Improved Auxiliary Basis Sets

```
$jbas
*
h universal
h def2-SV(P)
h def2-SVP
h def2-TZVP
h def2-TZVPP
h def2-QZVP
h def2-QZVPP
# h     (5s2p1d) / [3s1p1d]     {311/2/1}
*
    3  s
       15.6752927        0.0186886
        3.6063578        0.0631670
        1.2080016        0.1204609
    1  s
        0.4726794        0.0592485
    1  s
        0.2018100        0.0051272
    2  p
        2.0281365        1.0
        0.5358730        1.0
    1  d
        2.2165124        0.0033116
*
he universal
he def2-SV(P)
he def2-SVP
he def2-TZVP
he def2-TZVPP
he def2-QZVP
he def2-QZVPP
# he     (5s2p1d) / [3s1p1d]     {311/2/1}
*
    3  s
       50.6720580        0.0651007
       12.6182260        0.2103093
        3.8995171        0.3791436
    1  s
        1.4088465        0.2938041
    1  s
        0.5393970        0.0661606
    2  p
        4.0              1.0
        1.0              1.0
    1  d
        4.0              1.0
*
li universal
li def2-SV(P)
li def2-SVP
li def2-TZVP
li def2-TZVPP
li def2-QZVP
li def2-QZVPP
# li    (12s5p4d2f1g) / [6s4p3d1f1g]     {711111/2111/211/2/1}
*
    7  s
      498.3689730        0.0207908
      162.9342738        0.0542177
       57.3246735        0.1776783
       21.6427314        0.4181150
        8.7345375        0.6535245
```

```
        3.7491039        0.5492618
        1.7006754        0.1701425
    1  s
        0.8090859       -0.0097548
    1  s
        0.4000933       -0.0050152
    1  s
        0.2035793        0.0232200
    1  s
        0.1054201        0.0134535
    1  s
        0.0549139        0.0006647
    2  p
       10.7024696        0.0072923
        3.6551543        0.0060940
    1  p
        1.2464013        0.0172529
    1  p
        0.4246282       -0.0160026
    1  p
        0.1446192       -0.0195111
    2  d
        1.1510647       -0.0014314
        0.6019112        0.0038969
    1  d
        0.3109573        0.0024683
    1  d
        0.1600032        0.0036451
    2  f
        0.5967918        0.0010494
        0.1790687        0.0006468
    1  g
        1.0460130       -0.0001971
*
be universal
be def2-SV(P)
be def2-SVP
be def2-TZVP
be def2-TZVPP
be def2-QZVP
be def2-QZVPP
# be    (12s5p4d2f1g) / [6s4p3d1f1g]     {711111/2111/211/2/1}
*
    7  s
      931.3932020        0.0339736
      309.1384767        0.0769224
      109.7579334        0.2770466
       41.5609052        0.6423826
       16.7186235        1.0888458
        7.1095250        0.9162473
        3.1768417        0.2832563
    1  s
        1.4810941       -0.0784363
    1  s
        0.7146066        0.0169349
    1  s
        0.3536015        0.0938089
    1  s
        0.1776945        0.0544796
    1  s
        0.0897625        0.0056480
    2  p
        4.8768490        0.0006466
```

```
        1.8686000        0.0169061
    1  p
        0.7059119       -0.0271994
    1  p
        0.2644480        0.0190199
    1  p
        0.0987920        0.0054201
    2  d
        1.5703852        0.0036075
        0.6733684        0.0208788
    1  d
        0.3299827        0.0084999
    1  d
        0.1697927        0.0039819
    2  f
        2.2794515       -0.0005539
        0.9215384        0.0035407
    1  g
        1.3893341       -0.0006334
*
b universal
b def2-SV(P)
b def2-SVP
b def2-TZVP
b def2-TZVPP
b def2-QZVP
b def2-QZVPP
# b     (12s5p4d2f1g) / [6s4p3d1f1g]     {711111/2111/211/2/1}
*
    7  s
     1322.2016723        0.0542834
      458.2370653        0.1167149
      168.0023641        0.4020230
       64.9577690        0.9377941
       26.3871856        1.5869087
       11.2108611        1.3566478
        4.9554460        0.3199019
    1  s
        2.2652825       -0.1340611
    1  s
        1.0638086        0.0498171
    1  s
        0.5095187        0.2553537
    1  s
        0.2469859        0.0800208
    1  s
        0.1202089        0.0163658
    2  p
        9.3560736       -0.0130117
        3.9743131       -0.0114013
    1  p
        1.6645147        0.0309850
    1  p
        0.6913035       -0.0037719
    1  p
        0.2863135        0.0449188
    2  d
        2.1120313        0.0228072
        0.7780769        0.0405259
    1  d
        0.3277101        0.0082013
    1  d
        0.1449465        0.0024471
```

```
    2  f
        1.0582718        0.0087498
        0.4010000        0.0036145
    1  g
        0.6514300       -0.0012389
*
c universal
c def2-SV(P)
c def2-SVP
c def2-TZVP
c def2-TZVPP
c def2-QZVP
c def2-QZVPP
# c     (12s5p4d2f1g) / [6s4p3d1f1g]     {711111/2111/211/2/1}
*
    7  s
     1861.0916331        0.0744171
      642.9939764        0.1653957
      235.1105725        0.5576484
       90.7028894        1.3108298
       36.7794552        2.1694681
       15.6046273        1.7668846
        6.8907294        0.2930769
    1  s
        3.1478850       -0.1708702
    1  s
        1.4777287        0.1641553
    1  s
        0.7076466        0.4149941
    1  s
        0.3430122        0.1624366
    1  s
        0.1669453        0.0207675
    2  p
       13.5472892       -0.0206477
        5.4669419       -0.0115282
    1  p
        2.1751721        0.0455914
    1  p
        0.8582194        0.0028360
    1  p
        0.3376720        0.0181875
    2  d
        5.9287253       -0.0225948
        1.9809209       -0.0476827
    1  d
        0.8055417       -0.0365372
    1  d
        0.3531244       -0.0145417
    2  f
        1.6755626        0.0088798
        0.5997536        0.0069903
    1  g
        1.0024600       -0.0022192
*
n universal
n def2-SV(P)
n def2-SVP
n def2-TZVP
n def2-TZVPP
n def2-QZVP
n def2-QZVPP
# n     (12s5p4d2f1g) / [6s4p3d1f1g]     {711111/2111/211/2/1}
```

```
*
    7  s
     2542.9401785        0.0904668
     1029.5472946        0.1455675
      424.9053546        0.4594090
      178.4573708        1.1392859
       76.1362742        2.1795891
       32.9338653        2.7604305
       14.4155436        1.2837451
    1  s
        6.3718891       -0.1702642
    1  s
        2.8381742        0.0504472
    1  s
        1.2711793        0.6634588
    1  s
        0.5712407        0.4116559
    1  s
        0.2569887        0.0489167
    2  p
       17.8975990       -0.0330656
        6.5346319        0.0041582
    1  p
        2.3523645        0.0525824
    1  p
        0.8397377        0.0017058
    1  p
        0.2989335        0.0122960
    2  d
        7.6909870        0.0035820
        2.3044972        0.0180403
    1  d
        0.8403987        0.0194441
    1  d
        0.3303797        0.0002361
    2  f
        2.3331076        0.0067248
        0.8446137        0.0054427
    1  g
        1.4037700       -0.0023051
*
o universal
o def2-SV(P)
o def2-SVP
o def2-TZVP
o def2-TZVPP
o def2-QZVP
o def2-QZVPP
# o     (12s5p4d2f1g) / [6s4p3d1f1g]     {711111/2111/211/2/1}
*
    7  s
     2876.8216605        0.1443558
     1004.7443032        0.2920041
      369.7579954        1.0258517
      142.9442404        2.2875516
       57.8366425        3.6080237
       24.3864983        2.3737865
       10.6622662        0.0489414
    1  s
        4.8070437       -0.1295186
    1  s
        2.2210770        0.7747158
    1  s
```

```
        1.0447795        0.7647816
    1  s
        0.4968425        0.2369803
    1  s
        0.2371384        0.0208099
    2  p
       64.2613382       -0.0126659
       16.3006076       -0.0378744
    1  p
        4.3550542        0.0638078
    1  p
        1.2019554        0.0169516
    1  p
        0.3354196        0.0065743
    2  d
        9.2146611       -0.0597914
        2.8435251       -0.0846724
    1  d
        0.9955759       -0.0466066
    1  d
        0.3649441       -0.0096978
    2  f
        2.6420115        1.0
        0.7345613        1.0
    1  g
        1.3931000       -0.0016533
*
f universal
f def2-SV(P)
f def2-SVP
f def2-TZVP
f def2-TZVPP
f def2-QZVP
f def2-QZVPP
# f     (12s5p4d2f1g) / [6s4p3d1f1g]     {711111/2111/211/2/1}
*
    7  s
     3514.9201549        0.1805835
     1231.2458815        0.3676084
      454.1367336        1.2707881
      175.8376258        2.8274164
       71.2081775        4.3588226
       30.0316883        2.7180994
       13.1259023       -0.0804726
    1  s
        5.9126861       -0.0023370
    1  s
        2.7284431        1.1236274
    1  s
        1.2813993        0.9999042
    1  s
        0.6082793        0.3119579
    1  s
        0.2897894        0.0312295
    2  p
       49.3740409       -0.0346332
       13.4874956       -0.0096069
    1  p
        3.9664900        0.0762067
    1  p
        1.2226629       -0.0103329
    1  p
        0.3830317        0.0018853
```

```
    2  d
       29.9719140       -0.0113316
        6.7860915       -0.0467639
    1  d
        1.8137313       -0.0167604
    1  d
        0.5157840       -0.0050777
    2  f
        2.8301877        1.0
        0.9155962        1.0
    1  g
        1.6097500       -0.0005411
*
ne universal
ne def2-SV(P)
ne def2-SVP
ne def2-TZVP
ne def2-TZVPP
ne def2-QZVP
ne def2-QZVPP
# ne    (12s5p4d2f1g) / [6s4p3d1f1g]     {711111/2111/211/2/1}
*
    7  s
     4165.3443917        0.2215380
     1475.2326437        0.4503030
      549.2884359        1.5166656
      214.3631494        3.3680211
       87.3657300        5.1165136
       37.0296590        3.1485977
       16.2441770       -0.1945455
    1  s
        7.3360628        0.1247267
    1  s
        3.3907965        1.5785951
    1  s
        1.5939747        1.2555710
    1  s
        0.7570527        0.3695086
    1  s
        0.3608023        0.0368256
    2  p
       61.2             -0.0346332
       16.7             -0.0096069
    1  p
        4.92             0.0762067
    1  p
        1.52             1.0
    1  p
        0.48             1.0
    2  d
       37.17            -0.0113316
        8.41            -0.0467639
    1  d
        2.25             1.0
    1  d
        0.64             1.0
    2  f
        3.51             1.0
        1.14             1.0
    1  g
        2.00             1.0
*
na universal
```

```
na def2-SV(P)
na def2-SVP
na def2-TZVP
na def2-TZVPP
na def2-QZVP
na def2-QZVPP
# na    (14s5p5d2f1g) / [8s4p4d1f1g]     {71111111/2111/2111/2/1}
*
    7  s
     3754.9468758        0.3681280
     1406.4560878        0.6386505
      543.4611528        2.1314027
      216.2389118        4.4341952
       88.4180110        6.0193186
       37.0700801        2.6066659
       15.8976971       -0.6617046
    1  s
        6.9557845        1.0910786
    1  s
        3.0964156        2.3362969
    1  s
        1.3983233        0.9741825
    1  s
        0.6386578        0.0619929
    1  s
        0.2940844       -0.0076913
    1  s
        0.1360866        0.0263452
    1  s
        0.0630775        0.0027263
    2  p
       19.2914768        0.0091163
        5.8156595       -0.0286151
    1  p
        1.7285804        0.0155463
    1  p
        0.5094901        0.0133567
    1  p
        0.1497524       -0.0194810
    2  d
       14.0911593        0.0025046
        3.9826616        0.0012793
    1  d
        1.3285602       -0.0023986
    1  d
        0.4969388       -0.0006677
    1  d
        0.1937075        0.0049815
    2  f
        0.1873532        0.0012141
        0.0980271       -0.0004706
    1  g
        0.0701600        0.0001161
*
mg universal
mg def2-SV(P)
mg def2-SVP
mg def2-TZVP
mg def2-TZVPP
mg def2-QZVP
mg def2-QZVPP
# mg    (14s5p5d2f1g) / [8s4p4d1f1g]     {71111111/2111/2111/2/1}
*
```

```
    7  s
     4618.7144348        0.4062037
     1715.8572368        0.7248204
      660.3662172        2.4015050
      262.7772421        5.0268089
      107.8796646        6.8807535
       45.5809298        3.0930185
       19.7676678       -0.8061330
    1  s
        8.7738606        1.2834607
    1  s
        3.9730763        2.9682392
    1  s
        1.8294222        1.2081584
    1  s
        0.8535432       -0.0228789
    1  s
        0.4020431        0.0060268
    1  s
        0.1904672        0.0852479
    1  s
        0.0904075        0.0238626
    2  p
        4.2335270       -0.0089796
        1.3598327        0.0169486
    1  p
        0.5026752       -0.0127300
    1  p
        0.2043109        0.0127291
    1  p
        0.0858908        0.0069646
    2  d
       15.3639340        0.0072298
        3.9275269        0.0022521
    1  d
        1.1824901       -0.0081411
    1  d
        0.3985299        0.0134364
    1  d
        0.1398822        0.0062003
    2  f
        2.2586461       -0.0009518
        0.4740262        0.0022316
    1  g
        0.8087604       -0.0004005
*
al universal
al def2-SV(P)
al def2-SVP
al def2-TZVP
al def2-TZVPP
al def2-QZVP
al def2-QZVPP
# al    (14s5p5d2f1g) / [8s4p3d1f1g]     {71111111/2111/311/2/1}
*
    7  s
     4875.9816108        0.5248525
     1839.4838989        0.8958282
      715.5582316        2.9427043
      286.4958622        5.9976464
      117.8265577        7.7609764
       49.6666399        2.8641690
       21.4066429       -1.0464290
```

```
    1  s
        9.4098725        2.2627888
    1  s
        4.2071557        3.6026980
    1  s
        1.9077330        0.8061044
    1  s
        0.8747225       -0.1790388
    1  s
        0.4042979        0.1555884
    1  s
        0.1877731        0.1366505
    1  s
        0.0873510        0.0104116
    2  p
       10.9820947        0.0163880
        3.3106913       -0.0029350
    1  p
        0.9840322       -0.0059291
    1  p
        0.2900384        0.0303071
    1  p
        0.0852498        0.0068614
    3  d
       21.5501974        0.0114463
        5.9277503        0.0082803
        1.8822054       -0.0133523
    1  d
        0.6586442        0.0135944
    1  d
        0.2385982        0.0185676
    2  f
        0.5382976        0.0072119
        0.1976728        0.0039371
    1  g
        0.3262000       -0.0020989
*
si universal
si def2-SV(P)
si def2-SVP
si def2-TZVP
si def2-TZVPP
si def2-QZVP
si def2-QZVPP
# si    (14s5p5d2f1g) / [8s4p3d1f1g]     {71111111/2111/311/2/1}
*
    7  s
     5826.7657660        0.5677983
     2173.1214409        1.0118069
      839.4966509        3.2799844
      335.2659622        6.7361713
      138.1170978        8.6949143
       58.5516054        3.2431556
       25.4744274       -1.2520738
    1  s
       11.3418415        2.6706099
    1  s
        5.1513356        4.3474757
    1  s
        2.3788654        0.8729007
    1  s
        1.1130498       -0.3244603
    1  s
```

```
        0.5257427        0.2956979
    1  s
        0.2497578        0.1946885
    1  s
        0.1188768        0.0318632
    2  p
        8.7836931        0.0242245
        2.6158248       -0.0153268
    1  p
        0.8266040        0.0061588
    1  p
        0.2711487        0.0428066
    1  p
        0.0900870        0.0015544
    3  d
       10.8892767        0.0240593
        2.6605925       -0.0189904
        0.8067528        0.0242108
    1  d
        0.2859848        0.0317147
    1  d
        0.1074329        0.0020599
    2  f
        0.8103816        0.0088216
        0.1988529        0.0020248
    1  g
        0.4014900       -0.0016684
*
p universal
p def2-SV(P)
p def2-SVP
p def2-TZVP
p def2-TZVPP
p def2-QZVP
p def2-QZVPP
# p     (14s5p5d2f1g) / [8s4p3d1f1g]     {71111111/2111/311/2/1}
*
    7  s
     7402.6405628        0.6312551
     2444.3806296        1.0410015
     1031.0485275        3.5177235
      387.5215861        7.8577024
      159.3342518        9.3323916
       72.5438912        3.5808385
       29.2976155       -1.1039880
    1  s
       13.1685047        2.8706692
    1  s
        6.4235268        4.9937953
    1  s
        3.1479365        1.2003750
    1  s
        1.4941282       -0.4895877
    1  s
        0.6745215        0.3794973
    1  s
        0.3252877        0.3625040
    1  s
        0.1527285        0.0512179
    2  p
       10.6100703        0.0333958
        3.3972489       -0.0239301
    1  p
```

```
        1.0821336        0.0194214
    1  p
        0.3436265        0.0184052
    1  p
        0.1090044        0.0008768
    3  d
        5.5575593        0.0066400
        2.6033240       -0.0123559
        1.2378589        0.0087029
    1  d
        0.5939646        0.0072180
    1  d
        0.2858732       -0.0025575
    2  f
        1.0262041        0.0104661
        0.2959414        0.0038742
    1  g
        0.5510844       -0.0032181
*
s universal
s def2-SV(P)
s def2-SVP
s def2-TZVP
s def2-TZVPP
s def2-QZVP
s def2-QZVPP
# s     (14s5p5d2f1g) / [8s4p3d1f1g]     {71111111/2111/311/2/1}
*
    7  s
     7399.0303145        0.7227933
     2710.1675859        1.3706745
     1034.3279062        4.3217500
      410.4645411        8.7624644
      168.9762502       10.5289909
       71.9687889        3.0836598
       31.6172683       -1.5821203
    1  s
       14.2796836        4.4920092
    1  s
        6.6060948        5.6247567
    1  s
        3.1181477        0.2331133
    1  s
        1.4954039       -0.4527401
    1  s
        0.7254779        0.6731617
    1  s
        0.3544216        0.4015653
    1  s
        0.1735525        0.0610369
    2  p
       12.6998799        0.0457971
        4.4295784       -0.0394968
    1  p
        1.5232889        0.0357338
    1  p
        0.5194667       -0.0040859
    1  p
        0.1766547       -0.0036880
    3  d
       16.8546461        0.0263236
        5.0810461       -0.0190773
        1.5102323        0.0213668
```

```
    1  d
        0.4451331        0.0219369
    1  d
        0.1308362        0.0016925
    2  f
        1.0809860        1.0
        0.4161474        1.0
    1  g
        0.6707100       -0.0044361
*
cl universal
cl def2-SV(P)
cl def2-SVP
cl def2-TZVP
cl def2-TZVPP
cl def2-QZVP
cl def2-QZVPP
# cl    (14s5p5d2f1g) / [8s4p3d1f1g]     {71111111/2111/311/2/1}
*
    7  s
     8044.2766240        0.8306605
     2924.5123954        1.6146203
     1110.8168739        5.0051398
      439.9050761        9.9863273
      181.1987287       11.3443970
       77.4148302        2.6726629
       34.1977273       -1.6043227
    1  s
       15.5648397        5.7539291
    1  s
        7.2707873        6.0638907
    1  s
        3.4711900       -0.3199326
    1  s
        1.6860808       -0.3947320
    1  s
        0.8293125        0.9334036
    1  s
        0.4110124        0.4864175
    1  s
        0.2042190        0.0781778
    2  p
       12.2564993        0.0563086
        4.8922575       -0.0563007
    1  p
        1.9265460        0.0469222
    1  p
        0.7525989       -0.0071758
    1  p
        0.2932189       -0.0162325
    3  d
       28.4370504       -0.0265404
        7.2772298        0.0134848
        2.3111621       -0.0136452
    1  d
        0.8580943       -0.0131608
    1  d
        0.3376227       -0.0045372
    2  f
        1.2035685        1.0
        0.4700000        1.0
    1  g
        0.7521100       -0.0026699
```

```
*
ar universal
ar def2-SV(P)
ar def2-SVP
ar def2-TZVP
ar def2-TZVPP
ar def2-QZVP
ar def2-QZVPP
# ar    (14s5p5d2f1g) / [8s4p3d1f1g]     {71111111/2111/311/2/1}
*
    7  s
     9188.5309157        0.8877141
     3279.0428273        1.8231585
     1227.6297914        5.6127323
      481.1823792       11.2156190
      196.9697695       12.2962961
       83.9606192        2.3552090
       37.1435409       -1.5769042
    1  s
       16.9892190        7.1038677
    1  s
        8.0003093        6.4548370
    1  s
        3.8606959       -0.9952810
    1  s
        1.8996439       -0.1889378
    1  s
        0.9480149        1.2108212
    1  s
        0.4771798        0.5527940
    1  s
        0.2408781        0.0788216
    2  p
       14.10             0.0563086
        5.63            -0.0563007
    1  p
        2.22             1.0
    1  p
        0.87             1.0
    1  p
        0.34             1.0
    3  d
       32.70            -0.0265404
        8.37             0.0134848
        2.66            -0.0136452
    1  d
        0.99             1.0
    1  d
        0.39             1.0
    2  f
        1.38             1.0
        0.54             1.0
    1  g
        0.87             1.0
*
k universal
k def2-SV(P)
k def2-SVP
k def2-TZVP
k def2-TZVPP
k def2-QZVP
k def2-QZVPP
# k     (19s5p5d3f1g) / [8s4p4d1f1g]     {(12)1111111/2111/2111/3/1}
```

```
*
    12 s
    15600.4998000        0.6051572
     6840.8316412        0.5813049
     3055.5125810        2.2844173
     1389.0430931        4.7624289
      642.1465666        9.1248263
      301.6119674       12.2016392
      143.7961476        7.5846370
       69.5181492       -0.9813327
       34.0447209        0.1827059
       16.8706410        8.6437278
        8.4499772        5.8265076
        4.2728448       -1.6665361
    1  s
        2.1786969        0.0049863
    1  s
        1.1188238        1.5636047
    1  s
        0.5779194        0.6232905
    1  s
        0.2998881        0.0075801
    1  s
        0.1561261        0.0132062
    1  s
        0.0814421        0.0115103
    1  s
        0.0425117        0.0015798
    2  p
       35.0867756       -0.0129960
        8.2256301        0.0042675
    1  p
        1.9013059       -0.0148988
    1  p
        0.4358032        0.0356020
    1  p
        0.0996141       -0.0146255
    2  d
        4.3574288        0.0014449
        1.4555147       -0.0021214
    1  d
        0.4793580       -0.0045251
    1  d
        0.1565521        0.0065329
    1  d
        0.0509859        0.0004860
    3  f
        2.2961175       -0.0019497
        0.6766476       -0.0019950
        0.1981564        0.0021994
    1  g
        0.2814606       -0.0007654
*
ca universal
ca def2-SV(P)
ca def2-SVP
ca def2-TZVP
ca def2-TZVPP
ca def2-QZVP
ca def2-QZVPP
# ca    (19s5p5d3f1g) / [8s4p4d1f1g]     {(12)1111111/2111/2111/3/1}
*
    12 s
```

```
    17917.6370280        0.6831653
     8061.4596925        0.3918308
     3601.3424667        2.6391299
     1620.0122645        4.3734240
      778.4284854        9.5722795
      357.7554238       13.1715185
      172.7026048        8.9978572
       84.9193850       -0.4545484
       41.0281476       -0.4987409
       20.1494249        9.2079374
       10.2489427        7.2301219
        5.0555149       -1.9039492
    1  s
        2.6223894       -0.1384725
    1  s
        1.3458864        2.1173709
    1  s
        0.6963381        0.6153236
    1  s
        0.3565069       -0.0138892
    1  s
        0.1853829        0.0025927
    1  s
        0.0975465        0.0548225
    1  s
        0.0508517        0.0078906
    2  p
       12.5452782       -0.0060069
        3.5025409       -0.0066064
    1  p
        1.0011018        0.0257326
    1  p
        0.2902721       -0.0017144
    1  p
        0.0845726        0.0173409
    2  d
        9.5006987        0.0012657
        3.0210015        0.0029405
    1  d
        0.9763668       -0.0070814
    1  d
        0.3186918        0.0032026
    1  d
        0.1043687        0.0052962
    3  f
        2.4531931       -0.0083306
        0.7229365       -0.0006437
        0.2117121        0.0021253
    1  g
        0.9854875       -0.0019534
*
sc universal
sc def2-SV(P)
sc def2-SVP
sc def2-TZVP
sc def2-TZVPP
sc def2-QZVP
sc def2-QZVPP
# sc    (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12  s
    98612.7465040        0.2881537
     7210.3125501        3.0971477
```

```
     4075.8639445       -3.0468547
     2501.5115273        7.8667177
      846.2830005       10.7908312
      497.8135157        6.5247306
      298.0167777       11.8190682
      162.6523616        5.8011585
       59.6033884       -1.9154412
       35.0608157        2.5873650
       20.6240087        8.5944447
       12.1317695        6.9837735
    1  s
        4.4902120       -2.2231724
    1  s
        2.4506794        1.0865928
    1  s
        1.4817371        1.7596148
    1  s
        0.8376001        0.8693169
    1  s
        0.1765263        0.0611055
    1  s
        0.0997872        0.0229913
    1  s
        0.0606353        0.0108648
    1  p
       10.8099871       -0.0162612
    1  p
        3.2058514        0.0095104
    1  p
        0.9739254        0.0216819
    1  p
        0.3002684        0.0008927
    1  p
        0.0930355        0.0237489
    1  d
       15.0102726        0.0001270
    1  d
        4.2489449        0.0007224
    1  d
        1.2496854        0.0012863
    1  d
        0.3763665        0.0004464
    1  d
        0.1142632       -0.0000425
    2  f
        3.3095160       -0.0030594
        1.7054297       -0.0127954
    1  f
        0.8769316        0.0067473
    1  g
        5.4407205        0.0317423
    1  g
        1.7246112        0.0352184
    1  g
        0.5581653        0.0120819
*
ti universal
ti def2-SV(P)
ti def2-SVP
ti def2-TZVP
ti def2-TZVPP
ti def2-QZVP
ti def2-QZVPP
```

```
# ti    (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12 s
    19204.6235570        0.9150506
     8781.0703955        0.4699773
     4148.7833952        3.0298523
     1906.8876382        5.4371020
      908.9650422       11.0298634
      431.5745483       14.8132612
      211.1642070       10.3626783
      102.2548133       -0.5837071
       50.7017530       -0.6326340
       25.0892871       11.5043968
       12.7562921        8.4908452
        6.3986226       -3.0065313
    1  s
        3.2036391        0.4229386
    1  s
        1.6645345        2.7911389
    1  s
        0.8426907        0.7010768
    1  s
        0.4321995        0.0393570
    1  s
        0.2216023        0.0613957
    1  s
        0.1143336        0.0464437
    1  s
        0.0588697        0.0053964
    1  p
       16.7078840       -0.0072975
    1  p
        4.4154511       -0.0061159
    1  p
        1.2395226        0.0288908
    1  p
        0.3614638       -0.0035596
    1  p
        0.1067894        0.0242905
    1  d
       10.7607651        0.0008272
    1  d
        3.6392680       -0.0053072
    1  d
        1.3695124       -0.0115937
    1  d
        0.5931772       -0.0046652
    1  d
        0.2569230        0.0075375
    2  f
        3.1724794       -0.0155587
        1.1137039       -0.0010250
    1  f
        0.3885240        0.0064951
    1  g
        6.9650158       -0.0719791
    1  g
        2.1773896       -0.0829719
    1  g
        0.6876369       -0.0250650
*
v universal
v def2-SV(P)
```

```
v def2-SVP
v def2-TZVP
v def2-TZVPP
v def2-QZVP
v def2-QZVPP
# v     (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12 s
    11942.0842430        2.3430425
     2430.7110193        8.8888994
      841.0764301       14.7776882
      494.7508273        7.1901959
      291.0298903       13.5563769
      171.1940483        2.2742542
       59.2366916       -2.0798226
       34.8451117        7.1058855
       20.4971240       11.0294860
       12.0571314        4.4034789
        7.0924300       -2.8965426
        4.1720176       -0.6430604
    1  s
        2.4541279        2.6822253
    1  s
        1.4436046        1.6657641
    1  s
        0.8491792        0.5747589
    1  s
        0.2938336        0.0898967
    1  s
        0.1728433        0.0335229
    1  s
        0.1016725        0.0338678
    1  s
        0.0598074        0.0024470
    1  p
       16.7130979       -0.0067910
    1  p
        4.7454037       -0.0065330
    1  p
        1.3889998        0.0295173
    1  p
        0.4142440       -0.0035054
    1  p
        0.1243234        0.0236494
    1  d
        7.7143225        0.0046868
    1  d
        3.1170731        0.0011054
    1  d
        1.2767950       -0.0036313
    1  d
        0.5273386        0.0020859
    1  d
        0.2184050        0.0056681
    2  f
        3.1309344       -0.0188627
        1.0419780        0.0031524
    1  f
        0.3559044        0.0055024
    1  g
        8.7130110        0.0338121
    1  g
        2.7493872        0.0411332
```

```
    1  g
        0.8775089        0.0133622
*
cr universal
cr def2-SV(P)
cr def2-SVP
cr def2-TZVP
cr def2-TZVPP
cr def2-QZVP
cr def2-QZVPP
# cr    (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12 s
    22068.3284240        1.2311186
    10310.8895880       -0.1803545
     5874.1996884        3.0996748
     3056.7316460        3.3857089
     1578.4919380        8.9414617
      809.3861699       12.2195628
      438.3568734       15.0612186
      220.5886040        9.9023470
      115.7826755       -2.5664082
       50.5886272        2.0386762
       26.0501639       15.6667257
       13.2120964        5.6715887
    1  s
        7.0565191       -4.1324257
    1  s
        3.2438287        2.5134865
    1  s
        1.6625711        2.9303082
    1  s
        0.7341156        0.4812524
    1  s
        0.3736963        0.0398902
    1  s
        0.1924875        0.0948590
    1  s
        0.0837506        0.0209393
    1  p
       19.1759031       -0.0162825
    1  p
        4.7052443        0.0058134
    1  p
        1.2925721        0.0328032
    1  p
        0.3825208       -0.0085505
    1  p
        0.1161954        0.0104898
    1  d
       31.2759498       -0.0008406
    1  d
        7.1528914       -0.0242658
    1  d
        1.8136115       -0.0434567
    1  d
        0.4919052       -0.0034061
    1  d
        0.1365942        0.0036109
    2  f
        2.8679160       -0.0195047
        0.5851052        0.0115724
    1  f
```

```
        0.1339202        0.0014336
    1  g
       12.4142739        0.0193619
    1  g
        4.4448953        0.0312836
    1  g
        1.6427198        0.0145788
*
mn universal
mn def2-SV(P)
mn def2-SVP
mn def2-TZVP
mn def2-TZVPP
mn def2-QZVP
mn def2-QZVPP
# mn    (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12 s
    17733.2246460        2.0292530
     3609.4490442        7.9031521
     1299.6563311       12.7657954
      749.4399737       10.3339893
      440.8470310       14.0664479
      254.2121170        8.7966524
       89.7307132       -2.0086132
       52.7827710        2.3261543
       31.6727660       13.1659295
       17.9040623       10.1098077
       10.7434900       -2.4278177
        6.3196998       -2.1609521
    1  s
        3.7921915        2.0643421
    1  s
        2.2307008        3.3646654
    1  s
        1.2609763        1.1171104
    1  s
        0.7417507        0.2966517
    1  s
        0.2670826        0.0932427
    1  s
        0.1540118        0.0256140
    1  s
        0.0905952        0.0345786
    1  p
        2.7199275       -0.0169210
    1  p
        1.1743733        0.0478257
    1  p
        0.5068762       -0.0275246
    1  p
        0.2187287        0.0104273
    1  p
        0.0943798        0.0149334
    1  d
       11.5225001       -0.0037389
    1  d
        3.7793049        0.0204126
    1  d
        1.2528632       -0.0153393
    1  d
        0.4180182        0.0027280
    1  d
```

```
        0.1397732        0.0059124
    2  f
        6.9646522       -0.0024120
        2.4170922       -0.0049219
    1  f
        0.8415789        0.0029075
    1  g
        5.9366152        0.0015904
    1  g
        1.4312160       -0.0012821
    1  g
        0.3465192        0.0000505
*
fe universal
fe def2-SV(P)
fe def2-SVP
fe def2-TZVP
fe def2-TZVPP
fe def2-QZVP
fe def2-QZVPP
# fe    (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12 s
    22231.1675350        1.5463792
