

On differences in substituent effects in substituted ethene and acetylene derivatives and their boranyl analogs

SUPPORTING INFORMATION

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Received: date / Accepted: date

Abstract This article is the first attempt to present different influence of substituent effects on double and triple bonds and, conversely, to present the impact of these bonds on the electronic structure of substituents. For this purpose, quantum-mechanical calculations were made for X-substituted derivatives of ethene and acetylene with 27 diverse substituents representing a wide spectrum of electronic properties, from strongly electron-accepting to strongly electron-donating ones. In addition to these systems, their boranyl derivatives are also investigated. It turns out that the Hammett substituent constants do not correctly describe changes in the CC bond length in any of the considered family of systems. However, the relationships with the CB bond length are significantly better. It is shown that the triple bond in acetylene derivatives is much more resistant to external perturbations than the double bond in the analogs containing an ethene unit. As a consequence, in acetylene derivatives the substituent effects on CC bond length are about half of the substituent effects in ethene derivatives. We suggest that the observed lack of a clear linear correlation between the length of the CC triple bond in acetylene derivatives and the value of electron density on this bond is due to the disturbing additional interaction between the structure of the X substituent in the xy plane and the π bond being in the same plane in the acetylene unit – on the contrary, this interaction is not possible in ethene analogs.

Keywords Acetylene · Boranyl · Ethene · Substituent · Substituent Effect

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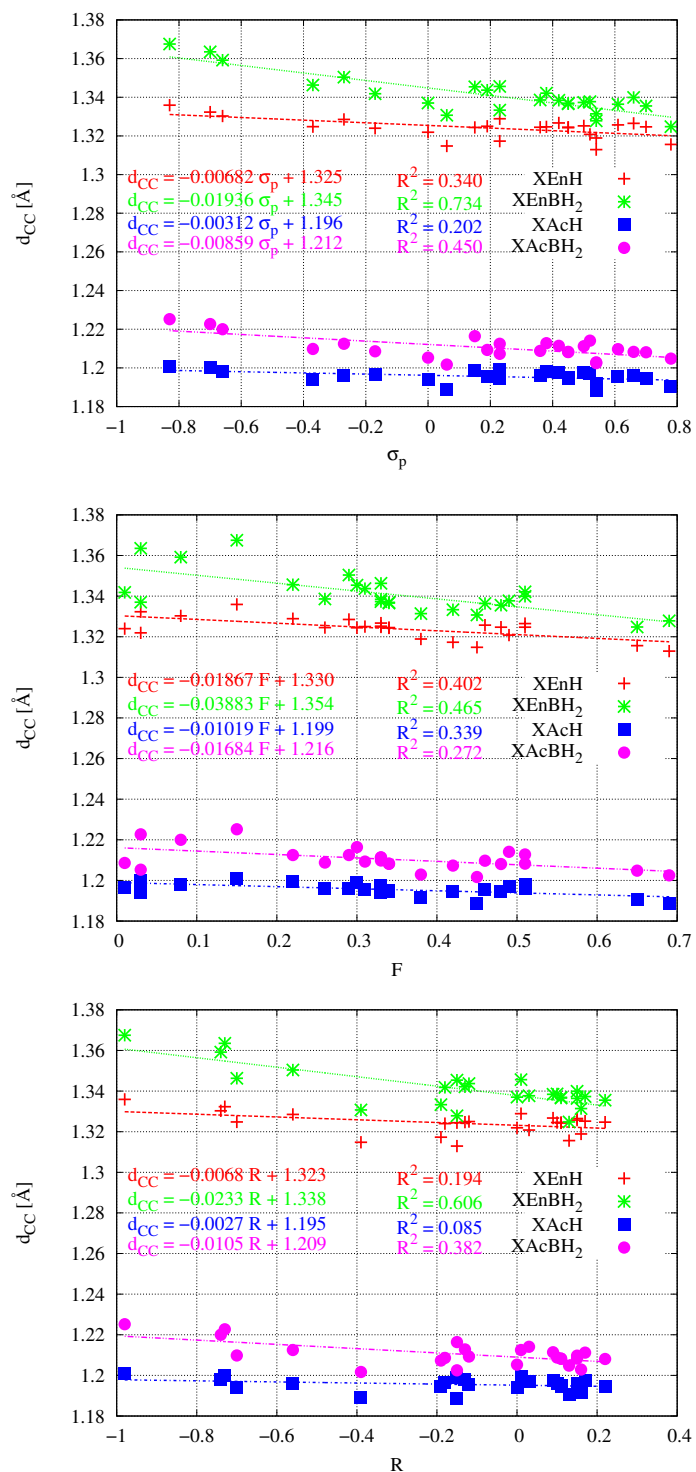
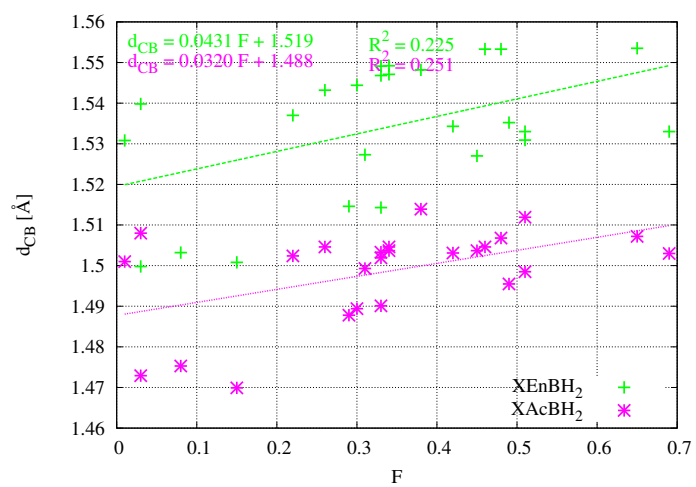


Fig. S1 Relationships between d_{CC} and σ_p , F and R .

**Fig. S2** Relationship between d_{CB} and F .

– HEnH

$$E_{\text{tot}} = -78.5859009$$

6 0.000000 0.000000 0.660965
 6 0.000000 0.000000 -0.660965
 1 0.000000 0.921892 1.228853
 1 0.000000 0.921892 -1.228853
 1 0.000000 -0.921892 -1.228853
 1 0.000000 -0.921892 1.228853

– HEnBH₂

$$E_{\text{tot}} = -104.0201945$$

6 0.000000 0.487536 0.000000
 6 -1.167741 -0.163593 0.000000
 1 -0.027964 1.573591 0.000000
 1 -2.125428 0.346560 0.000000
 1 -1.199223 -1.247830 0.000000
 5 1.332966 -0.283297 0.000000
 1 1.308018 -1.479336 0.000000
 1 2.386213 0.279843 0.000000

– HEnNO₂

$$E_{\text{tot}} = -283.0948463$$

6 -0.597434 -0.776201 0.000000
 6 0.157434 -1.853627 0.000000
 1 -1.674420 -0.735876 0.000000
 1 -0.300112 -2.832073 0.000000
 1 1.235392 -1.774800 0.000000
 7 0.000000 0.560040 0.000000
 8 -0.785187 1.486943 0.000000
 8 1.207580 0.663237 0.000000

