322129   0.0000000
   0.0000000   0.0000000  -0.4068986
atom C
      v1          v2          v3
  -1.1052741  -0.0005360   0.0000000
  -0.0002102  -0.4075686   0.0000000
   0.0000000   0.0000000  -0.4070112
atom C
      v1          v2          v3
```

```
  -0.4855135  -0.1099931  -0.1902966
  -0.1103326  -0.5621969  -0.2694254
  -0.1906188  -0.2695283  -0.8738739
atom C
      v1          v2          v3
  -0.4855135  -0.1099931   0.1902966
  -0.1103326  -0.5621969   0.2694253
   0.1906188   0.2695283  -0.8738739
atom H
      v1          v2          v3
  -0.7740279   0.0513560   0.0000000
   0.1198674  -0.5128784   0.0000000
   0.0000000   0.0000000  -0.4054088
atom H
      v1          v2          v3
  -0.4433135  -0.0033285   0.0638537
  -0.0375666  -0.6293831   0.1906693
   0.0836333   0.1346017  -0.6197671
atom H
      v1          v2          v3
  -0.4433135  -0.0033285  -0.0638537
  -0.0375666  -0.6293831  -0.1906693
  -0.0836333  -0.1346017  -0.6197671
atom H
      v1          v2          v3
  -0.5959339   0.1830324   0.0000000
   0.1143709  -0.6915039   0.0000000
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   0.0000000   0.0000000  -0.4053469
atom H
      v1          v2          v3
  -0.5957922  -0.0915435  -0.1584653
  -0.0572027  -0.4769435  -0.1239066
  -0.0990358  -0.1239450  -0.6200586
atom H
      v1          v2          v3
  -0.5957922  -0.0915435   0.1584653
  -0.0572027  -0.4769435   0.1239066
   0.0990358   0.1239450  -0.6200586
atom H
      v1          v2          v3
  -0.4434179  -0.0537216   0.0351697
  -0.0537960  -0.4812756   0.0490265
   0.0749076   0.1049876  -0.7678999
atom H
      v1          v2          v3
  -0.7743249  -0.0252005  -0.0446274
  -0.0596219  -0.4319981  -0.0465509
  -0.1040286  -0.0464614  -0.4860850
atom H
      v1          v2          v3
  -0.4432888   0.0567181  -0.0292231
   0.0908940  -0.7633245  -0.0571493
  -0.0095316  -0.1133199  -0.4859907
atom H
```

```
      v1          v2          v3
  -0.4434179  -0.0537216  -0.0351697
  -0.0537960  -0.4812756  -0.0490265
  -0.0749076  -0.1049876  -0.7678999
atom H
      v1          v2          v3
  -0.4432888   0.0567181   0.0292230
   0.0908940  -0.7633245   0.0571494
   0.0095316   0.1133199  -0.4859907
atom H
      v1          v2          v3
  -0.7743249  -0.0252005   0.0446274
  -0.0596219  -0.4319981   0.0465509
   0.1040286   0.0464614  -0.4860850

pNA
atom C
      v1          v2          v3
  -0.7852878   0.5895783  -0.0121810
   0.7261700  -0.0342528  -0.0959464
  -0.0489802  -0.0073232  -3.2969274
atom C
      v1          v2          v3
   0.8244713   0.0000871  -0.2218750
  -0.0000770  -0.0822032  -0.0000663
   0.0434841  -0.0000625  -2.1741817
atom C
```