    10088.6252560        0.5616730
     4961.4420234        4.8306560
     2333.9778892        7.2162778
     1195.0581566       13.7667481
      605.7548994       17.3953035
      312.9849847       13.5974545
      146.2270422       -0.1052884
       73.1574429       -1.5186939
       37.1905224       16.4954218
       18.7270618       11.2685887
        9.8648356       -5.1127291
    1  s
        4.9921254        1.3183030
    1  s
        2.5312760        4.6550254
    1  s
        1.2321766        1.3101855
    1  s
        0.6265715        0.1513152
    1  s
        0.3212932        0.0845107
    1  s
        0.1627967        0.0694777
    1  s
        0.0808724        0.0157801
    1  p
       19.0489263       -0.0062879
    1  p
        5.1364325       -0.0049488
    1  p
        1.3971534        0.0270354
    1  p
        0.3820476       -0.0123603
    1  p
        0.1046543        0.0199595
    1  d
       13.4494385       -0.0256685
    1  d
        4.6650265       -0.0262829
```

```
    1  d
        1.5953692       -0.0486537
    1  d
        0.5410331       -0.0025964
    1  d
        0.1829694        0.0085806
    2  f
        4.4300720       -0.0066965
        0.6208564        0.0038112
    1  f
        0.0884909       -0.0000953
    1  g
       11.9744409       -0.0555001
    1  g
        3.6312678       -0.0560530
    1  g
        1.0943052       -0.0150572
*
co universal
co def2-SV(P)
co def2-SVP
co def2-TZVP
co def2-TZVPP
co def2-QZVP
co def2-QZVPP
# co    (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12 s
    22984.7412470        1.8791745
    11624.1099270       -0.1009719
     5640.3127898        5.4867635
     2645.0376429        6.3829372
     1371.0418944       15.3176605
      651.5910470       19.3841517
      339.5908122       13.7760601
      160.5957974        0.4301535
       80.4014754       -2.4807282
       42.1316835       17.1669735
       21.1733240       12.7549558
       10.6983797       -5.3364495
    1  s
        5.3718887        1.8124877
    1  s
        2.7108298        4.9363750
    1  s
        1.3406445        1.4812423
    1  s
        0.6844781        0.3053361
    1  s
        0.3500673        0.1431234
    1  s
        0.1771067        0.0358756
    1  s
        0.0899548        0.0006055
    1  p
        2.4895098       -0.0477884
    1  p
        1.1178371        0.0779946
    1  p
        0.5057605       -0.0161107
    1  p
        0.2298817       -0.0180766
    1  p
```

```
        0.1046479        0.0010136
    1  d
       39.1009947        0.0120719
    1  d
       13.4136581       -0.0618794
    1  d
        4.5931057       -0.1016032
    1  d
        1.5710363       -0.0720917
    1  d
        0.5371633        0.0069216
    2  f
        6.3589028       -0.0139407
        1.8418252       -0.0015213
    1  f
        0.5359683        0.0085099
    1  g
       18.1954609        0.0650677
    1  g
        6.0833764        0.0994221
    1  g
        2.0211729        0.0493786
*
ni universal
ni def2-SV(P)
ni def2-SVP
ni def2-TZVP
ni def2-TZVPP
ni def2-QZVP
ni def2-QZVPP
# ni    (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12 s
    22563.9787840        2.3471633
     4592.7085051        9.4929055
     1589.1724040       16.2456582
      934.8072702       11.2020312
      549.8866141       16.9261542
      323.4627051       10.1481287
      111.9248052       -2.8026798
       65.8381188        4.5460584
       38.7283041       16.3485067
       22.7813547       10.6984945
       13.4007965       -3.9670080
        7.8828213       -1.7808478
    1  s
        4.6369536        3.6269036
    1  s
        2.7276197        4.3527387
    1  s
        1.6044821        1.1235414
    1  s
        0.9438130        0.6940712
    1  s
        0.5551841       -0.1256659
    1  s
        0.3265789        0.2262361
    1  s
        0.1130031        0.0396414
    1  p
        3.1875428       -0.0135476
    1  p
        1.2896458        0.0487879
```

```
    1  p
        0.5289442       -0.0368103
    1  p
        0.2187477        0.0141467
    1  p
        0.0907155        0.0114606
    1  d
        9.7032658        0.0023627
    1  d
        3.9764688        0.0179281
    1  d
        1.6295856       -0.0173793
    1  d
        0.6723272        0.0048241
    1  d
        0.2785147        0.0118576
    2  f
        2.2394071       -0.0066692
        0.6523378        0.0083570
    1  f
        0.1910373        0.0000690
    1  g
       15.9627506        0.0567298
    1  g
        5.1321451        0.0600436
    1  g
        1.6619205        0.0201898
*
cu universal
cu def2-SV(P)
cu def2-SVP
cu def2-TZVP
cu def2-TZVPP
cu def2-QZVP
cu def2-QZVPP
# cu    (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12 s
    22760.1575320        2.0757355
     7272.8802874        5.0748858
     2725.0817134       12.1893535
     1480.3337422       10.7340332
      870.7845298       16.9779033
      533.0245964       14.5404854
      313.5438715        8.6537292
      112.8979167       -4.1810761
       66.4105374        8.1507841
       39.0650209       16.8724469
       22.9794234        9.7250596
       13.5173075       -5.7359384
    1  s
        4.3193796        4.8879037
    1  s
        2.5408114        3.6509306
    1  s
        1.5552814        0.9780872
    1  s
        0.9148714        0.6622433
    1  s
        0.3294183        0.1696094
    1  s
        0.1139855        0.0204929
    1  s
```

```
        0.0670503       -0.0018056
    1  p
       10.4327236        0.0125183
    1  p
        4.0251086       -0.0626251
    1  p
        1.5534382        0.0553108
    1  p
        0.5996423        0.0049618
    1  p
        0.2314823       -0.0265968
    2  d
       19.6140080       -0.0211366
        7.2975860        0.0263009
    1  d
        2.7500946       -0.0031456
    1  d
        1.0444408       -0.0146906
    1  d
        0.3976934        0.0008400
    1  f
        5.8169042       -0.0043051
    1  f
        0.7156542        0.0031524
    1  f
        0.0892019       -0.0001229
    1  g
       15.3794722        0.0065104
    1  g
        4.2631148        0.0047914
    1  g
        1.1926492       -0.0006660
*
zn universal
zn def2-SV(P)
zn def2-SVP
zn def2-TZVP
zn def2-TZVPP
zn def2-QZVP
zn def2-QZVPP
# zn    (19s5p5d3f3g) / [8s5p5d2f3g]     {(12)1111111/11111/11111/21/111}
*
    12 s
    30551.9544690        2.1427401
     6218.5939138        8.8047088
     2151.7624792       16.0008682
     1265.7425993       11.2584053
      744.5544493       19.5302706
      437.9731932       13.5622422
      257.6312829        3.0481957
      151.5478092       -2.5872090
       52.4386854       17.8287839
       30.8462846       14.3096651
       10.6734543       -5.5459298
        6.2785024        4.7543194
    1  s
        3.6932366        4.7018703
    1  s
        2.1724920        3.0337446
    1  s
        1.2779365        0.4322469
    1  s
        0.7517273        0.3677663
```

```
    1  s
        0.2601132        0.1189962
    1  s
        0.1530078        0.0319696
    1  s
        0.0900046        0.0110124
    1  p
        3.2312922       -0.0273613
    1  p
        1.3537231        0.0327360
    1  p
        0.5635201       -0.0173812
    1  p
        0.2336862        0.0156617
    1  p
        0.0967846        0.0066581
    1  d
       15.2191565       -0.0039712
    1  d
        5.1494048        0.0267318
    1  d
        1.7418300       -0.0226252
    1  d
        0.5890930        0.0091283
    1  d
        0.1992225        0.0094735
    2  f
        6.3320732        0.0043183
        2.2893036       -0.0028012
    1  f
        0.8347658        0.0013646
    1  g
       13.7400089        0.0011933
    1  g
        3.3877103        0.0005860
    1  g
        0.8352674       -0.0004519
*
ga universal
ga def2-SV(P)
ga def2-SVP
ga def2-TZVP
ga def2-TZVPP
ga def2-QZVP
ga def2-QZVPP
# ga    (19s5p5d3f1g) / [8s4p3d2f1g]     {(12)1111111/2111/311/21/1}
*
    12 s
    22118.8686370        3.6312148
    11563.1894470       -1.1372003
     6066.9073717        8.7100393
     3064.1629886        7.9912451
     1582.3294729       20.7576561
      785.5319670       22.0229881
      420.5746558       15.8971216
      218.3678189       -1.8721945
      107.8151898       -0.1109626
       51.4202463       24.3297099
       27.1061684       10.8281431
       13.4767963       -7.2300603
    1  s
        6.6121251        5.6014149
    1  s
```

```
        3.3168950        6.9420357
    1  s
        1.5368355        1.3608401
    1  s
        0.8029702        0.1002162
    1  s
        0.3746460        0.2175493
    1  s
        0.1924527        0.0867454
    1  s
        0.0894794        0.0132891
    2  p
        6.4816513        1.0
        1.9990599        1.0
    1  p
        0.6508461        0.0110696
    1  p
        0.2192172        0.0461054
    1  p
        0.0746963        0.0015543
    3  d
       23.3115125       -0.0026250
        6.5778878        0.0200621
        1.8734606       -0.0169174
    1  d
        0.5365944        0.0187423
    1  d
        0.1539803        0.0052865
    2  f
        2.0365377       -0.0012599
        0.5063106        0.0032855
    1  f
        0.1257500        0.0008062
    1  g
        0.9825567       -0.0007256
*
ge universal
ge def2-SV(P)
ge def2-SVP
ge def2-TZVP
ge def2-TZVPP
ge def2-QZVP
ge def2-QZVPP
# ge    (19s5p5d3f1g) / [8s4p3d2f1g]     {(12)1111111/2111/311/21/1}
*
    12 s
    28796.4428680        2.8646544
    14646.9616880       -0.4061824
     7471.7899835        7.2992336
     3895.3057027        7.0744512
     2011.5304056       18.8178893
     1021.2184280       22.5492061
      530.7010175       21.3994917
      255.3655914        1.6377927
      131.8672763       -3.2635898
       62.5282421       21.6195717
       33.3202533       17.5304788
       16.2383651       -7.4182512
    1  s
        7.8587116        3.4606933
    1  s
        4.2116039        8.7192549
    1  s
```

```
        2.0601257        2.3311726
    1  s
        1.0018843       -0.0201682
    1  s
        0.4972238        0.3303515
    1  s
        0.2356806        0.1861312
    1  s
        0.1116319        0.0254341
    2  p
        7.6822072        1.0
        2.4152641        1.0
    1  p
        0.7834626        0.0166683
    1  p
        0.2590749        0.0404441
    1  p
        0.0862290        0.0021630
    3  d
        6.0738920       -0.0201057
        1.9956548        0.0227678
        0.7038653       -0.0238263
    1  d
        0.2596990       -0.0153831
    1  d
        0.0973145       -0.0006119
    2  f
        2.4274828       -0.0023660
        0.7006729        0.0061731
    1  f
        0.2019000        0.0012003
    1  g
        0.8994605       -0.0024009
*
as universal
as def2-SV(P)
as def2-SVP
as def2-TZVP
as def2-TZVPP
as def2-QZVP
as def2-QZVPP
# as    (19s5p5d3f1g) / [8s4p3d2f1g]     {(12)1111111/2111/311/21/1}
*
    12 s
    26349.9022630        3.0537145
     9117.6127284        5.5690714
     3154.8831200       22.1466660
     1091.6549976       35.2107294
      642.1499806        6.7189378
      377.7352721       16.8044997
      222.1972126       -7.5350959
       76.8848444       13.2913279
       45.2263778       23.1205976
       26.6037509        3.5902044
       15.6492648       -7.8992726
        9.2054496        3.3276883
    1  s
        5.4149702        8.1289430
    1  s
        3.1852765        4.6135976
    1  s
        1.8736920        0.5288351
    1  s
```

```
        0.6483363        0.1749183
    1  s
        0.3813743        0.3997195
    1  s
        0.2243378        0.1053646
    1  s
        0.1319634        0.0371426
    2  p
        7.2637315        0.0100015
        2.4151705       -0.0279590
    1  p
        0.8192826        0.0291851
    1  p
        0.2813347        0.0246331
    1  p
        0.0970052        0.0001270
    3  d
       22.8613405       -0.0028615
        7.4219103        0.0114491
        2.4809102       -0.0120303
    1  d
        0.8443001        0.0114339
    1  d
        0.2890752       -0.0069375
    2  f
        2.8008427       -0.0029300
        0.9558538        0.0064388
    1  f
        0.3262074        0.0025260
    1  g
        0.8920726       -0.0029234
*
se universal
se def2-SV(P)
se def2-SVP
se def2-TZVP
se def2-TZVPP
se def2-QZVP
se def2-QZVPP
# se    (19s5p5d3f1g) / [8s4p3d2f1g]     {(12)1111111/2111/311/21/1}
*
    12 s
   182587.1093200        0.7871683
    20799.6860920        2.8434576
    10963.6341210        4.8057763
     3793.6448116       18.7809406
     1539.6773146       26.6954015
      836.2676977       20.3863962
      491.9221613       15.1527499
      176.2716372       -3.8835832
      100.1266273        5.9543421
       58.8980144       26.3213790
       33.4555214       11.6714825
       19.0063819       -8.6271219
    1  s
        7.0518801        8.2612206
    1  s
        4.1481646        7.5205447
    1  s
        2.3920173        0.9466243
    1  s
        0.8443241        0.0226109
    1  s
```

```
        0.4966612        0.6347290
    1  s
        0.2821158        0.2060473
    1  s
        0.1602725        0.0603877
    2  p
        8.7516826        0.0107828
        2.8944407       -0.0295335
    1  p
        0.9766426        0.0340864
    1  p
        0.3335879        0.0121968
    1  p
        0.1144109        0.0021419
    3  d
        7.8807486       -0.0168739
        2.6611416        0.0192822
        0.9250344       -0.0220267
    1  d
        0.3273259       -0.0087679
    1  d
        0.1165229       -0.0001791
    2  f
        3.0536409       -0.0031967
        0.8481417        0.0110377
    1  f
        0.2355400        0.0016419
    1  g
        0.9616190       -0.0038648
*
br universal
br def2-SV(P)
br def2-SVP
br def2-TZVP
br def2-TZVPP
br def2-QZVP
br def2-QZVPP
# br    (19s5p5d3f1g) / [8s4p3d2f1g]     {(12)1111111/2111/311/21/1}
*
    12 s
   181929.6907400        0.9703820
    21782.5062350        3.1341819
     7843.2391724       11.0443801
     2608.0271777       24.6916778
     1564.9696465       12.3123948
      920.5703545       24.6284398
      552.3963380       16.2668646
      191.1405907       -3.1865943
      108.0484426        5.1797612
       64.8354183       25.8419691
       38.1384803       15.5771030
       22.4343995       -9.1953776
    1  s
       13.1967052       -1.3048405
    1  s
        7.9187991        8.5738870
    1  s
        4.6581170        9.2928352
    1  s
        2.6331523        0.5617368
    1  s
        0.5577180        0.8600521
    1  s
```

```
        0.3152683        0.2596004
    1  s
        0.1854519        0.0721463
    2  p
        8.4481854        0.0134690
        3.0812881       -0.0389777
    1  p
        1.1536778        0.0500453
    1  p
        0.4389478       -0.0087970
    1  p
        0.1679158        0.0062473
    3  d
        8.7933629       -0.0194411
        3.5598266        0.0201204
        1.4866514       -0.0158267
    1  d
        0.6328484       -0.0103896
    1  d
        0.2711415       -0.0137988
    2  f
        3.4681858       -0.0029576
        0.8708007        0.0124094
    1  f
        0.2186427        0.0004936
    1  g
        1.1078575       -0.0027251
*
kr universal
kr def2-SV(P)
kr def2-SVP
kr def2-TZVP
kr def2-TZVPP
kr def2-QZVP
kr def2-QZVPP
# kr    (19s5p5d3f1g) / [8s4p3d2f1g]     {(12)1111111/2111/311/21/1}
*
    12  s
    25124.7655573        5.4122684
     5113.9351604       23.8184381
     3008.1970688       -8.4029924
     1769.5276379       45.6087554
      612.2932660       36.4135060
      360.1724993       -9.8041476
      211.8661701        2.6373869
      124.6271554       -0.1448996
       73.3100894       27.9730114
       43.1235808       18.4639348
       25.3668115       -8.3616758
       14.9216534       -3.2585745
    1  s
        8.7774429        9.6168737
    1  s
        5.1632016       10.6493759
    1  s
        3.0371773        0.1799607
    1  s
        1.0509263        0.0519737
    1  s
        0.6181920        1.0828540
    1  s
        0.3636423        0.2804390
    1  s
```

```
        0.2139072        0.1074628
    2  p
        9.72             0.0134690
        3.54            -0.0389777
    1  p
        1.33             1.0
    1  p
        0.50             1.0
    1  p
        0.19             1.0
    3  d
       10.11            -0.0194411
        4.09             0.0201204
        1.71            -0.0158267
    1  d
        0.73             1.0
    1  d
        0.31             1.0
    2  f
        3.99            -0.0029576
        1.00             0.0124094
    1  f
        0.25             1.0
    1  g
        1.27             1.0
*
rb universal-ecp28
rb def2-SV(P)
rb def2-SVP
rb def2-TZVP
rb def2-TZVPP
rb def2-QZVP
rb def2-QZVPP
# rb    (11s5p5d3f1g) / [8s4p4d1f1g]     {41111111/2111/2111/3/1}
*
    4  s
       14.8277116        0.0608401
        8.7221830       -0.4741652
        5.1306958        1.5852121
        3.0180562       -1.8427056
    1  s
        1.7753272       -0.7055656
    1  s
        1.0443101        1.0825966
    1  s
        0.6143000        0.9039138
    1  s
        0.3613529        0.2340875
    1  s
        0.0735504        0.0190446
    1  s
        0.0432649       -0.0010159
    1  s
        0.0254499        0.0007439
    2  p
        3.0726016        0.0090140
        1.1369353       -0.0358530
    1  p
        0.4569368        0.0387502
    1  p
        0.1936542        0.0104052
    1  p
        0.0835914       -0.0155420
```

```
    2  d
        1.3411819        0.0009034
        0.4379095       -0.0071483
    1  d
        0.1567271        0.0054534
    1  d
        0.0595258        0.0020127
    1  d
        0.0230791       -0.0000857
    3  f
        0.8445587       -0.0026174
        0.3153454       -0.0002409
        0.1184513        0.0017392
    1  g
        0.1808175       -0.0005805
*
sr universal-ecp28
sr def2-SV(P)
sr def2-SVP
sr def2-TZVP
sr def2-TZVPP
sr def2-QZVP
sr def2-QZVPP
# sr    (11s5p5d3f1g) / [8s4p4d1f1g]     {41111111/2111/2111/3/1}
*
    4  s
       31.8879343        0.0098846
        9.4301300       -0.4292237
        5.6307588        1.8718426
        3.3787864       -2.2401775
    1  s
        1.9875213       -1.0459798
    1  s
        1.1926297        1.5872570
    1  s
        0.6877236        1.0628047
    1  s
        0.4045433        0.1207048
    1  s
        0.1399804       -0.0014185
    1  s
        0.0823414        0.0523519
    1  s
        0.0416009        0.0055320
    2  p
        1.2481443       -0.0208349
        0.6134265        0.0441633
    1  p
        0.2972469       -0.0117882
    1  p
        0.1428327        0.0034458
    1  p
        0.0684432        0.0121751
    2  d
        6.8818940       -0.0017912
        2.2949967        0.0041742
    1  d
        0.7554207       -0.0072096
    1  d
        0.2467349        0.0030798
    1  d
        0.0803815        0.0033670
    3  f
```

```
        1.1408701       -0.0079217
        0.3641675        0.0018987
        0.1173184        0.0014617
    1  g
        0.5831166       -0.0019680
*
y universal-ecp28
y def2-SV(P)
y def2-SVP
y def2-TZVP
y def2-TZVPP
y def2-QZVP
y def2-QZVPP
# y     (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       18.4228114        0.0772748
       10.8369476       -0.6623447
        6.3746749        2.2907103
        3.7498086       -2.6367675
    1  s
        2.2278274       -1.2630679
    1  s
        1.3104867        2.1090354
    1  s
        0.7632421        1.0378195
    1  s
        0.4489659        0.0761421
    1  s
        0.1569050        0.0391803
    1  s
        0.0922971        0.0750974
    1  s
        0.0537548        0.0067681
    1  p
        1.9203007       -0.0189987
    1  p
        0.7990992        0.0569819
    1  p
        0.3478309       -0.0332631
    1  p
        0.1557017        0.0293924
    1  p
        0.0703636        0.0078524
    1  d
        5.7534743       -0.0019703
    1  d
        1.5794103        0.0085600
    1  d
        0.5341157        0.0058071
    1  d
        0.2098183       -0.0109252
    1  d
        0.0871171       -0.0012422
    2  f
        1.4562045       -0.0211924
        0.4296594        0.0072121
    1  f
        0.1278076        0.0057355
    1  g
        1.2949792       -0.0069217
    1  g
        0.3816201       -0.0034052
```

```
    1  g
        0.1117575       -0.0001238
*
zr universal-ecp28
zr def2-SV(P)
zr def2-SVP
zr def2-TZVP
zr def2-TZVPP
zr def2-QZVP
zr def2-QZVPP
# zr    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       31.9496472        0.0195674
       11.3910710       -0.5829896
        6.7006298        2.5436590
        3.9415468       -3.3335860
    1  s
        2.2841235       -1.1025801
    1  s
        1.3981576        2.4449632
    1  s
        0.8224456        0.9442535
    1  s
        0.4580096        0.2849803
    1  s
        0.1716120        0.0927324
    1  s
        0.0984717        0.0408062
    1  s
        0.0579245        0.0061353
    1  p
        4.1403511        0.0046965
    1  p
        1.8165899       -0.0261014
    1  p
        0.7885726        0.0484164
    1  p
        0.3401489       -0.0181762
    1  p
        0.1464135        0.0222905
    1  d
        2.3340737        0.0057914
    1  d
        1.0436609       -0.0117083
    1  d
        0.4601097       -0.0029746
    1  d
        0.2011495       -0.0048693
    1  d
        0.0876937        0.0011630
    2  f
        1.3813732       -0.0193482
        0.4572625        0.0096168
    1  f
        0.1536990        0.0035806
    1  g
        1.7041213        0.0409467
    1  g
        0.6942669        0.0321446
    1  g
        0.2810797        0.0088093
*
```

```
nb universal-ecp28
nb def2-SV(P)
nb def2-SVP
nb def2-TZVP
nb def2-TZVPP
nb def2-QZVP
nb def2-QZVPP
# nb    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       23.6097510        0.0912480
       12.9971517       -0.8368562
        7.6453831        2.7528925
        4.2087782       -3.5380896
    1  s
        2.5422363       -1.1550316
    1  s
        1.5561536        2.3966300
    1  s
        0.9153844        1.2961509
    1  s
        0.4653603        0.4380934
    1  s
        0.2045671        0.1218763
    1  s
        0.1112405        0.0160331
    1  s
        0.0687820        0.0028044
    1  p
        5.9462204        0.0130780
    1  p
        2.0624858       -0.0372894
    1  p
        0.7053392        0.0384440
    1  p
        0.2391997        0.0099773
    1  p
        0.0808938        0.0003522
    1  d
        2.7449282        0.0046132
    1  d
        1.1660024       -0.0368833
    1  d
        0.4883430       -0.0006567
    1  d
        0.2028178       -0.0019691
    1  d
        0.0840000       -0.0001161
    2  f
        1.3761326       -0.0164750
        0.6115734        0.0087170
    1  f
        0.2755593        0.0013529
    1  g
        1.8119518        0.0174156
    1  g
        0.6678930        0.0089653
    1  g
        0.2446494        0.0024517
*
mo universal-ecp28
mo def2-SV(P)
mo def2-SVP
```

```
mo def2-TZVP
mo def2-TZVPP
mo def2-QZVP
mo def2-QZVPP
# mo    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       22.6901662        0.1949917
       13.6509970       -1.4097522
        8.3560478        3.9693529
        4.9153221       -3.9889833
    1  s
        3.0020634       -1.8916027
    1  s
        1.7008034        2.8537224
    1  s
        1.0004726        1.3330890
    1  s
        0.5585539        0.5294105
    1  s
        0.2467601        0.1825446
    1  s
        0.1197869        0.0350951
    1  s
        0.0704629        0.0030547
    1  p
        1.7973997       -0.0280976
    1  p
        0.8392010        0.0586922
    1  p
        0.3863176       -0.0142975
    1  p
        0.1763512        0.0101649
    1  p
        0.0802794        0.0001163
    1  d
        2.5392437        0.0080985
    1  d
        1.1855659       -0.0103385
    1  d
        0.5457631       -0.0056162
    1  d
        0.2491370       -0.0102279
    1  d
        0.1134133       -0.0016306
    2  f
        1.7005722       -0.0210507
        0.7055475        0.0101358
    1  f
        0.2986974        0.0029125
    1  g
        2.0378148        0.0090181
    1  g
        0.7511470        0.0014579
    1  g
        0.2751454        0.0008835
*
tc universal-ecp28
tc def2-SV(P)
tc def2-SVP
tc def2-TZVP
tc def2-TZVPP
tc def2-QZVP
```

```
tc def2-QZVPP
# tc    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       24.8047177        0.1969662
       14.8842890       -1.3943496
        8.7554639        4.4802534
        5.2537931       -4.9671050
    1  s
        3.0753955       -1.8426465
    1  s
        1.7821012        3.4225978
    1  s
        1.0482948        1.2785008
    1  s
        0.5837533        0.6932854
    1  s
        0.2253937        0.1894790
    1  s
        0.1255127        0.0020034
    1  s
        0.0738310        0.0098414
    1  p
        7.6664708        0.0114058
    1  p
        2.6591660       -0.0353321
    1  p
        0.9093949        0.0508359
    1  p
        0.3084006       -0.0059814
    1  p
        0.1042965        0.0023174
    1  d
        5.6542827       -0.0077142
    1  d
        2.3987947        0.0119366
    1  d
        1.0009673        0.0293466
    1  d
        0.4136089        0.0093865
    1  d
        0.1703531        0.0019693
    2  f
        1.5866517       -0.0186055
        0.6286164        0.0125267
    1  f
        0.2618564       -0.0001327
    1  g
        2.2280694        0.0331682
    1  g
        0.8126598        0.0129781
    1  g
        0.2951546        0.0029686
*
ru universal-ecp28
ru def2-SV(P)
ru def2-SVP
ru def2-TZVP
ru def2-TZVPP
ru def2-QZVP
ru def2-QZVPP
# ru    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
```

```
    4  s
       26.6762856        0.2165048
       15.6919322       -1.6924857
        9.5102427        5.1491315
        5.5942603       -5.8321471
    1  s
        3.2101693       -1.6589959
    1  s
        1.8788006        3.7136026
    1  s
        1.1051768        1.5250798
    1  s
        0.5884287        0.7380653
    1  s
        0.2485272        0.1692541
    1  s
        0.1323232        0.0214899
    1  s
        0.0778372        0.0047811
    1  p
        8.7134989        0.0113560
    1  p
        2.8784139       -0.0343923
    1  p
        0.9374995        0.0488087
    1  p
        0.3027920       -0.0027843
    1  p
        0.0975236       -0.0016201
    1  d
        2.2115508        0.0078913
    1  d
        1.0869127       -0.0041759
    1  d
        0.5266832        0.0029830
    1  d
        0.2530812       -0.0066125
    1  d
        0.1212725       -0.0003084
    2  f
        1.7397365       -0.0181947
        0.7482841        0.0122301
    1  f
        0.3542304       -0.0007698
    1  g
        2.5071456        0.0729714
    1  g
        0.9241443        0.0347206
    1  g
        0.3385144        0.0042387
*
rh universal-ecp28
rh def2-SV(P)
rh def2-SVP
rh def2-TZVP
rh def2-TZVPP
rh def2-QZVP
rh def2-QZVPP
# rh    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       29.3101190        0.2308387
       17.2412460       -1.6855742
```

```
      10.1419091        5.4619560
       5.9658287       -6.5704893
    1  s
       3.3723789       -1.5692224
    1  s
       1.9837523        4.1042386
    1  s
       1.1496062        1.6157725
    1  s
       0.6728683        0.7715724
    1  s
       0.3958049        0.1915225
    1  s
       0.2282225        0.1354333
    1  s
       0.0907871        0.0031274
    1  p
       4.4734721       -0.0001018
    1  p
       2.1985809       -0.0346250
    1  p
       1.0653622        0.0806528
    1  p
       0.5119266       -0.0171196
    1  p
       0.2453071       -0.0152897
    1  d
       6.5749622        0.0235711
    1  d
       2.8104159       -0.0567584
    1  d
       1.2629928       -0.0593122
    1  d
       0.5856334        0.0099826
    1  d
       0.2744598        0.0050638
    2  f
       1.7971363       -0.0240558
       0.7726280        0.0164170
    1  f
       0.3300935        0.0041275
    1  g
       7.0667397        0.0081334
    1  g
       2.4807901        0.0572796
    1  g
       0.8654422        0.0167799
*
pd universal-ecp28
pd def2-SV(P)
pd def2-SVP
pd def2-TZVP
pd def2-TZVPP
pd def2-QZVP
pd def2-QZVPP
# pd    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
      51.0211803        0.0538811
      17.6543867       -1.3608599
      10.3849330        5.9322863
       6.2315704       -7.8659686
    1  s
```

```
        3.6656295       -1.3215872
    1  s
        2.1995933        4.1735311
    1  s
        1.2683839        2.2689133
    1  s
        0.7461081        0.6712480
    1  s
        0.4477087        0.3367069
    1  s
        0.2581689        0.0896295
    1  s
        0.1518640        0.0380638
    1  p
        5.6999676        0.0141426
    1  p
        2.5155374       -0.0569343
    1  p
        1.1229524        0.0732647
    1  p
        0.5047808       -0.0021359
    1  p
        0.2274325       -0.0233875
    1  d
        3.8006002        0.0012299
    1  d
        1.5882692       -0.0485992
    1  d
        0.6550157       -0.0041355
    1  d
        0.2680210        0.0031650
    1  d
        0.1093843       -0.0006315
    2  f
        2.0106185       -0.0150205
        0.8268460        0.0105330
    1  f
        0.3451253        0.0027275
    1  g
        7.5375072        0.0047006
    1  g
        2.7664349        0.0340131
    1  g
        1.0133462        0.0097463
*
ag universal-ecp28
ag def2-SV(P)
ag def2-SVP
ag def2-TZVP
ag def2-TZVPP
ag def2-QZVP
ag def2-QZVPP
# ag    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       33.0003921        0.2038586
       19.4119948       -1.6877257
       11.0829946        6.6111686
        6.5194084       -9.3277547
    1  s
        3.7221609       -0.4582552
    1  s
        2.2558505        4.4241274
```

```
    1  s
        1.3269709        2.3916529
    1  s
        0.7982463        0.7922029
    1  s
        0.3973142        0.3672976
    1  s
        0.1459674        0.0505674
    1  s
        0.0619668        0.0003115
    1  p
        8.6302966        0.0181446
    1  p
        2.6201449       -0.0579345
    1  p
        0.8433914        0.0710520
    1  p
        0.2816572       -0.0287439
    1  p
        0.0952523       -0.0047699
    1  d
        7.2207512       -0.0100289
    1  d
        3.2511233        0.0337244
    1  d
        1.4866000       -0.0143934
    1  d
        0.6861688       -0.0134013
    1  d
        0.3177130        0.0001632
    2  f
        4.3005188       -0.0015244
        1.6452068       -0.0021536
    1  f
        0.6333305        0.0034774
    1  g
        4.3915496        0.0028464
    1  g
        2.0620255        0.0033503
    1  g
        0.9729182       -0.0008695
*
cd universal-ecp28
cd def2-SV(P)
cd def2-SVP
cd def2-TZVP
cd def2-TZVPP
cd def2-QZVP
cd def2-QZVPP
# cd    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       51.9694461        0.0883266
       20.2189912       -1.7697622
