

Electronic Supplementary Information

An Atoms-In-Molecules Description Of Bond Energy

Distributions In Polyatomic Molecules

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MP2/6-311G(d,p) // MP2/6-311G(d,p) Energies, Topological Analyses And Atoms-In-Molecules Properties Of CHN compounds (atomic units)

Carbon atom ground state energy: -37.745020
Nitrogen atom ground state energy: -54.475050
Hydrogen atom ground state energy: -0.499810

C 1N 0H 4 Methane

Molecular Kinetic Energy = 40.32985
Molecular Total Energy = -40.37923
Virial = 2.00122
Carbon basin kinetic energies: 37.8722
Carbon basin populations: 6.0169
Carbon basin dipole magnitudes: 0.0000
Hydrogen basin kinetic energies: 0.6148 0.6148 0.6148 0.6148
Hydrogen basin populations: 0.9965 0.9965 0.9965 0.9965
Hydrogen basin dipole magnitudes: 0.1527 0.1527 0.1527 0.1527

C 2N 0H 6 Ethane

Molecular Kinetic Energy = 79.48498
Molecular Total Energy = -79.57089
Virial = 2.00108
Carbon basin kinetic energies: 37.8693 37.8693
Carbon basin populations: 5.9730 5.9730
Carbon basin dipole magnitudes: 0.0506 0.0506
Hydrogen basin kinetic energies: 0.6250 0.6250 0.6250 0.6250 0.6250 0.6250
Hydrogen basin populations: 1.0099 1.0099 1.0099 1.0099 1.0099 1.0099
Hydrogen basin dipole magnitudes: 0.1572 0.1572 0.1572 0.1572 0.1572 0.1572
C-C bond CP densities: 0.2398
C-C bond laplacians: -0.558

C 2N 0H 4 Ethene

Molecular Kinetic Energy = 78.28425
Molecular Total Energy = -78.34429
Virial = 2.00077
Carbon basin kinetic energies: 37.9197 37.9197
Carbon basin populations: 6.0440 6.0440
Carbon basin dipole magnitudes: 0.0732 0.0732
Hydrogen basin kinetic energies: 0.6118 0.6118 0.6118 0.6118
Hydrogen basin populations: 0.9792 0.9792 0.9792 0.9792
Hydrogen basin dipole magnitudes: 0.1436 0.1436 0.1436 0.1436
C-C bond CP densities: 0.3354
C-C bond laplacians: -0.979

C 2N 0H 2 Ethyne

Molecular Kinetic Energy = 77.09111
Molecular Total Energy = -77.11124
Virial = 2.00026
Carbon basin kinetic energies: 37.9942 37.9942
Carbon basin populations: 6.1519 6.1519
Carbon basin dipole magnitudes: 0.1622 0.1622
Hydrogen basin kinetic energies: 0.5522 0.5522
Hydrogen basin populations: 0.8496 0.8496
Hydrogen basin dipole magnitudes: 0.1215 0.1215
C-C bond CP densities: 0.3888
C-C bond laplacians: -1.081

C 3N 0H 8 Propane

Molecular Kinetic Energy = 118.64342
Molecular Total Energy = -118.76605
Virial = 2.00103
Carbon basin kinetic energies: 37.8700 37.8866 37.8866
Carbon basin populations: 5.9392 5.9860 5.9860
Carbon basin dipole magnitudes: 0.0527 0.0456 0.0456
Hydrogen basin kinetic energies: 0.6334 0.6334 0.6224 0.6237 0.6237 0.6224
0.6237 0.6237
Hydrogen basin populations: 1.0195 1.0195 1.0076 1.0112 1.0112 1.0076
1.0112 1.0112
Hydrogen basin dipole magnitudes: 0.1609 0.1609 0.1571 0.1602 0.1602 0.1571
0.1602 0.1602
C-C bond CP densities: 0.2417 0.2417
C-C bond laplacians: -0.562 -0.562

C 3N 0H 6 Propene

Molecular Kinetic Energy = 117.44714
Molecular Total Energy = -117.54365
Virial = 2.00082
Carbon basin kinetic energies: 37.9418 37.9282 37.8889
Carbon basin populations: 6.0236 6.0556 5.9873
Carbon basin dipole magnitudes: 0.0564 0.0902 0.0773
Hydrogen basin kinetic energies: 0.6186 0.6158 0.6158 0.6177 0.6117 0.6128
Hydrogen basin populations: 0.9915 0.9928 0.9928 0.9956 0.9812 0.9868
Hydrogen basin dipole magnitudes: 0.1484 0.1545 0.1545 0.1556 0.1454 0.1480
C-C bond CP densities: 0.3349 0.2535
C-C bond laplacians: -0.970 -0.627

C 3N 0H 4 Propyne

Molecular Kinetic Energy = 116.25788
Molecular Total Energy = -116.31410
Virial = 2.00048
Carbon basin kinetic energies: 37.8453 38.0743 37.9731
Carbon basin populations: 5.9321 6.1827 6.1451
Carbon basin dipole magnitudes: 0.2119 0.0098 0.2239
Hydrogen basin kinetic energies: 0.6044 0.6044 0.6044 0.5552
Hydrogen basin populations: 0.9623 0.9623 0.9623 0.8588
Hydrogen basin dipole magnitudes: 0.1470 0.1470 0.1470 0.1250
C-C bond CP densities: 0.2614 0.3851
C-C bond laplacians: -0.677 -1.046

C 3N 0H 4 Allene

Molecular Kinetic Energy = 116.24707
Molecular Total Energy = -116.30512
Virial = 2.00050
Carbon basin kinetic energies: 37.8388 38.2025 37.8388
Carbon basin populations: 5.9448 6.3446 5.9448
Carbon basin dipole magnitudes: 0.3259 0.0000 0.3259
Hydrogen basin kinetic energies: 0.5926 0.5926 0.5926 0.5926
Hydrogen basin populations: 0.9429 0.9429 0.9429 0.9429
Hydrogen basin dipole magnitudes: 0.1412 0.1412 0.1412 0.1412
C-C bond CP densities: 0.3393 0.3393
C-C bond laplacians: -0.996 -0.996