```
      v1          v2          v3
  -0.7849038  -0.5894752  -0.0120573
  -0.7261432  -0.0342872   0.0957873
  -0.0490395   0.0073242  -3.2969060
atom C
      v1          v2          v3
   0.3317436   0.5741726  -0.0169794
  -0.2122209   0.0593672   0.0103951
  -0.0171863  -0.0044495  -2.8184487
atom C
      v1          v2          v3
  -1.0070584   0.0001559  -0.0004757
   0.0002977  -0.1115539   0.0000946
   0.0038882   0.0000258  -3.0786341
atom C
      v1          v2          v3
   0.3316152  -0.5737051  -0.0171712
   0.2123687   0.0598105  -0.0103225
  -0.0172524   0.0045022  -2.8184596
atom H
      v1          v2          v3
  -0.5399596  -0.1592085   0.0000730
  -0.1979045  -0.7913976   0.0113939
  -0.0035196  -0.0010077  -0.4515624
atom H
      v1          v2          v3
  -0.5399226   0.1591302   0.0000577
```

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   0.1979273  -0.7914217  -0.0113741
  -0.0035359   0.0010154  -0.4515675
atom H
      v1          v2          v3
  -0.1820085  -0.0358651  -0.0033873
  -0.1245994  -0.7023299   0.0009525
   0.0015385   0.0005252  -0.4784755
atom H
      v1          v2          v3
  -0.1823642   0.0358513  -0.0034288
   0.1244065  -0.7023103  -0.0009836
   0.0015361  -0.0005365  -0.4784708
atom N
      v1          v2          v3
  -2.2163719  -0.0000712   0.3912763
   0.0000026   0.0482039   0.0000536
   2.2658329  -0.0001141  -2.3757073
atom H
      v1          v2          v3
  -0.3521522  -0.0082129   0.0393171
  -0.0191707  -0.2117556   0.0628752
  -0.0591238  -0.0183683  -0.2547445
atom H
      v1          v2          v3
  -0.3521482   0.0081839   0.0393005
   0.0192123  -0.2116875  -0.0628736
  -0.0591096   0.0183488  -0.2547434
```

```
atom N
      v1          v2          v3
   0.5301672  -0.0004516  -0.0107681
   0.0017070   1.3352426   0.0003453
  -0.0081292   0.0000802  -1.7986905
atom O
      v1          v2          v3
  -1.9841765   0.0067786  -0.0025616
  -0.1617140  -1.0734985   0.0001737
  -0.0000396   0.0000770  -2.1782327
atom O
      v1          v2          v3
  -1.9827962  -0.0074158  -0.0023579
   0.1637613  -1.0742059   0.0001842
  -0.0000318  -0.0000236  -2.1782265


thymine
atom N
      v1          v2          v3
  -0.2375400   0.5494737  -0.9193050
  -0.0123591  -1.9483788  -0.9108052
  -0.1178844  -0.9222372  -1.7714308
atom C
      v1          v2          v3
   0.5252991  -0.0773412  -0.3813346
  -0.1467767  -1.5241090  -1.4434956
  -0.3328247  -1.4903307  -1.1052357
```

```
atom H
      v1          v2          v3
  -0.7827293  -0.0159548   0.0521281
   0.1140899  -0.4874883  -0.0537869
  -0.0836965  -0.0319652  -0.4755524
atom C
      v1          v2          v3
  -1.0800032  -0.1607748  -0.1425105
   0.0739944  -1.6346286  -1.4199328
  -0.3779449  -1.4330107  -1.2007801
atom C
      v1          v2          v3
  -0.1687116   0.1521563  -0.2268859
  -0.1637441  -1.1207958   0.6043085
   0.1110756   0.5394299  -1.2012485
atom H
      v1          v2          v3
  -0.3613145   0.0234785   0.0217701
  -0.0305208  -0.6039648   0.0615796
   0.0739786  -0.0109949  -0.7033955
atom H
      v1          v2          v3
  -0.3890676  -0.0739539  -0.0528853
  -0.1449667  -0.6371598   0.0236943
   0.0193074   0.0896968  -0.5951065
atom H
      v1          v2          v3
```

```
  -0.6475179   0.0736271  -0.0243121
   0.1203212  -0.5616516   0.0894805
  -0.0740479   0.1124644  -0.5454462
atom C
      v1          v2          v3
   0.5797149  -0.2306882  -0.1583796
   0.0339864  -1.1631990  -1.1537461
  -0.5602424  -1.1554632  -0.7463966
atom O
      v1          v2          v3
  -1.7542815   0.0716505  -0.0613082
   0.1385938  -2.1914733  -0.4000239
  -0.3146469  -0.4404155  -2.0530199
atom N
      v1          v2          v3
  -0.1861247  -0.6723471   0.2458863
  -0.6595277  -1.9538741  -1.0674575
   0.1091562  -0.9478245  -1.9055316
atom H
      v1          v2          v3
  -0.2278718   0.0135404  -0.0178598
   0.0363100  -0.2199793  -0.0449999
  -0.0391157  -0.0390474  -0.2043565
atom C
      v1          v2          v3
  -0.0605850  -0.2544561   0.0194748
  -0.1494353  -0.5269580  -1.6705614
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  -0.1249271  -1.5716560  -0.2722819
atom O
      v1          v2          v3
  -1.9952043  -0.0264576  -0.0721446
  -0.0999438  -2.2300514  -0.5671693
  -0.0016438  -0.5305117  -2.1137176
atom H
      v1          v2          v3
  -0.1443628   0.0338938  -0.0533539
  -0.0488832  -0.2474265  -0.0109870
   0.0337417  -0.0161359  -0.2428430

uracil
atom N
      v1          v2          v3
  -2.7153069  -0.3510627  -0.1352221
  -0.4305687  -0.0282316  -0.4662412
  -0.3780478   0.3819299  -1.2128114
atom C
      v1          v2          v3
  -2.4619570  -0.7685600  -0.3908359
  -0.8287393   0.4230222   0.2221700
  -0.2051004  -0.1259027   0.1529999
atom H
      v1          v2          v3
  -0.5552888   0.0567770   0.0274960
   0.0183722  -0.6126771  -0.0846078
```