       11.8935239        7.5473655
        7.1368136      -10.1983309
    1  s
        4.0343163       -1.0927616
    1  s
        2.4208270        5.3174660
    1  s
        1.4240158        2.6936134
    1  s
```

```
        0.7450006        0.8771888
    1  s
        0.2949185        0.1850001
    1  s
        0.1704979        0.0405807
    1  s
        0.1002929        0.0268722
    1  p
        1.8931176       -0.0250445
    1  p
        0.8838914        0.0320446
    1  p
        0.4068903       -0.0152044
    1  p
        0.1857425        0.0150557
    1  p
        0.0845546        0.0034040
    1  d
        8.6400749       -0.0050684
    1  d
        3.0268264        0.0281445
    1  d
        1.0897690       -0.0279352
    1  d
        0.3989943        0.0110911
    1  d
        0.1469111        0.0058711
    2  f
        3.2884486        0.0037392
        1.3487599       -0.0029125
    1  f
        0.5670248        0.0011575
    1  g
        5.9447998        0.0006741
    1  g
        2.0610067        0.0012980
    1  g
        0.7189977       -0.0009113
*
in universal-ecp28
in def2-SV(P)
in def2-SVP
in def2-TZVP
in def2-TZVPP
in def2-QZVP
in def2-QZVPP
# in    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/311/21/1}
*
    4  s
       49.9211080        0.1736250
       29.3653568       -0.8112730
       11.7138181        6.3143059
        6.8904810      -12.3674999
    1  s
        4.0937562        1.8377240
    1  s
        2.4080918        5.2955492
    1  s
        1.4815213        2.5377656
    1  s
        0.7966937        0.7816533
    1  s
        0.2883217        0.2330778
```

```
    1  s
        0.1696010        0.0610977
    1  s
        0.0856835        0.0154366
    2  p
        3.7832538        1.0
        1.3534047        1.0
    1  p
        0.5058912        0.0168893
    1  p
        0.1943310        0.0376631
    1  p
        0.0753446        0.0026298
    3  d
        9.5381158       -0.0036902
        3.3034566        0.0200371
        1.1799064       -0.0213596
    1  d
        0.4294894        0.0160099
    1  d
        0.1573383        0.0057634
    2  f
        1.1653200       -0.0017274
        0.3487082        0.0022936
    1  f
        0.1039500        0.0005247
    1  g
        0.6332593       -0.0007994
*
sn universal-ecp28
sn def2-SV(P)
sn def2-SVP
sn def2-TZVP
sn def2-TZVPP
sn def2-QZVP
sn def2-QZVPP
# sn    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/311/21/1}
*
    4  s
       31.2387916       -0.4647563
       19.1218880        0.7746856
       11.2481691        4.9426802
        6.8852289      -13.7382140
    1  s
        4.1524054        4.5680214
    1  s
        2.2894704        5.7429605
    1  s
        1.3467473        2.0193063
    1  s
        0.5371532        0.3276598
    1  s
        0.2741191        0.2086801
    1  s
        0.1612465        0.0989278
    1  s
        0.0782836        0.0102271
    2  p
        4.2249132        1.0
        1.5867453        1.0
    1  p
        0.5870916        0.0256092
    1  p
```

```
        0.2153060        0.0322861
    1  p
        0.0787283        0.0016698
    3  d
        3.1923180       -0.0186449
        1.3067780        0.0245523
        0.5384098       -0.0179147
    1  d
        0.2227010       -0.0124363
    1  d
        0.0922357       -0.0007457
    2  f
        1.4966252       -0.0014873
        0.6167066        0.0017655
    1  f
        0.2536500        0.0025646
    1  g
        0.5747157       -0.0024205
*
sb universal-ecp28
sb def2-SV(P)
sb def2-SVP
sb def2-TZVP
sb def2-TZVPP
sb def2-QZVP
sb def2-QZVPP
# sb    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/311/21/1}
*
    4  s
       57.7143676        0.2216592
       33.9496271       -0.9373366
       13.1424655        7.5699431
        7.7308618      -15.5941282
    1  s
        4.6853613        2.9492367
    1  s
        2.7560948        6.8939008
    1  s
        1.6703571        2.8356894
    1  s
        0.8567648        0.2973843
    1  s
        0.3459747        0.4399703
    1  s
        0.1941107        0.1407647
    1  s
        0.1141828        0.0306082
    2  p
        4.8928790        0.0161202
        1.7252227       -0.0430711
    1  p
        0.6206252        0.0346402
    1  p
        0.2260065        0.0211668
    1  p
        0.0826410        0.0018079
    3  d
        3.1261744        0.0079150
        1.3258246       -0.0129211
        0.5750726        0.0118939
    1  d
        0.2528859       -0.0085159
    1  d
```

```
        0.1117206       -0.0016314
    2  f
        1.8404045        0.0032631
        0.9629380       -0.0072133
    1  f
        0.5029600        0.0087065
    1  g
        0.7040401       -0.0033090
*
te universal-ecp28
te def2-SV(P)
te def2-SVP
te def2-TZVP
te def2-TZVPP
te def2-QZVP
te def2-QZVPP
# te    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/311/21/1}
*
    4  s
       45.8923171        0.2824062
       25.9421266       -2.6481348
       15.2600740       10.3488865
        8.9765139      -15.0383635
    1  s
        5.2803021       -1.1878378
    1  s
        3.1684917        9.4677160
    1  s
        1.8638186        2.9347566
    1  s
        1.1184008        0.2761735
    1  s
        0.3869899        0.6025633
    1  s
        0.2276411        0.1700390
    1  s
        0.1339065        0.0616018
    2  p
        5.5689637        0.0192092
        2.0332966       -0.0471192
    1  p
        0.7319547        0.0394711
    1  p
        0.2612903        0.0128218
    1  p
        0.0930153        0.0011498
    3  d
        4.1438402        0.0169742
        1.6316912       -0.0193454
        0.6537365        0.0174281
    1  d
        0.2646969        0.0186739
    1  d
        0.1075556        0.0018136
    2  f
        1.7885159       -0.0030102
        0.7768242        0.0046119
    1  f
        0.3367900        0.0038150
    1  g
        0.7345132       -0.0041990
*
i  universal-ecp28
```

```
i def2-SV(P)
i def2-SVP
i def2-TZVP
i def2-TZVPP
i def2-QZVP
i def2-QZVPP
# i    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/311/21/1}
*
    4  s
      129.9537471        0.0331547
       25.6994960       -2.2540948
       15.6359930       10.9929981
        9.2032587      -17.9755829
    1  s
        5.4136814        1.3660383
    1  s
        3.1529885       10.6040521
    1  s
        1.8546991        1.8140037
    1  s
        0.6481820        0.2070696
    1  s
        0.3812835        0.7208308
    1  s
        0.2220638        0.1550170
    1  s
        0.1306257        0.0479420
    2  p
        6.3414007        0.0175949
        2.2502515       -0.0450366
    1  p
        0.7853950        0.0437747
    1  p
        0.2714491        0.0026449
    1  p
        0.0935145       -0.0009715
    3  d
       14.1399698        0.0037566
        5.2162306       -0.0186363
        1.9554103        0.0143662
    1  d
        0.7402137       -0.0132379
    1  d
        0.2811242       -0.0194808
    2  f
        1.8878261       -0.0038611
        0.7736294        0.0075270
    1  f
        0.3166600        0.0033025
    1  g
        0.9097867       -0.0028599
*
xe universal-ecp28
xe def2-SV(P)
xe def2-SVP
xe def2-TZVP
xe def2-TZVPP
xe def2-QZVP
xe def2-QZVPP
# xe    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/311/21/1}
*
    4  s
       50.8073424        0.5191416
```

```
      29.8866712       -3.6511464
      17.5803943       12.5652412
      10.3414081      -17.1144379
   1  s
       6.0831811       -2.8948770
   1  s
       3.5783417       13.6089205
   1  s
       2.1049068        1.7498122
   1  s
       0.7283414        0.2203818
   1  s
       0.4284361        0.8932188
   1  s
       0.2520212        0.2312029
   1  s
       0.1482478        0.0509501
   2  p
       7.17             0.0175949
       2.54            -0.0450366
   1  p
       0.89             1.0
   1  p
       0.31             1.0
   1  p
       0.11             1.0
   3  d
      15.98             0.0037566
       5.89            -0.0186363
       2.21             0.0143662
   1  d
       0.84             1.0
   1  d
       0.32             1.0
   2  f
       2.13            -0.0038611
       0.87             0.0075270
   1  f
       0.36             1.0
   1  g
       1.03             1.0
*
cs universal-ecp46
cs def2-SV(P)
cs def2-SVP
cs def2-TZVP
cs def2-TZVPP
cs def2-QZVP
cs def2-QZVPP
# cs    (11s5p5d3f1g) / [8s4p4d1f1g]     {41111111/2111/2111/3/1}
*
   4  s
      16.5325652       -0.0169720
       9.7250381        0.1460652
       5.7344868       -0.6702244
       3.3315825        1.7636965
   1  s
       1.9992444       -1.6178066
   1  s
       1.1528537       -0.9975717
   1  s
       0.6849307        1.2318250
   1  s
```

```
        0.4029004        0.6410558
    1  s
        0.2297292        0.1327203
    1  s
        0.0489643        0.0092818
    1  s
        0.0274712       -0.0006899
    2  p
        2.5056618        0.0117986
        0.8678690       -0.0355306
    1  p
        0.2966131        0.0475536
    1  p
        0.1005740       -0.0065267
    1  p
        0.0340126       -0.0019562
    2  d
        1.1521088        0.0016446
        0.4611706       -0.0096583
    1  d
        0.1881060        0.0032943
    1  d
        0.0776108        0.0025833
    1  d
        0.0321450        0.0001444
    3  f
        0.6157554       -0.0045421
        0.2296413        0.0003306
        0.0867322        0.0007464
    1  g
        0.2855416       -0.0009947
*
ba universal-ecp46
ba def2-SV(P)
ba def2-SVP
ba def2-TZVP
ba def2-TZVPP
ba def2-QZVP
ba def2-QZVPP
# ba    (11s5p5d3f1g) / [8s4p4d1f1g]     {41111111/2111/2111/3/1}
*
    4  s
       17.6467454       -0.2043885
       10.8570096        0.9988078
        6.5148441       -2.6422189
        3.8322611        4.5348196
    1  s
        2.2995820       -3.5333857
    1  s
        1.2999136       -0.7745134
    1  s
        0.7800246        1.2728578
    1  s
        0.4588380        0.9855216
    1  s
        0.0933926        0.0219396
    1  s
        0.0549368        0.0240349
    1  s
        0.0194505        0.0008734
    2  p
        3.3090543        0.0084477
        1.2476719       -0.0279101
```

```
    1  p
        0.4630816        0.0352309
    1  p
        0.1702794        0.0029967
    1  p
        0.0624200        0.0168317
    2  d
        1.3764634        0.0029492
        0.6669676       -0.0080408
    1  d
        0.3208320        0.0034124
    1  d
        0.1536602       -0.0047668
    1  d
        0.0734882       -0.0005866
    3  f
        2.0118372        0.0046272
        0.9229160       -0.0111932
        0.4226647        0.0000323
    1  g
        0.5296055       -0.0028225
*
la universal-ecp46
la def2-SV(P)
la def2-SVP
la def2-TZVP
la def2-TZVPP
la def2-QZVP
la def2-QZVPP
# la    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       17.6099386       -0.0360198
       10.3587871        0.2868368
        6.0934040       -1.2729320
        3.5843552        3.3276739
    1  s
        2.1084442       -3.8722091
    1  s
        0.7368611        1.7684916
    1  s
        0.4334477        0.4497990
    1  s
        0.2524448        0.0822052
    1  s
        0.1484969        0.0291853
    1  s
        0.0873511        0.0442031
    1  s
        0.0513830        0.0098434
    1  p
        4.2941634        0.0118889
    1  p
        1.5678515       -0.0340976
    1  p
        0.5644018        0.0424354
    1  p
        0.2014779        0.0042923
    1  p
        0.0717230        0.0107286
    1  d
        1.3700039        0.0051491
    1  d
```

```
        0.7087546       -0.0049203
    1  d
        0.3615157       -0.0068229
    1  d
        0.1828580       -0.0113111
    1  d
        0.0922343       -0.0036977
    2  f
        0.9957125       -0.0092472
        0.4731394       -0.0027479
    1  f
        0.2234196        0.0040615
    1  g
        1.6277423        0.0013551
    1  g
        0.5999926        0.0123505
    1  g
        0.2197775        0.0046045
*
hf universal-ecp60
hf def2-SV(P)
hf def2-SVP
hf def2-TZVP
hf def2-TZVPP
hf def2-QZVP
hf def2-QZVPP
# hf    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       22.7379198        0.3386767
       13.9893113       -1.8152067
        8.3944093        4.0726485
        4.9378877       -3.1262643
    1  s
        2.8474069       -2.2962445
    1  s
        1.7086116        2.1211369
    1  s
        1.0050656        1.6206345
    1  s
        0.5090252        0.2149525
    1  s
        0.2005007        0.1244491
    1  s
        0.1203369        0.0588904
    1  s
        0.0707864        0.0196081
    1  p
        8.6876159        0.0044404
    1  p
        2.9520544       -0.0177117
    1  p
        0.9882283        0.0337688
    1  p
        0.3279003       -0.0133848
    1  p
        0.1084804        0.0329225
    1  d
        5.3853247       -0.0078752
    1  d
        1.8910042        0.0251620
    1  d
        0.7054322       -0.0162403
```

```
    1  d
        0.2733923       -0.0096680
    1  d
        0.1073454        0.0033310
    2  f
        1.5856277       -0.0163882
        0.5025690        0.0070772
    1  f
        0.1806953        0.0004404
    1  g
        1.5143193       -0.0150935
    1  g
        0.6169406       -0.0141241
    1  g
        0.2497735       -0.0025013
*
ta universal-ecp60
ta def2-SV(P)
ta def2-SVP
ta def2-TZVP
ta def2-TZVPP
ta def2-QZVP
ta def2-QZVPP
# ta    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       22.8527132        0.3259813
       13.7139915       -2.0490751
        8.4118450        4.8778884
        5.2011925       -3.6263453
    1  s
        2.9545148       -2.6165030
    1  s
        1.8085175        2.1737443
    1  s
        1.0638338        1.6708589
    1  s
        0.5459089        0.5223169
    1  s
        0.2367153        0.1950698
    1  s
        0.1273732        0.0434717
    1  s
        0.0749254        0.0028228
    1  p
        4.9406412        0.0186019
    1  p
        1.8988299       -0.0516289
    1  p
        0.7195251        0.0482579
    1  p
        0.2703718       -0.0021739
    1  p
        0.1013138        0.0038548
    1  d
        2.7629851        0.0070240
    1  d
        1.1049374       -0.0353551
    1  d
        0.4659311        0.0028396
    1  d
        0.2031096       -0.0005468
    1  d
```

```
        0.0895480       -0.0009639
    2  f
        1.1163028       -0.0135587
        0.4585788        0.0111379
    1  f
        0.1960556        0.0002303
    1  g
        1.4844387        0.0158316
    1  g
        0.5603502        0.0076635
    1  g
        0.2110499        0.0021677
*
w universal-ecp60
w def2-SV(P)
w def2-SVP
w def2-TZVP
w def2-TZVPP
w def2-QZVP
w def2-QZVPP
# w     (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       23.3623178        0.4033255
       14.3384253       -2.2969338
        8.6473457        5.4965831
        5.2932130       -4.3250365
    1  s
        3.1136546       -2.5431511
    1  s
        1.7817313        2.6046978
    1  s
        1.0773891        1.4503417
    1  s
        0.6337583        0.4700192
    1  s
        0.3727990        0.2286580
    1  s
        0.2192935        0.1647729
    1  s
        0.1080597        0.0280397
    1  p
        1.7902753       -0.0284183
    1  p
        0.8321368        0.0614570
    1  p
        0.3852473       -0.0276493
    1  p
        0.1779303        0.0276737
    1  p
        0.0821137        0.0011607
    1  d
        2.4029601        0.0110485
    1  d
        1.1219355       -0.0169485
    1  d
        0.5164715       -0.0056947
    1  d
        0.2357655       -0.0124397
    1  d
        0.1073263       -0.0014511
    2  f
        1.4801525       -0.0249226
```

```
        0.6352033        0.0149743
    1  f
        0.2766107        0.0029713
    1  g
        1.6963435        0.0104289
    1  g
        0.6692890        0.0028665
    1  g
        0.2671445        0.0018391
*
re universal-ecp60
re def2-SV(P)
re def2-SVP
re def2-TZVP
re def2-TZVPP
re def2-QZVP
re def2-QZVPP
# re    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       25.3049480        0.4805131
       15.2611343       -2.6865851
        9.3416450        5.8254490
        5.4950851       -4.3673994
    1  s
        3.1062758       -3.3092765
    1  s
        1.9014134        3.4285862
    1  s
        1.1184785        1.5101625
    1  s
        0.5851929        0.6972014
    1  s
        0.2559532        0.2231023
    1  s
        0.1339158        0.0426337
    1  s
        0.0787740        0.0208274
    1  p
        2.2033341       -0.0420046
    1  p
        1.0225949        0.1026822
    1  p
        0.4813040       -0.0514707
    1  p
        0.2284716        0.0024308
    1  p
        0.1087638        0.0204922
    1  d
        6.4096346       -0.0075077
    1  d
        2.3402359        0.0228025
    1  d
        0.8424480       -0.0144468
    1  d
        0.3007337       -0.0132026
    1  d
        0.1070565        0.0005463
    2  f
        5.9179950        0.0027189
        1.9083953       -0.0176365
    1  f
        0.6243117        0.0094236
```

```
    1  g
        1.8573388        0.0041593
    1  g
        0.8348138       -0.0021146
    1  g
        0.3813500        0.0005980
*
os universal-ecp60
os def2-SV(P)
os def2-SVP
os def2-TZVP
os def2-TZVPP
os def2-QZVP
os def2-QZVPP
# os    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       26.0004809        0.4711836
       15.9154135       -2.4793345
        9.3620077        5.8099433
        5.3039968       -5.3265065
    1  s
        3.1130468       -2.5947463
    1  s
        1.9055581        3.5118664
    1  s
        1.1209165        1.5682106
    1  s
        0.5864575        0.8187971
    1  s
        0.2565159        0.2727158
    1  s
        0.1342077        0.0326954
    1  s
        0.0789457        0.0010249
    1  p
        9.5838254        0.0170831
    1  p
        3.1659172       -0.0445201
    1  p
        1.0311393        0.0620311
    1  p
        0.3330356       -0.0153384
    1  p
        0.1072645        0.0023930
    1  d
        8.0476299        0.0036460
    1  d
        2.3090979       -0.0121265
    1  d
        0.7062430        0.0121501
    1  d
        0.2249058        0.0042197
    1  d
        0.0726195       -0.0000666
    2  f
        1.6056776       -0.0197608
        0.5636757        0.0153960
    1  f
        0.1966425        0.0002588
    1  g
        1.9148331        0.0690279
    1  g
```

```
        0.7411062        0.0285502
    1  g
        0.2850409        0.0025849
*
ir universal-ecp60
ir def2-SV(P)
ir def2-SVP
ir def2-TZVP
ir def2-TZVPP
ir def2-QZVP
ir def2-QZVPP
# ir    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       26.6307757        0.5177215
       16.0607263       -2.9928774
        9.8310912        6.7312034
        5.7829947       -5.3059791
    1  s
        3.2690260       -3.7224154
    1  s
        2.0010361        4.0557144
    1  s
        1.1770800        1.6057191
    1  s
        0.6490030        1.1003734
    1  s
        0.2810451        0.3067754
    1  s
        0.1409322        0.0240663
    1  s
        0.0829013       -0.0011294
    1  p
        8.1966999        0.0218374
    1  p
        3.0002158       -0.0600483
    1  p
        1.0827372        0.0802816
    1  p
        0.3874799       -0.0256075
    1  p
        0.1382825        0.0030556
    1  d
        3.9845055        0.0159746
    1  d
        1.4679208       -0.0885892
    1  d
        0.5748278        0.0114514
    1  d
        0.2339323       -0.0006577
    1  d
        0.0964630       -0.0007168
    2  f
        1.5804788       -0.0166654
        0.5284091        0.0154318
    1  f
        0.1755614       -0.0007255
    1  g
        2.0107759        0.0476884
    1  g
        0.7782394        0.0157387
    1  g
        0.2993228        0.0022449
```

```
*
pt universal-ecp60
pt def2-SV(P)
pt def2-SVP
pt def2-TZVP
pt def2-TZVPP
pt def2-QZVP
pt def2-QZVPP
# pt    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       27.3032355        0.4254407
       16.0607263       -2.8743600
        9.7344766        7.4335236
        5.7829947       -6.8140678
    1  s
        3.4017615       -2.9580148
    1  s
        2.0208964        4.1765425
    1  s
        1.1311508        1.8607076
    1  s
        0.6653828        0.8189852
    1  s
        0.3914016        0.3621985
    1  s
        0.2302363        0.1005450
    1  s
        0.1126025        0.0131958
    1  p
        6.1685356        0.0264002
    1  p
        2.7429261       -0.0836981
    1  p
        1.2025503        0.1053993
    1  p
        0.5228149       -0.0362309
    1  p
        0.2266651        0.0190001
    1  d
        3.0954010        0.0146421
    1  d
        1.3785036       -0.0540360
    1  d
        0.6220505        0.0043368
    1  d
        0.2829541       -0.0188703
    1  d
        0.1290536       -0.0013434
    2  f
        1.6832598       -0.0198753
        0.7163718        0.0180265
    1  f
        0.3083391       -0.0047508
    1  g
        2.1558237        0.0318404
    1  g
        0.8343779        0.0085873
    1  g
        0.3209146        0.0028695
*
au universal-ecp60
au def2-SV(P)
```

```
au def2-SVP
au def2-TZVP
au def2-TZVPP
au def2-QZVP
au def2-QZVPP
# au    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       28.2452505        0.4467851
       16.5778354       -3.0662858
       10.1476241        7.7959203
        5.9691905       -7.0482833
    1  s
        3.6538607       -3.2757558
    1  s
        2.1445411        4.1629636
    1  s
        1.2614947        2.2725427
    1  s
        0.7146933        0.9834560
    1  s
        0.4204078        0.3795078
    1  s
        0.2199551        0.1545322
    1  s
        0.0962081        0.0097466
    1  p
        7.5722886        0.0189551
    1  p
        2.6998544       -0.0609335
    1  p
        0.9635729        0.0823214
    1  p
        0.3441024       -0.0380237
    1  p
        0.1229071       -0.0058157
    1  d
        6.8027810       -0.0159795
    1  d
        2.9625600        0.0464398
    1  d
        1.3082794       -0.0265724
    1  d
        0.5826481       -0.0166250
    1  d
        0.2602216       -0.0055737
    2  f
        1.9754530       -0.0124600
        0.8157566        0.0106630
    1  f
        0.3408128        0.0015514
    1  g
        2.3463119        0.0098587
    1  g
        0.8956940        0.0008294
    1  g
        0.3442127        0.0002724
*
hg universal-ecp60
hg def2-SV(P)
hg def2-SVP
hg def2-TZVP
hg def2-TZVPP
```

```
hg def2-QZVP
hg def2-QZVPP
# hg    (11s5p5d3f3g) / [8s5p5d2f3g]     {41111111/11111/11111/21/111}
*
    4  s
       27.8729499        0.3331174
       16.3958524       -2.5730499
        9.6446188        8.4196819
        5.6733050      -10.6735979
    1  s
        1.9630812        4.2385175
    1  s
        1.1547536        2.1493341
    1  s
        0.6792668        0.6605303
    1  s
        0.3995687        0.3641900
    1  s
        0.2350404        0.1092528
    1  s
        0.1382591        0.0400156
    1  s
        0.0813289        0.0037425
    1  p
        1.6943070       -0.0184145
    1  p
        0.8362763        0.0260387
    1  p
        0.4059931       -0.0189702
    1  p
        0.1951779        0.0188931
    1  p
        0.0935262        0.0025395
    1  d
        8.3848824       -0.0084800
    1  d
        2.9083518        0.0300474
    1  d
        0.9946128       -0.0293901
    1  d
        0.3373002        0.0089540
    1  d
        0.1140699        0.0017339
    2  f
        3.7826413        0.0014967
        0.8757371       -0.0000768
    1  f
        0.2037884       -0.0006129
    1  g
        5.1623898        0.0003994
    1  g
        1.9992876        0.0033125
    1  g
        0.7792167       -0.0013159
*
tl universal-ecp60
tl def2-SV(P)
tl def2-SVP
tl def2-TZVP
tl def2-TZVPP
tl def2-QZVP
tl def2-QZVPP
# tl    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/131/21/1}
```

```
*
    4  s
       28.5237942        0.5451875
       16.9909666       -3.7517060
       10.2982993       10.5302531
        6.1795851      -11.2564261
    1  s
        3.6350500       -1.9626116
    1  s
        2.1812437        5.5760147
    1  s
        1.2578027        2.2023740
    1  s
        0.7398839        0.8787837
    1  s
        0.4541143        0.2896401
    1  s
        0.2357894        0.2238820
    1  s
        0.0866223        0.0146728
    2  p
        3.1078607        1.0
        1.2541619        1.0
    1  p
        0.4990026        0.0316199
    1  p
        0.1968827        0.0331157
    1  p
        0.0774648        0.0011608
    1  d
        6.8126425       -0.0043372
    3  d
        2.6804781        0.0216744
        1.0546514       -0.0246906
        0.4149594        0.0145071
    1  d
        0.1632685        0.0064427
    2  f
        1.0581890       -0.0008685
        0.4302107       -0.0012987
    1  f
        0.1747600        0.0013458
    1  g
        0.5623024       -0.0007528
*
pb universal-ecp60
pb def2-SV(P)
pb def2-SVP
pb def2-TZVP
pb def2-TZVPP
pb def2-QZVP
pb def2-QZVPP
# pb    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/131/21/1}
*
    4  s
       29.5485529        0.7353872
       18.1581268       -4.3747100
       10.9509655       11.7080215
        6.7033046      -11.4066284
    1  s
        3.9431203       -3.9493257
    1  s
        2.4167925        6.8862889
```

```
    1  s
        1.3325968        2.6098502
    1  s
        0.7327981        0.8901670
    1  s
        0.3018818        0.3647306
    1  s
        0.1633603        0.0578416
    1  s
        0.0960943        0.0300960
    2  p
        9.9012410        1.0
        3.9873925        1.0
    1  p
        1.5850638       -0.0680275
    1  p
        0.6252510        0.0297323
    1  p
        0.2460090        0.0343536
    3  d
        2.5385939       -0.0187104
        1.1178518        0.0268522
        0.5013434       -0.0164630
    1  d
        0.2273702       -0.0114406
    1  d
        0.1035045       -0.0018401
    2  f
        1.2755120        0.0006869
        0.5727848       -0.0030805
    1  f
        0.2584277        0.0032450
    1  g
        0.5880719       -0.0022264
*
bi universal-ecp60
bi def2-SV(P)
bi def2-SVP
bi def2-TZVP
bi def2-TZVPP
bi def2-QZVP
bi def2-QZVPP
# bi    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/131/21/1}
*
    4  s
       51.8020205       -0.2855255
       32.1121772        1.5761605
       19.0788827       -5.7114949
       11.3351005       13.6149056
    1  s
        6.6677060      -15.1911297
    1  s
        2.1778861        6.9883162
    1  s
        1.1696389        1.8934141
    1  s
        0.5448910        0.4982552
    1  s
        0.2762376        0.3268082
    1  s
        0.1624927        0.0964518
    1  s
        0.0881553        0.0131968
```

```
    2  p
        3.8557206        0.0289384
        1.5122274       -0.0641238
    1  p
        0.5833643        0.0499577
    1  p
        0.2228465        0.0150693
    1  p
        0.0848520        0.0006925
    3  d
        2.4355837        0.0063489
        1.1371674       -0.0112341
        0.5234833        0.0096554
    1  d
        0.2389664       -0.0092493
    1  d
        0.1087834       -0.0011776
    2  f
        1.4889569        0.0010265
        0.7030956       -0.0030812
    1  f
        0.3321300        0.0042284
    1  g
        0.6087002       -0.0028321
*
po universal-ecp60
po def2-SV(P)
po def2-SVP
po def2-TZVP
po def2-TZVPP
po def2-QZVP
po def2-QZVPP
# po    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/131/21/1}
*
    4  s
       31.3175589        0.7608235
       19.1251422       -4.9725625
       11.5341618       14.6710182
        7.0602907      -16.7007606
    1  s
        4.1531121       -1.0134009
    1  s
        2.4430070        8.1406266
    1  s
        1.4370629        1.6385569
    1  s
        0.7805294        0.8796028
    1  s
        0.3329869        0.5581481
    1  s
        0.1720601        0.1310083
    1  s
        0.1012118        0.0195393
    2  p
        5.0763703        0.0240603
        1.8637706       -0.0504364
    1  p
        0.6746659        0.0429801
    1  p
        0.2421813        0.0028049
    1  p
        0.0866931        0.0000694
    3  d
```

```
        3.1636527        0.0144840
        1.3438700       -0.0171571
        0.5628372        0.0149380
    1   d
        0.2337566        0.0151916
    1   d
        0.0968137        0.0014631
    2   f
        1.5891020        0.0023563
        0.8314513       -0.0059191
    1   f
        0.4345900        0.0069739
    1   g
        0.6841917       -0.0034581
*
at universal-ecp60
at def2-SV(P)
at def2-SVP
at def2-TZVP
at def2-TZVPP
at def2-QZVP
at def2-QZVPP
# at    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/131/21/1}
*
    4   s
       58.2038317       -0.1848414
       34.0669993        1.3286913
       20.0394108       -6.1129447
       12.1767940       15.6815457
    1   s
        7.1628198      -18.3107100
    1   s
        2.5537111        8.5932950
    1   s
        1.5021830        2.0720593
    1   s
        0.5816041        0.6620779
    1   s
        0.3057567        0.5336767
    1   s
        0.1798569        0.1184714
    1   s
        0.0998997        0.0185245
    2   p
        4.9506786        0.0303578
        1.8979309       -0.0665855
    1   p
        0.7173865        0.0601145
    1   p
        0.2688942       -0.0026528
    1   p
        0.1005083       -0.0008925
    3   d
       10.1118169        0.0067863
        4.0805739       -0.0229907
        1.6235678        0.0185183
    1   d
        0.6405826       -0.0148890
    1   d
        0.2520414       -0.0187209
    2   f
        1.5362787       -0.0014670
        0.7613943        0.0002276
```

```
    1  f
        0.3770300        0.0059035
    1  g
        0.8223522       -0.0028128
*
rn universal-ecp60
rn def2-SV(P)
rn def2-SVP
rn def2-TZVP
rn def2-TZVPP
rn def2-QZVP
rn def2-QZVPP
# rn    (11s5p5d3f1g) / [8s4p3d2f1g]     {41111111/2111/131/21/1}
*
    4  s
       97.3217241       -0.0611041
       57.2480714        0.2276353
       19.8090201       -3.3477431
       11.6523645       14.3525060
    1  s
        6.8543318      -22.8927171
    1  s
        4.0319598        6.6716344
    1  s
        2.3717410        7.2744033
    1  s
        1.3951417        1.0544772
    1  s
        0.4827480        0.9623629
    1  s
        0.2839694        0.3508958
    1  s
        0.1670408        0.1282619
    2  p
        4.9506786        0.0303578
        1.8979309       -0.0665855
    1  p
        0.7173865        1.0
    1  p
        0.2688942        1.0
    1  p
        0.1005083        1.0
    3  d
       10.1118169        0.0067863
        4.0805739       -0.0229907
        1.6235678        0.0185183
    1  d
        0.6405826        1.0
    1  d
        0.2520414        1.0
    2  f
        1.5362787       -0.0014670
        0.7613943        0.0002276
    1  f
        0.3770300        1.0
    1  g
        0.8223522        1.0
*
$end
```