C 4N 0H10 n-Butane

Molecular Kinetic Energy = 157.80525
Molecular Total Energy = -157.96114
Virial = 2.00099
Carbon basin kinetic energies: 37.8854 37.8866 37.8866 37.8854
Carbon basin populations: 5.9869 5.9487 5.9487 5.9869
Carbon basin dipole magnitudes: 0.0483 0.0486 0.0486 0.0483
Hydrogen basin kinetic energies: 0.6218 0.6234 0.6234 0.6328 0.6328 0.6328
0.6328 0.6218 0.6234 0.6234
Hydrogen basin populations: 1.0066 1.0104 1.0104 1.0213 1.0213 1.0213
1.0213 1.0066 1.0104 1.0104
Hydrogen basin dipole magnitudes: 0.1574 0.1602 0.1602 0.1635 0.1635 0.1635
0.1635 0.1574 0.1602 0.1602
C-C bond CP densities: 0.2414 0.2436 0.2414
C-C bond laplacians: -0.561 -0.567 -0.561

C 4N 0H10 iso-Butane

Molecular Kinetic Energy = 157.805180000000
Molecular Total Energy = -157.964180000000
Virial = 2.00100757148783
Carbon basin kinetic energies: 37.8709 37.9014 37.9014 37.9014
Carbon basin populations: 5.9159 5.9951 5.9951 5.9951
Carbon basin dipole magnitudes: 0.0464 0.0436 0.0436 0.0436
Hydrogen basin kinetic energies: 0.6394 0.6222 0.6222 0.6220 0.6222 0.6222
0.6220 0.6222 0.6222 0.6220
Hydrogen basin populations: 1.0252 1.0088 1.0088 1.0113 1.0088 1.0088
1.0113 1.0088 1.0088 1.0113
Hydrogen basin dipole magnitudes: 0.1645 0.1593 0.1593 0.1637 0.1593 0.1593
0.1637 0.1593 0.1593 0.1637
C-C bond CP densities: 0.2426 0.2426 0.2426
C-C bond laplacians: -0.563 -0.563 -0.563

C 4N 0H 8 iso-Butene

Molecular Kinetic Energy = 156.61427
Molecular Total Energy = -156.74434
Virial = 2.00083
Carbon basin kinetic energies: 37.9344 37.9603 37.8994 37.8994
Carbon basin populations: 6.0618 6.0058 5.9962 5.9962
Carbon basin dipole magnitudes: 0.1047 0.0542 0.0691 0.0691
Hydrogen basin kinetic energies: 0.6139 0.6139 0.6173 0.6162 0.6162 0.6173
0.6162 0.6162
Hydrogen basin populations: 0.9885 0.9885 0.9944 0.9962 0.9962 0.9944
0.9962 0.9962
Hydrogen basin dipole magnitudes: 0.1490 0.1490 0.1552 0.1576 0.1576 0.1552
0.1576 0.1576
C-C bond CP densities: 0.3335 0.2525 0.2525
C-C bond laplacians: -0.955 -0.617 -0.617

C 4N 0H 8 But-2-ene

Molecular Kinetic Energy = 156.60819
Molecular Total Energy = -156.74271
Virial = 2.00086
Carbon basin kinetic energies: 37.8847 37.9502 37.9502 37.8847
Carbon basin populations: 5.9851 6.0321 6.0321 5.9851
Carbon basin dipole magnitudes: 0.0751 0.0538 0.0538 0.0751
Hydrogen basin kinetic energies: 0.6199 0.6199 0.6167 0.6167 0.6183 0.6167
0.6167 0.6183
Hydrogen basin populations: 0.9988 0.9988 0.9957 0.9957 0.9976 0.9957
0.9957 0.9976
Hydrogen basin dipole magnitudes: 0.1523 0.1523 0.1558 0.1558 0.1564 0.1558
0.1558 0.1564
C-C bond CP densities: 0.2527 0.3343 0.2527
C-C bond laplacians: -0.621 -0.959 -0.621

C 4N 0H 6 1,3-Butadiene

Molecular Kinetic Energy = 155.41289
Molecular Total Energy = -155.52248
Virial = 2.00071
Carbon basin kinetic energies: 37.9264 37.9522 37.9522 37.9264
Carbon basin populations: 6.0548 6.0162 6.0162 6.0548
Carbon basin dipole magnitudes: 0.0944 0.0683 0.0683 0.0944
Hydrogen basin kinetic energies: 0.6082 0.6094 0.6131 0.6131 0.6082 0.6094
Hydrogen basin populations: 0.9731 0.9791 0.9814 0.9814 0.9731 0.9791
Hydrogen basin dipole magnitudes: 0.1443 0.1470 0.1474 0.1474 0.1443 0.1470
C-C bond CP densities: 0.3319 0.2743 0.3319
C-C bond laplacians: -0.961 -0.728 -0.961

C 6N 0H10 Hexa-2,4-diene

Molecular Kinetic Energy = 233.73869
Molecular Total Energy = -233.92193
Virial = 2.00078
Carbon basin kinetic energies: 37.9482 37.9601 37.9601 37.9482 37.8846
37.8846
Carbon basin populations: 6.0323 6.0243 6.0243 6.0323 5.9854
5.9854
Carbon basin dipole magnitudes: 0.0561 0.0631 0.0631 0.0561 0.0816
0.0816
Hydrogen basin kinetic energies: 0.6173 0.6155 0.6155 0.6173 0.6174 0.6153
0.6153 0.6153 0.6174 0.6153
Hydrogen basin populations: 0.9936 0.9912 0.9912 0.9936 0.9957 0.9924
0.9924 0.9924 0.9957 0.9924
C-C bond CP densities: 0.3308 0.2745 0.3308 0.2535 0.2535
C-C bond laplacians: -0.948 -0.724 -0.948 -0.623 -0.623