– HEnCFO

$$E_{\text{tot}} = -291.1842739$$

6 0.401612 0.918943 0.000000
 6 -0.517552 1.872819 0.000000
 1 1.461325 1.130640 0.000000
 1 -0.240614 2.917833 0.000000
 1 -1.571118 1.624455 0.000000
 6 0.000000 -0.499976 0.000000
 8 -1.087426 -0.961680 0.000000
 9 1.082829 -1.303356 0.000000

– HEnCN

$$E_{\text{tot}} = -170.8214084$$

6 0.000000 -0.774864 0.000000
 6 1.311411 -0.974311 0.000000

1 -0.699847 -1.600367 0.000000
 1 1.714089 -1.977259 0.000000
 1 2.010842 -0.149721 0.000000
 6 -0.578442 0.532640 0.000000
 7 -1.060414 1.575222 0.000000

– HEnCClO

$E_{\text{tot}} = -651.5382009$

6 1.059157 -0.681517 0.000000
 6 2.334189 -0.318500 0.000000
 1 0.747559 -1.715427 0.000000
 1 3.123720 -1.057187 0.000000
 1 2.614179 0.726935 0.000000
 6 0.000000 0.349442 0.000000
 8 0.139344 1.522890 0.000000
 17 -1.644722 -0.366705 0.000000

– HEnCF₃

$E_{\text{tot}} = -415.6636685$

6 -0.985375 0.642772 -0.000005
 6 -2.105344 -0.053683 0.000003
 1 -0.972163 1.724781 -0.000023
 1 -3.064946 0.443768 -0.000008
 1 -2.101113 -1.135043 0.000018
 6 0.373250 0.017840 0.000000
 9 1.077912 0.398815 -1.076721
 9 1.077940 0.398895 1.076679
 9 0.337819 -1.317163 0.000046

– HEnOCN

$E_{\text{tot}} = -246.0174853$

6 0.887120 0.520516 0.000000
 6 2.180898 0.297208 0.000000
 1 0.406048 1.488591 0.000000
 1 2.857750 1.137014 0.000000
 1 2.585076 -0.704668 0.000000
 8 0.000000 -0.560473 0.000000
 6 -1.256166 -0.289925 0.000000
 7 -2.388570 -0.086279 0.000000

– HEnSCN

$E_{\text{tot}} = -569.0131764$

6 1.113551 -0.510555 0.238904
 6 2.348207 -0.379284 -0.211605
 1 0.770614 -1.377672 0.786308
 1 3.076609 -1.156404 -0.026132
 1 2.674581 0.491759 -0.764586

16 -0.066491 0.803417 0.074353
 6 -1.485923 -0.105183 -0.059563
 7 -2.473281 -0.691745 -0.141664

– HEnCMeO

$$E_{\text{tot}} = -231.2347806$$

6 0.802550 -0.659097 -0.000012
 6 2.004324 -0.100686 0.000010
 1 0.686839 -1.736992 -0.000033
 1 2.907905 -0.695021 0.000006
 1 2.101021 0.978099 0.000032
 6 -0.442757 0.167022 -0.000004
 8 -0.407816 1.374316 -0.000006
 6 -1.742068 -0.597047 0.000009
 1 -2.583920 0.088983 0.000012
 1 -1.790816 -1.245380 -0.877406
 1 -1.790803 -1.245373 0.877429

– HEnCOOH

$$E_{\text{tot}} = -267.1728173$$

6 0.804150 0.676571 0.000000
 6 0.287128 1.896024 0.000000
 1 1.871609 0.504347 0.000000
 1 0.924585 2.769879 0.000000
 1 -0.782634 2.055122 0.000000
 6 0.000000 -0.564103 0.000000
 8 -1.328016 -0.351943 0.000000
 8 0.476443 -1.668329 0.000000
 1 -1.748650 -1.218125 0.000000

– HEnCOOMe

$$E_{\text{tot}} = -306.4715385$$

6 -1.479799 -0.404751 0.000000
 6 -2.172078 0.724177 0.000000
 1 -1.962994 -1.372393 0.000000
 1 -3.253730 0.712605 0.000000
 1 -1.679584 1.686978 0.000000
 6 0.000000 -0.481423 0.000000
 8 0.592620 0.717937 0.000000
 8 0.606895 -1.521132 0.000000
 6 2.016668 0.704863 0.000000
 1 2.321884 1.746635 0.000000
 1 2.394782 0.197271 0.886029
 1 2.394782 0.197271 -0.886029

– HEnCHO

$$E_{\text{tot}} = -191.9079376$$

6	0.000000	0.893478	0.000000
6	1.321875	0.779980	0.000000
1	-0.484311	1.862886	0.000000
1	1.967269	1.647698	0.000000
1	1.784809	-0.199157	0.000000
6	-0.883499	-0.297603	0.000000
8	-0.491161	-1.435514	0.000000
1	-1.968737	-0.082436	0.000000

– HEnNCS
 $E_{\text{tot}} = -569.0331239$

6	0.757536	1.666902	0.000000
6	0.227653	2.881038	0.000000
1	1.829415	1.505071	0.000000
1	0.871835	3.747018	0.000000
1	-0.842434	3.031310	0.000000
7	0.000000	0.518269	0.000000
6	-0.144664	-0.655867	0.000000
16	-0.431373	-2.203982	0.000000

– HEnCONH₂
 $E_{\text{tot}} = -247.3000512$

6	0.849998	-0.585958	0.183465
6	1.924050	0.119799	-0.136800
1	0.934725	-1.607957	0.529590
1	2.916916	-0.297477	-0.036606
1	1.858496	1.124333	-0.537169
6	-0.563092	-0.132323	0.024708
7	-0.782738	1.212321	0.046018
8	-1.457745	-0.934866	-0.140367
1	-1.737999	1.520103	0.004469
1	-0.096751	1.844571	0.412285

– HEnCl
 $E_{\text{tot}} = -538.1991004$

6	0.000000	0.757798	0.000000
6	1.287319	1.037434	0.000000
1	-0.778346	1.506292	0.000000
1	1.605028	2.070881	0.000000
1	2.045217	0.266884	0.000000
17	-0.623283	-0.859732	0.000000

– HEnAc
 $E_{\text{tot}} = -154.725168$

6	-0.586514	-0.556013	0.000000
6	0.113685	-1.685508	0.000000
1	-1.670196	-0.588791	0.000000

1 -0.385148 -2.644598 0.000000
 1 1.195293 -1.680080 0.000000
 6 0.000000 0.743173 0.000000
 6 0.467940 1.846849 0.000000
 1 0.889383 2.822465 0.000000