Cartesian Coordinates of Test Set Molecules

```
#BaF
    0.00000000000000      0.00000000000000     -2.07069892703602      ba
    0.00000000000000      0.00000000000000      2.07069892703602      f
#BaF2
    0.00000000000000      0.00000000000000      1.55847796152849      ba
    3.50406263138391      0.00000000000000     -0.77923898076424      f
   -3.50406263138391      0.00000000000000     -0.77923898076424      f
#BaH2
    0.00000000000000      0.00000000000000      1.68536306424487      ba
    3.48553102731125      0.00000000000000     -0.84268153212243      h
   -3.48553102731125      0.00000000000000     -0.84268153212243      h
#BaO
    0.00000000000000      0.00000000000000     -1.92962468481039      ba
    0.00000000000000      0.00000000000000      1.92962468481039      o
#BaS
    0.00000000000000      0.00000000000000     -2.42999531404145      ba
    0.00000000000000      0.00000000000000      2.42999531404145      s
#Be2F4
   -2.13361594547065      0.00000000000000      0.00000000000000      be
    2.13361594547065      0.00000000000000      0.00000000000000      be
    0.00000000000000      2.13211302712278      0.00000000000000      f
    0.00000000000000     -2.13211302712278      0.00000000000000      f
   -4.78939030299712      0.00000000000000      0.00000000000000      f
    4.78939030299712      0.00000000000000      0.00000000000000      f
#Be2H4
    0.00000000000000      0.00000000000000     -1.92929449970282      be
    0.00000000000000      0.00000000000000      1.92931071700141      be
    2.05284948165387      0.00000000000000     -0.00000554462538      h
   -2.05284948165387      0.00000000000000     -0.00000554462538      h
    0.00000000000000      0.00000000000000     -4.46632923721534      h
    0.00000000000000      0.00000000000000      4.46632410916751      h
#Be4
    1.98239336244068     -1.40175406475758      0.00000000000000      be
   -1.98240276048822     -1.40176820517744      0.00000000000000      be
    0.00000469902377      1.40176113496751     -1.98238088228083      be
    0.00000469902377      1.40176113496751      1.98238088228083      be
#BeC2H6
    0.00000000000000      0.00000000000000      0.00000000000000      be
   -0.00020044556495      3.18689981828802      0.00000000000000      c
    0.00020044556495     -3.18689981828802      0.00000000000000      c
    1.94277443489397      3.99483630431448      0.00000000000000      h
    0.97131508976867     -3.99480784611534     -1.68303202724579      h
   -0.97131508976866      3.99480784611534     -1.68303202724579      h
   -1.94277443489397     -3.99483630431448      0.00000000000000      h
   -0.97131508976866      3.99480784611534      1.68303202724579      h
    0.97131508976867     -3.99480784611534      1.68303202724579      h
#BeF2O2H4
   -0.00000032363640     -0.00000008566633     -0.88438717282531      be
    0.00000013544101     -2.55923932656878     -2.01794116529110      f
   -0.00000415512240      2.55924102532360     -2.01793952586888      f
    2.70021194774609     -0.00000008523155      1.18317601953195      o
   -2.70021065005859      0.00000715003053      1.18318161817594      o
    3.67189018000387      1.47880857364976      0.63847717253928      h
   -3.67189013209522     -1.47881214872542      0.63847438690258      h
    3.67189002508221     -1.47880764617565      0.63847412415729      h
   -3.67188702736059      1.47880254336382      0.63848454267826      h
#BeH2
    0.00000000000000      0.00000000000000      0.00000000000000      be
    0.00000000000000      0.00000000000000      2.54057183216976      h
    0.00000000000000      0.00000000000000     -2.54057183216976      h
#BeS
    0.00000000000000      0.00000000000000     -1.67244267945864      be
    0.00000000000000      0.00000000000000      1.67244267945864      s
```

```
#CaCl2
    0.00000000000000      0.00000000000000      0.00000000000000      ca
    0.00000000000000      0.00000000000000     -4.87191849109726      cl
    0.00000000000000      0.00000000000000      4.87191849109726      cl
#CaF2
    0.00000000000000      0.00000000000000      0.00000000000000      ca
    0.00000000000000      0.00000000000000     -3.97143043764854      f
    0.00000000000000      0.00000000000000      3.97143043764854      f
#CaH2
    0.00000000000000      0.00000000000000      0.00000000000000      ca
    0.00000000000000      0.00000000000000      4.04362377931292      h
    0.00000000000000      0.00000000000000     -4.04362377931292      h
#CsF
    0.00000000000000      0.00000000000000     -2.43002010389848      f
    0.00000000000000      0.00000000000000      2.43002010389848      cs
#CsH
    0.00000000000000      0.00000000000000     -2.51401278411792      cs
    0.00000000000000      0.00000000000000      2.51401278411792      h
#CsO
    0.00000000000000      0.00000000000000     -2.61735090985010      o
    0.00000000000000      0.00000000000000      2.61735090985010      cs
#K2S
    0.00000000000000      0.00000000000000      1.75493373992356      s
   -4.68812462132366      0.00000000000000     -0.87746686996178      k
    4.68812462132366      0.00000000000000     -0.87746686996178      k
#K3P
    0.00000000000000      0.00000000000000      1.89749417626207      p
    2.58580346543032     -4.47874298051299     -0.63249805875402      k
    2.58580346543032      4.47874298051299     -0.63249805875402      k
   -5.17160693086064      0.00000000000000     -0.63249805875402      k
#KBr
    0.00000000000000      0.00000000000000     -2.75588742538509      k
    0.00000000000000      0.00000000000000      2.75588742538509      br
#KCl
    0.00000000000000      0.00000000000000     -2.59307106746649      k
    0.00000000000000      0.00000000000000      2.59307106746649      cl
#KF
    0.00000000000000      0.00000000000000     -2.13462007168556      k
    0.00000000000000      0.00000000000000      2.13462007168556      f
#KH
    0.00000000000000      0.00000000000000     -2.20252950247800      k
    0.00000000000000      0.00000000000000      2.20252950247800      h
#KI
    0.00000000000000      0.00000000000000     -3.00693295045154      k
    0.00000000000000      0.00000000000000      3.00693295045154      i
#Li2
    0.00000000000000      0.00000000000000      2.64099487417752      li
    0.00000000000000      0.00000000000000     -2.64099487417752      li
#Li2O
    0.00000000000000      0.00000000000000      0.00000000000000      o
    0.00000000000000      0.00000000000000      3.07886917104883      li
    0.00000000000000      0.00000000000000     -3.07886917104883      li
#Li4C4H12
    1.64706365185023     -1.64706414193258      1.64706544369022      li
   -1.64706403016091      1.64706609392631      1.64705887225055      li
   -1.64706511498339     -1.64706283357271     -1.64706684500640      li
    1.64706611886332      1.64706488898669     -1.64706698536379      li
   -2.43039744530168     -2.43039421024393      2.43039371335858      c
   -2.43039481981438      2.43039861558535     -2.43039404610143      c
    2.43041016795889     -2.43037962486503     -2.43040830076453      c
    2.43039584881608      2.43039712925517      2.43039442430495      c
   -3.75314966263209     -3.75314808906104      1.42781762772074      h
   -3.75315152314663      1.42782582005728     -3.75315082553213      h
```

```
    3.75314761464945     -3.75315658904388     -1.42781372983920      h
    3.75314887684819      1.42782119712603      3.75314726754457      h
    3.75315353972696     -1.42784583286734     -3.75312947798914      h
   -1.42781763382581      3.75315092168214     -3.75315637933721      h
   -1.42782024327477     -3.75314815761710      3.75314688009472      h
    3.75314899897099      3.75315138842044      1.42781694923781      h
    1.42781612597795     -3.75315104845671     -3.75315272040008      h
   -3.75315006597704     -1.42781843578250      3.75314714040825      h
    1.42782002306320      3.75315047748770      3.75314651403628      h
   -3.75316042760865      3.75314243091576     -1.42779552231280      h
#Li4Cl4
    2.74433107302748     -1.94051594179951      0.00000000000000      li
    0.00000067632057      1.94051446095008      2.74434044508148      li
   -2.74434673087586     -1.94050438549579      0.00000000000000      li
    0.00000067632057      1.94051446095008     -2.74434044508148      li
    3.45559531815124      2.44348827432849      0.00000000000000      cl
   -0.00000377172669     -2.44349841628354      3.45558889743391      cl
   -3.45557361860438      2.44349993543522      0.00000000000000      cl
   -0.00000377172669     -2.44349841628354     -3.45558889743391      cl
#Li4H4
    1.70080534683096      1.70080537092335      1.70080629791783      li
   -1.70080500921405      1.70080539807377     -1.70080575731674      li
   -1.70080602667080     -1.70080602949547      1.70080562105870      li
    1.70080538482293     -1.70080498514297     -1.70080576838347      li
   -1.85949824812399      1.85949816528516      1.85949815526986      h
   -1.85949848558192     -1.85949846568449     -1.85949840131317      h
    1.85949821284325     -1.85949826186725      1.85949814331282      h
    1.85949882509361      1.85949880790790     -1.85949829054584      h
#Li8
    2.74131108923626      2.74132478269676      2.74117649987501      li
   -2.74132095967384      2.74139733087893      2.74123662814823      li
   -2.74141505700265     -2.74140311587089      2.74132801066027      li
    2.74142424897969     -2.74136699425814      2.74128552508306      li
    2.74120592621730     -2.74115999255214     -2.74129238641303      li
    2.74113282151043      2.74114762466293     -2.74121705828456      li
   -2.74113063835797      2.74118015543297     -2.74125140645887      li
   -2.74120743090921     -2.74111979099044     -2.74126581261013      li
#LiBH4
   -0.00024869116689     -0.69457330488353      0.00000000000000      b
    0.00086758333408     -2.99344227721830      0.00000000000000      h
    1.10203755028072      0.22558430838791     -1.90940541026977      h
    1.10203755028072      0.22558430838791      1.90940541026977      h
   -2.20471760670618      0.22450989127912      0.00000000000000      h
    0.00002361397754      3.01233707404689      0.00000000000000      li
#LiCl
    0.00000000000000      0.00000000000000     -1.93849439881658      li
    0.00000000000000      0.00000000000000      1.93849439881658      cl
#LiF
    0.00000000000000      0.00000000000000     -1.48697136026104      li
    0.00000000000000      0.00000000000000      1.48697136026103      f
#LiH
    0.00000000000000      0.00000000000000      1.54697769798700      li
    0.00000000000000      0.00000000000000     -1.54697769798700      h
#LiSLi
    0.00000000000000      0.00000000000000      0.00000000000000      s
    0.00000000000000      0.00000000000000      3.94716240337943      li
    0.00000000000000      0.00000000000000     -3.94716240337943      li
#Mg4
    2.14509045506480     -2.14509045506480      2.14509045506480      mg
   -2.14509045506480      2.14509045506480      2.14509045506480      mg
   -2.14509045506480     -2.14509045506480     -2.14509045506480      mg
    2.14509045506480      2.14509045506480     -2.14509045506480      mg
#MgCl2
```

```
    0.00000000000000      0.00000000000000      0.00000000000000      mg
    0.00000000000000      0.00000000000000      4.14223402210192      cl
    0.00000000000000      0.00000000000000     -4.14223402210192      cl
#MgF
    0.00000000000000      0.00000000000000     -1.67915451808357      mg
    0.00000000000000      0.00000000000000      1.67915451808357      f
#MgF2
    0.00000000000000      0.00000000000000      0.00000000000000      mg
    0.00000000000000      0.00000000000000      3.32239429304949      f
    0.00000000000000      0.00000000000000     -3.32239429304949      f
#MgH2
    0.00000000000000      0.00000000000000      0.00000000000000      mg
    0.00000000000000      0.00000000000000      3.23157098894782      h
    0.00000000000000      0.00000000000000     -3.23157098894782      h
#Na2O
    0.00000000000000      0.00000000000000     -0.00125987003817      o
    3.76616708679694      0.00000000000000      0.00062993501909      na
   -3.76616708679694      0.00000000000000      0.00062993501909      na
#Na2S
    0.00000000000000      0.00000000000000      0.00000000000000      s
    0.00000000000000      0.00000000000000     -4.54664766104049      na
    0.00000000000000      0.00000000000000      4.54664766104049      na
#Na3N
    0.00000000000000      0.00000000000000      0.98846813029527      n
   -1.94602685234149      3.37061738114880     -0.32948937676509      na
   -1.94602685234149     -3.37061738114880     -0.32948937676509      na
    3.89205370468299      0.00000000000000     -0.32948937676509      na
#Na3P
    0.02166950952763     -0.00927750719924      1.85753834100637      p
    1.53863108521887     -3.99579517958087     -0.62708109943298      na
    2.65769485647032      3.35118326979984     -0.62224016723425      na
   -4.21799545121683      0.65388941698028     -0.60821707433915      na
#NaCl
    0.00000000000000      0.00000000000000     -2.23125548600731      na
    0.00000000000000      0.00000000000000      2.23125548600731      cl
#NaF
    0.00000000000000      0.00000000000000     -1.81647944104883      na
    0.00000000000000      0.00000000000000      1.81647944104883      f
#NaH
    0.00000000000000      0.00000000000000     -1.79420308214526      na
    0.00000000000000      0.00000000000000      1.79420308214526      h
#PLi3
   -0.00040508715227      1.96231380420593      0.00000000000000      p
    3.47020495828402     -0.65597305055359      0.00000000000000      li
   -1.73489993556587     -0.65317037682617      3.00666083679482      li
   -1.73489993556587     -0.65317037682617     -3.00666083679482      li
#RbF
    0.00000000000000      0.00000000000000     -2.29684487633273      f
    0.00000000000000      0.00000000000000      2.29684487633273      rb
#RbH
    0.00000000000000      0.00000000000000     -2.33735012066011      rb
    0.00000000000000      0.00000000000000      2.33735012066011      h
#RbO
    0.00000000000000      0.00000000000000     -2.46235472688576      o
    0.00000000000000      0.00000000000000      2.46235472688576      rb
#SrF
    0.00000000000000      0.00000000000000     -1.95487637299250      sr
    0.00000000000000      0.00000000000000      1.95487637299250      f
#SrF2
    0.00000000000000      0.00000000000000      1.21686253050211      sr
    3.54167198526231      0.00000000000000     -0.60843126525105      f
   -3.54167198526231      0.00000000000000     -0.60843126525105      f
#SrH2
```

```
    0.00000000000000      0.00000000000000      1.36780798604125      sr
   -3.52443250853761      0.00000000000000     -0.68390399302062      h
    3.52443250853761      0.00000000000000     -0.68390399302062      h
#SrO
    0.00000000000000      0.00000000000000     -1.83598401421036      sr
    0.00000000000000      0.00000000000000      1.83598401421036      o
#SrS
    0.00000000000000      0.00000000000000     -2.31673677279564      sr
    0.00000000000000      0.00000000000000      2.31673677279564      s
#B2H6
    0.00000000000000      0.00000000000000      1.68149280660034      b
    0.00000000000000      0.00000000000000     -1.68149280660034      b
    0.00000000000000     -1.88412562931544      0.00000000000000      h
    0.00000000000000      1.88412562931544      0.00000000000000      h
    1.99832414844106      0.00000000000000      2.79335654905377      h
   -1.99832414844106      0.00000000000000      2.79335654905377      h
   -1.99832414844106      0.00000000000000     -2.79335654905377      h
    1.99832414844106      0.00000000000000     -2.79335654905377      h
#B3N3H6
    2.75503008971104     -0.00000323939483      0.00000000000000      b
    1.33708167162979      2.31531468226869      0.00000000000000      n
   -1.37762869492974      2.38537342180479      0.00000000000000      b
   -2.67435276602476      0.00000211824938      0.00000000000000      n
   -1.37764337777651     -2.38537456910514      0.00000000000000      b
    1.33706851342589     -2.31531512981732      0.00000000000000      n
    5.05300245977585     -0.00000804976266      0.00000000000000      h
    2.30183999853162      3.98629277576524      0.00000000000000      h
   -2.52609075956054      4.37610354836293      0.00000000000000      h
   -4.60403920406282      0.00000416958359      0.00000000000000      h
   -2.52610296250991     -4.37610284086748      0.00000000000000      h
    2.30183503179008     -3.98628688708722      0.00000000000000      h
#B4H4
    1.13513007545606      1.13512970003633      1.13512888659479      b
   -1.13512170839976      1.13512235099020     -1.13512294487928      b
   -1.13512831829025     -1.13512872380334      1.13512812346088      b
    1.13513271243326     -1.13513209595804     -1.13513301541142      b
    2.45171101991862      2.45170873428443      2.45170917853944      h
   -2.45171753891449      2.45171830786967     -2.45171888582538      h
   -2.45170898165818     -2.45171133452650      2.45171018828927      h
    2.45170273945477     -2.45170693889277     -2.45170153076831      h
#BF3
    0.00057162011753      0.00000112131525      0.00000000000000      b
    2.50269790165942      0.00000463627076      0.00000000000000      f
   -1.25162960237501      2.16558024460409      0.00000000000000      f
   -1.25163991940193     -2.16558600219009      0.00000000000000      f
#BH3
    0.00000000000000      0.00000000000000     -0.00001716605107      b
    0.00000000000000      0.00000000000000      2.29252379962527      h
    1.98536152775083      0.00000000000000     -1.14625331603055      h
   -1.98536152775083      0.00000000000000     -1.14625331603055      h
#BH3CO
   -0.00003267004886      1.01111329216265      0.00000000000000      b
    2.24066059731720      1.62213805210289      0.00000000000000      h
   -1.12023754948246      1.62311914581523      1.94044267338909      h
   -1.12023754948246      1.62311914581523     -1.94044267338909      h
   -0.00018198607045     -1.85414688329676      0.00000000000000      c
    0.00002915776702     -4.02534275259922      0.00000000000000      o
#BH3NH3
   -0.00005391609667     -0.00000006055366      1.59755328544083      b
    0.00003677556503     -0.00000004984535     -1.51922811870669      n
   -1.12198704238829      1.94345823821240      2.21019712023369      h
   -1.81066670598354     -0.00000007552669     -2.23620407950898      h
   -1.12200568324154     -1.94345788468772      2.21023739863948      h
```

```
    0.90537147089552     -1.56819423165877     -2.23633381411281      h
    2.24393364900982     -0.00000003812768      2.21011203996588      h
    0.90537145223968      1.56819410218746     -2.23633383195137      h
#C2H2
    0.00000000000000      0.00000000000000      1.15246217269357      c
    0.00000000000000      0.00000000000000     -1.15237758930046      c
    0.00000000000000      0.00000000000000      3.19592252631204      h
    0.00000000000000      0.00000000000000     -3.19600710970514      h
#C2H3N
    1.88736354706722     -0.38569072500046      0.00000000000000      n
   -0.71824807664584     -0.19471094953120     -1.22023694426924      c
   -0.71824807664584     -0.19471094953120      1.22023694426924      c
    2.62906670020725      1.44277863614961      0.00000000000000      h
   -1.53996704699139     -0.33383300604337     -3.10934257471802      h
   -1.53996704699139     -0.33383300604337      3.10934257471802      h
#C2H4
   -0.00000595240645     -1.26733455985489      0.00000000000000      c
   -0.00001103692376      1.26733990808114      0.00000000000000      c
    1.77139591530185     -2.36353680346697      0.00000000000000      h
   -1.77135302848125     -2.36354228611354      0.00000000000000      h
    1.77143988920888      2.36354006871598      0.00000000000000      h
   -1.77146578669927      2.36353367263826      0.00000000000000      h
#C2H6
   -0.00004769714133      0.00000349348608      1.44636083928208      c
    0.00000804691144      0.00000483284596     -1.44638600827020      c
    0.00000507341384      1.94903094277111      2.21977150357274      h
   -1.68811904618790      0.97442869763498     -2.21944595476968      h
   -1.68812247614916     -0.97443046693153      2.21943006405761      h
    0.00000720306362     -1.94903334377391     -2.21978760781604      h
    1.68813497191566     -0.97443316442446      2.21950311354087      h
    1.68813392417380      0.97442900839179     -2.21944594959735      h
#C4H4
    0.99384594007199      0.99384464702096      0.99383622488147      c
   -0.99383778119390      0.99384857359297     -0.99384786547507      c
   -0.99383837692231     -0.99383758446481      0.99383909184982      c
    0.99384393287549     -0.99383406319256     -0.99384192088452      c
    2.18053060627208      2.18052818251503      2.18055255481919      h
   -2.18053790501712      2.18055083059018     -2.18055040079725      h
   -2.18053792505281     -2.18054059788475      2.18054096602118      h
    2.18053150896658     -2.18055998817700     -2.18052865041484      h
#C6H6
    2.65617581771435     -0.00001755566762      0.00000000000000      c
    1.32809320450038      2.30036580039517      0.00000000000000      c
   -1.32814289699474      2.30032454944275      0.00000000000000      c
   -2.65616474222357     -0.00002947176151      0.00000000000000      c
   -1.32814664832257     -2.30031670879657      0.00000000000000      c
    1.32804572900546     -2.30030596170580      0.00000000000000      c
    4.73697603254869     -0.00001003497658      0.00000000000000      h
    2.36858554692983      4.10225225927773      0.00000000000000      h
   -2.36858598921966      4.10217914017551      0.00000000000000      h
   -4.73684964271648     -0.00000987434447      0.00000000000000      h
   -2.36856197133617     -4.10217066208403      0.00000000000000      h
    2.36857556011450     -4.10226147995460      0.00000000000000      h
#CF4
    0.00000072798427     -0.00000084127378      0.00000134823270      c
    1.45612263947210      1.45612426874410      1.45612670863342      f
   -1.45612382956586      1.45612744820956     -1.45611634123477      f
   -1.45611302972194     -1.45611774949082      1.45611910063923      f
    1.45611349183143     -1.45613312618904     -1.45613081627060      f
#CH2O
    0.00001136906018     -0.00680178712325      0.00000000000000      c
    0.00001124892632     -2.29137576741941      0.00000000000000      o
   -1.79950764336418      1.14910699652609      0.00000000000000      h
```

```
    1.79948502537768      1.14907055801657      0.00000000000000      h
#CH2O2
   -0.00257696271985     -0.00029911539700      0.43566389538811      c
    0.91809787651456      1.10119962920547     -1.77030267443462      o
   -0.89638419996679     -1.09806893130047     -1.78331456460493      o
    1.35822195950510     -1.13175262110298      1.56631140453024      h
   -1.37735867333304      1.12892103859498      1.55164193912118      h
#CH3N
   -0.51099882579378     -1.72615900810017      0.00000000000000      n
   -0.28199635256966      0.67673092847568      0.00000000000000      c
    1.26548359579527     -2.55925182755683      0.00000000000000      h
    1.54014071938432      1.74203610207273      0.00000000000000      h
   -2.01262913681617      1.86664380510858      0.00000000000000      h
#CH3OH
   -0.60943318920949      0.23208453617070      0.00000000000000      c
   -1.40349374228799     -0.73023655246102     -1.70457168393205      h
   -1.40349374228799     -0.73023655246102      1.70457168393205      h
   -1.34535487704355      2.19364844386480      0.00000000000000      h
    2.05720432204887      0.37903865616194      0.00000000000000      o
    2.70457122878014     -1.34429853127539      0.00000000000000      h
#CH4
    0.00000365772543     -0.00000430204539     -0.00000303470922      c
    1.20635474089927      1.20638206443483      1.20635809459961      h
   -1.20637417661767      1.20636079380735     -1.20635435342573      h
   -1.20635629114801     -1.20637256903187      1.20636439312342      h
    1.20637206914099     -1.20636598716490     -1.20636509958807      h
#CO
    0.00000000000000      0.00000000000000     -1.07901367410215      c
    0.00000000000000      0.00000000000000      1.07901367410215      o
#CO2
    0.00000000000000      0.00000000000000      0.00002806040915      c
    0.00000000000000      0.00000000000000      2.21994735057408      o
    0.00000000000000      0.00000000000000     -2.21997541098322      o
#F2
    0.00000000000000      0.00000000000000     -1.33472243762606      f
    0.00000000000000      0.00000000000000      1.33472243762606      f
#H2
    0.00000000000000      0.00000000000000      0.72490772298399      h
    0.00000000000000      0.00000000000000     -0.72490772298399      h
#H2CO3
   -0.00000072368405      0.22080394668051      0.00000000000000      c
   -0.00000085983362      2.51789433031705      0.00000000000000      o
    2.06907082035747     -1.26682714026337      0.00000000000000      o
   -2.06907034454166     -1.26683026979785      0.00000000000000      o
    3.50618225374280     -0.10251893084200      0.00000000000000      h
   -3.50618114604093     -0.10252193609435      0.00000000000000      h
#H2O
   -0.00000092153086      0.77139067871094      0.00000000000000      o
    1.43408493447591     -0.38569466553748      0.00000000000000      h
   -1.43408401294505     -0.38569601317346      0.00000000000000      h
#H2O2
    1.37391573291828     -0.11754325013582      0.47481512973650      o
   -1.37391573291828      0.11754325013582      0.47481512973650      o
    1.81764940640807      1.41027485517298     -0.47481512973649      h
   -1.81764940640807     -1.41027485517298     -0.47481512973649      h
#HCN
    0.00000000000000      0.00000000000000     -2.10459881646616      h
    0.00000000000000      0.00000000000000     -0.05057148541107      c
    0.00000000000000      0.00000000000000      2.15517030187723      n
#HF
    0.00000000000000      0.00000000000000      0.88143111896247      h
    0.00000000000000      0.00000000000000     -0.88143111896247      f
#HNC
```

```
    0.00000000000000      0.00000000000000     -2.02196172790527      h
    0.00000000000000      0.00000000000000     -0.10820520253614      n
    0.00000000000000      0.00000000000000      2.13016693044140      c
#HNO
   -1.79661507816673      0.48943320881840      0.00000000000000      o
    0.47454096973458      0.69971484027459      0.00000000000000      n
    1.32207410843215     -1.18914804909299      0.00000000000000      h
#HNO2
   -0.00005991769124      0.00467141411420      0.00000000000000      n
    0.00050822247803     -2.00908183598864      0.00000000000000      h
    2.08688969332883      1.00263775985379      0.00000000000000      o
   -2.08733799811562      1.00177266202064      0.00000000000000      o
#HNO3
   -0.84920495946036     -0.15764648097179      0.00000000000000      n
   -1.28916831029594      2.10044345874920      0.00000000000000      o
    1.78029964374549     -0.83073113266367      0.00000000000000      o
   -2.25079424696181     -1.94859046351144      0.00000000000000      o
    2.60886787297262      0.83652461839769      0.00000000000000      h
#N2
    0.00000000000000      0.00000000000000     -1.05078974035833      n
    0.00000000000000      0.00000000000000      1.05078974035833      n
#N2H2
   -1.17672812398851      0.92386039472759      0.00000000000000      n
    1.17661864072211      0.92396010505874      0.00000000000000      n
   -1.95539025873620     -0.92400022187768      0.00000000000000      h
    1.95549974200260     -0.92382027790864      0.00000000000000      h
#N2H4
    1.34301342554004      0.11487732805038      0.44262664845470      n
   -1.34301342554004     -0.11487732805038      0.44262664845470      n
    2.06079980354008      0.61078546738212     -1.30448136798935      h
   -2.06079980354008     -0.61078546738212     -1.30448136798935      h
    2.08747379308132     -1.63000779480150      0.86185471953465      h
   -2.08747379308132      1.63000779480150      0.86185471953465      h
#N4
    0.97352637877574      0.97353427649995      0.97350854749399      n
   -0.97347107666161      0.97345970934768     -0.97348952076396      n
   -0.97352288698680     -0.97351512802877      0.97348592757745      n
    0.97346758487266     -0.97347885781885     -0.97350495430747      n
#NF3
   -0.00023917863373      0.86723125260972      0.00000000000000      n
    2.36152560364088     -0.29019299685791      0.00000000000000      f
   -1.18064321250358     -0.28851912787590      2.04401593693485      f
   -1.18064321250358     -0.28851912787590     -2.04401593693485      f
#NH3
   -0.00002996273382      0.60419573896846      0.00000000000000      n
    1.77459787410351     -0.20146478753319      0.00000000000000      h
   -0.88728395568485     -0.20136547571764      1.53702086353764      h
   -0.88728395568485     -0.20136547571764     -1.53702086353764      h
#NH4F
    0.00035295142012      0.99586270905472      0.00000000000000      n
    1.79756586681634      1.73917600761303      0.00000000000000      h
   -0.89974980156668      1.73568143900128      1.55739131188531      h
   -0.89974980156668      1.73568143900128     -1.55739131188531      h
    0.00153471995548     -2.18853841134706      0.00000000000000      h
    0.00004606494142     -4.01786318332326      0.00000000000000      f
#OF2
    0.00000000000000      0.00000000000000      1.08966458588793      o
   -2.12636045821744      0.00000000000000     -0.54483229294396      f
    2.12636045821744      0.00000000000000     -0.54483229294396      f
#Al2O3
    0.00000000000000      0.00000000000000      0.00000000000000      o
    0.00000000000000      0.00000000000000     -3.20592451951933      al
    0.00000000000000      0.00000000000000      3.20592451951933      al
```

```
    0.00000000000000      0.00000000000000     -6.26442328261665      o
    0.00000000000000      0.00000000000000      6.26442328261665      o
#Al2S3
    0.00000000000000      0.00000000000000      3.16034259123655      s
   -6.05680384209421      0.00000000000000     -2.01213979070925      s
    6.05680384209421      0.00000000000000     -2.01213979070925      s
   -3.12156733278024      0.00000000000000      0.43196849509098      al
    3.12156733278024      0.00000000000000      0.43196849509098      al
#AlCl3
    0.00000000000000      0.00000000000000      0.00000000000000      al
    1.98010837147193     -3.42964830388186      0.00000000000000      cl
    1.98010837147193      3.42964830388186      0.00000000000000      cl
   -3.96021674294387      0.00000000000000      0.00000000000000      cl
#AlF3
    0.00000000000000      0.00000000000000      0.00000000000000      al
    1.56643211516439     -2.71314001007231      0.00000000000000      f
    1.56643211516439      2.71314001007231      0.00000000000000      f