C 4N 0H 2 1,3-Butadiyne

Molecular Kinetic Energy = 153.02951
Molecular Total Energy = -153.05998
Virial = 2.00020
Carbon basin kinetic energies: 37.9472 38.0259 38.0259 37.9472
Carbon basin populations: 6.0870 6.0831 6.0831 6.0870
Carbon basin dipole magnitudes: 0.2665 0.1274 0.1274 0.2665
Hydrogen basin kinetic energies: 0.5434 0.5434
Hydrogen basin populations: 0.8327 0.8327
Hydrogen basin dipole magnitudes: 0.1220 0.1220
C-C bond CP densities: 0.3824 0.3018 0.3824
C-C bond laplacians: -1.050 -0.863 -1.050

C 4N 0H 6 But-2-yne

Molecular Kinetic Energy = 155.42005
Molecular Total Energy = -155.51588
Virial = 2.00062
Carbon basin kinetic energies: 37.8398 38.0513 38.0513 37.8398
Carbon basin populations: 5.9303 6.1671 6.1671 5.9303
Carbon basin dipole magnitudes: 0.2005 0.0610 0.0610 0.2005
Hydrogen basin kinetic energies: 0.6071 0.6071 0.6071 0.6071 0.6071 0.6071
Hydrogen basin populations: 0.9689 0.9689 0.9689 0.9689 0.9689 0.9689
Hydrogen basin dipole magnitudes: 0.1492 0.1492 0.1492 0.1492 0.1492 0.1492
C-C bond CP densities: 0.2601 0.3816 0.2601
C-C bond laplacians: -0.666 -1.013 -0.666

C 4N 0H 4 Butatriene

Molecular Kinetic Energy = 154.20548
Molecular Total Energy = -154.26951
Virial = 2.00042
Carbon basin kinetic energies: 37.8340 38.0865 38.0865 37.8340
Carbon basin populations: 5.9418 6.1813 6.1813 5.9418
Carbon basin dipole magnitudes: 0.2984 0.1799 0.1799 0.2984
Hydrogen basin kinetic energies: 0.5922 0.5922 0.5922 0.5922
Hydrogen basin populations: 0.9403 0.9403 0.9403 0.9403
Hydrogen basin dipole magnitudes: 0.1420 0.1420 0.1420 0.1420
C-C bond CP densities: 0.3316 0.3563 0.3316
C-C bond laplacians: -0.964 -1.028 -0.964

C 5N 0H12 neo-Pentane

Molecular Kinetic Energy = 196.97205
Molecular Total Energy = -197.16465
Virial = 2.00098
Carbon basin kinetic energies: 37.8730 37.9136 37.9136 37.9136 37.9136
Carbon basin populations: 5.9060 6.0008 6.0008 6.0008 6.0008
Carbon basin dipole magnitudes: 0.0000 0.0437 0.0437 0.0437 0.0437
Hydrogen basin kinetic energies: 0.6215 0.6215 0.6215 0.6215 0.6215 0.6215 0.6215 0.6215 0.6215 0.6215 0.6215
Hydrogen basin populations: 1.0093 1.0093 1.0093 1.0093 1.0093 1.0093 1.0093 1.0093 1.0093 1.0093 1.0093
Hydrogen basin dipole magnitudes: 0.1621 0.1621 0.1621 0.1621 0.1621 0.1621 0.1621 0.1621 0.1621 0.1621 0.1621
C-C bond CP densities: 0.2425 0.2425 0.2425 0.2425
C-C bond laplacians: -0.558 -0.558 -0.558 -0.558

C 5N 0H 4 Pentatetraene

Molecular Kinetic Energy = 192.17524
Molecular Total Energy = -192.23769
Virial = 2.00032
Carbon basin kinetic energies: 37.8274 38.0901 37.9972 38.0901 37.8274
Carbon basin populations: 5.9363 6.1814 6.0469 6.1814 5.9363
Carbon basin dipole magnitudes: 0.3439 0.2146 0.0000 0.2146 0.3439
Hydrogen basin kinetic energies: 0.5870 0.5870 0.5870 0.5870
Hydrogen basin populations: 0.9316 0.9316 0.9316 0.9316
Hydrogen basin dipole magnitudes: 0.1412 0.1412 0.1412 0.1412
C-C bond CP densities: 0.3328 0.3508 0.3508 0.3328
C-C bond laplacians: -0.968 -1.012 -1.012 -0.968

C 6N 0H 8 1,3,5-Hexatriene

Molecular Kinetic Energy = 232.54445
Molecular Total Energy = -232.70271
Virial = 2.00068
Carbon basin kinetic energies: 37.9248 37.9492 37.9614 37.9614 37.9492
37.9248
Carbon basin populations: 6.0552 6.0132 6.0240 6.0240 6.0132
6.0552
Carbon basin dipole magnitudes: 0.0980 0.0745 0.0641 0.0641 0.0745
0.0980
Hydrogen basin kinetic energies: 0.6078 0.6089 0.6129 0.6115 0.6115 0.6129
0.6089 0.6078
Hydrogen basin populations: 0.9724 0.9786 0.9812 0.9824 0.9824 0.9812
0.9786 0.9724
Hydrogen basin dipole magnitudes: 0.1446 0.1473 0.1475 0.1502 0.1502 0.1475
0.1473 0.1446
C-C bond CP densities: 0.3305 0.2768 0.3275 0.2768 0.3305
C-C bond laplacians: -0.955 -0.736 -0.940 -0.736 -0.955