– HEnNCO

$E_{\text{tot}} = -246.0699562$

6 -1.331265 -0.301606 0.000000
 6 -1.757436 0.952980 0.000000
 1 -2.020919 -1.133863 0.000000
 1 -2.817864 1.156090 0.000000
 1 -1.076777 1.793645 0.000000
 7 0.000000 -0.700159 0.000000
 6 1.108361 -0.245520 0.000000
 8 2.224700 0.081264 0.000000

– HEnSH

$E_{\text{tot}} = -476.7915912$

6 0.000000 0.759762 0.000000
 6 1.279303 1.102254 0.000000
 1 -0.773913 1.517880 0.000000
 1 1.562147 2.145615 0.000000
 1 2.076740 0.370243 0.000000
 16 -0.688054 -0.854649 0.000000
 1 0.468076 -1.531443 0.000000

– HEnF

$E_{\text{tot}} = -177.8330701$

6 0.000000 0.430837 0.000000
 6 1.180467 -0.148014 0.000000
 1 -0.181959 1.497392 0.000000
 1 2.067311 0.466659 0.000000
 1 1.284033 -1.223428 0.000000
 9 -1.139131 -0.270840 0.000000

– HEnAcF

$E_{\text{tot}} = -253.9463476$

6 1.419186 -0.376092 0.000000
 6 2.277467 0.637923 0.000000
 1 1.786951 -1.395881 0.000000
 1 3.343292 0.457524 0.000000
 1 1.940626 1.665774 0.000000
 6 0.000000 -0.224204 0.000000
 6 -1.188859 -0.129880 0.000000
 9 -2.457515 -0.019322 0.000000

– HEnMe

$$E_{\text{tot}} = -117.905431$$

6 -1.274088 -0.220683 -0.000005
6 -0.134485 0.453275 -0.000006
6 1.228405 -0.161860 0.000005
1 -0.168780 1.538911 0.000010
1 -2.230728 0.284651 0.000015
1 -1.289770 -1.304720 0.000022
1 1.797910 0.153531 -0.876781
1 1.797905 0.153531 0.876784
1 1.174469 -1.250294 -0.000018

– HEnOMe

$$E_{\text{tot}} = -193.1182905$$

6 0.000000 0.927324 0.000000
6 -1.322344 0.799489 0.000000
1 0.478847 1.898128 0.000000
1 -1.927907 1.692561 0.000000
1 -1.831135 -0.152755 0.000000
8 0.927199 -0.046906 0.000000
6 0.457824 -1.375402 0.000000
1 1.336294 -2.014263 0.000000
1 -0.143287 -1.578446 0.890572
1 -0.143287 -1.578446 -0.890572

– HEnOH

$$E_{\text{tot}} = -153.8178815$$

6 0.000000 0.439561 0.000000
6 1.206483 -0.107813 0.000000
1 -0.150313 1.511148 0.000000
1 2.081395 0.523186 0.000000
1 1.353629 -1.181041 0.000000
8 -1.185800 -0.210690 0.000000
1 -1.037213 -1.158270 0.000000

– HEnNH₂

$$E_{\text{tot}} = -133.9514846$$

6 0.069718 0.427085 -0.001225
6 1.244739 -0.196459 0.013557
1 0.032533 1.510584 -0.007337
1 2.161180 0.372586 0.010086
1 1.320803 -1.276785 0.014436
7 -1.177847 -0.169373 -0.078246
1 -1.214062 -1.151422 0.137667
1 -1.942271 0.346894 0.318883

– HEnNMeH

$$E_{\text{tot}} = -173.2553801$$

6 -0.652980 -0.361331 -0.104840
 6 -1.896307 0.064442 0.114194
 1 -0.460811 -1.420730 -0.243878
 1 -2.715968 -0.636754 0.125359
 1 -2.126323 1.112224 0.262938
 7 0.476535 0.420212 -0.236573
 1 0.344906 1.385171 0.018650
 6 1.763387 -0.127707 0.132858
 1 2.555275 0.535840 -0.211098
 1 1.880561 -0.280077 1.212320
 1 1.902009 -1.089580 -0.361557

– HEnNMe₂

$$E_{\text{tot}} = -212.5642819$$

6 0.793201 -0.665586 -0.113115
 6 1.989333 -0.114889 0.112046
 1 0.719411 -1.740679 -0.237921
 1 2.865870 -0.744067 0.129275
 1 2.133356 0.945008 0.263575
 7 -0.416153 -0.020593 -0.249444
 6 -0.451875 1.398363 -0.002119
 6 -1.604269 -0.751495 0.130155
 1 -2.477740 -0.318707 -0.358312
 1 -1.516647 -1.788479 -0.191532
 1 -1.777183 -0.742969 1.214891
 1 -1.440796 1.782900 -0.246730
 1 -0.228800 1.647008 1.045127
 1 0.277259 1.905782 -0.634069

– H₂BE_nBH₂

$$E_{\text{tot}} = -129.4493031$$

6 -0.000008 -0.674510 0.000000
 6 0.000000 0.674499 0.000000
 1 0.969946 -1.167919 0.000000
 5 1.312198 1.507613 0.000000
 1 -0.969947 1.167921 0.000000
 5 -1.312187 -1.507605 0.000000
 1 -2.359320 -0.932484 0.000000
 1 -1.293785 -2.700853 0.000000
 1 1.293778 2.700851 0.000000
 1 2.359325 0.932509 0.000000