   -3.13286423032878      0.00000000000000      0.00000000000000      f
#AlH3
    0.00000000000000      0.00000000000000      0.00000000000000      al
    1.51111027824900     -2.61731977776682      0.00000000000000      h
    1.51111027824900      2.61731977776682      0.00000000000000      h
   -3.02222055649801      0.00000000000000      0.00000000000000      h
#AlN
    0.00000000000000      0.00000000000000      1.70183203298110      n
    0.00000000000000      0.00000000000000     -1.70183203298110      al
#CS2
    0.00000000000000      0.00000000000000     -0.00042370317242      c
    0.00000000000000      0.00000000000000      2.96976471283164      s
    0.00000000000000      0.00000000000000     -2.96934100965921      s
#Cl2
    0.00000000000000      0.00000000000000      1.94562946845339      cl
    0.00000000000000      0.00000000000000     -1.94562946845339      cl
#ClF
    0.00000000000000      0.00000000000000     -1.58509614282258      cl
    0.00000000000000      0.00000000000000      1.58509614282258      f
#ClF3
   -0.00003067860727     -0.83736782989924      0.00000000000000      cl
   -3.32968626746479     -0.75728391745932      0.00000000000000      f
    3.32967523209023     -0.75719934611368      0.00000000000000      f
    0.00004171398183      2.35185109347225      0.00000000000000      f
#H2SO4
   -0.00001618652064      0.00000532998352      0.57726346501965      s
    2.40449042802622      0.00000119792204      1.95483853136064      o
   -2.40446876756433      0.00000117641825      1.95482480979171      o
   -0.00000130197438      2.22843215334819     -1.58826869332215      o
   -0.00000131291374     -2.22844560147121     -1.58825020322016      o
   -0.00000143369034      3.83405981964557     -0.65522713489551      h
   -0.00000142536279     -3.83405407584636     -0.65518077473415      h
#H3PO4
    0.00025271029759      0.00000002775195      0.18378624273833      p
    2.75771513369481      0.00000046305733     -1.18697263987526      o
   -1.38058842041890      2.38580178738371     -1.18704930153066      o
   -1.38058701560059     -2.38580233754762     -1.18704935129008      o
    0.00141162249612      0.00000008197607      3.01262148875343      o
    4.05947580693281     -0.00000015128153      0.12202776723928      h
   -2.02883988453177      3.51548597828379      0.12131791511576      h
   -2.02883995287005     -3.51548584962367      0.12131787884917      h
#HCP
    0.00000000000000      0.00000000000000     -2.64853987727355      p
    0.00000000000000      0.00000000000000      2.35551089579161      h
    0.00000000000000      0.00000000000000      0.29302898148195      c
#HCl
```

```
    0.00000000000000      0.00000000000000     -1.22530682104886      cl
    0.00000000000000      0.00000000000000      1.22530682104886      h
#HSH
   -0.00000891346937      1.19653856768716      0.00000000000000      s
    1.84307080535555     -0.59826448731836      0.00000000000000      h
   -1.84306189188618     -0.59827408036881      0.00000000000000      h
#HSSH
    1.98198459838609     -0.07543787142517      0.90366573347496      s
   -1.98198459838609      0.07543787142517      0.90366573347496      s
    2.42926401991953      1.72380811808687     -0.90366607995143      h
   -2.42926401991953     -1.72380811808687     -0.90366607995143      h
#P2
    0.00000000000000      0.00000000000000      1.81038834147637      p
    0.00000000000000      0.00000000000000     -1.81038834147637      p
#PF3
    0.00190593228732      0.00000637856307     -1.13522248396255      p
    2.65740159746508      0.00000628935462      0.38170793256163      f
   -1.32964926884328      2.29968766474854      0.37675740109626      f
   -1.32965826090911     -2.29970033266624      0.37675715030465      f
#PF5
    0.00093568540199      0.00000556340549      0.00000000000000      p
    0.00115403835462     -3.04805754510344      0.00000000000000      f
    0.00115453827044      3.04805857150255      0.00000000000000      f
    3.00853565827311     -0.00000245516935      0.00000000000000      f
   -1.50588996015008     -0.00000206731762      2.60331280562780      f
   -1.50588996015008     -0.00000206731762     -2.60331280562780      f
#PH3
    0.00021868262881      0.00000408524970     -1.13254033248507      p
    2.26639108333582      0.00000455950564      0.37803102689817      h
   -1.13330963847505      1.96296552283309      0.37726390137846      h
   -1.13330012748958     -1.96297416758843      0.37724540420844      h
#S2
    0.00000000000000      0.00000000000000     -1.82795217547776      s
    0.00000000000000      0.00000000000000      1.82795217547776      s
#S5
   -1.01219286085597      0.91031071217532      2.78939529359939      s
    2.56254320877922     -0.26701145071347      2.27262712733185      s
    2.56256180032893     -0.26700825963793     -2.27262274065567      s
   -1.01216802810249      0.91029852260584     -2.78940508703009      s
   -3.10074412014967     -1.28658952442978      0.00000540675450      s
#SF2
    0.00000000000000      0.00000000000000      1.32266337773884      s
    2.37880811467657      0.00000000000000     -0.66133188418768      f
   -2.37880811467657      0.00000000000000     -0.66133188418768      f
#SF4
   -0.00000226380055     -0.00002431422764      0.84926009844488      s
   -3.18886562268367     -0.00001733471558      0.66640784370306      f
    3.18886006659826     -0.00001733422028      0.66642737569287      f
    0.00000390405808      2.35445661105741     -1.09097973125881      f
    0.00000391582787     -2.35439762789392     -1.09111558658199      f
#SF6
    0.00000000000000      0.00000000000000      0.00000118515990      s
   -2.15172851914079     -2.15172851914079     -0.00000033099473      f
    0.00000000000000      0.00000000000000      3.04300291311907      f
   -2.15172851914079      2.15172851914079     -0.00000033099473      f
    0.00000000000000      0.00000000000000     -3.04300276329175      f
    2.15172851914079     -2.15172851914079     -0.00000033099473      f
    2.15172851914079      2.15172851914079     -0.00000033099473      f
#SiCl4
    0.00000000000000      0.00000000000000      0.00000000000000      si
    2.24180189786400     -2.24180189786400      2.24180189786400      cl
   -2.24180189786400      2.24180189786400      2.24180189786400      cl
   -2.24180189786400     -2.24180189786400     -2.24180189786400      cl
```

```
    2.24180189786400      2.24180189786400     -2.24180189786400      cl
#SiF4
    0.00000000000000      0.00000000000000      0.00000000000000      si
    1.74748733068482     -1.74748733068482      1.74748733068482      f
   -1.74748733068482      1.74748733068482      1.74748733068482      f
   -1.74748733068482     -1.74748733068482     -1.74748733068482      f
    1.74748733068482      1.74748733068482     -1.74748733068482      f
#SiH4
    0.00000000000000      0.00000000000000      0.00000000000000      si
    1.63806238513397     -1.63806238513397      1.63806238513397      h
   -1.63806238513397      1.63806238513397      1.63806238513397      h
   -1.63806238513397     -1.63806238513397     -1.63806238513397      h
    1.63806238513397      1.63806238513397     -1.63806238513397      h
#SiO2
    0.00000000000000      0.00000000000000      0.00000000000000      si
    0.00000000000000      0.00000000000000     -2.90863957585795      o
    0.00000000000000      0.00000000000000      2.90863957585795      o
#SiS2
    0.00000000000000      0.00000000000000      0.00000000000000      si
    0.00000000000000      0.00000000000000     -3.68153174204543      s
    0.00000000000000      0.00000000000000      3.68153174204543      s
#As4
    1.64900717955662     -1.64900717955662      1.64900717955662      as
   -1.64900717955662      1.64900717955662      1.64900717955662      as
   -1.64900717955662     -1.64900717955662     -1.64900717955662      as
    1.64900717955662      1.64900717955662     -1.64900717955662      as
#As4S4
   -1.41083883866857     -1.41083883866857      4.46081971940384      s
    1.41083883866857      1.41083883866857      4.46081971940384      s
   -1.41083883866857      1.41083883866857     -4.46081971940384      s
    1.41083883866857     -1.41083883866857     -4.46081971940384      s
    0.00000000000000      3.30253054743472      0.00000000000000      as
    3.30253054743472      0.00000000000000      0.00000000000000      as
    0.00000000000000     -3.30253054743472      0.00000000000000      as
   -3.30253054743472      0.00000000000000      0.00000000000000      as
#AsCl3
    0.00000000000000      0.00000000000000      1.45363897308538      as
   -1.85326772975506      3.20995386796359     -0.48454632436179      cl
   -1.85326772975506     -3.20995386796359     -0.48454632436179      cl
    3.70653545951011      0.00000000000000     -0.48454632436179      cl
#AsCl6-
    0.00000000000000      0.00000000000000      0.00000000000000      as
    0.00000000000000      4.35128874572739      0.00000000000000      cl
    0.00000000000000      0.00000000000000      4.35128874572739      cl
    4.35128874572739      0.00000000000000      0.00000000000000      cl
    0.00000000000000      0.00000000000000     -4.35128874572739      cl
   -4.35128874572739      0.00000000000000      0.00000000000000      cl
    0.00000000000000     -4.35128874572739      0.00000000000000      cl
#AsH3
    0.00000000000000      0.00000000000000      1.23244998693740      as
   -1.20159017904000      2.08121523997307     -0.41081666231247      h
   -1.20159017904000     -2.08121523997307     -0.41081666231247      h
    2.40318035808001      0.00000000000000     -0.41081666231247      h
#Br2
    0.00000000000000      0.00000000000000     -2.20336345967580      br
    0.00000000000000      0.00000000000000      2.20336345967580      br
#BrCl
    0.00000000000000      0.00000000000000     -2.07645102410186      br
    0.00000000000000      0.00000000000000      2.07645102410186      cl
#BrO4-
    0.00000000000000      0.00000000000000      0.00000000000000      br
    1.80474294078758     -1.80474294078758      1.80474294078758      o
   -1.80474294078758      1.80474294078758      1.80474294078758      o
```

```
   -1.80474294078758     -1.80474294078758     -1.80474294078758      o
    1.80474294078758      1.80474294078758     -1.80474294078758      o
#GaCl
    0.00000000000000      0.00000000000000     -2.11198999351902      ga
    0.00000000000000      0.00000000000000      2.11198999351902      cl
#GaCl3
    0.00000000000000      0.00000000000000      0.00000000000000      ga
    2.02363708334148     -3.50504224442794      0.00000000000000      cl
    2.02363708334148      3.50504224442794      0.00000000000000      cl
   -4.04727416668296      0.00000000000000      0.00000000000000      cl
#GaF
    0.00000000000000      0.00000000000000     -1.69732010119943      ga
    0.00000000000000      0.00000000000000      1.69732010119943      f
#GaF2
    0.00000000000000      0.00000000000000      1.16213096204235      ga
   -2.87257490857190      0.00000000000000     -0.58106548102118      f
    2.87257490857190      0.00000000000000     -0.58106548102118      f
#GaH3
    0.00000000000000      0.00000000000000      0.00000000000000      ga
    1.49230772481659     -2.58475279990984      0.00000000000000      h
    1.49230772481659      2.58475279990984      0.00000000000000      h
   -2.98461544963317      0.00000000000000      0.00000000000000      h
#GaO
    0.00000000000000      0.00000000000000     -1.61698641616867      ga
    0.00000000000000      0.00000000000000      1.61698641616867      o
#GeCl4
    0.00000000000000      0.00000000000000      0.00000000000000      ge
    2.34720419578646     -2.34720419578646      2.34720419578646      cl
   -2.34720419578646      2.34720419578646      2.34720419578646      cl
   -2.34720419578646     -2.34720419578646     -2.34720419578646      cl
    2.34720419578646      2.34720419578646     -2.34720419578646      cl
#GeF3
    0.00000000000000      0.00000000000000      0.93844457989423      ge
    1.53348366776395     -2.65607162514423     -0.31281485996474      f
    1.53348366776395      2.65607162514423     -0.31281485996474      f
   -3.06696733552790      0.00000000000000     -0.31281485996474      f
#GeF4
    0.00000000000000      0.00000000000000      0.00000000000000      ge
    1.87482477759343     -1.87482477759343      1.87482477759343      f
   -1.87482477759343      1.87482477759343      1.87482477759343      f
   -1.87482477759343     -1.87482477759343     -1.87482477759343      f
    1.87482477759343      1.87482477759343     -1.87482477759343      f
#GeH4
    0.00000000000000      0.00000000000000      0.00000000000000      ge
    1.69283500661777     -1.69283500661777      1.69283500661777      h
   -1.69283500661777      1.69283500661777      1.69283500661777      h
   -1.69283500661777     -1.69283500661777     -1.69283500661777      h
    1.69283500661777      1.69283500661777     -1.69283500661777      h
#GeO
    0.00000000000000      0.00000000000000     -1.55696412775958      ge
    0.00000000000000      0.00000000000000      1.55696412775958      o
#GeO2
    0.00000000000000      0.00000000000000      0.00000000000000      ge
    0.00000000000000      0.00000000000000      3.09562411619127      o
    0.00000000000000      0.00000000000000     -3.09562411619127      o
#HBr
    0.00000000000000      0.00000000000000     -1.35667371651595      h
    0.00000000000000      0.00000000000000      1.35667371651595      br
#HCBr3
    0.00000000000000      0.00000000000000      0.22579559169999      c
    0.00000000000000      0.00000000000000      2.30613641574210      h
    1.76507167530612     -3.05719382063092     -0.84397733581403      br
    1.76507167530612      3.05719382063092     -0.84397733581403      br
```

```
   -3.53014335061225      0.00000000000000     -0.84397733581403      br
#Se8
    4.73473332107232     -1.96119075580796      1.08203483157154      se
    1.96119075580796      4.73473332107232      1.08203483157154      se
   -4.73473332107232      1.96119075580796      1.08203483157154      se
   -1.96119075580796     -4.73473332107232      1.08203483157154      se
    4.73473332107232      1.96119075580796     -1.08203483157154      se
   -1.96119075580796      4.73473332107232     -1.08203483157154      se
   -4.73473332107232     -1.96119075580796     -1.08203483157154      se
    1.96119075580796     -4.73473332107232     -1.08203483157154      se
#SeH2
    0.00000000000000      0.00000000000000      1.31443756714499      se
   -1.99442696033084      0.00000000000000     -0.65721878357249      h
    1.99442696033084      0.00000000000000     -0.65721878357249      h
#SeO
    0.00000000000000      0.00000000000000     -1.58117857273827      se
    0.00000000000000      0.00000000000000      1.58117857273827      o
#SeO2
    0.00000000000000      0.00000000000000      1.10091950638887      se
   -2.61260008861725      0.00000000000000     -0.55045975319444      o
    2.61260008861725      0.00000000000000     -0.55045975319444      o
#I2
    0.00000000000000      0.00000000000000     -2.58717910006003      i
    0.00000000000000      0.00000000000000      2.58717910006003      i
#ICl
    0.00000000000000      0.00000000000000     -2.27749291163188      i
    0.00000000000000      0.00000000000000      2.27749291163189      cl
#IH
    0.00000000000000      0.00000000000000     -1.54901575226915      i
    0.00000000000000      0.00000000000000      1.54901575226915      h
#IO4-
    0.00000000000000      0.00000000000000      0.00000000000000      i
    2.03119023188409     -2.03119023188409      2.03119023188409      o
   -2.03119023188409      2.03119023188409      2.03119023188409      o
   -2.03119023188409     -2.03119023188409     -2.03119023188409      o
    2.03119023188409      2.03119023188409     -2.03119023188409      o
#InCl
    0.00000000000000      0.00000000000000     -2.28501380453881      in
    0.00000000000000      0.00000000000000      2.28501380453881      cl
#InCl3
    0.00000000000000      0.00000000000000      0.00000000000000      in
   -2.18888514352907      3.79126028052504      0.00000000000000      cl
   -2.18888514352907     -3.79126028052504      0.00000000000000      cl
    4.37777028705814      0.00000000000000      0.00000000000000      cl
#InH
    0.00000000000000      0.00000000000000     -1.77323971157117      in
    0.00000000000000      0.00000000000000      1.77323971157117      h
#InH3
    0.00000000000000      0.00000000000000      0.00000000000000      in
   -1.65719731255026      2.87034994350365      0.00000000000000      h
   -1.65719731255026     -2.87034994350365      0.00000000000000      h
    3.31439462510052      0.00000000000000      0.00000000000000      h
#InO
    0.00000000000000      0.00000000000000     -1.77046376816122      in
    0.00000000000000      0.00000000000000      1.77046376816122      o
#SbCl6-
    0.00000000000000      0.00000000000000      0.00000000000000      sb
    0.00000000000000      4.64447503829980      0.00000000000000      cl
    0.00000000000000      0.00000000000000      4.64447503829980      cl
    4.64447503829980      0.00000000000000      0.00000000000000      cl
    0.00000000000000      0.00000000000000     -4.64447503829980      cl
   -4.64447503829980      0.00000000000000      0.00000000000000      cl
    0.00000000000000     -4.64447503829980      0.00000000000000      cl
```

```
#SbF
    0.00000000000000      0.00000000000000     -1.86318815100045      sb
    0.00000000000000      0.00000000000000      1.86318815100045      f
#SbF3
    0.00000000000000      0.00000000000000      1.41635010067847      sb
   -1.57661128992144      2.73077085793065     -0.47211670022616      f
   -1.57661128992144     -2.73077085793065     -0.47211670022616      f
    3.15322257984289      0.00000000000000     -0.47211670022616      f
#SbH3
    0.00000000000000      0.00000000000000      1.40288124678412      sb
    1.34916589534128     -2.33682387857025     -0.46762708226138      h
    1.34916589534128      2.33682387857025     -0.46762708226138      h
   -2.69833179068256      0.00000000000000     -0.46762708226138      h
#SbO2
    0.00000000000000      0.00000000000000      1.18120858212824      sb
    3.08998758817836      0.00000000000000     -0.59060429106412      o
   -3.08998758817836      0.00000000000000     -0.59060429106412      o
#SnF3
    0.00000000000000      0.00000000000000      1.07456818814013      sn
    1.71243475756358     -2.96602400474702     -0.35818939604671      f
    1.71243475756358      2.96602400474702     -0.35818939604671      f
   -3.42486951512717      0.00000000000000     -0.35818939604671      f
#SnH4
    0.00000000000000      0.00000000000000      0.00000000000000      sn
    1.89044177023958     -1.89044177023958      1.89044177023958      h
   -1.89044177023958      1.89044177023958      1.89044177023958      h
   -1.89044177023958     -1.89044177023958     -1.89044177023958      h
    1.89044177023958      1.89044177023958     -1.89044177023958      h
#SnO
    0.00000000000000      0.00000000000000     -1.76719363698803      sn
    0.00000000000000      0.00000000000000      1.76719363698803      o
#SnO2
    0.00000000000000      0.00000000000000      0.00163548812459      sn
   -3.51460840178293      0.00000000000000     -0.00081774406230      o
    3.51460840178293      0.00000000000000     -0.00081774406230      o
#TeF3
    0.00000000000000      0.00000000000000      0.35475666747305      te
   -1.87725312652868      3.25149779381520     -0.11825222249101      f
   -1.87725312652868     -3.25149779381520     -0.11825222249101      f
    3.75450625305736      0.00000000000000     -0.11825222249101      f
#TeH2
    0.00000000000000      0.00000000000000      1.49820193039170      te
   -2.24906865611118      0.00000000000000     -0.74910096519585      h
    2.24906865611118      0.00000000000000     -0.74910096519585      h
#TeO
    0.00000000000000      0.00000000000000     -1.77896181226445      te
    0.00000000000000      0.00000000000000      1.77896181226445      o
#TeO2
    0.00000000000000      0.00000000000000      1.29984292231352      te
   -2.88498675314837      0.00000000000000     -0.64992146115676      o
    2.88498675314837      0.00000000000000     -0.64992146115676      o
#XeF2
    0.00000000000000      0.00000000000000      0.00000000000000      xe
    0.00000000000000      0.00000000000000      3.90757878328295      f
    0.00000000000000      0.00000000000000     -3.90757878328295      f
#XeF4
    0.00000000000000      0.00000000000000      0.00000000000000      xe
    2.72236103703447     -2.72236103703447      0.00000000000000      f
    2.72236103703447      2.72236103703447      0.00000000000000      f
   -2.72236103703447      2.72236103703447      0.00000000000000      f
   -2.72236103703447     -2.72236103703447      0.00000000000000      f
#XeOF4
    0.00000000000000      0.00000000000000     -0.39099828949089      xe
```

```
    0.00000000000000      0.00000000000000      3.04665434896357      o
    2.70138310369918     -2.70138310369918     -0.66391401486817      f
    2.70138310369918      2.70138310369918     -0.66391401486817      f
   -2.70138310369918      2.70138310369918     -0.66391401486817      f
   -2.70138310369918     -2.70138310369918     -0.66391401486817      f
#BiCl6-
    0.00000000000000      0.00000000000000      0.00000000000000      bi
    0.00000000000000      4.82554937284918      0.00000000000000      cl
    0.00000000000000      0.00000000000000      4.82554937284918      cl
    0.00000000000000     -4.82554937284918      0.00000000000000      cl
    0.00000000000000      0.00000000000000     -4.82554937284918      cl
    4.82554937284918      0.00000000000000      0.00000000000000      cl
   -4.82554937284918      0.00000000000000      0.00000000000000      cl
#BiF
    0.00000000000000      0.00000000000000     -1.93137769997131      bi
    0.00000000000000      0.00000000000000      1.93137769997131      f
#BiF3
    0.00000000000000      0.00000000000000      1.46232798160630      bi
    1.63662897536318     -2.83472453846842     -0.48744266053543      f
    1.63662897536318      2.83472453846842     -0.48744266053543      f
   -3.27325795072636      0.00000000000000     -0.48744266053543      f
#BiH3
    0.00000000000000      0.00000000000000      1.47386771700502      bi
    1.40843659350503     -2.43948373918995     -0.49128923900167      h
    1.40843659350503      2.43948373918995     -0.49128923900167      h
   -2.81687318701006      0.00000000000000     -0.49128923900167      h
#BiO2
    0.00000000000000      0.00000000000000      1.37289088296138      bi
   -3.15041062335303      0.00000000000000     -0.68644544148069      o
    3.15041062335303      0.00000000000000     -0.68644544148069      o
#PbF3
    0.00000000000000      0.00000000000000      1.10329818701537      pb
   -1.78036242435008      3.08367817486085     -0.36776606233846      f
   -1.78036242435008     -3.08367817486085     -0.36776606233846      f
    3.56072484870017      0.00000000000000     -0.36776606233846      f
#PbH4
    0.00000000000000      0.00000000000000      0.00000000000000      pb
    1.91301550123300     -1.91301550123300      1.91301550123300      h
   -1.91301550123300      1.91301550123300      1.91301550123300      h
   -1.91301550123300     -1.91301550123300     -1.91301550123300      h
    1.91301550123300      1.91301550123300     -1.91301550123300      h
#PbO
    0.00000000000000      0.00000000000000     -1.80754257937630      pb
    0.00000000000000      0.00000000000000      1.80754257937630      o
#PbO2
    0.00000000000000      0.00000000000000      0.00000000000000      pb
    0.00000000000000      0.00000000000000      3.61357863592328      o
    0.00000000000000      0.00000000000000     -3.61357863592328      o
#TlCl
    0.00000000000000      0.00000000000000     -2.38342001986092      tl
    0.00000000000000      0.00000000000000      2.38342001986092      cl
#TlCl3
    0.00000000000000      0.00000000000000     -0.01443837177572      tl
   -2.26117878730255      3.91647654460500      0.00481279059057      cl
   -2.26117878730255     -3.91647654460500      0.00481279059057      cl
    4.52235757460510      0.00000000000000      0.00481279059057      cl
#TlH
    0.00000000000000      0.00000000000000     -1.81347675018980      tl
    0.00000000000000      0.00000000000000      1.81347675018980      h
#TlH3
    0.00000000000000      0.00000000000000      0.00000000000000      tl
   -1.64536913789863      2.84986294404622      0.00000000000000      h
   -1.64536913789863     -2.84986294404622      0.00000000000000      h
```

```
    3.29073827579725      0.00000000000000      0.00000000000000      h
#TlO
    0.00000000000000      0.00000000000000     -1.81795601245970      tl
    0.00000000000000      0.00000000000000      1.81795601245970      o
#CoCl3
    0.00000000000000      0.00000000000000      0.00000000000000      co
    2.00502719350387     -3.47280896970594      0.00000000000000      cl
    2.00502719350387      3.47280896970594      0.00000000000000      cl
   -4.01005438700775      0.00000000000000      0.00000000000000      cl
#CoF2
    0.00000000000000      0.00000000000000     -0.01591379082412      co
    3.26355789294746      0.00000000000000      0.00795689541206      f
   -3.26355789294746      0.00000000000000      0.00795689541206      f
#CoF3
    0.00000000000000      0.00000000000000      0.00000000000000      co
    1.65123154872552     -2.86001693745324      0.00000000000000      f
    1.65123154872552      2.86001693745324      0.00000000000000      f
   -3.30246309745104      0.00000000000000      0.00000000000000      f
#CrCO6
    0.00000000000000      0.00000000000000      0.00000000000000      cr
    0.00000000000000      3.59171681854581      0.00000000000000      c
    0.00000000000000      0.00000000000000      3.59171681854581      c
    3.59171681854581      0.00000000000000      0.00000000000000      c
    0.00000000000000      0.00000000000000     -3.59171681854581      c
   -3.59171681854581      0.00000000000000      0.00000000000000      c
    0.00000000000000     -3.59171681854581      0.00000000000000      c
    0.00000000000000      5.77973936611907      0.00000000000000      o
    0.00000000000000      0.00000000000000      5.77973936611907      o
    5.77973936611907      0.00000000000000      0.00000000000000      o
    0.00000000000000      0.00000000000000     -5.77973936611907      o
   -5.77973936611907      0.00000000000000      0.00000000000000      o
    0.00000000000000     -5.77973936611907      0.00000000000000      o
#CrCl3
    0.00000000000000      0.00000000000000      0.00000000000000      cr
    2.02495084056461     -3.50731773868720      0.00000000000000      cl
    2.02495084056461      3.50731773868720      0.00000000000000      cl
   -4.04990168112921      0.00000000000000      0.00000000000000      cl
#CrF3
    0.00000000000000      0.00000000000000      0.00000000000000      cr
    1.63137792162153     -2.82562944659461      0.00000000000000      f
    1.63137792162153      2.82562944659461      0.00000000000000      f
   -3.26275584324306      0.00000000000000      0.00000000000000      f
#CrO3
    0.00000000000000      0.00000000000000      0.00000000000000      cr
   -1.50063115995876      2.59916941246959      0.00000000000000      o
   -1.50063115995876     -2.59916941246959      0.00000000000000      o
    3.00126231991752      0.00000000000000      0.00000000000000      o
#Cu2
    0.00000000000000      0.00000000000000     -2.07387116344728      cu
    0.00000000000000      0.00000000000000      2.07387116344728      cu
#Cu2O
    0.00000000000000      0.00000000000000      1.63312192704579      o
    2.28854347532692      0.00000000000000     -0.81656096352289      cu
   -2.28854347532692      0.00000000000000     -0.81656096352289      cu
#Cu2S
    0.00000000000000      0.00000000000000      2.19080233145777      s
   -2.28384138036123      0.00000000000000     -1.09540116572889      cu
    2.28384138036123      0.00000000000000     -1.09540116572889      cu
#CuCN
    0.00000000000000      0.00000000000000     -3.01968451426437      cu
    0.00000000000000      0.00000000000000      0.39611548720036      c
    0.00000000000000      0.00000000000000      2.62356902706402      n
#CuCl
```

```
    0.00000000000000      0.00000000000000     -1.95954303758138      cu
    0.00000000000000      0.00000000000000      1.95954303758138      cl
#CuF
    0.00000000000000      0.00000000000000     -1.64676654637877      cu
    0.00000000000000      0.00000000000000      1.64676654637877      f
#CuH
    0.00000000000000      0.00000000000000     -1.37926640891550      cu
    0.00000000000000      0.00000000000000      1.37926640891550      h
#FeCO5
    0.00000000000000      0.00000000000000      0.00000000000000      fe
    1.70357480283978     -2.95067811301262      0.00000000000000      c
    1.70357480283978      2.95067811301262      0.00000000000000      c
   -3.40714960567955      0.00000000000000      0.00000000000000      c
    0.00000000000000      0.00000000000000      3.40816318478371      c
    0.00000000000000      0.00000000000000     -3.40816318478371      c
    2.79922085086665     -4.84839273530721      0.00000000000000      o
    2.79922085086665      4.84839273530721      0.00000000000000      o
   -5.59844170173329      0.00000000000000      0.00000000000000      o
    0.00000000000000      0.00000000000000      5.59447063964439      o
    0.00000000000000      0.00000000000000     -5.59447063964439      o
#FeF2
   0.00000000000000      0.00000000000000      0.00000000000000      fe
   3.29988416615965       0.00000000000000      0.00000000000000      f
  -3.29988416615965      0.00000000000000      0.00000000000000      f
#FeF3
    0.00000000000000      0.00000000000000      0.00000000000000      fe
    1.67360598116772     -2.89877059123365      0.00000000000000      f
    1.67360598116772      2.89877059123365      0.00000000000000      f
   -3.34721196233544      0.00000000000000      0.00000000000000      f
#FeO
   -0.66907143281002      0.00000000000000      0.00000000000000      fe
    2.33556505384199      0.00000000000000      0.00000000000000      o
#Ferrocen
    0.00000000000000      0.00000000000000      0.00000000000000      fe
    2.31561104541701      0.00000000000000      3.09927116392114      c
    0.71556316539619      2.20227697394888      3.09927116392114      c
   -1.87336868810470      1.36108202254167      3.09927116392114      c
   -1.87336868810470     -1.36108202254167      3.09927116392114      c
    0.71556316539619     -2.20227697394888      3.09927116392114      c
    2.31561104541701      0.00000000000000     -3.09927116392114      c
    0.71556316539619     -2.20227697394888     -3.09927116392114      c
   -1.87336868810470     -1.36108202254167     -3.09927116392114      c
   -1.87336868810470      1.36108202254167     -3.09927116392114      c