C 6N 0H14 n-Hexane

Molecular Kinetic Energy = 236.12576
Molecular Total Energy = -236.35128
Virial = 2.00096
Carbon basin kinetic energies: 37.8846 37.8844 37.9032 37.9032 37.8844
37.8846
Carbon basin populations: 5.9867 5.9489 5.9613 5.9613 5.9489
5.9867
Carbon basin dipole magnitudes: 0.0488 0.0502 0.0362 0.0362 0.0502
0.0488
Hydrogen basin kinetic energies: 0.6218 0.6233 0.6233 0.6323 0.6323 0.6318
0.6318 0.6318 0.6318 0.6323 0.6323 0.6218
0.6233 0.6233
Hydrogen basin populations: 1.0068 1.0102 1.0102 1.0203 1.0203 1.0222
1.0222 1.0222 1.0222 1.0203 1.0203 1.0068
1.0102 1.0102
C-C bond CP densities: 0.2410 0.2431 0.2428 0.2431 0.2410
C-C bond laplacians: -0.558 -0.564 -0.562 -0.564 -0.558

C 7N 0H 4 HC(CCH)₃ (C3v)

Number of C-C bonds : 6
Number of C-H bonds : 4
Number of C-N bonds : 0
Number of N-H bonds : 0
Molecular Kinetic Energy = 268.09095
Molecular Total Energy = -268.17738
Virial = 2.00032
Carbon basin kinetic energies: 37.7640 38.0729 37.9600 38.0729 37.9600
38.0729 37.9600
Carbon basin populations: 5.7890 6.1474 6.1130 6.1474 6.1130
6.1474 6.1130
Carbon basin dipole magnitudes: 0.1815 0.0456 0.2377 0.0456 0.2377
0.0456 0.2377
Hydrogen basin kinetic energies: 0.5887 0.5489 0.5489 0.5489
Hydrogen basin populations: 0.9074 0.8446 0.8446 0.8446
C-C bond CP densities: 0.2594 0.3838 0.2594 0.3838 0.2594 0.3838
C-C bond laplacians: -0.658 -1.038 -0.658 -1.038 -0.658 -1.038

C 9N 0H 4 C(CCH)₄ (Td)

Number of C-C bonds : 8

Number of C-H bonds : 4

Number of C-N bonds : 0

Number of N-H bonds : 0

Molecular Kinetic Energy = 343.99768

Molecular Total Energy = -344.10755

Virial = 2.00032

Carbon basin kinetic energies: 37.7067 38.0742 37.9539 38.0742 37.9539
38.0742 37.9539 38.0742 37.9539

Carbon basin populations: 5.7213 6.1324 6.1007 6.1324 6.1007
6.1324 6.1007 6.1324 6.1007

Carbon basin dipole magnitudes: 0.0000 0.0685 0.2435 0.0685 0.2435
0.0685 0.2435 0.0685 0.2435

Hydrogen basin kinetic energies: 0.5469 0.5469 0.5469 0.5469

Hydrogen basin populations: 0.8401 0.8401 0.8401 0.8401

C-C bond CP densities: 0.2585 0.3828 0.2585 0.3828 0.2585 0.3828
0.2585 0.3828

C-C bond laplacians: -0.650 -1.032 -0.650 -1.032 -0.650 -1.032
-0.650 -1.032

C10N 0H 4 (HCC)₂C=C(CCH)₂

Molecular Kinetic Energy = 382.02283

Molecular Total Energy = -382.12145

Virial = 2.00026

Carbon basin kinetic energies: 37.9633 38.0684 37.8617 37.8617 38.0684
37.9633 38.0684 37.9633 38.0684 37.9633

Carbon basin populations: 6.1158 6.1284 5.8433 5.8433 6.1284
6.1158 6.1284 6.1158 6.1284 6.1158

Carbon basin dipole magnitudes: 0.2307 0.0244 0.1051 0.1051 0.0244
0.2307 0.0244 0.2307 0.0244 0.2307

Hydrogen basin kinetic energies: 0.5457 0.5457 0.5457 0.5457

Hydrogen basin populations: 0.8382 0.8382 0.8382 0.8382

Hydrogen basin dipole magnitudes: 0.1228 0.1228 0.1228 0.1228

C-C bond CP densities: 0.3827 0.2825 0.3100 0.2825 0.3827 0.2825
0.3827 0.2825 0.3827

C-C bond laplacians: -1.051 -0.767 -0.842 -0.767 -1.051 -0.767
-1.051 -0.767 -1.051

C 0N 1H 3 Ammonia

Molecular Kinetic Energy = 56.43094

Molecular Total Energy = -56.40879

Virial = 1.99961

Nitrogen basin kinetic energies: 54.9475

Nitrogen basin populations: 8.0052

Nitrogen basin dipole magnitudes: 0.2039

Hydrogen basin kinetic energies: 0.4948 0.4948 0.4948

Hydrogen basin populations: 0.6654 0.6654 0.6654

Hydrogen basin dipole magnitudes: 0.1830 0.1830 0.1830

C 1N 1H 5 Methylamine

Molecular Kinetic Energy = 95.56367
Molecular Total Energy = -95.58746
Virial = 2.00025
Carbon basin kinetic energies: 37.6869
Carbon basin populations: 5.6344
Carbon basin dipole magnitudes: 0.4244
Nitrogen basin kinetic energies: 54.9832
Nitrogen basin populations: 7.9922
Nitrogen basin dipole magnitudes: 0.2519
Hydrogen basin kinetic energies: 0.5022 0.5022 0.6268 0.6268 0.6386
Hydrogen basin populations: 0.6723 0.6723 1.0006 1.0006 1.0321
Hydrogen basin dipole magnitudes: 0.1855 0.1855 0.1507 0.1507 0.1574
C-N bond CP densities: 0.2621
C-N bond laplacians: -0.709

