Supporting Information for Bootstrap Embedding for Molecules

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Note: figures and tables in the main text are referred as Figure Mxxx and Table Mxxx.

1 Supplementary figures

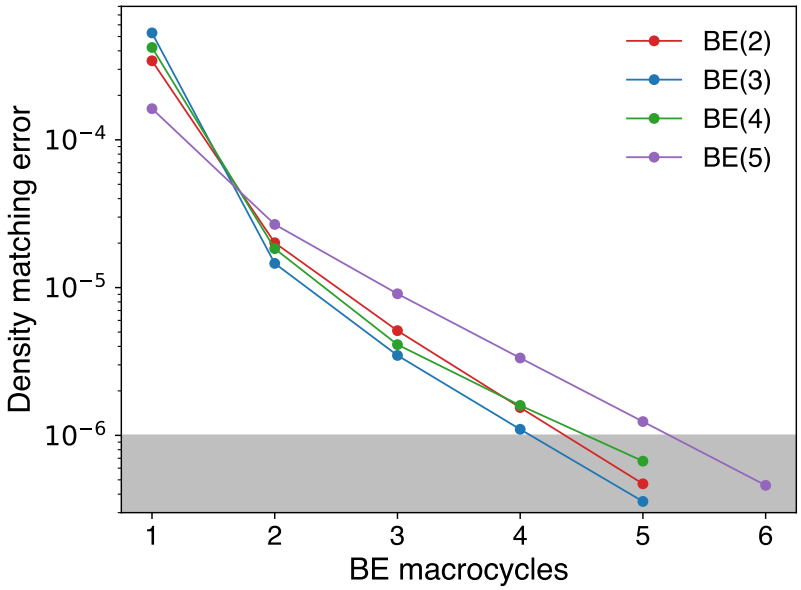

Figure S1: Variation of the BE matching error as defined in eqn (M14) with the number of iterations for the all-electron calculations on hexacene, which is the largest molecules tested in this work. A threshold of 10^{-6} is used for convergence (grey shaded region).

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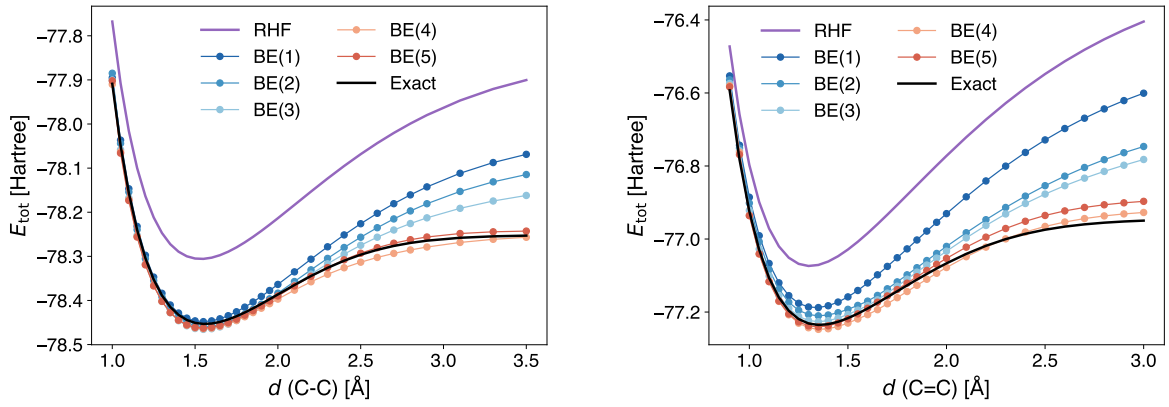

(a) (b)

Figure S2: Energy curves of homolytic cleavage of (a) the C−C single bond in C_2H_6 and (b) the C=C double bond in C_2H_4 computed by BE without density matching. For both molecules, fragments determined at their respective equilibrium geometries are used for all bond lengths. All calculations are performed using the STO-3G basis.