    0.71556316539619      2.20227697394888     -3.09927116392114      c
    4.38900985665904      0.00000000000000      3.08518706538327      h
    1.35627863418680      4.17419642425924      3.08518706538327      h
   -3.55078356251632      2.57979526591049      3.08518706538327      h
   -3.55078356251632     -2.57979526591049      3.08518706538327      h
    1.35627863418680     -4.17419642425924      3.08518706538327      h
    4.38900985665904      0.00000000000000     -3.08518706538327      h
    1.35627863418680     -4.17419642425924     -3.08518706538327      h
   -3.55078356251632     -2.57979526591049     -3.08518706538327      h
   -3.55078356251632      2.57979526591049     -3.08518706538327      h
    1.35627863418680      4.17419642425924     -3.08518706538327      h
#MnF2
    0.00000000000000      0.00000000000000      0.00000000000000      mn
    0.00000000000000      0.00000000000000      3.36165918231541      f
    0.00000000000000      0.00000000000000     -3.36165918231541      f
#MnO
    0.00000000000000      0.00000000000000     -1.52065965443162      mn
    0.00000000000000      0.00000000000000      1.52065965443162      o
#MnO2
    0.00000000000000      0.00000000000000      0.91350357143973      mn
```

```
    2.66795187804954      0.00000000000000     -0.45675178571986      o
   -2.66795187804954      0.00000000000000     -0.45675178571986      o
#MnO3F
    0.00000000000000      0.00000000000000     -0.07330413800993      mn
    0.00000000000000      0.00000000000000      3.16649627047248      f
    1.40721736620792     -2.43737197556538     -1.03106404415419      o
    1.40721736620792      2.43737197556538     -1.03106404415419      o
   -2.81443473241584      0.00000000000000     -1.03106404415419      o
#MnO4-
    0.00000000000000      0.00000000000000      0.00000000000000      mn
    1.75938547049818     -1.75938547049818      1.75938547049818      o
   -1.75938547049818      1.75938547049818      1.75938547049818      o
   -1.75938547049818     -1.75938547049818     -1.75938547049818      o
    1.75938547049818      1.75938547049818     -1.75938547049818      o
#MnS
    0.00000000000000      0.00000000000000     -1.92619713055598      mn
    0.00000000000000      0.00000000000000      1.92619713055598      s
#NiCO4
    0.00000000000000      0.00000000000000      0.00000000000000      ni
    1.98326378231725     -1.98326378231725      1.98326378231725      c
   -1.98326378231725      1.98326378231725      1.98326378231725      c
   -1.98326378231725     -1.98326378231725     -1.98326378231725      c
    1.98326378231725      1.98326378231725     -1.98326378231725      c
    3.24273654096679     -3.24273654096679      3.24273654096679      o
   -3.24273654096679      3.24273654096679      3.24273654096679      o
   -3.24273654096679     -3.24273654096679     -3.24273654096679      o
    3.24273654096679      3.24273654096679     -3.24273654096679      o
#NiCl2
    0.00000000000000      0.00000000000000      0.00232084864856      ni
   -3.96670138124145      0.00000000000000     -0.00116042432428      cl
    3.96670138124145      0.00000000000000     -0.00116042432428      cl
#NiF2
    0.00000000000000      0.00000000000000      0.00000000000000      ni
    0.00000000000000      0.00000000000000     -3.26603962131760      f
    0.00000000000000      0.00000000000000      3.26603962131760      f
#NiF3
    0.00000000000000      0.00000000000000      0.00152306552660      ni
   -1.66351766562508      2.88129711615101     -0.00050768850887      f
   -1.66351766562508     -2.88129711615101     -0.00050768850887      f
    3.32703533125016      0.00000000000000     -0.00050768850887      f
#NiO
    0.00000000000000      0.00000000000000     -1.51749092920855      ni
    0.00000000000000      0.00000000000000      1.51749092920855      o
#NiS
    0.00000000000000      0.00000000000000     -1.85681514730456      ni
    0.00000000000000      0.00000000000000      1.85681514730456      s
#ScCl3
    0.00000000000000      0.00000000000000      0.00000000000000      sc
    2.15416668810895     -3.73112615177708      0.00000000000000      cl
    2.15416668810895      3.73112615177708      0.00000000000000      cl
   -4.30833337621790      0.00000000000000      0.00000000000000      cl
#ScF3
    0.00000000000000      0.00000000000000      0.00000000000000      sc
    1.73202055035891     -2.99994759297505      0.00000000000000      f
    1.73202055035891      2.99994759297505      0.00000000000000      f
   -3.46404110071783      0.00000000000000      0.00000000000000      f
#ScH3
    0.00000000000000      0.00000000000000      0.00000000000000      sc
    1.71347214324408     -2.96782080945268      0.00000000000000      h
    1.71347214324408      2.96782080945268      0.00000000000000      h
   -3.42694428648816      0.00000000000000      0.00000000000000      h
#ScO
    0.00000000000000      0.00000000000000     -1.57175591846256      sc
```

```
    0.00000000000000      0.00000000000000      1.57175591846256      o
#TiCO4
    0.00000000000000      0.00000000000000      0.00000000000000      ti
    2.25209609785139     -2.25209609785139      2.25209609785139      c
   -2.25209609785139      2.25209609785139      2.25209609785139      c
   -2.25209609785139     -2.25209609785139     -2.25209609785139      c
    2.25209609785139      2.25209609785139     -2.25209609785139      c
    3.52294080235074     -3.52294080235074      3.52294080235074      o
   -3.52294080235074      3.52294080235074      3.52294080235074      o
   -3.52294080235074     -3.52294080235074     -3.52294080235074      o
    3.52294080235074      3.52294080235074     -3.52294080235074      o
#TiCl4
    0.00000000000000      0.00000000000000      0.00000000000000      ti
    2.38225918250055     -2.38225918250055      2.38225918250055      cl
   -2.38225918250055      2.38225918250055      2.38225918250055      cl
   -2.38225918250055     -2.38225918250055     -2.38225918250055      cl
    2.38225918250055      2.38225918250055     -2.38225918250055      cl
#TiF3
    0.00000000000000      0.00000000000000      0.00000000000000      ti
    1.67141378359608     -2.89497359365934      0.00000000000000      f
    1.67141378359608      2.89497359365934      0.00000000000000      f
   -3.34282756719215      0.00000000000000      0.00000000000000      f
#TiF4
    0.00000000000000      0.00000000000000      0.00000000000000      ti
    1.91049002205680     -1.91049002205680      1.91049002205680      f
   -1.91049002205680      1.91049002205680      1.91049002205680      f
   -1.91049002205680     -1.91049002205680     -1.91049002205680      f
    1.91049002205680      1.91049002205680     -1.91049002205680      f
#TiH4
    0.00000000000000      0.00000000000000      0.00000000000000      ti
    1.85401673992524     -1.85401673992524      1.85401673992524      h
   -1.85401673992524      1.85401673992524      1.85401673992524      h
   -1.85401673992524     -1.85401673992524     -1.85401673992524      h
    1.85401673992524      1.85401673992524     -1.85401673992524      h
#TiO
    0.00000000000000      0.00000000000000     -1.52666508702031      ti
    0.00000000000000      0.00000000000000      1.52666508702031      o
#TiO2
    0.00000000000000      0.00000000000000      1.20428895304113      ti
   -2.52745691819368      0.00000000000000     -0.60214447652056      o
    2.52745691819368      0.00000000000000     -0.60214447652056      o
#TiS2
    0.00000000000000      0.00000000000000      1.47408703528939      ti
   -3.26474084717958      0.00000000000000     -0.73704351764470      s
    3.26474084717958      0.00000000000000     -0.73704351764470      s
#VH5
    0.19112681055705      0.02226992514811     -0.53930273355572      v
    1.21909073594429      0.14802719321707     -3.48934725444155      h
    1.35539695757176     -1.88711320691551      1.52413775854092      h
    1.36313902267154      1.74011620101324      1.68211209473418      h
   -2.05809542406512      1.79208170165047      0.49003911695103      h
   -2.07065810267952     -1.81538181411337      0.33236101777113      h
#VO
    0.00000000000000      0.00000000000000     -1.49605986356322      v
    0.00000000000000      0.00000000000000      1.49605986356322      o
#VOF3
    0.00000000000000      0.00000000000000      0.02138488636646      v
    0.00000000000000      0.00000000000000      2.99447623694060      o
   -1.54851197430779      2.68210141562988     -1.00528704110235      f
   -1.54851197430779     -2.68210141562988     -1.00528704110235      f
    3.09702394861558      0.00000000000000     -1.00528704110235      f
#ZnCl2
    0.00000000000000      0.00000000000000      0.00000000000000      zn
```

```
    0.00000000000000      0.00000000000000      3.97259040076298      cl
    0.00000000000000      0.00000000000000     -3.97259040076298      cl
#ZnF2
    0.00000000000000      0.00000000000000      0.00000000000000      zn
    0.00000000000000      0.00000000000000      3.28287621534218      f
    0.00000000000000      0.00000000000000     -3.28287621534218      f
#ZnH2
    0.00000000000000      0.00000000000000      0.00000000000000      zn
    0.00000000000000      0.00000000000000     -2.92711569055511      h
    0.00000000000000      0.00000000000000      2.92711569055511      h
#ZnMe2
    3.68342584557891      0.00005713689622      0.00026506182462      c
   -3.68356713887322      0.00023772392501      0.00027909608166      c
    4.44876667227890      1.40886676936816     -1.35377226518157      h
    4.44905348065180     -1.87650086846691     -0.54356099559000      h
    4.45013283461305      0.46800749693417      1.89658631099636      h
   -4.44857871394426      1.21933922067696     -1.52675501888773      h
   -4.45004569978716      0.71048953578705      1.82005490636899      h
   -4.44913036491722     -1.93120927472341     -0.29420173043471      h
   -0.00005691560083      0.00071225960275      0.00110463482239      zn
#Ag2
    0.00000000000000      0.00000000000000     -2.43284975341900      ag
    0.00000000000000      0.00000000000000      2.43284975341900      ag
#AgCl
    0.00000000000000      0.00000000000000     -2.17427221124677      ag
    0.00000000000000      0.00000000000000      2.17427221124677      cl
#CdF2
    0.00000000000000      0.00000000000000      0.00000000000000      cd
    0.00000000000000      0.00000000000000      3.65399698977701      f
    0.00000000000000      0.00000000000000     -3.65399698977701      f
#CdMe2
   -0.01552765207821     -0.00211074960291     -0.00256455209819      cd
   -0.00518470223702     -0.00014740649893      4.03174197678488      c
   -0.00362618205013     -0.00022460589332     -4.02970589844624      c
    1.03909570930236      1.66912049287321      4.74981657043364      h
    0.94231936085281     -1.72490849239420      4.75261331167082      h
   -1.95136186467702      0.05616956014136      4.80782591209543      h
   -1.54974432309212     -1.20222871244731     -4.77501608328692      h
    1.81386811131603     -0.73818341030734     -4.76612177697937      h
   -0.26983845733673      1.94251332412944     -4.76858946017406      h
#MoCO6
    0.00000000000000      0.00000000000000      0.00000000000000      mo
    0.00000000000000      3.90295652556995      0.00000000000000      c
    0.00000000000000      0.00000000000000      3.90295652556995      c
    3.90295652556995      0.00000000000000      0.00000000000000      c
    0.00000000000000      0.00000000000000     -3.90295652556995      c
   -3.90295652556995      0.00000000000000      0.00000000000000      c
    0.00000000000000     -3.90295652556995      0.00000000000000      c
    0.00000000000000      6.09006160839460      0.00000000000000      o
    0.00000000000000      0.00000000000000      6.09006160839460      o
    6.09006160839460      0.00000000000000      0.00000000000000      o
    0.00000000000000      0.00000000000000     -6.09006160839460      o
   -6.09006160839460      0.00000000000000      0.00000000000000      o
    0.00000000000000     -6.09006160839460      0.00000000000000      o
#MoF3
    0.00000000000000      0.00000000000000     -0.00159671171885      mo
    1.77637872237622     -3.07677820063990      0.00053223723962      f
    1.77637872237622      3.07677820063990      0.00053223723962      f
   -3.55275744475244      0.00000000000000      0.00053223723962      f
#MoH
    0.00000000000000      0.00000000000000     -1.62042478286011      mo
    0.00000000000000      0.00000000000000      1.62042478286011      h
#MoO2
```

```
    0.00000000000000      0.00000000000000      1.20329050676615      mo
    2.70432477568260      0.00000000000000     -0.60164525338307      o
   -2.70432477568260      0.00000000000000     -0.60164525338307      o
#MoO3
    0.00000000000000      0.00000000000000     -0.87497023552764      mo
   -1.52984968466562      2.64977738178409      0.29165674517588      o
   -1.52984968466562     -2.64977738178409      0.29165674517588      o
    3.05969936933125      0.00000000000000      0.29165674517588      o
#NbF3
    0.00000000000000      0.00000000000000      0.00000000000000      nb
   -1.76123486076723      3.05054826291034      0.00000000000000      f
   -1.76123486076723     -3.05054826291034      0.00000000000000      f
    3.52246972153446      0.00000000000000      0.00000000000000      f
#NbO
    0.00000000000000      0.00000000000000      1.61827909896555      nb
    0.00000000000000      0.00000000000000     -1.61827909896555      o
#NbO2
    0.00000000000000      0.00000000000000      1.35090407793570      nb
    2.58725120191969      0.00000000000000     -0.67545203896785      o
   -2.58725120191969      0.00000000000000     -0.67545203896785      o
#NbO2F
   -0.02610891780556      0.86342528822632      0.06758988948919      nb
    2.62395976524113      0.01237672503655     -1.69666564370223      o
   -2.62102600254883     -0.14687228651066     -1.69136676770083      o
    0.02317515511327     -0.72892972675222      3.32044252191387      f
#PdCO4
    0.00000919143467      0.00000531380106     -0.00001191622877      pd
    2.18351277656177      2.18350949811326      2.18351805760958      c
   -2.18350195361372     -2.18350090015659      2.18350128273601      c
    2.18351494366302     -2.18352263605300     -2.18351671330313      c
   -2.18351964856344      2.18351087841231     -2.18351593700892      c
    3.44064404148229      3.44064088770018      3.44067413451479      o
   -3.44064406985283     -3.44062025793711      3.44067735832652      o
    3.44066163241694     -3.44068081079362     -3.44066336280415      o
   -3.44067691352870      3.44065802691347     -3.44066290384197      o
#PdF
    0.00000000000000      0.00000000000000     -1.82090621303246      pd
    0.00000000000000      0.00000000000000      1.82090621303246      f
#PdO2
    0.00000000000000      0.00000000000000      0.00368780697011      pd
   -3.56296972714997      0.00000000000000     -0.00184390348506      o
    3.56296972714997      0.00000000000000     -0.00184390348506      o
#RhF
    0.00000000000000      0.00000000000000     -1.80303434766506      rh
    0.00000000000000      0.00000000000000      1.80303434766506      f
#RhF4
    0.00000000000000      0.00000000000000      0.00000000000000      rh
    2.11095283269456     -2.11095283269456      2.11095283269456      f
   -2.11095283269456      2.11095283269456      2.11095283269456      f
   -2.11095283269456     -2.11095283269456     -2.11095283269456      f
    2.11095283269456      2.11095283269456     -2.11095283269456      f
#RhF6
    0.00000000000000      0.00000000000000      0.00000000000000      rh
    2.51299833250292     -2.51299833250292      0.00000000000000      f
    2.51299833250292      2.51299833250292      0.00000000000000      f
   -2.51299833250292      2.51299833250292      0.00000000000000      f
   -2.51299833250292     -2.51299833250292      0.00000000000000      f
    0.00000000000000      0.00000000000000      3.55393480343994      f
    0.00000000000000      0.00000000000000     -3.55393480343994      f
#RhO
    0.00000000000000      0.00000000000000     -1.63450098884323      rh
    0.00000000000000      0.00000000000000      1.63450098884323      o
#RuCO5
```

```
    0.00000000000000      0.00000000000000      0.00000000000000      ru
    1.84480011535838     -3.19528752960964      0.00000000000000      c
    1.84480011535838      3.19528752960964      0.00000000000000      c
   -3.68960023071676      0.00000000000000      0.00000000000000      c
    0.00000000000000      0.00000000000000      3.69125554048716      c
    0.00000000000000      0.00000000000000     -3.69125554048716      c
    2.94039490193387     -5.09291336446596      0.00000000000000      o
    2.94039490193387      5.09291336446596      0.00000000000000      o
   -5.88078980386773      0.00000000000000      0.00000000000000      o
    0.00000000000000      0.00000000000000      5.87379294085885      o
    0.00000000000000      0.00000000000000     -5.87379294085885      o
#RuF
    0.00000000000000      0.00000000000000     -1.79559672059692      ru
    0.00000000000000      0.00000000000000      1.79559672059692      f
#RuO
    0.00000000000000      0.00000000000000     -1.63370929862074      ru
    0.00000000000000      0.00000000000000      1.63370929862074      o
#RuO2
    0.00000000000000      0.00000000000000      0.00000000000000      ru
    0.00000000000000      0.00000000000000      3.22936844775946      o
    0.00000000000000      0.00000000000000     -3.22936844775946      o
#RuO4
   -0.00003901512132     -0.00004974867915      0.00003175074579      ru
    1.87142850130396      1.87147977103538      1.87148905199029      o
   -1.87142232278019     -1.87137312944410      1.87142093412647      o
    1.87151789303364     -1.87153124203117     -1.87151937514838      o
   -1.87148505643610      1.87147434911906     -1.87142236171416      o
#Tc2O7
    0.00000000000000      0.00000000000000      0.00000000000000      o
    0.00000000000000      0.00000000000000      3.55098914866315      tc
    0.00000000000000      0.00000000000000     -3.55098914866315      tc
    2.62571861860354     -1.51595935126696      4.65860875354015      o
    2.62571861860354      1.51595935126696     -4.65860875354015      o
    0.00000000000000      3.03191870253393      4.65860875354015      o
   -2.62571861860354      1.51595935126696     -4.65860875354015      o
   -2.62571861860354     -1.51595935126696      4.65860875354015      o
    0.00000000000000     -3.03191870253393     -4.65860875354015      o
#TcO
    0.00000000000000      0.00000000000000     -1.65131440458535      tc
    0.00000000000000      0.00000000000000      1.65131440458535      o
#TcO3F
    0.00000000000000      0.00000000000000     -0.03575380241616      tc
    0.00000000000000      0.00000000000000      3.47832150786421      f
    1.51189127548743     -2.61867250466434     -1.14752256848268      o
    1.51189127548743      2.61867250466434     -1.14752256848268      o
   -3.02378255097485      0.00000000000000     -1.14752256848268      o
#YF
    0.00000000000000      0.00000000000000     -1.84234806551158      y
    0.00000000000000      0.00000000000000      1.84234806551158      f
#YF3
    0.00000000000000      0.00000000000000      0.00977112603694      y
   -1.89922978387516      3.28956248091983     -0.00325704201177      f
   -1.89922978387516     -3.28956248091983     -0.00325704201177      f
    3.79845956775031      0.00000000000000     -0.00325704201177      f
#YO
    0.00000000000000      0.00000000000000     -1.72806290572366      y
    0.00000000000000      0.00000000000000      1.72806290572366      o
#ZrF
    0.00000000000000      0.00000000000000     -1.78049044438309      zr
    0.00000000000000      0.00000000000000      1.78049044438309      f
#ZrF3
    0.00000000000000      0.00000000000000      0.00444657710922      zr
   -1.82070257365541      3.15354936304259     -0.00148219236669      f
```

```
   -1.82070257365541     -3.15354936304259     -0.00148219236669      f
    3.64140514731082      0.00000000000000     -0.00148219236669      f
#ZrO
    0.00000000000000      0.00000000000000     -1.66498802952802      zr
    0.00000000000000      0.00000000000000      1.66498802952802      o
#ZrO2
    0.00000000000000      0.00000000000000      1.36096020616404      zr
   -2.71171774062042      0.00000000000000     -0.68048010308202      o
    2.71171774062042      0.00000000000000     -0.68048010308202      o
#Au2
    0.00000000000000      0.00000000000000     -2.42327065240856      au
    0.00000000000000      0.00000000000000      2.42327065240856      au
#Au3-
    0.00000000000000      0.00000000000000      0.00000000000000      au
    0.00000000000000      0.00000000000000      4.97146253204511      au
    0.00000000000000      0.00000000000000     -4.97146253204511      au
#AuCl
    0.00000000000000      0.00000000000000     -2.15000661513040      au
    0.00000000000000      0.00000000000000      2.15000661513040      cl
#AuCl3
    0.00000000000000      0.00000000000000      0.00000000000000      au
    2.21054988848081     -3.82878471951448      0.00000000000000      cl
    2.21054988848081      3.82878471951448      0.00000000000000      cl
   -4.42109977696162      0.00000000000000      0.00000000000000      cl
#HfF
    0.00000000000000      0.00000000000000      1.78068737689156      hf
    0.00000000000000      0.00000000000000     -1.78068737689156      f
#HfF3
    0.00000000000000      0.00000000000000      0.00000000000000      hf
    1.81947112203196     -3.15141642626371      0.00000000000000      f
    1.81947112203196      3.15141642626371      0.00000000000000      f
   -3.63894224406392      0.00000000000000      0.00000000000000      f
#HfO
    0.00000000000000      0.00000000000000     -1.66226332616427      hf
    0.00000000000000      0.00000000000000      1.66226332616427      o
#HfO2
    0.00000000000000      0.00000000000000      1.37910110648005      hf
    2.72240351204331      0.00000000000000     -0.68955055324002      o
   -2.72240351204331      0.00000000000000     -0.68955055324002      o
#HgF2
    0.00000000000000      0.00000000000000      0.00000000000000      hg
    0.00000000000000      0.00000000000000     -3.69723523229824      f
    0.00000000000000      0.00000000000000      3.69723523229824      f
#HgMe2
    0.00000000000000      0.00000000000000      0.00000000000000      hg
    0.00000000000000      0.00000000000000      4.03656130521134      c
    0.00000000000000      0.00000000000000     -4.03656130521134      c
    1.70138176612670     -0.98229322066757      4.76366724761748      h
    1.70138176612670      0.98229322066757     -4.76366724761748      h
    0.00000000000000      1.96458644133514      4.76366724761748      h
   -1.70138176612670      0.98229322066757     -4.76366724761748      h
   -1.70138176612670     -0.98229322066757      4.76366724761748      h
    0.00000000000000     -1.96458644133514     -4.76366724761748      h
#Hg2Cl2
   -0.00092289111444     -2.49971029372210      0.00000000000000      hg
    0.00086843425201      2.49894980264274      0.00000000000000      hg
    0.00005416705884     -6.97426742991672      0.00000000000000      cl
    0.00000028980360      6.97502792099608      0.00000000000000      cl
#IrF6
    0.00000000000000      0.00000000000000      0.00000000000000      ir
    0.00000000000000      0.00000000000000      3.59726293025323      f
    0.00000000000000      0.00000000000000     -3.59726293025323      f
    2.54361009647590     -2.54361009647590      0.00000000000000      f
```

```
    2.54361009647590      2.54361009647590      0.00000000000000      f
   -2.54361009647590      2.54361009647590      0.00000000000000      f
   -2.54361009647590     -2.54361009647590      0.00000000000000      f
#OsCO5
    0.00000000000000      0.00000000000000      0.00000000000000      os
    1.86245714222963     -3.22587039726125      0.00000000000000      c
    1.86245714222963      3.22587039726125      0.00000000000000      c
   -3.72491428445925      0.00000000000000      0.00000000000000      c
    0.00000000000000      0.00000000000000      3.74847701997556      c
    0.00000000000000      0.00000000000000     -3.74847701997556      c
    2.95959230898802     -5.12616424885734      0.00000000000000      o
    2.95959230898802      5.12616424885734      0.00000000000000      o
   -5.91918461797604      0.00000000000000      0.00000000000000      o
    0.00000000000000      0.00000000000000      5.93170395303675      o
    0.00000000000000      0.00000000000000     -5.93170395303675      o
#OsO2
    0.00000000000000      0.00000000000000     -0.90139173199185      os
    2.96334365356516      0.00000000000000      0.45069586599592      o
   -2.96334365356516      0.00000000000000      0.45069586599592      o
#OsO3
    0.00000000000000      0.00000000000000      0.00000000000000      os
    1.63177166219432     -2.82631142527168      0.00000000000000      o
    1.63177166219432      2.82631142527168      0.00000000000000      o
   -3.26354332438864      0.00000000000000      0.00000000000000      o
#OsO4
    0.00000000000000      0.00000000000000      0.00000000000000      os
    1.90033009057400     -1.90033009057400      1.90033009057400      o
   -1.90033009057400      1.90033009057400      1.90033009057400      o
   -1.90033009057400     -1.90033009057400     -1.90033009057400      o
    1.90033009057400      1.90033009057400     -1.90033009057400      o
#OsOF5
    0.00000000000000      0.00000000000000      0.22822360502953      os
    0.00000000000000      0.00000000000000      3.47998909744502      o
    0.00000000000000      0.00000000000000     -3.39562990080580      f
   -2.53530418774888      2.53530418774888     -0.07814570041718      f
   -2.53530418774888     -2.53530418774888     -0.07814570041718      f
    2.53530418774888     -2.53530418774888     -0.07814570041718      f
    2.53530418774888      2.53530418774888     -0.07814570041718      f
#PtCO4
    0.00000000000000      0.00000000000000      0.00000000000000      pt
    2.17219503977633     -2.17219503977633      2.17219503977633      c
   -2.17219503977633      2.17219503977633      2.17219503977633      c
   -2.17219503977633     -2.17219503977633     -2.17219503977633      c
    2.17219503977633      2.17219503977633     -2.17219503977633      c
    3.43196912076035     -3.43196912076035      3.43196912076035      o
   -3.43196912076035      3.43196912076035      3.43196912076035      o
   -3.43196912076035     -3.43196912076035     -3.43196912076035      o
    3.43196912076035      3.43196912076035     -3.43196912076035      o
#PtO
    0.00000000000000      0.00000000000000     -1.67069134020836      pt
    0.00000000000000      0.00000000000000      1.67069134020836      o
#PtO2
    0.00000000000000      0.00000000000000      0.00000000000000      pt
    0.00000000000000      0.00000000000000     -3.28869598692728      o
    0.00000000000000      0.00000000000000      3.28869598692728      o
#ReH
    0.00000000000000      0.00000000000000     -1.56532428006416      re
    0.00000000000000      0.00000000000000      1.56532428006416      h
#ReO
    0.00000000000000      0.00000000000000     -1.67864437842535      re
    0.00000000000000      0.00000000000000      1.67864437842535      o
#ReO2
    0.00000000000000      0.00000000000000      0.00000000000000      re
```

```
    0.00000000000000      0.00000000000000     -3.36557123070835      o
    0.00000000000000      0.00000000000000      3.36557123070835      o
#ReO3
    0.00000000000000      0.00000000000000      0.00000000000000      re
   -1.64935415797960      2.85676520129566      0.00000000000000      o
   -1.64935415797960     -2.85676520129566      0.00000000000000      o
    3.29870831595921      0.00000000000000      0.00000000000000      o
#ReO3F
    0.00000000000000      0.00000000000000     -0.00862182543285      re
    0.00000000000000      0.00000000000000      3.55207214412449      f
   -1.52651151621215      2.64399550441844     -1.18115010623055      o
   -1.52651151621215     -2.64399550441844     -1.18115010623055      o
    3.05302303242429      0.00000000000000     -1.18115010623055      o
#TaF
    0.00000000000000      0.00000000000000     -1.73663852825574      ta
    0.00000000000000      0.00000000000000      1.73663852825574      f
#TaF3
    0.00000000000000      0.00000000000000     -0.00088004990885      ta
   -1.76481713541870      3.05675294461335      0.00029334996962      f
   -1.76481713541870     -3.05675294461335      0.00029334996962      f
    3.52963427083740      0.00000000000000      0.00029334996962      f
#TaO2F
    0.00000000000000      0.00000000000000      0.03006542312973      ta
    0.00000000000000      0.00000000000000      3.72739793762169      f
    2.74274130577697      0.00000000000000     -1.87873168037571      o
   -2.74274130577697      0.00000000000000     -1.87873168037571      o
#WCO6
    0.00000000000000      0.00000000000000      0.00000000000000      w
    0.00000000000000      3.93720141856123      0.00000000000000      c
    0.00000000000000      0.00000000000000      3.93720141856123      c
    3.93720141856123      0.00000000000000      0.00000000000000      c
    0.00000000000000      0.00000000000000     -3.93720141856123      c
   -3.93720141856123      0.00000000000000      0.00000000000000      c
    0.00000000000000     -3.93720141856123      0.00000000000000      c
    0.00000000000000      6.12568593744740      0.00000000000000      o
    0.00000000000000      0.00000000000000      6.12568593744740      o
    6.12568593744740      0.00000000000000      0.00000000000000      o
    0.00000000000000      0.00000000000000     -6.12568593744740      o
   -6.12568593744740      0.00000000000000      0.00000000000000      o
    0.00000000000000     -6.12568593744740      0.00000000000000      o
#WF3
    0.00000000000000      0.00000000000000      0.00187166361740      w
   -1.79324602416154      3.10599322431868     -0.00062388787247      f
   -1.79324602416154     -3.10599322431868     -0.00062388787247      f
    3.58649204832309      0.00000000000000     -0.00062388787247      f
#WH
    0.00000000000000      0.00000000000000     -1.62254316912897      w
    0.00000000000000      0.00000000000000      1.62254316912897      h
#WO
    0.00000000000000      0.00000000000000     -1.58822148469933      w
    0.00000000000000      0.00000000000000      1.58822148469933      o
#WO2
    0.00000000000000      0.00000000000000      1.21145734769756      w
   -2.74201323107353      0.00000000000000     -0.60572867384878      o
    2.74201323107353      0.00000000000000     -0.60572867384878      o
#WO3
    0.00000000000000      0.00000000000000      0.00000000000000      w
    1.67015014718729     -2.89278491119702      0.00000000000000      o
    1.67015014718729      2.89278491119702      0.00000000000000      o
   -3.34030029437458      0.00000000000000      0.00000000000000      o
```