C 2N 1H 7 Dimethylamine

Molecular Kinetic Energy = 134.70549
Molecular Total Energy = -134.77258
Virial = 2.00050
Carbon basin kinetic energies: 37.7037 37.7037
Carbon basin populations: 5.6415 5.6415
Carbon basin dipole magnitudes: 0.4367 0.4367
Nitrogen basin kinetic energies: 55.0356
Nitrogen basin populations: 7.9953
Nitrogen basin dipole magnitudes: 0.2666
Hydrogen basin kinetic energies: 0.5070 0.6251 0.6251 0.6325 0.6325 0.6236
0.6236
Hydrogen basin populations: 0.6744 1.0003 1.0003 1.0310 1.0310 0.9975
0.9975
Hydrogen basin dipole magnitudes: 0.1858 0.1540 0.1540 0.1690 0.1690 0.1506
0.1506
C-N bond CP densities: 0.2677 0.2677
C-N bond laplacians: -0.731 -0.731

C 3N 1H 9 Trimethylamine

Molecular Kinetic Energy = 173.85898
Molecular Total Energy = -173.96267
Virial = 2.00060
Carbon basin kinetic energies: 37.7204 37.7204 37.7204
Carbon basin populations: 5.6483 5.6483 5.6483
Carbon basin dipole magnitudes: 0.4511 0.4511 0.4511
Nitrogen basin kinetic energies: 55.0915
Nitrogen basin populations: 8.0072
Nitrogen basin dipole magnitudes: 0.2732
Hydrogen basin kinetic energies: 0.6252 0.6234 0.6234 0.6252 0.6234 0.6234 0
0.6252 0.6234 0.6234
Hydrogen basin populations: 1.0275 0.9966 0.9966 1.0275 0.9966 0.9966
1.0275 0.9966 0.9966
Hydrogen basin dipole magnitudes: 0.1814 0.1525 0.1525 0.1814 0.1525 0.1525
0.1814 0.1525 0.1525
C-N bond CP densities: 0.2706 0.2706 0.2706
C-N bond laplacians: -0.742 -0.742 -0.742

C 1N 2H 6 Diaminomethane

Molecular Kinetic Energy = 150.80893
Molecular Total Energy = -150.80969
Virial = 2.00001
Carbon basin kinetic energies: 37.4932
Carbon basin populations: 5.2680
Carbon basin dipole magnitudes: 0.5252
Nitrogen basin kinetic energies: 55.0236 55.0236
Nitrogen basin populations: 8.0143 8.0143
Nitrogen basin dipole magnitudes: 0.2379 0.2379
Hydrogen basin kinetic energies: 0.6474 0.6474 0.4922 0.4971 0.4922 0.4971
Hydrogen basin populations: 1.0307 1.0307 0.6568 0.6674 0.6568 0.6674
C-N bond CP densities: 0.2710 0.2710
C-N bond laplacians: -0.764 -0.764

C 1N 3H 7 Triaminomethane

Molecular Kinetic Energy = 206.05201
Molecular Total Energy = -206.04330
Virial = 1.99996
Carbon basin kinetic energies: 37.3166
Carbon basin populations: 4.9468
Carbon basin dipole magnitudes: 0.4383
Nitrogen basin kinetic energies: 55.0527 55.0466 55.0449
Nitrogen basin populations: 8.0261 8.0298 8.0275
Nitrogen basin dipole magnitudes: 0.2509 0.2380 0.2416
Hydrogen basin kinetic energies: 0.6463 0.4883 0.4903 0.4976 0.4883 0.4969
0.4904
Hydrogen basin populations: 1.0155 0.6505 0.6590 0.6697 0.6509 0.6712
0.6612
C-N bond CP densities: 0.2819 0.2716 0.2720
C-N bond laplacians: -0.827 -0.763 -0.764

C 4N 1H11 t-Butylamine

Molecular Kinetic Energy = 213.04951
Molecular Total Energy = -213.18809
Virial = 2.00065
Carbon basin kinetic energies: 37.9218 37.7003 37.9218 37.9285
Carbon basin populations: 5.9982 5.6054 5.9982 6.0105
Carbon basin dipole magnitudes: 0.0635 0.3857 0.0635 0.0240
Nitrogen basin kinetic energies: 55.0078
Nitrogen basin populations: 7.9982
Nitrogen basin dipole magnitudes: 0.2521
Hydrogen basin kinetic energies: 0.4992 0.4992 0.6202 0.6228 0.6228 0.6212 0.6137 0.6232 0.6212 0.6137 0.6232
Hydrogen basin populations: 0.6761 0.6761 1.0072 1.0136 1.0136 1.0075 0.9884 1.0140 1.0075 0.9884 1.0140
C-C bond CP densities: 0.2467 0.2467 0.2441
C-C bond laplacians: -0.583 -0.583 -0.566
C-N bond CP densities: 0.2611
C-N bond laplacians: -0.693

C 2N 2H 6 1,1-diaminoethene

Molecular Kinetic Energy = 188.77602
Molecular Total Energy = -188.80506
Virial = 2.00015
Carbon basin kinetic energies: 37.5245 37.9060
Carbon basin populations: 5.2368 6.0726
Carbon basin dipole magnitudes: 0.7452 0.2368
Nitrogen basin kinetic energies: 55.1039 55.1039
Nitrogen basin populations: 8.0933 8.0933
Nitrogen basin dipole magnitudes: 0.1511 0.1511
Hydrogen basin kinetic energies: 0.6137 0.6137 0.4778 0.4802 0.4778 0.4802
Hydrogen basin populations: 0.9930 0.9930 0.6297 0.6329 0.6297 0.6329
Hydrogen basin dipole magnitudes: 0.1521 0.1521 0.1732 0.1713 0.1732 0.1713
C-C bond CP densities: 0.3271
C-C bond laplacians: -0.921
C-N bond CP densities: 0.2969 0.2969
C-N bond laplacians: -0.915 -0.915