– H₂BE_nNO₂

$$E_{\text{tot}} = -308.5269506$$

6 0.000000 0.581483 0.000000

```

6 -1.323198 0.516459 0.000000
1 0.602014 1.477955 0.000000
5 -2.144095 1.835340 0.000000
1 -1.773186 -0.469870 0.000000
7 0.844258 -0.625311 0.000000
8 2.041975 -0.424149 0.000000
8 0.310030 -1.711518 0.000000
1 -3.333856 1.814466 0.000000
1 -1.561150 2.875603 0.000000

- H2BEnCFO
Etot = -316.6150695

6 0.000000 0.577472 0.000000
6 -1.332354 0.669595 0.000000
1 0.635581 1.454038 0.000000
5 -2.029982 2.057462 0.000000
1 -1.891046 -0.261543 0.000000
6 0.686354 -0.736814 0.000000
8 0.205690 -1.814756 0.000000
9 2.022835 -0.579404 0.000000
1 -3.217295 2.151404 0.000000
1 -1.352359 3.039952 0.000000

- H2BEnCN
Etot = -196.2541447

6 0.000000 -0.452608 0.000000
6 -1.024230 0.411238 0.000000
1 -0.171649 -1.523114 0.000000
5 -2.481115 -0.112723 0.000000
1 -0.791181 1.470866 0.000000
6 1.372441 -0.049800 0.000000
7 2.478607 0.259960 0.000000
1 -3.407431 0.635711 0.000000
1 -2.663680 -1.292551 0.000000

- H2BEnCClO
Etot = -676.9692251

6 0.197183 -0.782304 0.000000
6 1.422363 -1.315967 0.000000
1 -0.695395 -1.393838 0.000000
5 1.608561 -2.858109 0.000000
1 2.263263 -0.629261 0.000000
6 0.000000 0.691718 0.000000
8 0.842097 1.519645 0.000000
17 -1.729269 1.146863 0.000000
1 2.694317 -3.347715 0.000000

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1 0.638533 -3.553155 0.000000

– H₂BEnCF₃

$E_{\text{tot}} = -441.096086$

6 -0.640969 0.456817 0.000028
 6 -1.679926 -0.375842 0.000001
 1 -0.769482 1.533392 0.000063
 5 -3.123856 0.182671 0.000003
 1 -1.476006 -1.441401 -0.000030
 6 0.797947 0.027796 0.000003
 9 1.431498 0.509950 -1.078328
 9 1.431513 0.509836 1.078360
 9 0.954076 -1.295442 -0.000056
 1 -4.068953 -0.543205 -0.000054
 1 -3.282374 1.366135 0.000042

– H₂BEnOCN

$E_{\text{tot}} = -271.4570602$

6 0.000000 -0.491275 0.000000
 6 -0.870294 -1.494036 0.000000
 1 1.078132 -0.597914 0.000000
 5 -0.318008 -2.924100 0.000000
 1 -1.926862 -1.251110 0.000000
 8 -0.437232 0.823329 0.000000
 6 0.458175 1.751223 0.000000
 7 1.227015 2.605853 0.000000
 1 -1.045341 -3.867423 0.000000
 1 0.865577 -3.086135 0.000000

– H₂BEnSCN

$E_{\text{tot}} = -594.4513714$

6 0.000000 -0.753398 0.000000
 6 -0.776754 -1.842420 0.000000
 1 1.081637 -0.808508 0.000000
 5 -0.117295 -3.228728 0.000000
 1 -1.855753 -1.715944 0.000000
 16 -0.669885 0.874065 0.000000
 6 0.754354 1.785096 0.000000
 7 1.701487 2.438721 0.000000
 1 -0.772587 -4.224640 0.000000
 1 1.075334 -3.299029 0.000000

– H₂BEnCMeO

$E_{\text{tot}} = -256.6669753$

6 0.411035 -0.424290 -0.000001
 6 1.511812 0.335129 -0.000010
 1 0.492823 -1.507420 0.000006

5 2.920435 -0.303911 0.000004
 1 1.356730 1.410506 -0.000016
 6 -0.976505 0.151307 0.000001
 8 -1.161156 1.343312 0.000002
 6 -2.106447 -0.843543 0.000001
 1 -3.063336 -0.330212 -0.000003
 1 -2.030633 -1.489898 -0.877057
 1 -2.030638 -1.489892 0.877065
 1 3.908607 0.363988 0.000041
 1 3.014154 -1.495627 -0.000020

– H₂BE_nCOOH

$$E_{\text{tot}} = -292.6045859$$

6 0.000000 -0.642501 0.000000
 6 1.335983 -0.600949 0.000000
 1 -0.537583 -1.583027 0.000000
 5 2.161643 -1.911735 0.000000
 1 1.808995 0.375480 0.000000
 6 -0.897090 0.542637 0.000000
 8 -0.245973 1.715169 0.000000
 8 -2.096210 0.461205 0.000000
 1 -0.913004 2.410163 0.000000
 1 3.353779 -1.893429 0.000000
 1 1.583706 -2.956621 0.000000

– H₂BE_nCOOMe

$$E_{\text{tot}} = -331.9038847$$

6 1.079575 -0.298319 0.000000
 6 0.897440 -1.622733 0.000000
 1 2.073284 0.133824 0.000000
 5 2.112425 -2.580446 0.000000
 1 -0.123928 -1.988574 0.000000
 6 0.000000 0.727265 0.000000
 8 -1.226087 0.202366 0.000000
 8 0.223702 1.909718 0.000000
 6 -2.301854 1.137518 0.000000
 1 -3.209727 0.542888 0.000000
 1 -2.258280 1.768368 0.886309
 1 -2.258280 1.768368 -0.886309
 1 1.969637 -3.764664 0.000000
 1 3.213285 -2.117048 0.000000

– H₂BE_nCHO

$$E_{\text{tot}} = -217.3395539$$

6 0.000000 0.640194 0.000000
 6 0.996835 -0.252961 0.000000
 1 0.209877 1.705525 0.000000

5 2.477361 0.202739 0.000000
 1 0.710242 -1.300970 0.000000
 6 -1.438589 0.249682 0.000000
 8 -1.823263 -0.889106 0.000000
 1 -2.161328 1.086538 0.000000
 1 3.371244 -0.586103 0.000000
 1 2.719784 1.372669 0.000000

– H₂BE_nNCS

$E_{\text{tot}} = -594.4719021$

6 1.136416 0.598485 0.000000
 6 2.379512 0.092559 0.000000
 1 0.963436 1.670696 0.000000
 5 3.576312 1.047230 0.000000
 1 2.479304 -0.987404 0.000000
 7 0.000000 -0.159729 0.000000
 6 -1.176544 -0.315833 0.000000
 16 -2.714620 -0.620017 0.000000
 1 4.697638 0.641310 0.000000
 1 3.375686 2.226363 0.000000

– H₂BE_nCONH₂

$E_{\text{tot}} = -272.7337893$

6 0.410006 -0.453458 0.169567
 6 1.424694 0.355990 -0.157510
 1 0.600713 -1.462011 0.518917
 5 2.887177 -0.111312 -0.001920
 1 1.192608 1.343475 -0.549129
 6 -1.050587 -0.156422 0.022384
 7 -1.419393 1.147915 0.092620
 8 -1.839781 -1.057064 -0.170975
 1 -2.398184 1.364062 0.031725
 1 -0.782585 1.862585 0.388570
 1 3.801004 0.609758 -0.263847
 1 3.099885 -1.216873 0.396183

– H₂BE_nCl

$E_{\text{tot}} = -563.6376638$

6 0.000000 0.413363 0.000000
 6 1.163576 -0.237654 0.000000
 1 -0.073107 1.492642 0.000000
 5 2.459719 0.583407 0.000000
 1 1.147995 -1.321873 0.000000
 17 -1.545591 -0.351319 0.000000
 1 3.528261 0.053620 0.000000
 1 2.391840 1.776737 0.000000

– H₂BE_nAc

$$E_{\text{tot}} = -180.1610435$$

6 0.000000 -0.449146 0.000000
6 1.103390 0.320978 0.000000
1 0.104174 -1.530065 0.000000
5 2.499419 -0.321980 0.000000
1 0.961035 1.397060 0.000000
6 -1.333535 0.042761 0.000000
6 -2.465413 0.438928 0.000000
1 -3.466729 0.796278 0.000000
1 3.492078 0.340296 0.000000
1 2.585697 -1.514794 0.000000

– H₂BE_nNCO

$$E_{\text{tot}} = -271.5102836$$

6 0.000000 -0.951240 0.000000
6 1.312718 -0.664228 0.000000
1 -0.343836 -1.977709 0.000000
5 2.325567 -1.807407 0.000000
1 1.606335 0.381408 0.000000
7 -1.036736 -0.040510 0.000000
6 -1.193620 1.153423 0.000000
8 -1.471972 2.277928 0.000000
1 3.500381 -1.598897 0.000000
1 1.927623 -2.935356 0.000000

– H₂BE_nSH

$$E_{\text{tot}} = -502.233271$$

6 0.000000 0.404032 0.000000
6 1.193490 -0.216886 0.000000
1 -0.044145 1.488484 0.000000
5 2.474630 0.609299 0.000000
1 1.206335 -1.303482 0.000000
16 -1.589536 -0.291986 0.000000
1 -1.212296 -1.578368 0.000000
1 3.551199 0.091917 0.000000
1 2.397395 1.803851 0.000000

– H₂BE_nF

$$E_{\text{tot}} = -203.2744919$$

6 0.000000 -0.583735 0.000000
6 0.035750 0.746514 0.000000
1 -0.903817 -1.182100 0.000000
5 -1.294462 1.496273 0.000000
1 1.008060 1.226213 0.000000
9 1.089500 -1.340116 0.000000
1 -1.338123 2.688053 0.000000

1 -2.313806 0.870835 0.000000

– H₂BEnAcF
 $E_{\text{tot}} = -279.3828254$

6 0.727079 -0.578234 0.000000
6 0.176031 -1.805820 0.000000
1 1.808615 -0.482140 0.000000
5 1.069223 -3.054721 0.000000
1 -0.907691 -1.867982 0.000000
6 0.000000 0.643948 0.000000
6 -0.588470 1.682379 0.000000
9 -1.222048 2.782239 0.000000
1 0.606318 -4.154742 0.000000
1 2.257226 -2.915322 0.000000