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   0.0615871  -0.2025399  -0.6184461
atom C
      v1          v2          v3
  -3.6281939  -0.5499822  -0.2625024
  -0.5851197  -1.4698827  -0.5941246
  -0.1647911  -1.0284257  -0.1594806
atom H
      v1          v2          v3
  -0.4237899  -0.0024380   0.0219497
   0.0036237  -0.4683989   0.0464931
   0.0023292   0.1588890  -0.6760367
atom C
      v1          v2          v3
  -1.7754704  -0.9150820  -0.2151053
  -0.9911041   0.6394519  -0.1175074
  -0.1251841  -0.2236992   0.0264742
atom O
      v1          v2          v3
  -2.5750770  -0.3434712  -0.0586571
  -0.3070157  -1.6167587  -0.0868532
  -0.0029177  -0.2494304  -1.9276638
atom N
      v1          v2          v3
  -2.6576154  -0.7536020  -0.6674022
  -0.6914951  -1.0665680   0.4780825
  -0.6054464   0.5032073  -0.4553523
atom H
```

```
      v1          v2          v3
  -0.2356406  -0.0158762   0.0071012
  -0.0500750  -0.1635739  -0.0411815
  -0.0294644  -0.0425573  -0.2139297
atom C
      v1          v2          v3
  -1.8809433  -0.4041455  -0.4010490
  -0.3915894   0.0694848  -0.4385627
  -0.4363576  -0.5322807   0.8032767
atom O
      v1          v2          v3
  -2.6809266  -0.1630570  -0.1312088
  -0.1807169  -1.9313465  -0.2266208
  -0.0816929  -0.1867116  -1.6978637
atom H
      v1          v2          v3
  -0.2598922  -0.0328926  -0.0092164
   0.0360011  -0.1941970  -0.0097028
  -0.0259048   0.0771380  -0.2049679


val dipeptide
atom N
      v1          v2          v3
  -1.1130550   0.2362157   0.0392677
   0.1966503  -1.7722501  -0.8702194
   0.0976382  -0.9658576  -0.6476496
atom H
```

```
      v1          v2          v3
  -0.0488399  -0.0470546   0.0375299
  -0.0587386  -0.2241103  -0.0081240
   0.0869643  -0.0885241  -0.2567515
atom C
      v1          v2          v3
  -0.6105217  -0.1151229  -0.1123570
   0.1481781  -0.7135311   0.1236088
   0.0092150  -0.0128020  -0.0275549
atom H
      v1          v2          v3
  -0.2699115   0.0098765  -0.0160384
  -0.0544812  -0.5759818  -0.0818651
   0.0914181  -0.0485491  -0.5902324
atom C
      v1          v2          v3
  -0.1946318  -0.2816823   0.0753950
  -0.1055007  -0.3692553  -0.1530868
   0.2152396   0.0013112  -0.5531250
atom C
      v1          v2          v3
  -0.0438441  -0.7749514  -0.3391142
  -0.6918519  -1.4045655  -0.7832120
  -0.4879825  -0.9521172   0.1157890
atom H
      v1          v2          v3
  -0.5059515   0.1940248   0.0417943
```