C 2N 2H 6 1,2-diaminoethene

Molecular Kinetic Energy = 188.76112
Molecular Total Energy = -188.78891
Virial = 2.00015
Carbon basin kinetic energies: 37.7408 37.7408
Carbon basin populations: 5.6605 5.6605
Carbon basin dipole magnitudes: 0.5279 0.5279
Nitrogen basin kinetic energies: 55.0442 55.0442
Nitrogen basin populations: 8.0489 8.0489
Nitrogen basin dipole magnitudes: 0.1763 0.1763
Hydrogen basin kinetic energies: 0.6189 0.6189 0.4896 0.4899 0.4896 0.4899
Hydrogen basin populations: 0.9917 0.9917 0.6496 0.6531 0.6496 0.6531
Hydrogen basin dipole magnitudes: 0.1476 0.1476 0.1782 0.1802 0.1782 0.1802
C-C bond CP densities: 0.3320
C-C bond laplacians: -0.937
C-N bond CP densities: 0.2838 0.2838
C-N bond laplacians: -0.823 -0.823

C 1N 1H 3 HN=CH₂

Molecular Kinetic Energy = 94.35385
Molecular Total Energy = -94.37576
Virial = 2.00023
Carbon basin kinetic energies: 37.5019
Carbon basin populations: 5.3098
Carbon basin dipole magnitudes: 0.7169
Nitrogen basin kinetic energies: 55.1162
Nitrogen basin populations: 8.0534
Nitrogen basin dipole magnitudes: 0.2653
Hydrogen basin kinetic energies: 0.5013 0.6172 0.6204
Hydrogen basin populations: 0.6707 0.9761 0.9932
Hydrogen basin dipole magnitudes: 0.1793 0.1370 0.1448
C-N bond CP densities: 0.3759
C-N bond laplacians: -0.869

C 3N 1H 7 HN=CMe₂

Molecular Kinetic Energy = 172.69194
Molecular Total Energy = -172.78300
Virial = 2.00053
Carbon basin kinetic energies: 37.5393 37.9261 37.9261
Carbon basin populations: 5.2970 6.0136 6.0229
Carbon basin dipole magnitudes: 0.6393 0.0893 0.0559
Nitrogen basin kinetic energies: 55.1345
Nitrogen basin populations: 8.0851
Nitrogen basin dipole magnitudes: 0.2493
Hydrogen basin kinetic energies: 0.5037 0.6042 0.6140 0.6140 0.6166 0.6101
0.6101
Hydrogen basin populations: 0.6831 0.9628 0.9925 0.9925 0.9944 0.9827
0.9827
Hydrogen basin dipole magnitudes: 0.1886 0.1537 0.1546 0.1546 0.1550 0.1537
0.1537
C-C bond CP densities: 0.2560 0.2526
C-C bond laplacians: -0.639 -0.616
C-N bond CP densities: 0.3754
C-N bond laplacians: -0.921

C 2N 1H 5 H₂C=N-Me

Molecular Kinetic Energy = 133.50152
Molecular Total Energy = -133.56526
Virial = 2.00048
Carbon basin kinetic energies: 37.7279 37.5124
Carbon basin populations: 5.6652 5.3198
Carbon basin dipole magnitudes: 0.4419 0.7476
Nitrogen basin kinetic energies: 55.1827
Nitrogen basin populations: 8.0832
Nitrogen basin dipole magnitudes: 0.3424
Hydrogen basin kinetic energies: 0.6153 0.6255 0.6153 0.6128 0.6153
Hydrogen basin populations: 0.9789 1.0145 0.9789 0.9696 0.9969
Hydrogen basin dipole magnitudes: 0.1481 0.1666 0.1481 0.1376 0.1600
C-N bond CP densities: 0.2684 0.3753
C-N bond laplacians: -0.741 -0.758

C 2N 1H 3 Aminoethyne

Molecular Kinetic Energy = 132.31579
Molecular Total Energy = -132.33234
Virial = 2.00013
Carbon basin kinetic energies: 37.8624 37.8976
Carbon basin populations: 6.0035 5.8390
Carbon basin dipole magnitudes: 0.4418 0.8477
Nitrogen basin kinetic energies: 55.0658
Nitrogen basin populations: 8.0849
Nitrogen basin dipole magnitudes: 0.1099
Hydrogen basin kinetic energies: 0.5543 0.4695 0.4695
Hydrogen basin populations: 0.8580 0.6096 0.6096
Hydrogen basin dipole magnitudes: 0.1271 0.1617 0.1617
C-C bond CP densities: 0.3781
C-C bond laplacians: -0.951

Physical Chemistry Chemical Physics
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C-N bond CP densities: 0.3134
C-N bond laplacians: -0.946

C 2N 1H 3 HN=C=CH₂
Molecular Kinetic Energy = 132.31822
Molecular Total Energy = -132.35268
Virial = 2.00026
Carbon basin kinetic energies: 37.7941 37.7026
Carbon basin populations: 5.9231 5.4664
Carbon basin dipole magnitudes: 0.4900 1.1111
Nitrogen basin kinetic energies: 55.1959
Nitrogen basin populations: 8.1564
Nitrogen basin dipole magnitudes: 0.3351
Hydrogen basin kinetic energies: 0.5837 0.5837 0.4583
Hydrogen basin populations: 0.9265 0.9265 0.6011
Hydrogen basin dipole magnitudes: 0.1407 0.1407 0.1608
C-C bond CP densities: 0.3271
C-C bond laplacians: -0.878
C-N bond CP densities: 0.4060
C-N bond laplacians: -0.863