– H₂BEnMe
 $E_{\text{tot}} = -143.3430862$

6 -0.667972 -0.444374 0.000003
6 0.401096 0.366521 0.000006
6 1.828538 -0.059241 -0.000002
1 0.228207 1.440431 0.000008
5 -2.088844 0.125204 -0.000001
1 -0.481078 -1.516226 0.000002
1 2.344921 0.342376 -0.874971
1 2.344922 0.342318 0.874989
1 1.928869 -1.143388 -0.000044
1 -3.052344 -0.582081 -0.000003
1 -2.239248 1.313115 -0.000016

– H₂BEnOMe
 $E_{\text{tot}} = -218.5642258$

6 0.000000 0.667400 0.000000
6 -1.060076 -0.169143 0.000000
1 -0.137429 1.742958 0.000000
5 -2.450487 0.431478 0.000000
1 -0.890461 -1.239471 0.000000
8 1.292636 0.371428 0.000000
6 1.664402 -0.996341 0.000000
1 2.749761 -1.014712 0.000000
1 1.284626 -1.498974 0.891027
1 1.284626 -1.498974 -0.891027
1 -3.429572 -0.254235 0.000000
1 -2.576160 1.623100 0.000000

– H₂BEnOH
 $E_{\text{tot}} = -179.2641643$

6 0.000000 -0.593140 0.000000

6 -0.006710 0.753117 0.000000
1 -0.917961 -1.169129 0.000000
5 -1.331652 1.486413 0.000000
1 0.953361 1.265557 0.000000
8 1.066111 -1.394003 0.000000
1 1.871350 -0.869341 0.000000
1 -1.388801 2.679684 0.000000
1 -2.348313 0.853329 0.000000

– H₂BEnNH₂
 $E_{\text{tot}} = -159.4019617$

6 -0.447762 0.343572 0.000006
6 0.647729 -0.460934 0.000012
1 -0.314149 1.420635 0.000009
5 2.021626 0.149095 -0.000007
1 0.478136 -1.535543 0.000010
7 -1.736741 -0.048981 -0.000002
1 -1.975085 -1.023629 -0.000020
1 -2.485401 0.615236 -0.000029
1 3.013863 -0.520241 -0.000035
1 2.131893 1.345109 0.000004

– H₂BEnNMeH
 $E_{\text{tot}} = -198.7072826$

6 -0.161694 -0.166020 -0.000014
6 -1.373752 0.458539 0.000004
1 -0.128983 -1.252016 -0.000029
5 -2.631673 -0.358241 0.000007
1 -1.375332 1.546550 0.000021
7 1.047180 0.417102 -0.000023
1 1.075521 1.422280 0.000007
6 2.305919 -0.288412 0.000017
1 2.895940 -0.049608 -0.886477
1 2.895797 -0.049792 0.886656
1 2.113216 -1.359181 -0.000112
1 -3.717711 0.146117 0.000030
1 -2.553179 -1.557507 -0.000012

– H₂BEnNMe₂
 $E_{\text{tot}} = -238.015731$

6 0.431714 -0.438233 -0.013281
6 1.544193 0.356717 0.006988
1 0.567906 -1.515173 -0.025139
5 2.902921 -0.280748 0.004803
1 1.409751 1.433053 0.027461
7 -0.852438 -0.051968 -0.023853
6 -1.191948 1.353730 -0.000583

6 -1.936009 -1.007908 0.014977
 1 -2.606048 -0.870898 -0.836596
 1 -1.534751 -2.017781 -0.023626
 1 -2.520049 -0.904480 0.933054
 1 -2.271250 1.463996 -0.072709
 1 -0.852093 1.826478 0.924164
 1 -0.730952 1.876284 -0.840627
 1 3.908695 0.369497 0.022623
 1 2.993554 -1.479296 -0.014261

– HAcH

$E_{\text{tot}} = -77.3248917$

6 0.000000 0.000000 0.597043
 6 0.000000 0.000000 -0.597043
 1 0.000000 0.000000 -1.660317
 1 0.000000 0.000000 1.660317

– HAcBH₂

$E_{\text{tot}} = -102.7713729$

6 0.000000 0.000000 0.111862
 6 0.000000 0.000000 1.317156
 1 0.000000 0.000000 2.381529
 5 0.000000 0.000000 -1.396151
 1 0.000000 1.033368 -1.987442
 1 0.000000 -1.033368 -1.987442

– HAcNO₂

$E_{\text{tot}} = -281.805218$

6 0.000002 -2.066755 0.000000
 6 0.000001 -0.876281 0.000000
 7 0.000000 0.526063 0.000000
 1 -0.000002 -3.130712 0.000000
 8 1.083304 1.069156 0.000000
 8 -1.083306 1.069154 0.000000

– HAcCFO

$E_{\text{tot}} = -289.9129279$

6 -0.526114 2.067888 0.000000
 6 -0.268067 0.901560 0.000000
 6 0.000000 -0.511894 0.000000
 1 -0.757571 3.106641 0.000000
 8 -0.789914 -1.386652 0.000000
 9 1.315774 -0.750973 0.000000

– HAcCN

$E_{\text{tot}} = -169.557390$

6 0.000000 0.000000 -1.830305
6 0.000000 0.000000 -0.634149
6 0.000000 0.000000 0.740911
1 0.000000 0.000000 -2.894479
7 0.000000 0.000000 1.890819

– HAcCClO

$$E_{\text{tot}} = -650.2673147$$

6 -2.308930 0.736889 0.000000
6 -1.255361 0.171913 0.000000
6 0.000000 -0.524327 0.000000
1 -3.248162 1.237111 0.000000
8 0.147570 -1.697124 0.000000
17 1.379609 0.590178 0.000000

– HAcCF₃

$$E_{\text{tot}} = -414.3920521$$

6 0.000000 0.000000 2.321081
6 0.000000 0.000000 1.129316
6 0.000000 0.000000 -0.334905
1 0.000000 0.000000 3.385017
9 0.000000 1.244045 -0.817703
9 1.077374 -0.622022 -0.817703
9 -1.077374 -0.622022 -0.817703

– HAcOCN

$$E_{\text{tot}} = -244.7287478$$

6 2.112486 -0.595462 0.000000
6 1.091440 0.012541 0.000000
8 0.000000 0.757207 0.000000
1 3.019446 -1.148419 0.000000
6 -1.147512 0.144937 0.000000
7 -2.193989 -0.325905 0.000000

– HAcCSCN

$$E_{\text{tot}} = -567.7450893$$

6 -2.220979 -0.923987 0.000000
1 -3.064173 -1.572225 0.000000
6 -1.264764 -0.203907 0.000000
16 0.000000 0.916553 0.000000
6 1.333507 -0.136729 0.000000
7 2.282513 -0.786411 0.000000

– HAcCMeO

$$E_{\text{tot}} = -229.9704464$$

6 2.176075 -0.163382 0.000004

6 0.991947 0.014128 -0.000006
 6 -0.456362 0.203501 -0.000003
 1 3.230645 -0.303075 0.000004
 8 -0.936001 1.308173 0.000001
 6 -1.272470 -1.059624 -0.000002
 1 -1.023502 -1.658126 -0.877629
 1 -1.023541 -1.658108 0.877652
 1 -2.330734 -0.813810 -0.000006

– HAcCOOH

$E_{\text{tot}} = -265.9035599$

6 -0.465340 2.110442 0.000000
 6 -0.226763 0.939798 0.000000
 6 0.000000 -0.490534 0.000000
 1 -0.677822 3.152785 0.000000
 8 1.305296 -0.785449 0.000000
 8 -0.873923 -1.310037 0.000000
 1 1.379458 -1.747133 0.000000

– HAcCOOMe

$E_{\text{tot}} = -305.2033436$

6 2.642239 0.197424 0.000000
 6 1.447535 0.219868 0.000000
 6 0.000000 0.314494 0.000000
 1 3.705639 0.176885 0.000000
 8 -0.560086 -0.893605 0.000000
 8 -0.602405 1.351776 0.000000
 6 -1.988211 -0.909297 0.000000
 1 -2.267855 -1.957557 0.000000
 1 -2.373619 -0.409812 0.887105
 1 -2.373619 -0.409812 -0.887105

– HAcCHO

$E_{\text{tot}} = -190.6424661$

6 0.364292 1.828700 0.000000
 6 0.000000 0.687921 0.000000
 6 -0.497596 -0.673258 0.000000
 1 0.705267 2.836602 0.000000
 8 0.211423 -1.642166 0.000000
 1 -1.596827 -0.759455 0.000000

– HAcNCS

$E_{\text{tot}} = -567.7654478$

6 0.000000 0.000000 -3.084709
 6 0.000000 0.000000 -1.886526
 7 0.000000 0.000000 -0.589897
 1 0.000000 0.000000 -4.146742

6 0.000000 0.000000 0.592159
16 0.000000 0.000000 2.159405

– HAcCONH₂

$E_{\text{tot}} = -246.0364243$

6 -0.557659 2.090710 0.000000
6 -0.292341 0.924646 0.000000
6 0.000000 -0.508353 0.000000
1 -0.808803 3.124255 0.000000
8 -0.873794 -1.343422 0.000000
7 1.325015 -0.797386 0.000000
1 2.019976 -0.075122 0.000000
1 1.604082 -1.762084 0.000000

– HAcCl

$E_{\text{tot}} = -536.9277832$

6 0.000000 0.000000 -1.807441
6 0.000000 0.000000 -0.613058
17 0.000000 0.000000 1.023102
1 0.000000 0.000000 -2.869735

– HAcAcH

$E_{\text{tot}} = -153.4679501$

6 0.000000 0.000000 1.885244
6 0.000000 0.000000 0.685996
6 0.000000 0.000000 -0.685996
1 0.000000 0.000000 2.948275
6 0.000000 0.000000 -1.885244
1 0.000000 0.000000 -2.948273

– HAcNCO

$E_{\text{tot}} = -244.8021142$

6 2.401056 -0.330178 0.000000
6 1.249034 -0.010671 0.000000
7 0.000000 0.410485 0.000000
1 3.420233 -0.627976 0.000000
6 -1.154994 0.091627 0.000000
8 -2.298851 -0.093761 0.000000

– HAcSH

$E_{\text{tot}} = -475.5299111$

6 0.039131 1.847129 0.000000
6 0.000000 0.648895 0.000000
16 0.060257 -1.040263 0.000000
1 0.067319 2.909501 0.000000