```
   0.1135757  -0.5527803   0.0284588
   0.0607998   0.0577898  -0.5024707
atom C
      v1          v2          v3
  -0.4479407  -0.0574248  -0.0631673
  -0.0943978  -0.3450296  -0.2876507
  -0.2866259  -0.1518752  -1.0703169
atom C
      v1          v2          v3
  -0.7866838  -0.2178570   0.1397264
  -0.3678557  -0.5960949   0.1866743
   0.2857095   0.1778109  -0.5217155
atom O
      v1          v2          v3
  -2.2029336   0.0330122  -0.1643162
  -0.1056019  -2.0794743  -0.2344827
   0.2322580  -0.4778911  -1.4114763
atom H
      v1          v2          v3
  -0.6143187   0.0575265  -0.0715801
   0.0164548  -0.3071842  -0.0353985
  -0.1320012   0.0077147  -0.5327521
atom H
      v1          v2          v3
  -0.4201165   0.0123085  -0.0175874
   0.0442936  -0.7621580  -0.0900803
  -0.0179051  -0.1938387  -0.5322433
```

```
atom H
      v1          v2          v3
  -0.5126588  -0.0618217   0.0766479
  -0.0426903  -0.3844192  -0.0089257
   0.1669105   0.0714246  -0.5976411
atom H
      v1          v2          v3
  -0.4731884  -0.0500743   0.0328424
  -0.0294124  -0.4516737   0.0332246
  -0.0200059  -0.0032600  -0.7612877
atom H
      v1          v2          v3
  -0.4865317  -0.0870851   0.0184821
  -0.0090114  -0.7856910  -0.0115684
   0.0533847   0.0336943  -0.4132223
atom H
      v1          v2          v3
  -0.7167392   0.0060741  -0.0176153
  -0.0996618  -0.3725579   0.0359238
   0.0155201   0.0659376  -0.4326534
atom C
      v1          v2          v3
   0.2956169   0.5991636   0.3778067
   0.1481511  -1.2247668  -1.0975889
   0.5212854  -0.9758263   0.0452551
atom O
      v1          v2          v3
```

```
  -2.2874352  -0.0811509   0.1145041
   0.0203360  -2.0862067  -0.5099642
  -0.2259531  -0.5074894  -1.4977572
atom C
      v1          v2          v3
  -1.3043423  -0.4735253   0.6521296
  -0.4666687  -1.1702542   0.1237520
   0.5295376   0.1184684  -0.8852106
atom H
      v1          v2          v3
  -0.5238709  -0.0553320   0.0802464
  -0.0289841  -0.5078278   0.1410649
  -0.0127778   0.1209065  -0.6148825
atom H
      v1          v2          v3
  -0.6469352   0.0302777   0.0090925
   0.0122831  -0.5577910  -0.0033932
   0.0716389  -0.0212597  -0.3987901
atom H
      v1          v2          v3
  -0.5794185  -0.0894698  -0.0297020
  -0.1073588  -0.5187153  -0.1230576
   0.0199222  -0.0870996  -0.5234503
atom N
      v1          v2          v3
  -1.1460635  -0.5735550   0.1834506
  -0.2237344  -1.6856985  -0.9695517
```

```
  -0.0794155  -0.6945296  -0.5865133
atom C
      v1          v2          v3
  -0.7846476   0.2808048  -0.4730298
   0.3197353  -0.4204358   0.1647032
  -0.1472497  -0.0086451  -0.1968057
atom H
      v1          v2          v3
  -0.2915498  -0.0084720  -0.0168700
  -0.0581320  -0.1934901  -0.0748975
   0.1233999  -0.0640526  -0.2045424
atom H
      v1          v2          v3
  -0.5581899   0.0013940  -0.1026894
   0.0234317  -0.5559596  -0.0516299
  -0.1621972  -0.0427038  -0.5074020
atom H
      v1          v2          v3
  -0.6377312   0.0244750   0.1825682
   0.0557518  -0.4712812  -0.0283552
   0.0920702  -0.0061409  -0.6332093
atom H
      v1          v2          v3
  -0.5055583  -0.0092566  -0.0660126
   0.0027386  -0.6880235  -0.0034615
  -0.0982969   0.0611458  -0.4233011
```

```
water
atom O
      v1          v2          v3
  -0.4797294  -0.0380068   0.0000000
  -0.0318763  -0.5245581  -0.0000001
   0.0000000   0.0000000  -2.3382428
atom H
      v1          v2          v3
  -0.1717541  -0.1223963   0.0000000
   0.0350637  -0.1019390   0.0000000
   0.0000000   0.0000000  -0.2503739
atom H
      v1          v2          v3
  -0.0885778   0.0918824   0.0000000
  -0.0656961  -0.1897621   0.0000000
   0.0000000   0.0000000  -0.2493776
```