C 1N 2H 2 HN=C=NH
Molecular Kinetic Energy = 148.41494
Molecular Total Energy = -148.41442
Virial = 2.00000
Carbon basin kinetic energies: 37.1379
Carbon basin populations: 4.4899
Carbon basin dipole magnitudes: 0.3103
Nitrogen basin kinetic energies: 55.1956 55.1956
Nitrogen basin populations: 8.1806 8.1806
Nitrogen basin dipole magnitudes: 0.2705 0.2705
Hydrogen basin kinetic energies: 0.4450 0.4450
Hydrogen basin populations: 0.5762 0.5762
Hydrogen basin dipole magnitudes: 0.1532 0.1532
C-N bond CP densities: 0.4057 0.4057
C-N bond laplacians: -0.993 -0.993

C 2N 2H 2 HN=C=C=NH
Molecular Kinetic Energy = 186.30921
Molecular Total Energy = -186.33053
Virial = 2.00011
Carbon basin kinetic energies: 37.5970 37.5970
Carbon basin populations: 5.3679 5.3679
Carbon basin dipole magnitudes: 0.9726 0.9726
Nitrogen basin kinetic energies: 55.0900 55.0900
Nitrogen basin populations: 8.0136 8.0136
Nitrogen basin dipole magnitudes: 0.2436 0.2436
Hydrogen basin kinetic energies: 0.4704 0.4704
Hydrogen basin populations: 0.6209 0.6209
Hydrogen basin dipole magnitudes: 0.1644 0.1644
C-C bond CP densities: 0.3277
C-C bond laplacians: -0.880
C-N bond CP densities: 0.3846 0.3846
C-N bond laplacians: -0.825 -0.825

C 2N 2H 4 H₂C=N-CH=NH

Molecular Kinetic Energy = 187.54343
Molecular Total Energy = -187.58427
Virial = 2.00022
Carbon basin kinetic energies: 37.5143 37.3391
Carbon basin populations: 5.3217 4.9373
Carbon basin dipole magnitudes: 0.7526 0.6374
Nitrogen basin kinetic energies: 55.2380 55.1507
Nitrogen basin populations: 8.1279 8.0743
Nitrogen basin dipole magnitudes: 0.2573 0.2550
Hydrogen basin kinetic energies: 0.6045 0.6081 0.6120 0.4838
Hydrogen basin populations: 0.9486 0.9761 0.9749 0.6461
Hydrogen basin dipole magnitudes: 0.1335 0.1532 0.1504 0.1760
C-N bond CP densities: 0.3724 0.2908 0.3854
C-N bond laplacians: -0.805 -0.868 -0.965

C 1N 3H 5 Guanidine

Molecular Kinetic Energy = 204.86560
Molecular Total Energy = -204.85899
Virial = 1.99997
Carbon basin kinetic energies: 37.0833
Carbon basin populations: 4.4875
Carbon basin dipole magnitudes: 0.0643
Nitrogen basin kinetic energies: 55.1343 55.1275 55.1333
Nitrogen basin populations: 8.1372 8.1128 8.1098
Nitrogen basin dipole magnitudes: 0.2152 0.1249 0.1412
Hydrogen basin kinetic energies: 0.5013 0.4768 0.4723 0.4767 0.4668
Hydrogen basin populations: 0.6809 0.6270 0.6180 0.6264 0.6074
Hydrogen basin dipole magnitudes: 0.1898 0.1697 0.1672 0.1696 0.1636
C-N bond CP densities: 0.3825 0.2987 0.3048
C-N bond laplacians: -1.141 -0.918 -0.969

C 3N 2H 6 HN=CH-CH=CH-NH₂

Molecular Kinetic Energy = 226.73406
Molecular Total Energy = -226.78640
Virial = 2.00023
Carbon basin kinetic energies: 37.5375 37.6630 37.9696
Carbon basin populations: 5.3189 5.5444 6.0396
Carbon basin dipole magnitudes: 0.6401 0.7124 0.1542
Nitrogen basin kinetic energies: 55.1067 55.1945
Nitrogen basin populations: 8.0777 8.2024
Nitrogen basin dipole magnitudes: 0.2265 0.1321
Hydrogen basin kinetic energies: 0.5042 0.6283 0.6031 0.6127 0.4602 0.4622
Hydrogen basin populations: 0.6794 1.0177 0.9705 0.9718 0.5942 0.5929
Hydrogen basin dipole magnitudes: 0.1853 0.1572 0.1532 0.1440 0.1586 0.1566
C-C bond CP densities: 0.2808 0.3245
C-C bond laplacians: -0.753 -0.925
C-N bond CP densities: 0.3703 0.3049
C-N bond laplacians: -0.960 -0.746

C 2N 1H 3 Acetonitrile

Molecular Kinetic Energy = 132.34237
Molecular Total Energy = -132.40726
Virial = 2.00049
Carbon basin kinetic energies: 37.8512 37.5435
Carbon basin populations: 5.9324 5.1977
Carbon basin dipole magnitudes: 0.2655 0.8991
Nitrogen basin kinetic energies: 55.1698
Nitrogen basin populations: 8.0605
Nitrogen basin dipole magnitudes: 0.4009
Hydrogen basin kinetic energies: 0.5942 0.5942 0.5942
Hydrogen basin populations: 0.9382 0.9382 0.9382
Hydrogen basin dipole magnitudes: 0.1407 0.1407 0.1407
C-C bond CP densities: 0.2597
C-C bond laplacians: -0.681
C-N bond CP densities: 0.4529
C-N bond laplacians: -0.263

C 1N 1H 1 HC≡N

Molecular Kinetic Energy = 93.17307
Molecular Total Energy = -93.20021
Virial = 2.00029
Carbon basin kinetic energies: 37.4885
Carbon basin populations: 5.1860
Carbon basin dipole magnitudes: 0.9727
Nitrogen basin kinetic energies: 55.1581
Nitrogen basin populations: 8.0136
Nitrogen basin dipole magnitudes: 0.4122
Hydrogen basin kinetic energies: 0.5294
Hydrogen basin populations: 0.8025
C-N bond CP densities: 0.4561
C-N bond laplacians: -0.247