```

1 -1.266215 -1.241435 0.000000

– HAcF
  Etot = -176.5475546
  6 0.000000 0.000000 -1.282055
  6 0.000000 0.000000 -0.093145
  9 0.000000 0.000000 1.177155
  1 0.000000 0.000000 -2.343198

– HAcAcF
  Etot = -252.6892791
  6 0.000000 0.000000 -2.630071
  6 0.000000 0.000000 -1.431153
  6 0.000000 0.000000 -0.059223
  1 0.000000 0.000000 -3.692949
  6 0.000000 0.000000 1.133977
  9 0.000000 0.000000 2.401308

– HAcMe
  Etot = -116.649977
  6 0.000000 0.000000 1.415476
  6 0.000000 0.000000 0.219017
  6 0.000000 0.000000 -1.236458
  1 0.000000 0.000000 2.478007
  1 0.000000 1.019358 -1.622071
  1 0.882790 -0.509679 -1.622071
  1 -0.882790 -0.509679 -1.622071

– HAcOMe
  Etot = -191.8425457
  6 -0.647481 1.747413 0.000000
  6 0.000000 0.741758 0.000000
  8 0.721838 -0.331341 0.000000
  1 -1.208291 2.647911 0.000000
  6 -0.019473 -1.557455 0.000000
  1 0.717924 -2.353929 0.000000
  1 -0.641306 -1.616777 0.893031
  1 -0.641306 -1.616777 -0.893031