Statistical Evaluation

RI-ERRORS PER ATOM IN COULOMB ENERGIES / 10**(-6) H

auxbasis:	NEW							NEW, UNCONTRACTED							OLD (LARGEST)						
	orbital basis (def2-)							orbital basis (def2-)							orbital basis (def2-)						
	Naux	SV(P)	SVP	TZVP	TZVPP	QZVP	QZVPP	Naux	SV(P)	SVP	TZVP	TZVPP	QZVP	QZVPP	Naux	SV(P)	SVP	TZVP	TZVPP	QZVP	QZVPP
Molecule	(e a r t h -) a l k a l i m e t a l c o m p o u n d s																				
BaF	105	43.9	43.9	15.1	15.1	24.9	23.3	151	24.8	24.8	5.1	5.1	6.4	6.8	96	81.7	81.7	67.4	67.3	68.2	67.5
BaF2	154	61.6	61.6	22.6	22.6	33.9	28.2	221	39.6	39.6	12.5	12.5	14.9	11.9	139	110.3	110.3	123.4	123.4	132.9	126.6
BaH2	78	55.1	48.4	33.2	58.7	72.3	79.0	113	24.9	23.8	18.4	18.7	22.1	23.9	81	75.9	77.0	116.2	124.5	127.1	126.6
BaO	105	70.8	70.8	62.9	62.9	65.1	56.0	151	43.8	43.8	39.6	39.6	40.8	34.9	91	184.7	184.7	269.0	269.0	250.6	232.6
BaS	107	59.3	59.3	39.1	40.0	42.1	38.7	158	36.5	36.5	26.1	26.9	28.9	26.4	93	157.4	157.4	268.3	269.5	304.4	288.2
Be2F4	294	27.5	27.5	6.9	6.9	13.5	13.5	420	19.1	19.1	2.9	2.9	3.4	3.4	232	43.7	43.7	36.2	36.2	44.2	44.2
Be2H4	142	9.7	8.8	9.4	10.4	11.9	11.9	204	2.1	4.3	4.0	4.2	4.6	4.6	116	12.7	13.6	10.9	11.8	17.7	17.7
Be4	196	26.9	26.9	37.7	37.7	34.2	34.2	280	16.5	16.5	17.1	17.1	10.2	10.2	1201	762.6	1762.6	2011.9	2012.0	1866.9	1866.9
BeC2H6	213	11.0	14.0	11.2	12.8	15.5	15.5	306	2.6	4.1	2.6	2.0	2.0	2.0	190	15.0	14.6	22.1	21.7	21.4	21.4
BeF2O2H4	289	24.4	27.0	28.5	33.0	40.3	40.3	414	13.0	13.6	7.1	5.8	6.2	6.2	248	44.9	53.9	41.2	35.8	42.4	42.4
BeH2	71	7.4	6.4	3.2	2.2	5.9	5.9	102	1.7	3.0	2.8	1.9	2.3	2.3	58	4.3	3.9	5.4	5.3	5.3	5.3
BeS	100	23.5	23.5	32.6	32.5	42.3	42.3	147	13.8	13.8	10.1	10.3	16.8	16.8	70	107.6	107.6	186.1	185.7	258.5	258.5
CaCl2	158	84.4	84.4	11.8	12.1	20.1	20.1	243	66.8	66.8	4.1	4.3	3.6	3.6	109	124.3	124.3	169.3	171.3	228.3	211.8
CaF2	154	43.0	42.9	12.1	12.1	18.9	18.5	229	32.4	32.4	4.9	4.9	4.1	3.4	115	55.6	55.6	27.3	27.3	29.9	34.0
CaH2	78	40.2	33.6	27.1	40.1	50.4	50.5	121	14.5	13.5	9.9	9.9	13.1	12.6	57	170.5	155.6	156.1	154.2	160.5	157.0
CsF	105	35.0	35.0	9.4	10.8	11.5	8.8	151	24.1	24.1	3.4	4.0	2.5	1.9	64	273.6	273.6	604.1	599.2	554.2	571.5
CsH	67	18.2	15.5	9.7	24.2	27.0	32.4	97	7.4	7.0	4.7	6.0	6.3	6.2	35	135.5	136.9	327.9	369.3	366.1	365.7
CsO	105	23.9	23.9	7.5	7.8	9.9	11.3	151	19.7	19.7	4.4	4.5	3.8	4.4	59	239.4	239.4	499.2	490.7	471.8	508.1
K2S	163	20.8	20.8	13.9	14.1	23.7	24.3	255	12.8	12.8	5.7	5.8	6.1	6.5	98	390.3	390.3	550.3	551.1	660.6	666.2
K3P	219	23.0	23.0	20.6	21.2	33.5	33.5	344	16.3	16.3	11.0	11.1	14.8	15.0	127	267.1	267.1	401.9	402.4	480.3	485.0
KBr	114	44.1	44.1	14.3	14.3	21.4	20.4	178	20.8	20.8	8.3	8.3	8.8	7.9	73	219.9	219.9	323.1	323.1	414.8	417.9
KCl	107	72.9	72.9	9.9	10.0	18.1	17.6	166	56.5	56.5	3.3	3.3	3.7	3.6	69	312.6	312.6	392.7	394.2	497.7	499.3
KF	105	50.0	50.0	21.0	21.0	25.1	23.7	159	28.6	28.6	4.3	4.3	2.6	2.7	72	406.7	406.7	544.0	544.0	632.1	631.9
KH	67	19.2	16.1	12.3	16.4	24.9	24.9	105	10.1	9.4	4.7	4.5	5.4	5.6	43	219.1	218.8	308.0	317.7	358.4	367.0
Li2	98	12.1	12.1	34.9	34.4	18.6	18.6	140	7.8	7.8	13.1	13.6	6.4	6.4	60	43.0	43.0	58.7	55.9	40.1	40.1
Li2O	147	6.8	6.8	9.9	9.9	9.8	9.8	210	3.4	3.4	0.7	0.8	0.9	0.9	98	126.5	126.5	142.3	146.2	163.1	163.1
Li4C4H12	524	7.9	9.6	10.2	11.9	12.2	12.2	752	2.2	3.1	2.5	2.4	2.3	2.3	440	19.4	19.7	27.3	27.7	29.3	29.3
Li4Cl4	400	33.2	33.2	10.0	9.7	11.4	11.4	588	25.2	25.2	2.3	2.2	1.7	1.7	280	30.4	30.4	83.4	83.9	128.2	128.2
Li4H4	240	3.0	2.8	7.7	13.1	10.9	10.9	344	0.5	0.7	0.7	0.4	0.6	0.6	176	22.3	22.0	23.6	27.9	33.9	33.9
Li8	392	9.2	9.2	26.6	28.5	22.9	22.9	560	2.4	2.4	5.6	5.6	4.0	4.0	240	65.7	65.7	92.3	104.0	79.3	79.3
LiBH4	142	8.0	9.1	7.0	10.2	10.5	10.5	204	3.5	4.9	2.9	2.1	2.6	2.6	124	17.5	18.3	23.1	23.8	28.1	28.1
LiCl	100	58.6	58.6	11.2	10.5	11.6	11.6	147	40.9	40.9	2.5	2.2	2.2	2.1	70	72.5	72.5	164.7	157.9	210.0	210.0
LiF	98	28.5	28.5	10.1	10.0	9.7	9.7	140	21.3	21.3	2.0	1.9	0.6	0.6	73	106.4	106.4	96.6	95.5	100.7	100.7
LiH	60	2.8	2.3	10.1	11.9	9.2	9.2	86	0.7	1.1	2.5	2.1	2.5	2.5	44	55.5	59.6	86.1	91.1	102.8	102.8
LiSLi	149	7.6	7.6	12.2	11.9	12.0	12.0	217	4.5	4.5	1.3	1.0	1.7	1.7	100	69.0	69.0	162.1	147.4	172.6	172.6
Mg4	224	33.5	33.5	26.4	26.4	27.9	28.0	308	30.7	30.7	25.6	25.6	23.5	23.6	112	105.2	105.2	66.0	66.0	66.6	67.1
MgCl2	158	77.6	77.6	7.2	7.4	12.5	12.6	231	60.9	60.9	5.3	5.4	4.2	4.2	108	90.2	90.2	154.3	156.3	204.8	203.7
MgF	105	34.7	34.7	5.7	5.7	10.8	10.9	147	25.7	25.7	2.9	2.8	2.8	2.7	71	105.6	105.6	103.4	103.4	102.8	102.2
MgF2	154	39.9	39.9	5.9	5.9	12.2	12.4	217	31.5	31.5	3.3	3.3	3.8	3.6	114	66.4	66.4	41.2	41.2	40.2	38.5
MgH2	78	13.0	9.8	5.7	6.5	8.8	9.0	109	4.4	4.6	3.1	2.9	2.3	2.4	56	39.2	36.0	30.2	31.1	33.5	32.1
Na2O	161	23.4	23.4	5.9	5.9	9.9	9.8	224	16.7	16.7	4.1	4.1	5.2	5.1	94	131.4	131.4	267.0	267.0	205.3	287.8
Na2S	163	15.8	15.8	4.8	4.9	7.6	7.4	231	11.3	11.3	3.5	3.4	2.8	2.6	96	126.3	126.3	190.9	191.3	187.3	237.7
Na3N	217	39.2	39.2	18.9	18.9	20.7	20.7	301	27.3	27.3	13.3	13.3	11.8	11.7	122	118.7	118.7	203.9	203.9	158.5	217.9
Na3P	219	23.7	23.7	15.4	16.1	17.8	17.8	308	18.2	18.2	12.7	12.8	11.1	11.1	124	79.4	79.4	134.3	135.0	138.1	171.1
NaCl	107	70.5	70.5	4.5	4.6	9.6	9.5	154	42.4	42.5	3.1	3.2	3.7	3.5	68	117.2	117.2	165.0	166.4	193.4	222.9
NaF	105	47.8	47.8	7.5	7.5	10.7	10.5	147	33.0	33.0	4.8	4.9	4.5	4.3	71	133.8	133.8	182.6	182.6	144.3	198.7
NaH	67	14.5	12.9	5.8	8.9	10.1	10.2	93	10.8	9.8	3.9	3.9	3.8	3.8	42	75.3	70.7	109.9	111.7	100.5	126.4
PLi3	198	5.3	5.3	17.9	17.5	15.1	15.1	287	2.8	2.8	5.7	5.6	4.4	4.4	130	73.3	73.3	111.9	111.8	137.6	137.6
RbF	105	39.4	39.4	6.0	9.0	13.2	9.6	151	29.5	29.5	2.3	3.2	2.7	2.2	64	270.6	270.6	346.0	346.5	467.2	472.4
RbH	67	12.3	10.8	4.9	14.9	18.7	18.9	97	6.9	7.6	2.7	3.5	3.6	3.6	35	140.6	143.2	181.4	198.5	267.8	268.6
RbO	105	36.5	36.5	5.4	6.1	10.0	9.3	151	32.5	32.5	3.5	3.6	3.5	3.3	59	219.4	219.4	310.8	306.7	395.4	413.9
SrF	105	43.3	43.3	11.8	11.3	19.3	14.2	151	21.7	21.7	3.3	3.1	4.1	2.9	96	51.7	51.7	55.0	51.6	57.9	59.3
SrF2	154	53.0	53.0	17.5	16.7	31.4	26.0	221	27.6	27.6	3.3	3.2	4.6	3.2	139	113.1	113.1	59.9	57.5	67.9	66.0
SrH2	78	45.8	35.0	23.5	40.2	50.2	54.3	113	12.6	10.8	8.5	7.8	8.5	9.0	81	255.4	241.2	191.7	183.6	195.9	204.0
SrO	105	36.9	36.9	30.1	34.5	43.0	34.2	151	18.8	18.8	13.1	16.1	13.1	9.7	911	002.3	1002.3	641.0	630.9	649.0	693.8
SrS	107	42.5	42.5	25.5	28.9	38.0	32.2	158	22.0	22.0	12.4	14.9	16.9	13.2	93	950.3	950.3	715.0	711.2	809.5	810.9
average	41	32.5	32.0	15.7	17.8	21.8	21.2	60	20.5	20.6	7.0	7.1	7.1	6.8	29	184.1	183.8	226.5	227.2	244.7	252.4
std-dev		20.7	20.6	11.4	13.1	14.6	14.4		15.3	15.2	7.1	7.2	7.5	6.9		280.3	280.2	295.8	295.5	290.9	292.5
maximum		84.4	84.4	62.9	62.9	72.3	79.0		66.8	66.8	39.6	39.6	40.8	34.9		1762.6	1762.6	2011.9	2012.0	1866.9	1866.9
typical		53.2	52.6	27.1	31.0	36.4	35.6		35.8	35.8	14.1	14.4	14.6	13.6		464.4	464.0	522.3	522.7	535.7	544.9
kJ/mol		0.140	0.138	0.071	0.081	0.096	0.093		0.094	0.094	0.037	0.038	0.038	0.036		1.219	1.218	1.371	1.372	1.406	1.430
Molecule	m a i n g r o u p c o m p o u n d s 2 p t o 4 p																				
B2H6	164	11.6	13.1	8.2	8.6	9.7	9.7	236	5.3	7.6	4.6	3.3	3.3	3.3	160	11.9	13.3	11.7	11.8	13.1	13.1
B3N3H6	360	21.2	22.9	14.0	16.2	19.5	19.5	516	7.4	8.1	2.9	2.6	3.4	3.4	312	36.0	37.6	26.7	26.6	27.8	27.8
B4H4	240	16.6	17.0	9.8	9.5	10.8	10.9	344	6.3	7.6	4.6	3.9	3.4	3.4	208	16.6	15.7	15.0	15.0	15.3	15.4
BF3	196	33.7	33.7	11.4	11.4	14.6	14.6	280	22.1	22.1	3.8	3.8	4.0	4.0	167	72.1	72.1	39.9	39.9	46.9	46.9

BH3	82	14.3	15.8	10.3	11.8	11.8	11.9	118	5.6	7.5	4.3	3.4	3.4	3.4	80	8.1	9.2	8.3	8.5	9.1	9.1
BH3CO	180	12.6	13.3	8.0	8.5	10.6	10.6	258	6.2	7.3	2.7	2.1	2.1	2.1	156	38.6	39.1	23.3	23.8	26.1	26.2
BH3NH3	164	16.6	20.2	15.7	20.0	21.9	22.0	236	5.6	6.8	3.2	2.8	3.1	3.2	160	17.1	18.3	16.2	16.6	18.1	18.1
C2H2	120	10.0	10.7	9.6	11.1	16.0	16.1	172	3.6	4.5	1.3	1.2	1.8	1.8	104	34.2	37.8	17.5	15.2	12.2	12.2
C2H3N	180	24.9	26.6	24.0	26.9	31.7	31.8	258	9.5	10.6	7.3	6.9	7.7	7.7	156	98.5	102.4	92.1	89.8	92.4	92.6
C2H4	142	14.2	18.0	17.7	20.1	21.8	21.9	204	5.0	7.2	5.1	4.4	4.4	4.4	132	36.2	40.1	41.2	39.5	39.8	39.8
C2H6	164	12.5	16.3	15.4	17.9	19.6	19.6	236	3.6	5.4	3.1	2.4	2.4	2.4	160	29.6	28.3	37.7	36.9	36.5	36.5
C4H4	240	24.1	24.8	24.0	25.4	31.2	31.2	344	5.6	6.1	8.1	7.8	7.4	7.4	208	75.6	74.0	60.6	58.5	55.0	55.2
C6H6	360	17.2	20.7	19.7	21.8	24.7	24.7	516	6.5	8.5	6.4	5.5	5.5	5.5	312	63.0	65.1	58.1	55.8	56.1	56.1
CF4	245	60.7	60.7	15.8	15.8	20.3	20.3	350	46.3	46.3	9.7	9.7	9.2	9.2	210	171.8	171.8	136.9	136.9	162.7	162.8
CH2O	120	22.6	26.3	17.4	19.4	20.8	20.8	172	10.6	12.4	6.3	5.6	4.9	5.0	104	70.8	73.6	55.6	55.4	59.6	59.8
CH2O2	169	34.1	37.3	26.4	26.9	29.3	29.3	242	24.5	26.1	15.2	14.8	14.1	14.1	142	159.9	159.8	154.1	154.3	158.2	158.3
CH3N	131	24.3	27.5	19.0	22.7	25.3	25.4	188	7.4	8.7	4.6	4.2	4.4	4.4	118	50.1	55.4	51.7	49.5	51.6	51.8
CH3OH	142	20.9	24.4	24.9	27.9	29.8	29.9	204	9.6	11.1	7.8	6.2	5.9	5.9	132	70.9	74.1	75.2	70.1	72.1	72.1
CH4	93	14.4	19.2	18.7	20.9	22.1	22.1	134	3.3	5.3	3.4	2.2	2.2	2.2	94	21.8	21.2	31.0	29.1	28.2	28.3
CO	98	20.8	20.8	12.6	12.6	17.5	17.5	140	12.8	12.8	4.3	4.3	3.6	3.6	76	108.2	108.2	60.7	60.7	63.8	64.2
CO2	147	18.0	18.0	7.3	7.3	12.3	12.3	210	12.6	12.6	2.0	2.0	1.6	1.6	114	125.0	125.0	66.5	66.5	70.5	70.9
F2	98	79.9	79.9	50.0	50.0	54.6	54.6	140	71.4	71.4	37.0	37.0	35.9	35.9	86	129.0	129.0	136.2	136.2	139.8	139.9
H2	22	30.4	65.8	53.2	56.3	52.4	52.5	32	6.4	12.6	5.8	2.6	2.6	2.5	28	1.5	1.3	2.7	4.8	7.2	7.2
H2CO3	218	36.6	38.3	30.3	33.3	37.5	37.5	312	20.1	20.1	9.5	8.5	7.8	7.8	180	107.5	114.6	91.3	86.3	94.1	94.1
H2O	71	27.1	29.1	43.0	48.3	51.6	51.6	102	13.5	12.2	10.4	7.6	6.8	6.8	66	47.6	60.3	68.5	51.2	58.1	58.1
H2O2	120	40.6	43.5	52.3	57.3	62.7	62.7	172	26.8	26.7	19.3	17.2	16.8	16.8	104	143.2	151.6	185.9	174.3	180.0	180.0
HCN	109	15.3	15.3	12.0	12.9	17.1	17.2	156	7.9	8.1	1.5	1.6	1.9	1.9	90	50.8	54.2	28.7	27.8	26.3	26.4
HF	60	32.3	34.5	26.5	32.9	39.3	39.4	86	24.9	23.0	5.3	4.8	4.6	4.6	57	55.2	54.8	38.5	32.9	39.7	40.0
HNC	109	18.9	19.8	15.5	17.3	20.0	20.0	156	9.2	10.0	3.3	3.2	2.6	2.6	90	41.9	44.4	32.5	31.2	29.7	29.8
HNO	109	51.2	54.9	43.2	46.9	51.4	51.5	156	19.2	19.6	11.5	11.0	10.8	10.8	90	171.1	176.4	174.9	170.8	176.8	177.9
HNO2	158	41.3	45.3	31.1	34.2	35.8	35.8	226	20.1	20.5	8.9	9.1	7.7	7.7	128	113.6	116.4	86.5	86.1	90.9	91.0
HNO3	207	44.4	45.9	36.1	37.4	41.8	41.8	296	22.6	23.1	10.5	9.6	8.5	8.5	166	151.5	155.6	120.1	117.1	123.6	123.6
N2	98	48.2	48.2	16.0	16.0	18.2	18.2	140	23.1	23.1	3.8	3.8	2.5	2.5	76	97.3	97.3	42.2	42.2	43.3	43.6
N2H2	120	60.1	66.4	46.8	51.3	56.6	56.7	172	16.0	16.6	9.6	8.7	9.2	9.2	104	105.7	114.1	116.0	108.4	111.9	112.1
N2H4	142	49.5	55.2	45.1	53.7	56.9	56.9	204	11.2	12.1	6.2	5.9	6.6	6.6	132	63.9	69.2	94.1	87.8	92.8	92.8
N4	196	59.0	59.0	24.9	24.9	28.7	28.8	280	52.5	52.5	14.8	14.8	15.8	15.8	152	449.7	449.7	415.4	415.4	425.7	426.5
NF3	196	73.9	73.9	32.4	32.4	41.0	41.0	280	52.1	52.1	13.7	13.7	14.3	14.3	167	208.4	208.4	188.0	188.0	206.8	207.0
NH3	82	33.8	37.8	29.0	35.9	39.4	39.4	118	7.8	8.1	4.1	3.5	5.3	5.3	80	27.3	36.5	55.0	46.7	54.1	54.1
NH4F	142	29.2	34.4	22.3	27.2	30.6	30.6	204	11.9	12.2	3.3	3.2	3.1	3.1	137	27.0	30.0	24.9	22.9	27.6	27.6
OF2	147	71.5	71.5	43.9	43.9	48.5	48.5	210	64.8	64.8	30.6	30.6	29.4	29.4	124	189.1	189.1	198.0	198.0	202.1	202.2
Al2O3	249	42.4	42.4	19.0	21.1	27.8	27.8	364	27.8	27.8	11.4	11.0	10.5	10.5	176	97.5	97.5	108.2	114.2	124.1	124.1
Al2S3	255	38.8	38.8	13.8	14.3	18.5	18.5	385	24.3	24.3	8.8	9.0	7.5	7.5	182	87.7	87.7	179.5	190.6	247.9	248.1
AlCl3	204	67.6	67.6	15.0	16.2	24.4	24.4	308	52.3	52.3	9.0	9.2	10.4	10.4	151	66.5	66.5	185.9	190.2	255.6	255.7
AlF3	198	48.0	48.0	13.2	13.9	26.2	26.2	287	36.4	36.4	7.1	7.2	9.2	9.2	160	72.6	72.6	61.4	63.2	74.2	74.2
AlH3	84	31.5	34.5	20.2	19.5	20.7	20.7	125	17.0	20.1	14.8	13.8	13.0	13.0	73	15.5	15.3	42.5	45.1	49.7	49.8
AlN	100	30.1	30.1	24.0	24.3	29.8	29.7	147	14.9	14.9	8.3	8.1	8.0	8.0	69	56.9	56.9	97.6	100.2	106.8	106.6
CS2	151	29.5	29.5	20.2	18.5	24.3	24.4	224	22.0	22.0	5.1	5.3	5.9	5.9	118	45.3	45.3	92.4	93.5	143.5	144.1
Cl2	102	118.5	118.5	42.3	43.9	52.1	52.2	154	93.4	93.4	36.5	35.7	36.5	36.5	80	164.4	164.4	457.0	458.8	548.3	548.6
ClF	100	103.7	103.7	49.2	49.4	60.0	60.0	147	72.1	72.1	33.8	33.4	35.5	35.6	83	116.2	116.2	231.9	230.6	281.6	281.8
ClF3	198	71.0	71.0	41.7	43.1	53.1	53.1	287	57.2	57.2	28.9	28.5	30.6	30.6	169	113.2	113.2	163.1	165.5	196.8	196.8
H2SO4	269	44.8	46.6	42.8	44.9	48.1	48.2	389	31.5	32.0	27.6	26.8	24.5	24.5	220	127.8	134.5	106.6	103.0	117.6	117.7
H3PO4	280	45.0	46.4	52.7	58.8	62.2	62.3	405	27.8	27.2	26.1	25.6	24.4	24.4	234	100.8	107.3	79.2	76.6	87.0	87.0
HCP	111	18.5	19.0	17.7	19.6	23.4	23.6	163	11.7	12.4	5.8	5.9	6.0	6.0	92	33.8	35.4	50.8	52.8	77.1	77.7
HCl	62	61.6	67.1	47.3	44.1	48.9	49.1	93	41.3	45.9	15.0	12.3	13.1	13.1	54	23.4	30.8	120.1	109.1	153.1	153.6
HSH	73	47.8	62.2	57.3	53.0	55.5	55.6	109	25.5	32.8	25.0	21.0	21.8	21.8	68	20.7	27.5	73.5	69.9	98.6	99.1
HSSH	124	55.4	67.9	61.5	60.1	63.6	63.6	186	36.9	42.9	32.9	29.9	31.5	31.5	108	77.4	82.2	163.4	163.3	203.6	203.7
P2	102	52.0	52.0	33.2	32.5	39.2	39.3	154	42.2	42.2	23.9	24.1	27.8	27.8	80	82.9	82.9	128.8	134.1	206.1	207.4
P4	204	123.2	123.2	78.9	82.4	90.3	90.3	308	75.2	75.2	27.4	27.3	31.3	31.3	160	219.5	219.5	257.7	260.2	334.9	334.9
PF3	198	53.9	53.9	38.1	41.9	54.7	54.7	287	40.8	40.8	25.9	26.3	32.2	32.2	169	110.5	110.5	80.2	84.6	104.0	104.0
PF5	296	57.9	57.9	42.8	43.6	54.9	54.9	427	41.7	41.7	23.1	23.7	27.8	27.8	255	118.4	118.4	81.1	81.9	98.6	98.6
PH3	84	66.5	81.0	51.6	47.8	50.8	50.8	125	40.4	52.3	38.0	34.7	38.6	38.6	82	19.3	23.3	31.5	33.4	52.8	52.8
S2	102	56.3	56.3	22.6	23.3	29.3	29.4	154	46.6	46.6	19.3	19.9	21.5	21.6	80	111.9	111.9	219.2	221.9	302.0	303.5
S5	255	71.7	71.7	49.3	52.9	58.7	58.7	385	62.8	62.8	41.7	42.1	43.6	43.6	200	197.6	197.6	371.6	376.7	464.3	464.4
SF2	149	92.1	92.1	55.9	56.2	66.1	66.1	217	69.3	69.3	37.6	37.6	43.2	43.2	126	138.4	138.4	156.6	158.7	197.0	197.2
SF4	247	66.4	66.4	48.6	51.3	62.5	62.5	357	50.7	50.7	28.3	28.0	32.3	32.3	212	132.9	132.9	116.5	122.8	145.6	145.6
SF6	345	53.6	53.6	18.9	19.0	27.1	27.1	497	46.2	46.2	13.8	13.9	16.4	16.4	298	140.8	140.8	86.0	86.2	103.1	103.1
SiCl4	255	88.6	88.6	30.5	31.6	42.2	42.2	385	73.5	73.5	16.2	16.8	21.0	21.0	200	97.2	97.2	213.4	216.0	289.2	289.2
SiF4	247	42.8	42.8	21.3	22.1	29.6	29.6	357	30.7	30.7	9.9	10.5	11.7	11.7	212	81.9	81.9	48.5	49.8	66.9	67.0
SiH4	95	45.4	49.7	33.7	31.4	34.3	34.3	141	28.9	35.9	27.8	26.9	30.4	30.4	96	18.1	20.1	23.5	25.7	42.1	42.2
SiO2	149	52.5	52.5	48.2	51.9	51.3	51.4	217	33.3	33.3	25.8	25.5	18.9	18.9	116	91.3	91.3	81.2	85.7	113.9	114.0
SiS2	153	52.3	52.3	24.4	27.1	28.4	28.5	231	30.6	30.6	11.7	11.9	9.7	9.7	120	87.2	87.2	141.9	147.8	221.2	221.7
As4	232	112.3	112.3	71.9	71.9	78.0	78.2	356	69.0	69.0	67.9	67.9	56.1	55.9	176	118.3	118.3	189.9	189.9	235.6	238.2
As4S4	436	116.1	116.1	101.8	104.7	110.0	109.2	664	84.6	84.6	88.4	89.0	83.0	82.7	336	192.2	192.2	323.8	326.7	398.3	40.0
AsCl3	211	99.0	99.0	50.6	51.5	59.3	55.7	320	72.2	72.2	32.6	32.7	30.7	30.3	164	76.0	76.0	237.9	239.7	306.5	309.7
AsCl6-	364	93.0	93.0	28.4	28.6	38.1	38.0	551	73.1	73.1	17.3	17.2	17.6	17.5	284	61.0	61.0	251.3	252.5	352.1	352.3
AsH3	91	54.7	64.7	46.2	43.1	45.8	45.5	137	36.0	45.8	42.5	39.5	38.5	38.0	86	30.7	34.0	44.0	43.8	54.5	55.0
Br2	116	119.7	119.7	64.1	64.1	71.4	70.2	178	77.9	77.9	54.1	54.1	57.8	56.8	88	113.6	113.6	289.4	289.4	427.9	420.2
BrCl	109	115.1	115.1	50.2	51.0	57.6	57.5	166	81.4	81.4	40.1	39.8	39.7	39.4	84	127.8	127.8	350.4	351.8	465.7	461.7
BrO4-	254	59.5	59.5	55.0	55.0	52.2	51.0	369	46.8	46.8	46.1	46.1	37.2	35.8	196	90.7	90.7	111.2	111.2	131.0	130.9
GaCl	109	86.4	86.4	29.9	29.8	51.1	54.0	166	59.2	59.2	15.6	15.6	11.0	10.7	75	41.8	41.8	143.1	143.8	213.7	214.1
GaCl3	211	95.6	95.6	38.6	38.3	52.2	48.6	320	75.3	75.3	25.9	25.8	23.4	22.4	155	76.6	76.6	207.9	208.9	275.9	275.3
GaF	107	71.8	71.8	41.8	41.8	62.3	62.4	159	45.6	45.6	25.0	25.0	20.1	19.3	78	67.9	67.9	75.3	75.3	105.7	103.6
GaF2	156	78.2	78.2	48.0	48.0	67.0	61.5	229	49.7	49.7	29.4	29.4	27.8	26.4	121	99.0	99.0	100.7	100.7	122.6	118.3
GaH3	91	50.6	51.3	47.2	45.7	49.4	46.2	137	36.6	40.1	39.9	39.9	31.3	29.8	77	42.7	45.8	60.4	61.4	73.7	71.7
GaO	107	60.4	60.4	39.5	39.5	57.7	55.5	159	36.6	36.6	24.7	24.7	18.6	17.7	73	110.6	110.6	143.1	143.1	166.7	161.7
GeCl4	262	94.4	94.4	45.0	45.1	54.4	53.1	397	80.3	80.3	30.6	30.5	28.0	26.9	204	62.8	62.8	207.7	208.8	262.8	262.7
GeF3	205	66.3	66.3	42.8	42.8	55.3	54.2	299	47.9	47.9	28.1	28.1	26.1	24.8	173	77.3	77.3	74.5	74.5	85.7	84.8
GeF4	254	63.7	63.7	45.1	45.1	56.5	54.2	369	52.2	52.2	35.4	35.4	33.0	30.5	216	85.5	85.5	81.4	81.4	88.8	87.2
GeH4	102	55.5	57.9	50.8	49.5	49.5	47.3	153	40.7	46.3	45.9	45.2	38.1	36.1	100	35.7	39.0	48.3	49.0	56.5	55.2
GeO	107	68.9	68.9	55.1	55.1	63.0	61.9	159	43.0	43.0	35.8	35.8	27.6	26.7	82	85.9	85.9	104.3	104.3	118.5	118.7
GeO2	156	80.3	80.3	65.6	65.6	69.6	70.2	229	33.0	33.0	27.7	27.7	20.7	20.7	120	148.2	148.2	163.7	163.7	168.5	167.7
HBr	69	58.6	66.6	28.4	25.5	24.8	23.8	105	35.8	43.3	22.8	20.8	18.7	18.5	58	25.0	29.7	78.8	74.6	126.8	125.3
HCBr3	234	82.4	83.9	36.3	37.0	39.3	38.6	353	50.0	50.5	23.9	23.3	21.0	20.8	184	65.1	63.2	129.5	129.2	189.2	186.9
Se8	464	109.8	109.8	96.3	96.3	122.2	113.3	712	81.6	81.6	68.9	68.9	69.7	68.8	352	106.5	106.5	211.5	211.5	280.7	280.7