C 1N 2H 2 N≡C-NH₂

Molecular Kinetic Energy = 148.40706
Molecular Total Energy = -148.42567
Virial = 2.00013
Carbon basin kinetic energies: 37.2951
Carbon basin populations: 4.7110
Carbon basin dipole magnitudes: 0.2232
Nitrogen basin kinetic energies: 55.1264 55.0756
Nitrogen basin populations: 8.0365 8.0826
Nitrogen basin dipole magnitudes: 0.3134 0.0881
Hydrogen basin kinetic energies: 0.4571 0.4571
Hydrogen basin populations: 0.5868 0.5868
Hydrogen basin dipole magnitudes: 0.1525 0.1525
C-N bond CP densities: 0.4465 0.3203
C-N bond laplacians: -0.317 -1.000

Physical Chemistry Chemical Physics

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C 3N 2H 6 N≡C-NMe₂ (Cs)

Molecular Kinetic Energy = 226.70202

Molecular Total Energy = -226.79716

Virial = 2.00042

Carbon basin kinetic energies: 37.3210 37.7043 37.7043

Carbon basin populations: 4.7244 5.6468 5.6468

Carbon basin dipole magnitudes: 0.2007 0.4958 0.4958

Nitrogen basin kinetic energies: 55.1852 55.1145

Nitrogen basin populations: 8.1099 8.0375

Nitrogen basin dipole magnitudes: 0.1542 0.3028

Hydrogen basin kinetic energies: 0.6173 0.6079 0.6158 0.6079 0.6173 0.6158

Hydrogen basin populations: 0.9895 0.9573 0.9758 0.9573 0.9895 0.9758

C-N bond CP densities: 0.3277 0.4429 0.2548 0.2548

C-N bond laplacians: -1.015 -0.348 -0.672 -0.672

C 2N 2H 0 Cyanogen N≡C-C≡N

Molecular Kinetic Energy = 185.15783

Molecular Total Energy = -185.22144

Virial = 2.00034

Carbon basin kinetic energies: 37.5001 37.5001

Carbon basin populations: 5.1106 5.1106

Carbon basin dipole magnitudes: 0.6810 0.6810

Nitrogen basin kinetic energies: 55.0813 55.0813

Nitrogen basin populations: 7.8915 7.8915

Nitrogen basin dipole magnitudes: 0.3494 0.3494

C-C bond CP densities: 0.2972

C-C bond laplacians: -0.865

C-N bond CP densities: 0.4474 0.4474

C-N bond laplacians: -0.301 -0.301

C 4N 3H 1 HC(C≡N)₃ (C_{3v})

Molecular Kinetic Energy = 316.31052

Molecular Total Energy = -316.43182

Virial = 2.00038

Carbon basin kinetic energies: 37.7729 37.5477 37.5477 37.5477

Carbon basin populations: 5.7922 5.1730 5.1730 5.1730

Carbon basin dipole magnitudes: 0.2236 0.7801 0.7801 0.7801

Nitrogen basin kinetic energies: 55.1138 55.1138 55.1138

Nitrogen basin populations: 7.9481 7.9481 7.9481

Nitrogen basin dipole magnitudes: 0.3772 0.3772 0.3772

Hydrogen basin kinetic energies: 0.5632

Hydrogen basin populations: 0.8535

C-C bond CP densities: 0.2589 0.2589 0.2589

C-C bond laplacians: -0.665 -0.665 -0.665

C-N bond CP densities: 0.4486 0.4486 0.4486

C-N bond laplacians: -0.203 -0.203 -0.203

C 5N 4H 0 C(C≡N)₄ (T_d)

Molecular Kinetic Energy = 408.27621

Molecular Total Energy = -408.43416

Virial = 2.00039

Carbon basin kinetic energies: 37.5546 37.7131 37.5546 37.5546 37.5546

Carbon basin populations: 5.1693 5.7246 5.1693 5.1693 5.1693

Carbon basin dipole magnitudes: 0.7371 0.0000 0.7371 0.7371 0.7371

Nitrogen basin kinetic energies: 55.0894 55.0894 55.0894 55.0894

Nitrogen basin populations: 7.9023 7.9023 7.9023 7.9023

Nitrogen basin dipole magnitudes: 0.3641 0.3641 0.3641 0.3641

C-C bond CP densities: 0.2578 0.2578 0.2578 0.2578

C-C bond laplacians: -0.655 -0.655 -0.655 -0.655

C-N bond CP densities: 0.4458 0.4458 0.4458 0.4458

C-N bond laplacians: -0.184 -0.184 -0.184 -0.184

C 4N 1H 11 Trimethyl ylidy

Physical Chemistry Chemical Physics

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Molecular Kinetic Energy = 212.95636

Molecular Total Energy = -213.05691

Virial = 2.00047

Carbon basin kinetic energies: 37.7354 37.7697 37.7836 37.7697

Carbon basin populations: 6.0805 5.7011 5.7224 5.7011

Carbon basin dipole magnitudes: 1.3063 0.4927 0.4380 0.4927

Nitrogen basin kinetic energies: 55.1265

Nitrogen basin populations: 7.9631

Nitrogen basin dipole magnitudes: 0.0533

Hydrogen basin kinetic energies: 0.6508 0.6508 0.6092 0.5938 0.6217 0.6084

0.6084 0.6192 0.5938 0.6092 0.6217

Hydrogen basin populations: 1.0836 1.0836 0.9613 0.9284 0.9958 0.9603

0.9603 0.9950 0.9284 0.9613 0.9958

C-N bond CP densities: 0.1990 0.2524 0.2505 0.2524

C-N bond laplacians: -0.219 -0.661 -0.637 -0.661