– HAcOH
  Etot = -152.5429383
  6 -0.099103 1.312147 0.000000
  6 0.000000 0.122198 0.000000
  8 0.181016 -1.168560 0.000000
  1 -0.190793 2.369142 0.000000

```

1 -0.662713 -1.626729 0.000000

– HAcNH₂

$E_{\text{tot}} = -132.6855083$

6 1.359884 -0.000010 0.011552

6 0.161919 0.000012 -0.004747

7 -1.183969 -0.000002 -0.081557

1 2.421037 0.000017 0.024553

1 -1.632026 -0.837508 0.252754

1 -1.632046 0.837490 0.252759

– HAcNMeH

$E_{\text{tot}} = -171.9897154$

6 1.906091 0.240769 0.018794

6 0.775421 -0.159711 -0.014378

7 -0.496108 -0.580738 -0.096090

1 2.910323 0.583221 0.038000

1 -0.674695 -1.451688 0.375720

6 -1.557390 0.409469 0.021408

1 -2.512612 -0.074466 -0.172805

1 -1.588746 0.883081 1.006967

1 -1.406245 1.181852 -0.730196

– HAcNMe₂

$E_{\text{tot}} = -211.2965327$

6 2.177905 0.000002 0.070828

6 0.986406 0.000003 -0.078634

7 -0.340497 0.000001 -0.269072

1 3.233595 -0.000004 0.178553

6 -1.040624 1.227747 0.071210

6 -1.040618 -1.227752 0.071210

1 -2.025956 -1.216044 -0.394548

1 -0.483695 -2.079462 -0.311613

1 -1.164598 -1.344889 1.154793

1 -2.025962 1.216036 -0.394548

1 -1.164606 1.344887 1.154793

1 -0.483707 2.079462 -0.311612

– H₂BAcBH₂

$E_{\text{tot}} = -128.2254801$

6 0.000000 0.000000 -0.611528

6 0.000000 0.000000 0.611528

5 0.000000 0.000000 2.101365

5 0.000000 0.000000 -2.101365

1 -0.732543 0.732568 -2.687264

1 0.732543 -0.732568 -2.687264

1 0.732543 0.732568 2.687264

1 -0.732543 -0.732568 2.687264

– H₂BACNO₂

$E_{\text{tot}} = -307.2547313$

6 -1.521849 0.000007 0.000001
 6 -0.317093 0.000004 -0.000005
 7 1.075773 -0.000001 -0.000001
 5 -3.029070 -0.000002 0.000001
 1 -3.606975 0.000016 -1.037694
 1 -3.606978 -0.000027 1.037695
 8 1.616407 -1.085032 -0.000001
 8 1.616412 1.085029 0.000004

– H₂BACFO

$E_{\text{tot}} = -315.3617598$

6 -1.580066 0.022036 -0.000004
 6 -0.372220 0.045730 -0.000008
 6 1.058039 0.123200 -0.000003
 5 -3.086576 -0.006819 0.000005
 1 -3.666912 -0.018384 1.036879
 1 -3.666931 -0.018326 -1.036859
 8 1.715486 1.102101 0.000007
 9 1.600924 -1.099089 -0.000001

– H₂BACCN

$E_{\text{tot}} = -195.0044793$

6 0.000000 0.000000 -1.159290
 6 0.000000 0.000000 0.048959
 6 0.000000 0.000000 1.420373
 5 0.000000 0.000000 -2.671212
 1 0.000000 1.036602 -3.252095
 1 0.000000 -1.036602 -3.252095
 7 0.000000 0.000000 2.571428

– H₂BACClO

$E_{\text{tot}} = -675.7168975$

6 -1.923700 -0.016817 -0.000003
 6 -0.741580 0.239952 0.000001
 6 0.648927 0.562617 0.000000
 5 -3.394863 -0.332212 0.000001
 1 -3.962370 -0.454270 1.037038
 1 -3.962384 -0.454261 -1.037030
 8 1.118069 1.648367 0.000001
 17 1.650155 -0.901874 0.000000

– H₂BACF₃

$E_{\text{tot}} = -439.8379566$

```

6 0 -0.243736 1.839276 0.000000
6 0 -0.080833 0.647485 0.000000
6 0 0.110097 -0.805036 0.000000
5 0 -0.447195 3.339435 0.000000
1 0 0.501156 4.055819 0.000000
1 0 -1.551834 3.777938 0.000000
9 0 1.402556 -1.136211 0.000000
9 0 -0.447195 -1.355300 1.079808
9 0 -0.447195 -1.355300 -1.079808

```

– H₂BACON

$E_{\text{tot}} = -270.1789886$

```

6 0.975418 1.294036 0.000000
6 0.000000 0.590741 0.000000
8 -1.115650 -0.100533 0.000000
5 2.207264 2.155195 0.000000
1 3.280047 1.641933 0.000000
1 2.093649 3.339186 0.000000
6 -1.025531 -1.402554 0.000000
7 -1.026306 -2.549452 0.000000

```

– H₂BACSCN

$E_{\text{tot}} = -593.1979489$

```

6 1.902007 0.109431 0.000004
5 3.311637 0.608957 -0.000004
6 0.753406 -0.283914 0.000010
16 -0.769416 -0.963589 -0.000002
6 -1.754877 0.429047 -0.000002
7 -2.481906 1.319571 0.000000
1 4.208451 -0.172567 -0.000010
1 3.514146 1.780833 -0.000006

```

– H₂BACMeO

$E_{\text{tot}} = -255.4200368$