SeH2	80	57.6	72.1	45.1	40.7	44.4	42.3	121	42.8	54.7	35.0	31.4	30.3	30.0	72	33.4	38.8	64.3	61.2	73.1	72.5
SeO	107	67.3	67.3	56.4	56.4	64.5	62.7	159	52.5	52.5	41.3	41.3	38.4	37.5	82	87.0	87.0	112.4	112.4	133.7	133.3
SeO2	156	74.3	74.3	66.6	66.6	71.3	69.2	229	56.9	56.9	49.7	49.7	45.8	44.5	120	101.2	101.2	113.5	113.5	128.4	128.5
average	38	53.7	55.9	35.7	36.8	42.6	42.2	56	35.7	36.9	20.4	19.9	19.3	19.1	31	87.9	89.5	117.0	116.7	142.2	138.4
std-dev		29.0	28.5	19.1	19.0	20.9	20.4		23.9	23.7	16.7	16.8	16.1	15.8		61.7	61.2	90.5	91.4	115.3	112.6
maximum		123.2	123.2	101.8	104.7	122.2	113.3		93.4	93.4	88.4	89.0	83.0	82.7		449.7	449.7	457.0	458.8	548.3	548.6
typical		82.7	84.4	54.8	55.9	63.5	62.5		59.7	60.6	37.2	36.7	35.4	34.9		149.6	150.7	207.5	208.1	257.6	251.0
kJ/mol		0.217	0.221	0.144	0.147	0.167	0.164		0.157	0.159	0.098	0.096	0.093	0.092		0.393	0.396	0.545	0.546	0.676	0.659

main group compounds 5 p to 6 p

I2	116	72.9	72.9	58.5	58.5	68.2	68.2	162	50.9	50.9	38.2	38.2	43.9	43.9
ICl	109	91.4	91.4	61.3	62.8	70.2	70.5	158	64.1	64.1	32.9	32.8	35.1	35.2
IH	69	41.3	52.0	37.8	32.9	33.8	34.0	97	35.4	46.1	34.8	31.0	30.5	30.7
KI	114	15.8	15.8	13.2	13.2	22.4	21.5	170	12.7	12.7	5.3	5.3	7.2	6.8
IO4-	254	48.6	48.6	56.0	56.0	53.0	53.0	361	38.5	38.5	42.9	42.9	33.3	33.3
InCl	109	88.6	88.6	38.4	38.4	43.1	43.1	158	52.7	52.7	12.4	12.4	12.0	12.0
InCl3	211	102.9	102.9	42.2	42.0	42.8	42.7	312	78.6	78.6	26.6	26.6	24.7	24.6
InH	69	42.2	41.4	38.0	38.8	39.9	40.1	97	23.4	24.2	23.2	23.5	23.0	23.1
InH3	91	53.9	52.8	51.8	51.9	48.9	49.0	129	40.1	41.8	41.0	41.4	37.5	37.5
InO	107	55.4	55.4	31.0	31.0	28.1	28.0	151	28.4	28.4	20.0	20.0	16.9	16.8
SbCl6-	364	86.0	86.0	23.1	23.4	34.1	34.1	543	72.0	72.0	12.4	12.4	13.9	13.9
SbF	107	36.2	36.2	22.9	22.9	28.7	28.8	151	26.6	26.6	17.0	17.0	18.3	18.4
SbF3	205	49.1	49.1	35.1	35.1	41.6	41.6	291	38.0	38.0	26.9	26.9	27.9	27.9
SbH3	91	30.6	35.8	30.1	28.7	30.5	30.5	129	22.1	29.2	28.5	27.1	29.0	29.0
SbO2	156	50.7	50.7	44.7	44.7	46.0	46.0	221	22.7	22.7	26.4	26.4	21.5	21.7
SnF3	205	76.9	76.9	47.3	47.3	53.5	53.4	291	48.1	48.1	26.3	26.3	23.8	23.8
SnH4	102	63.0	67.3	62.7	62.5	56.8	56.8	145	54.5	61.7	59.3	59.4	53.5	53.5
SnO	107	82.3	82.3	55.9	55.9	59.9	59.9	151	25.7	25.7	25.9	25.9	21.1	21.1
SnO2	156	86.6	86.6	50.6	50.6	67.3	67.3	221	23.5	23.5	24.9	24.9	23.8	23.8
TeF3	205	53.6	53.6	32.6	32.6	42.8	42.9	291	40.1	40.1	21.7	21.7	23.2	23.2
TeH2	80	42.9	53.7	40.9	38.2	40.4	40.5	113	32.9	43.6	37.9	35.7	38.0	38.1
TeO	107	41.3	41.3	43.5	43.5	46.3	46.1	151	28.7	28.7	32.0	32.0	29.5	29.4
TeO2	156	63.9	63.9	60.8	60.8	62.4	62.4	221	42.5	42.5	45.6	45.6	39.8	39.8
BiCl6-	364	78.3	78.3	17.3	17.4	26.0	26.0	543	65.9	65.9	10.2	10.2	10.3	10.3
BiF	107	41.0	41.0	29.7	29.7	38.9	39.0	151	34.5	34.5	19.5	19.5	20.8	20.9
BiF3	205	54.1	54.1	35.7	35.7	44.0	44.0	291	46.0	46.0	27.5	27.5	29.4	29.4
BiH3	91	36.1	42.7	41.7	40.5	43.4	43.5	129	29.8	37.9	38.5	37.4	39.7	39.8
BiO2	156	50.5	50.5	46.9	46.9	50.9	51.0	221	27.7	27.7	29.3	29.3	27.1	27.4
PbF3	205	72.6	72.6	38.9	38.9	44.0	44.0	291	53.7	53.7	26.6	26.6	26.1	26.2
PbH4	102	64.7	69.0	64.2	64.1	61.8	61.8	145	56.4	64.0	62.9	62.7	60.1	60.2
PbO	107	56.6	56.6	35.2	35.2	41.4	41.4	151	33.4	33.4	24.4	24.4	22.1	22.1
PbO2	156	109.5	109.5	80.2	80.2	92.8	92.8	221	41.4	41.4	49.2	49.2	50.1	50.1
TlCl	109	120.2	120.2	64.0	63.8	60.6	60.6	158	54.0	54.0	11.8	11.8	11.7	11.7
TlCl3	211	120.7	120.7	52.9	53.2	61.7	61.7	312	80.5	80.5	29.3	29.2	29.6	29.7
TlH	69	72.4	69.6	81.0	80.9	67.7	67.8	97	25.0	26.2	26.7	26.6	27.1	27.2
TlH3	91	66.4	69.3	55.1	54.7	53.9	53.9	129	50.2	52.9	51.4	51.3	49.5	49.6
TlO	107	92.8	92.8	75.0	75.0	83.4	17.6	151	30.8	30.8	21.2	21.2	20.9	20.9
average	44	65.2	66.3	45.8	45.6	49.5	47.7	63	41.4	43.0	29.5	29.3	28.4	28.5
std-dev		24.8	24.0	16.2	16.3	15.5	15.4		16.4	16.4	12.9	12.9	12.1	12.2
maximum		120.7	120.7	81.0	80.9	92.8	92.8		80.5	80.5	62.9	62.7	60.1	60.2
typical		90.0	90.3	62.0	62.0	65.0	63.1		57.8	59.4	42.4	42.1	40.6	40.6
kJ/mol		0.236	0.237	0.163	0.163	0.171	0.166		0.152	0.156	0.111	0.111	0.106	0.107
all p-compounds														
average	39	56.9	58.8	38.5	39.3	44.5	43.7	58	37.3	38.6	22.9	22.5	21.8	21.7
std-dev		28.4	27.7	18.9	18.8	19.8	19.3		22.3	22.1	16.3	16.4	15.6	15.5
maximum		123.2	123.2	101.8	104.7	122.2	113.3		93.4	93.4	88.4	89.0	83.0	82.7
typical		85.3	86.5	57.4	58.0	64.3	63.0		59.6	60.6	39.2	38.9	37.5	37.2
kJ/mol		0.224	0.227	0.151	0.152	0.169	0.165		0.156	0.159	0.103	0.102	0.098	0.098

transition metal compounds

CoCl3	242	75.9	75.5	26.7	28.2	34.1	33.1	338	56.1	56.1	15.2	17.3	18.1	17.4	192	67.8	69.4	148.6	151.2	216.9	215.8
CoF2	187	69.7	68.9	44.0	45.7	56.0	56.4	247	51.9	51.1	32.8	34.0	39.7	40.3	158	119.9	121.2	96.2	102.6	110.9	113.4
CoF3	236	55.2	54.1	26.7	29.5	41.4	39.1	317	36.7	36.6	12.9	15.3	21.1	19.2	201	77.5	78.5	51.8	54.9	61.4	60.6
CrCO6	677	21.5	21.3	13.8	13.6	17.0	16.9	947	10.6	10.6	3.6	3.5	2.8	2.8	523	85.5	85.7	70.6	71.0	70.4	70.3
CrCl3	242	87.4	81.2	28.8	27.5	32.3	32.3	338	63.2	64.2	23.4	22.5	21.7	21.8	187	58.4	53.7	196.8	207.9	254.1	254.9
CrF3	236	90.9	79.7	39.4	38.1	44.9	44.7	317	44.6	48.2	26.8	26.1	27.0	26.8	196	64.2	62.3	85.2	90.4	83.0	85.8
CrO3	236	65.5	63.6	78.8	73.0	72.2	72.3	317	45.0	54.5	47.9	40.9	41.9	41.2	181	99.2	105.1	175.5	175.4	154.7	156.9
Cu2	182	52.5	52.6	38.1	38.7	20.7	21.6	214	32.0	31.7	22.5	21.3	7.2	7.8	136	100.4	97.5	114.8	117.8	88.5	88.8
Cu2O	231	73.6	75.9	67.4	61.8	53.7	52.3	284	44.3	45.7	43.7	38.9	32.4	31.1	174	155.4	152.8	228.7	226.6	212.3	208.7
Cu2S	233	68.5	69.8	54.4	50.3	41.8	42.2	291	42.9	43.6	33.9	29.7	22.9	23.3	176	120.2	117.2	189.8	186.8	205.6	205.2
CuCN	189	33.0	33.3	18.0	18.3	17.4	17.6	247	19.1	19.1	7.8	7.3	4.2	4.4	144	93.3	92.8	107.4	105.2	96.8	95.9
CuCl	142	79.1	79.5	21.4	21.3	23.3	23.2	184	61.6	61.7	15.0	14.6	13.1	13.1	108	137.5	135.2	211.8	216.9	263.6	259.9
CuF	140	61.2	61.9	26.9	26.7	30.3	29.4	177	45.9	46.4	19.3	18.4	18.0	17.5	111	163.4	161.8	173.5	178.4	183.8	179.9
CuH	102	37.1	37.4	27.9	28.1	20.6	20.7	123	19.5	22.1	16.6	15.7	10.9	11.1	82	67.0	66.0	94.3	93.9	83.3	83.7
FeCO5	579	29.1	27.0	14.4	13.9	17.6	17.7	807	14.2	13.8	4.3	4.3	3.8	3.8	447	87.2	87.3	56.0	55.9	60.0	60.1
FeF2	187	49.3	49.4	18.5	-1.6	26.3	25.6	247	39.8	39.9	13.9	-6.7	14.8	14.3	153	60.5	59.7	56.8	45.1	80.6	82.6
FeF3	236	55.0	50.5	12.5	13.2	22.4	21.5	317	34.2	33.4	5.4	6.8	9.5	8.6	196	58.4	59.2	51.9	59.4	66.3	66.3
FeO	138	62.3	58.7	50.4	48.3	52.9	52.4	177	37.0	42.5	42.2	40.1	38.8	38.1	105	60.2	63.1	99.4	101.7	120.5	134.1
Ferrocen	689	22.3	24.8	16.3	17.5	20.8	20.8	967	10.0	11.5	6.4	6.0	5.6	5.6	587	57.1	58.3	51.6	50.9	52.6	52.4
MnF2	187	36.7	36.9	16.3	17.6	21.7	21.7	247	27.5	27.6	10.3	10.8	10.2	10.1	153	71.0	69.5	68.6	73.6	83.7	83.5
MnO	138	57.2	63.2	67.3	63.0	66.3	65.2	177	40.8	44.4	46.5	43.7	43.2	42.5	105	59.8	63.9	88.7	90.8	104.5	105.9
MnO2	187	52.9	56.8	61.3	57.2	57.2	56.5	247	36.6	38.4	39.1	37.5	35.8	35.6	143	89.0	94.6	120.5	122.9	124.6	127.7
MnO3F	285	43.6	47.0	50.5	47.6	48.7	47.7	387	24.9	26.2	21.8	21.2	20.2	19.9	224	61.5	62.3	100.4	103.7	103.7	106.9

MnO4-	285	39.5	42.6	46.7	43.3	43.7	42.4	387	18.9	19.8	16.9	15.9	14.7	14.3	219	55.6	56.0	103.3	106.1	101.0	104.1
MnS	140	36.9	38.0	36.0	36.2	43.8	43.4	184	27.7	28.1	27.4	27.4	30.7	30.6	107	50.0	50.1	122.6	129.1	197.4	197.3
NiCO4	481	82.8	81.1	53.8	50.6	53.5	52.8	667	63.0	63.0	41.3	39.8	37.9	37.4	372	80.7	80.6	53.8	54.0	57.5	57.7
NiCl2	191	83.9	83.3	26.8	28.3	36.7	36.9	261	68.8	68.3	19.5	20.3	20.5	21.0	148	177.5	168.4	219.9	227.7	295.1	293.2
NiF2	187	72.8	72.2	36.6	38.4	44.5	44.6	247	59.4	58.8	31.2	32.2	31.4	32.0	154	166.6	160.5	136.4	151.1	158.0	155.2
NiF3	236	51.7	50.7	18.5	20.1	28.5	27.1	317	36.1	36.0	11.8	13.0	14.3	13.6	197	58.9	58.4	54.8	60.3	57.5	57.8
NiO	138	81.0	78.1	62.8	65.4	66.9	67.5	177	67.7	66.6	54.5	55.1	51.2	51.5	106	183.6	175.8	160.2	166.1	170.9	168.7
NiS	140	63.1	61.0	42.0	46.2	51.7	52.5	184	47.1	46.2	33.5	34.0	33.3	33.6	108	140.0	131.4	141.2	145.1	193.4	189.9
ScCl3	242	71.7	72.0	17.3	19.3	27.5	27.1	338	56.7	58.3	7.8	8.5	9.4	9.4	192	48.7	49.2	162.1	169.0	222.0	221.4
ScF3	236	45.6	46.5	13.0	13.4	19.5	19.3	317	32.3	33.9	5.4	5.3	6.1	6.1	201	71.6	75.2	56.5	57.1	57.1	57.1
ScH3	122	76.8	63.5	67.5	82.9	87.5	87.6	155	32.4	39.3	42.5	44.6	50.4	50.5	114	45.0	44.7	61.3	66.8	67.6	67.2
ScO	138	26.0	29.0	44.2	38.3	40.9	42.2	177	18.4	22.1	28.7	23.3	19.9	20.6	110	109.2	109.1	115.2	123.7	117.9	119.6
TiCO4	481	36.2	33.8	34.5	35.4	41.4	41.8	667	19.2	18.5	16.7	17.2	17.7	18.1	371	90.3	91.5	73.4	73.6	79.5	79.9
TiCl4	293	53.9	51.0	17.0	15.3	21.0	20.7	415	34.8	35.2	9.5	7.7	8.9	8.6	227	30.5	30.5	134.1	140.7	197.6	198.0
TiF3	236	50.1	46.5	20.3	18.4	23.7	23.2	317	35.7	35.4	10.1	9.1	10.7	10.4	196	82.3	79.0	55.7	54.5	60.7	61.1
TiF4	285	43.3	40.8	24.3	22.1	27.8	26.9	387	27.5	28.5	9.0	7.9	10.2	9.6	239	51.6	51.6	52.9	51.2	51.4	51.7
TiH4	133	19.8	33.4	45.2	37.9	39.1	39.6	171	14.8	25.8	26.7	24.7	26.7	26.4	123	20.5	19.2	34.3	34.9	32.8	33.1
TiO	138	33.0	30.6	40.4	36.9	40.3	46.4	177	25.9	26.1	32.1	27.9	27.3	33.0	105	98.4	104.6	122.5	120.8	116.7	121.0
TiO2	187	37.2	35.1	26.0	23.7	27.4	27.4	247	28.9	29.2	18.5	15.9	15.6	15.4	143	150.9	152.4	156.8	167.8	165.7	166.6
TiS2	191	41.8	45.4	30.6	34.2	38.0	38.2	261	35.4	36.3	24.8	27.3	27.7	27.7	147	106.7	110.6	188.4	202.3	256.0	255.8
VH5	144	36.1	62.2	69.2	64.2	67.8	69.1	187	23.9	42.6	40.0	38.8	41.9	42.0	137	30.7	39.0	52.2	52.2	54.6	56.4
VO	138	26.6	23.9	31.1	30.8	32.9	33.6	177	19.3	19.7	18.1	17.2	15.6	15.8	105	103.9	104.7	118.3	109.6	116.1	116.9
VOF3	285	46.1	40.9	47.9	46.5	46.6	48.5	387	27.0	27.8	13.9	14.9	14.8	14.9	234	68.4	70.6	77.9	78.1	74.9	77.8
ZnCl2	191	71.1	71.1	19.3	19.2	22.5	22.9	261	57.4	57.5	13.6	13.6	11.5	11.5	148	80.0	79.9	185.5	187.6	238.6	239.1
ZnF2	187	59.7	59.9	22.6	22.6	24.9	24.3	247	48.1	48.4	16.6	16.6	13.7	13.3	154	81.5	80.2	88.1	85.0	77.9	76.3
ZnH2	111	27.4	26.8	19.6	18.6	13.5	13.6	139	16.6	19.1	12.7	12.1	8.2	8.2	96	76.4	67.8	99.2	102.1	79.9	80.5
ZnMe2	253	18.4	21.5	17.4	19.4	19.1	19.2	343	7.1	8.6	5.5	4.9	3.6	3.6	228	21.0	20.5	37.3	36.8	34.7	34.9
Ag2	178	31.7	30.1	16.1	17.3	7.8	7.9	198	18.6	17.0	12.5	13.6	5.3	5.4	146	22.6	33.0	41.2	37.1	46.3	46.2
AgCl	140	66.8	64.5	8.2	8.7	12.1	11.9	176	50.1	47.9	6.6	6.9	6.1	5.9	113	57.5	72.1	164.5	161.2	215.4	214.4
CdF2	187	44.3	44.4	9.0	9.5	15.5	13.7	239	33.3	33.4	6.0	6.4	7.5	6.2	154	89.8	90.1	77.4	82.1	93.2	88.7
CdMe2	253	15.1	18.3	13.6	15.6	16.8	16.7	335	4.5	6.1	3.3	2.6	2.7	2.7	228	29.7	29.7	39.6	39.2	41.7	41.6
MoCO6	677	19.0	18.6	8.8	9.1	13.4	13.4	939	11.2	11.1	2.9	3.0	2.4	2.4	523	86.2	90.9	51.8	51.8	55.6	55.4
MoF3	236	45.8	44.8	21.8	22.3	28.1	27.4	309	29.3	35.2	14.0	14.7	15.8	15.4	196	81.1	86.5	83.8	85.7	94.6	94.2
MoH	100	17.1	28.0	19.7	19.7	20.2	20.1	115	9.4	19.5	16.7	17.0	17.8	17.7	81	37.2	49.4	62.0	58.6	61.6	61.7
MoO2	187	36.1	28.8	27.3	23.8	25.5	25.4	239	19.3	22.3	19.7	17.0	15.5	15.6	143	130.1	144.0	145.5	135.6	139.7	140.7
MoO3	236	33.9	25.1	24.3	20.5	20.9	20.7	309	18.5	19.3	17.3	14.5	12.0	11.9	181	136.7	174.9	172.0	171.1	187.4	185.7
NbF3	236	52.9	44.6	23.2	23.1	27.6	26.8	309	38.0	38.2	18.3	18.8	18.9	18.3	201	156.4	150.8	132.0	130.2	135.7	132.4
NbO	138	45.3	36.2	46.3	34.1	38.2	38.7	169	18.6	24.8	30.5	22.0	21.3	21.7	110	92.0	111.7	113.3	93.9	100.3	101.5
NbO2	187	48.5	41.5	55.4	43.4	47.3	47.8	239	22.6	29.9	39.0	30.1	29.0	29.5	148	117.9	139.6	142.6	125.1	132.6	133.2
NbO2F	236	39.6	33.9	31.5	26.5	30.2	30.4	309	22.8	26.4	24.1	20.1	19.3	19.5	191	112.8	128.4	118.5	110.2	119.3	119.7
PdCO4	481	30.9	26.2	15.5	15.0	18.3	18.2	659	17.0	16.3	7.4	7.5	6.1	6.4	372	91.9	90.3	56.6	57.0	61.0	61.3
PdF	138	59.9	58.1	29.8	33.9	38.5	38.7	169	37.6	41.7	24.2	28.7	27.9	28.2	111	77.8	89.3	92.8	96.2	94.7	98.9
PdO2	187	25.9	25.5	18.9	19.6	22.1	21.4	239	18.6	18.2	13.7	14.0	12.5	11.8	144	88.7	81.0	79.1	82.8	91.2	96.5
RhF	138	59.0	83.5	16.1	18.3	22.5	21.5	169	45.1	67.7	13.7	14.4	17.0	16.2	116	98.7	118.1	101.1	110.4	109.2	114.0
RhF4	285	48.3	42.7	10.7	11.3	19.6	18.9	379	29.3	28.9	4.3	5.0	5.8	5.5	245	44.6	44.0	20.8	22.5	28.1	28.0
RhF6	383	30.9	30.9	16.8	18.8	23.4	22.9	519	24.3	24.3	10.9	11.9	11.6	11.0	331	51.2	53.9	41.2	43.4	45.0	43.9
RhO	138	44.9	44.1	32.1	30.2	30.5	29.2	169	28.1	36.7	26.4	22.9	22.0	21.0	111	186.1	192.9	205.2	178.6	177.0	170.3
RuCO5	579	22.2	21.1	10.3	10.5	14.6	14.7	799	13.5	13.2	4.0	4.1	3.4	3.5	453	83.9	85.8	51.0	51.6	55.1	55.7
RuF	138	51.4	55.4	17.4	18.9	22.5	22.5	169	37.3	44.6	14.6	15.5	16.5	16.3	116	67.8	80.2	99.9	97.6	100.9	103.4
RuO	138	41.1	45.5	49.1	42.4	45.0	45.9	169	27.9	39.7	41.2	35.8	36.2	36.7	111	65.4	82.1	90.5	85.3	87.5	92.8
RuO2	187	42.9	47.4	38.2	29.3	32.4	29.9	239	37.0	41.7	33.1	24.9	25.3	22.8	149	28.9	36.2	21.7	22.7	23.0	23.9
RuO4	285	28.5	29.7	25.9	20.8	21.8	21.2	379	19.5	22.5	16.8	13.3	11.4	11.1	225	63.5	70.4	61.4	59.8	59.6	60.4
Tc2O7	521	27.3	34.6	33.0	28.6	28.6	28.2	688	18.7	22.4	18.5	14.9	12.8	12.7	410	63.6	70.9	49.5	49.7	54.3	54.7
TcO	138	40.3	52.3	52.7	48.2	51.0	49.4	169	31.0	46.2	45.5	41.0	42.2	40.9	110	64.7	87.1	83.5	74.6	75.6	75.1
TcO3F	285	31.1	37.2	31.6	27.6	28.5	28.3	379	21.5	25.0	17.3	14.2	12.7	12.7	229	68.9	74.6	52.2	51.9	56.1	56.5
YF	138	31.0	29.6	13.9	12.4	18.4	17.4	169	20.3	21.2	6.8	6.7	7.0	6.3	110	241.7	243.8	259.6	248.5	229.0	228.7
YF3	236	52.8	52.9	19.8	16.9	29.7	28.8	309	27.3	30.8	3.6	3.4	4.3	4.2	196	72.3	85.7	50.3	57.9	56.0	59.0
YO	138	36.3	29.1	18.5	14.3	19.3	18.5	169	12.8	15.5	6.6	6.5	5.9	5.6	105	97.2	132.5	129.2	128.7	126.8	129.2
ZrF	138	42.1	35.8	7.1	7.9	11.3	10.9	169	29.3	29.2	4.5	4.7	4.2	4.2	115	67.3	71.6	59.9	50.6	57.7	58.1
ZrF3	236	43.2	36.7	12.1	13.0	20.2	19.6	309	28.8	28.7	6.6	6.3	6.9	6.9	201	72.0	76.5	51.1	49.0	49.6	49.8
ZrO	138	36.1	29.8	14.1	16.2	17.0	17.2	169	24.4	25.8	11.5	13.7	12.2	12.4	110	87.1	108.5	110.8	97.0	100.0	101.6
ZrO2	187	36.0	31.2	19.6	20.2	22.7	22.4	239	19.5	19.4	11.7	12.3	11.3	11.2	148	133.1	151.8	145.3	133.3	141.9	144.8
Au2	178	10.4	11.6	9.9	9.3	10.6	11.0	198	7.3	9.1	8.1	7.4	9.2	9.5	148	35.4	36.0	36.6	32.7	29.2	31.4
Au3-	267	9.1	8.8	9.0	8.2	7.0	7.4	297	4.8	5.9	6.5	5.7	4.5	4.7	222	27.9	29.4	38.1	35.5	39.1	46.4
AuCl	140	56.3	57.2	21.7	22.1	23.7	24.0	176	46.1	48.5	18.6	17.9	16.4	16.9	114	59.7	65.9	178.1	177.1	205.1	213.2
AuCl3	242	67.5	66.9	18.4	19.5	21.9	22.3	330	50.9	52.6	12.7	13.0	11.1	11.5	194	52.8	56.2	199.6	205.4	265.4	273.1
HfF	138	32.4	28.4	13.3	15.6	22.2	22.2	169	20.9	22.3	10.4	12.6	15.5	15.6	121	111.6	117.7	119.6	112.3	115.3	115.4
HfF3	236	45.5	41.8	15.5	15.0	25.6	25.2	309	29.9	31.4	5.6	4.8	5.8	6.0	207	69.0	72.0	58.1	58.0	60.2	61.7
HfO	138	39.4	24.6	18.5	17.0	18.5	18.6	169	16.1	18.9	14.3	13.5	12.3	12.4	116	116.1	140.3	151.5	148.1	144.8	147.7
HfO2	187	67.9	50.9	38.0	31.3	38.4	37.6	239	29.7	34.0	24.5	21.0	21.0	21.4	154	120.8	133.5	142.1	141.2	143.0	145.6
HgF2	187	35.0	34.2	20.9	21.8	26.9	26.3	239	26.9	26.1	11.0	11.2	11.6	11.2	159	66.6	62.5	46.9	46.0	48.5	48.7
HgMe2	253	16.4	20.2	18.7	20.9	21.8	21.8	335	4.2	6.4	4.0	2.9	2.9	2.9	233	22.0	20.9	27.7	26.2	25.3	25.5
IrF6	383	31.0	32.9	24.8	24.7	27.8	27.8	519	24.2	25.9	16.6	16.6	15.3	15.1	331	57.2	62.5	58.3	54.8	52.0	52.8
OsCO5	579	25.3	21.0	11.9	11.8	15.6	15.7	799	12.9	12.8	4.2	4.2	3.7	3.7	453	94.9	96.7	56.3	56.4	59.9	60.4
OsO2	187	44.5	44.9	60.4	55.2	55.5	54.3	239	27.2	33.2	45.0	40.0	38.1	37.5	149	106.2	111.3	97.9	92.9	96.6	98.2
OsO3	236	31.9	36.6	44.7	41.5	39.4	38.7	309	21.0	23.9	34.9	30.1	26.2	25.8	187	110.0	108.2	96.6	91.5	93.9	97.5
OsO4	285	27.7	35.4	33.0	34.3	31.8	31.6	379	20.6	20.2	16.3	15.8	12.8	12.9	225	80.0	88.7	81.4	76.2	77.3	77.6
OsOF5	383	30.1	36.4	31.8	30.5	33.0	33.0	519	22.9	26.4	20.0	18.9	17.4	17.2	326	71.4	84.5	81.7	72.4	70.0	71.5
PtCO4	481	25.7	20.6	13.3	13.4	16.5	16.8	659	12.2	11.9	4.9	4.9	4.3	4.3	377	84.1	83.5	52.9	53.4	57.3	58.2
PtO	138	55.6	42.4	46.7	44.0	41.4	43.8	169	32.4	36.4	37.7	35.2	31.4	33.7	111	194.1	206.9	226.3	209.7	210.1	221.1
PtO2	187	29.3	31.6	40.9	38.6	36.4	38.1	239	22.0	23.8	29.7	27.4	23.3	24.8	149	215.5	222.6	241.3	226.7	224.6	234.0
ReH	100	20.0	34.0	28.1	28.3	28.6	28.5	115	13.4	27.2	24.9	24.9	26.3	26.0	87	141.3	154.9	156.2	152.0	160.7	161.4
ReO	138	22.6	31.5	39.9	38.6	40.1	39.5	169	18.6	25.3	31.8	31.2	29.6	29.4	111	174.9	192.4	148.9	142.4	146.8	145.6
ReO2	187	16.0	16.1	12.8	10.6	11.3	10.8	239	11.4	11.8	8.2	6.1	4.1	3.8	149	96.4	99.7	80.1	76.7	80.5	82.1
ReO3	236	26.5	27.1	32.6	29.0	29.5	28.5	309	21.7	22.7	26.8	23.8	20.2	19.4	187	106.9	113.8	92.8	87.6	92.2	92.9
ReO3F	285	30.9	33.5	28.9	26.4	27.8	27.2	379	25.0	27.5	22.7	20.9	18.1	17.6	230	107.4	121.4	105.7	97.1	102.0	101.4
TaF	138	42.6	42.3	45.7	44.5	54.0	53.1	169	32.4	34.3	33.3	31.1	35.4	34.7	115	874.6	836.9	893.5	771.3	781.2	763.6
TaF3	236	55.5	56.2	48.5	47.9	56.1	55.3	309	45.5	48.4	37.6	36.1	37.2	36.6	201	172.8	176.9	169.3	147.0	152.0	144.1
TaO2F	236	30.4	35.4	28.5	29.0	30.9	31.2	309	24.2	26.6	22.6	22.4	21.0	21.3	191	78.3	88.1	75.1	77.8	82.8	82.5
WCO6	677	20.2	20.0	9.2	9.3	13.4	13.4	939	12.8	12.9	3.2	3.2	2.5	2.6	529	80.2	83.9	55.7	56.1	61.8	61.4

WF3	236	42.9	46.4	24.8	26.8	29.2	28.8	309	30.6	36.7	15.6	17.5	16.4	16.4	202	102.0	112.1	107.7	108.3	112.6	110.2
WH	100	12.6	25.1	23.4	22.7	22.8	22.9	115	8.5	17.5	17.4	18.5	19.0	19.2	87	45.0	52.8	56.7	56.9	59.4	59.4
WO	138	33.8	34.4	45.3	44.7	41.5	41.3	169	23.5	27.8	36.4	35.8	31.4	31.2	111	186.0	209.0	231.1	206.8	209.6	207.3
WO2	187	44.0	40.9	52.1	49.2	47.3	47.1	239	32.1	35.4	43.8	40.7	36.5	36.4	149	234.5	252.0	273.9	252.1	254.0	251.0
WO3	236	33.2	22.9	23.5	24.1	24.0	23.6	309	18.5	18.1	16.4	16.8	14.5	14.6	187	88.9	87.3	59.7	68.7	72.2	73.1
average	55	43.1	42.9	29.6	28.5	31.4	31.2	73	28.8	31.4	19.7	18.5	18.0	17.9	45	97.8	102.4	112.3	110.0	117.8	118.4
std-dev		18.3	17.6	16.1	15.4	14.9	15.0		14.4	14.6	12.6	11.9	11.7	11.7		84.9	82.7	92.1	82.7	88.8	87.6
maximum		90.9	83.5	78.8	82.9	87.5	87.6		68.8	68.3	54.5	55.1	51.2	51.5		874.6	836.9	893.5	771.3	781.2	763.6
typical		61.4	60.5	45.7	43.9	46.3	46.2		43.3	46.0	32.2	30.4	29.6	29.6		182.8	185.2	204.4	192.7	206.6	206.0
kJ/mol		0.161	0.159	0.120	0.115	0.121	0.121		0.114	0.121	0.085	0.080	0.078	0.078		0.480	0.486	0.537	0.506	0.542	0.541

s t a t i s t i c s f o r a l l m o l e c u l e s

auxbasis:	NEW							NEW, UNCONTRACTED							OLD (LARGEST)						
	orbital basis (def2-)							orbital basis (def2-)							orbital basis (def2-)						
	Naux	SV(P)	SVP	TZVP	TZVPP	QZVP	QZVPP	Naux	SV(P)	SVP	TZVP	TZVPP	QZVP	QZVPP	Naux	SV(P)	SVP	TZVP	TZVPP	QZVP	QZVPP
all																					
average	46	47.2	47.8	31.0	31.2	35.3	34.8	64	31.0	32.5	18.8	18.2	17.7	17.5							
std-dev		25.4	25.2	18.6	18.4	19.2	18.9		19.4	19.4	14.8	14.5	14.0	13.9							
maximum		123.2	123.2	101.8	104.7	122.2	113.3		93.4	93.4	88.4	89.0	83.0	82.7							
typical		72.5	73.0	49.5	49.6	54.6	53.7		50.4	52.0	33.6	32.7	31.7	31.5							
kJ/mol		0.190	0.192	0.130	0.130	0.143	0.141		0.132	0.136	0.088	0.086	0.083	0.083							
all except 5p-6p																					
average	46	44.7	45.3	28.9	29.3	33.4	33.1	64	29.6	31.1	17.3	16.7	16.2	16.0	37	112.1	114.6	137.6	136.6	152.8	153.3
std-dev		24.4	24.3	18.0	17.8	18.9	18.7		19.4	19.4	14.4	14.0	13.6	13.5		148.7	147.7	163.6	161.7	167.3	167.9
maximum		123.2	123.2	101.8	104.7	122.2	113.3		93.4	93.4	88.4	89.0	83.0	82.7		1762.6	1762.6	2011.9	2012.0	1866.9	1866.9
typical		69.1	69.6	46.9	47.1	52.3	51.7		49.0	50.5	31.7	30.7	29.8	29.5		260.8	262.3	301.2	298.3	320.1	321.2
kJ/mol		0.181	0.183	0.123	0.124	0.137	0.136		0.129	0.133	0.083	0.081	0.078	0.077		0.685	0.689	0.791	0.783	0.840	0.843
2p-4p,d																					
average	47	47.9	48.8	32.4	32.2	36.4	36.2	65	32.0	33.9	20.0	19.1	18.6	18.4	39	93.4	96.6	114.4	113.1	128.8	127.4
std-dev		24.3	24.0	17.8	17.6	18.7	18.4		19.6	19.4	14.6	14.3	13.8	13.7		75.5	74.1	91.4	86.8	102.4	100.2
maximum		123.2	123.2	101.8	104.7	122.2	113.3		93.4	93.4	88.4	89.0	83.0	82.7		874.6	836.9	893.5	771.3	781.2	763.6
typical		72.2	72.8	50.1	49.9	55.1	54.6		51.6	53.3	34.6	33.5	32.4	32.2		168.9	170.7	205.8	199.8	231.2	227.6
kJ/mol		0.190	0.191	0.132	0.131	0.145	0.143		0.135	0.140	0.091	0.088	0.085	0.084		0.443	0.448	0.540	0.525	0.607	0.597

Naux denotes the number of auxiliary basis functions per molecule, for the average the number of aux.bfn per atom is given.
"typical errors": average plus standard deviation