```

6 -1.622662 0.003759 -0.000004
6 -0.415277 -0.091874 -0.000002
6 1.033261 -0.192040 0.000000
5 -3.121383 0.101079 0.000001
1 -3.706420 0.141018 -1.035165
1 -3.706404 0.140980 1.035182
8 1.574699 -1.269381 -0.000001
6 1.771057 1.119002 0.000002
1 1.491301 1.701703 -0.878833
1 1.491315 1.701691 0.878849
1 2.841255 0.931178 -0.000005

```

– H₂BAcCOOH

$$E_{\text{tot}} = -291.352476$$

6 -1.603990 -0.005667 -0.000002
 6 -0.396009 0.014324 -0.000002
 6 1.043140 0.111811 0.000000
 5 -3.108324 -0.032367 0.000002
 1 -3.692373 -0.043323 -1.035757
 1 -3.692369 -0.043374 1.035762
 8 1.623395 -1.092986 -0.000002
 8 1.637864 1.152526 0.000004
 1 2.577448 -0.950594 0.000000

– H₂BAcCOOMe

$$E_{\text{tot}} = -330.6523001$$

6 2.123880 -0.096492 -0.000001
 6 0.927743 0.074571 -0.000001
 6 -0.489948 0.355717 0.000000
 5 3.612125 -0.311829 0.000001
 1 4.191645 -0.396430 1.035354
 1 4.191648 -0.396422 -1.035351
 8 -1.203976 -0.766743 -0.000001
 8 -0.941357 1.467620 0.000001
 6 -2.622872 -0.594010 0.000000
 1 -3.037212 -1.596546 0.000001
 1 -2.938427 -0.048593 0.887460
 1 -2.938428 -0.048594 -0.887459

– H₂BAcCHO

$$E_{\text{tot}} = -216.0918425$$

6 -1.230447 0.045242 -0.000002
 6 -0.026501 0.179241 0.000006
 6 1.398847 0.390965 -0.000005
 5 -2.721673 -0.145152 -0.000002
 1 -3.301135 -0.217857 -1.035905
 1 -3.301120 -0.217815 1.035914
 8 2.207867 -0.498126 0.000003
 1 1.696284 1.453751 -0.000017

– H₂BAcNCS

$$E_{\text{tot}} = -593.2162059$$

6 0.000000 0.000000 -2.483902
 6 0.000000 0.000000 -1.271123
 7 0.000000 0.000000 0.017187
 5 0.000000 0.000000 -3.982394
 1 0.000000 1.033947 -4.573670
 1 0.000000 -1.033947 -4.573670
 6 0.000000 0.000000 1.202519

16 0.000000 0.000000 2.765878

– H₂BACONH₂

$E_{\text{tot}} = -271.4847999$

6 1.607119 0.011590 0.000001
 6 0.399124 -0.031507 0.000001
 6 -1.053544 -0.138579 0.000000
 5 3.111350 0.046073 -0.000001
 1 3.698464 0.062068 1.034767
 1 3.698458 0.062011 -1.034771
 8 -1.603509 -1.215879 0.000003
 7 -1.703452 1.050807 -0.000004
 1 -1.209881 1.923414 0.000001
 1 -2.707751 1.044495 -0.000004

– H₂BACl

$E_{\text{tot}} = -562.3767781$

6 0.000000 0.000000 -1.215589
 6 0.000000 0.000000 -0.008249
 17 0.000000 0.000000 1.620977
 5 0.000000 0.000000 -2.718683
 1 0.000000 1.033655 -3.310087
 1 0.000000 -1.033655 -3.310087

– H₂BACAcH

$E_{\text{tot}} = -178.9169539$

6 0.000000 0.000000 -1.205172
 6 0.000000 0.000000 0.007301
 6 0.000000 0.000000 1.373103
 5 0.000000 0.000000 -2.707523
 1 0.000000 1.034349 -3.297075
 1 0.000000 -1.034349 -3.297075
 6 0.000000 0.000000 2.573870
 1 0.000000 0.000000 3.637154

– H₂BACNCO

$E_{\text{tot}} = -270.2523533$

6 0.501089 1.736521 0.000000
 6 0.000000 0.635911 0.000000
 7 -0.614924 -0.521227 0.000000
 5 1.145607 3.090256 0.000000
 1 2.333507 3.182260 0.000000
 1 0.467231 4.069671 0.000000
 6 -0.499982 -1.717163 0.000000
 8 -0.528869 -2.873280 0.000000

– H₂BACSH

$$E_{\text{tot}} = -500.9844671$$

6 -0.754225 -0.993809 0.000000
 6 0.000000 -0.039450 0.000000
 16 0.923592 1.348156 0.000000
 5 -1.666128 -2.171394 0.000000
 1 -1.209616 -3.271922 0.000000
 1 -2.845750 -2.004861 0.000000
 1 2.133874 0.762799 0.000000

– H₂BACF

$$E_{\text{tot}} = -201.9966204$$

6 0.000000 0.000000 -0.632269
 6 0.000000 0.000000 0.569448
 9 0.000000 0.000000 1.834737
 5 0.000000 0.000000 -2.135929
 1 0.000000 1.033217 -2.728031
 1 0.000000 -1.033217 -2.728031

– H₂BACAcF

$$E_{\text{tot}} = -278.1384882$$

6 0.000000 0.000000 -1.975543
 6 0.000000 0.000000 -0.763338
 6 0.000000 0.000000 0.602211
 5 0.000000 0.000000 -3.477151
 1 0.000000 1.034032 -4.067840
 1 0.000000 -1.034032 -4.067840
 6 0.000000 0.000000 1.797113
 9 0.000000 0.000000 3.062086

– H₂BACMe

$$E_{\text{tot}} = -142.0985415$$

6 -0.009172 -0.737193 0.000000
 6 0.000000 0.471372 0.000000
 6 0.019288 1.922639 0.000000
 5 -0.022634 -2.238095 0.000000
 1 -1.059927 -2.826192 0.000000
 1 1.003664 -2.845177 0.000000
 1 -0.987536 2.339132 0.000000
 1 0.548136 2.290901 0.879844
 1 0.548136 2.290901 -0.879844

– H₂BACOMe

$$E_{\text{tot}} = -217.2977737$$

6 -1.275734 0.060401 0.000000
 6 -0.091005 0.318258 0.000000

8 1.152130 0.618881 -0.000001
5 -2.730916 -0.249246 0.000000
1 -3.100379 -1.383968 -0.000004
1 -3.530595 0.635865 0.000005
6 2.065416 -0.495319 0.000001
1 3.060998 -0.064010 -0.000012
1 1.907733 -1.096365 0.893766
1 1.907717 -1.096382 -0.893750

– H₂BACOH

$$E_{\text{tot}} = -177.9972134$$

6 0.020853 0.661170 0.000000
6 0.000000 -0.548487 0.000000
8 0.062469 -1.837709 0.000000
5 0.026922 2.151243 0.000000
1 -1.003512 2.751950 0.000000
1 1.061959 2.743156 0.000000
1 -0.817927 -2.225745 0.000000

– H₂BACNH₂

$$E_{\text{tot}} = -158.1458398$$

6 0.000000 0.000000 -0.700829
6 0.000000 0.000000 0.519164
7 0.000000 0.000000 1.831231
5 0.000000 0.000000 -2.176111
1 0.000000 1.033658 -2.773210
1 0.000000 -1.033658 -2.773210
1 0.000000 0.859834 2.349171
1 0.000000 -0.859834 2.349171

– H₂BACNMeH

$$E_{\text{tot}} = -197.4515894$$

6 -1.338319 0.048778 -0.003355
6 -0.142763 0.304815 -0.007899
7 1.143310 0.543174 -0.033245
5 -2.780394 -0.250676 0.007846
1 -3.575539 0.637862 0.071589
1 -3.155686 -1.383094 -0.046163
1 1.454838 1.491499 0.087605
6 2.143952 -0.511206 0.015947
1 3.052051 -0.171421 -0.478658
1 2.381285 -0.795342 1.042861
1 1.764632 -1.382665 -0.511899

– H₂BACNMe₂

$$E_{\text{tot}} = -236.7596281$$

6 1.680756 -0.000006 -0.000014

6 0.455593 -0.000007 -0.000009
7 -0.847783 -0.000001 -0.000002
5 3.150664 0.000000 0.000009
1 3.749683 1.033676 0.000016
1 3.749690 -1.033672 0.000020
6 -1.609035 1.236931 0.000003
6 -1.609049 -1.236922 0.000003
1 -2.244537 -1.291028 -0.887059
1 -0.924873 -2.079736 -0.000011
1 -2.244512 -1.291039 0.887083
1 -2.244523 1.291043 -0.887059
1 -2.244497 1.291049 0.887084
1 -0.924848 2.079735 -0.000008