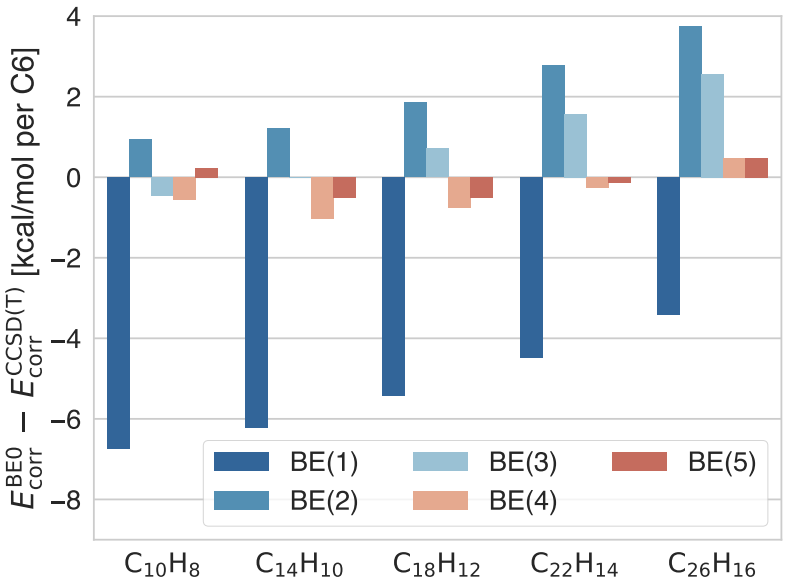

Figure S3: Error of active-space correlation energy (normalized to six carbons) computed by BE with increasing fragment size and without matching conditions compared to CCSD(T) for polyacene chains (from naphthalene to hexacene) at equilibrium geometry. The active space consists of symmetrically orthogonalized p_z orbitals from all carbon atoms. All calculations are performed using the STO-3G basis. Note that benzene (C_6H_6) is not included as it has only six orbitals and BE becomes exact for three-atom fragments.

2 Molecular structures

Shown below are the geometries (xyz format) used in the calculation in the main text.

- CH_3BH_2 (equilibrium):

```
7

C -5.8538351264 2.6281260008 -0.0105307690
B -4.2949320897 2.6522838442 -0.0061243396
H -6.2277104979 3.4026379925 -0.7099218576
H -6.2261530684 2.9645208238 0.9779354959
H -6.3272673222 1.6671325950 -0.2594765722
H -3.7183510002 3.6807612685 0.2644156231
H -3.6268708952 1.6766174752 -0.2562975805
```

- C_2H_6 (equilibrium):

```
8

C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.7588263823 -1.2028971530 -0.5562281523
H -0.7588263823 -1.2028971530 -1.6472811523
H -1.7992836344 -1.2028968825 -0.2278200192
H -0.3107836119 -2.1419365118 -0.2277953039
```

- C_2H_4 (equilibrium):

```
6

C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.1260810579 -0.0000000000 -0.6965844737
H -1.1260810579 -0.0000000000 -1.7791624737
H -2.0947595955 -0.0000000000 -0.2132221024
```

- C_2H_2 (equilibrium):

```
4

C -0.5980109316 0.0000000000 0.0000000000
H -1.6595966855 0.0000000000 0.0000000000
C 0.5980109403 0.0000000000 0.0000000000
H 1.6595966768 0.0000000000 0.0000000000
```

- CH_3NH_2 (equilibrium):

```
7

C -5.1194047373 2.6705378927 -0.0160180507
N -3.6555909405 2.6553237548 0.0093708081
H -5.4995250744 2.1621500029 0.8707286270
H -5.5789869858 2.2006522806 -0.8955352578
H -5.4691560026 3.7023474978 0.0320552242
H -3.2844290338 3.1262652268 -0.8066377287
H -3.3128872257 1.7032733444 -0.0298036220
```

- N_2H_4 (equilibrium):

```
6

N 1.6805041542 0.6665224509 -0.0248742799
N 3.1646858765 0.6671997949 0.0248743210
H 1.4254380685 1.4692165512 0.5634639245
H 1.4254443237 -0.1198466471 0.5851044882
H 3.4197456708 1.4535705392 -0.5851023281
H 3.4197519062 -0.1354926891 -0.5634661258
```

- C_2H_6 (homolytic dissociation of the C–C bond):

```
8
1.00
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.4968924884 -0.7876776211 -0.3642277037
H -0.4968924884 -0.7876776211 -1.4552807037
H -1.5373497404 -0.7876773506 -0.0358195706
H -0.0488497180 -1.7267169799 -0.0357948553

8
1.05
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.5217371128 -0.8270615022 -0.3824390888
H -0.5217371128 -0.8270615022 -1.4734920888
H -1.5621943649 -0.8270612316 -0.0540309558
H -0.0736943424 -1.7661008609 -0.0540062405

8
1.10
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.5465817373 -0.8664453832 -0.4006504740
H -0.5465817373 -0.8664453832 -1.4917034740
H -1.5870389893 -0.8664451127 -0.0722423410
H -0.0985389668 -1.8054847420 -0.0722176257

8
1.15
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.5714263617 -0.9058292643 -0.4188618592
H -0.5714263617 -0.9058292643 -1.5099148592
H -1.6118836137 -0.9058289937 -0.0904537261
H -0.1233835913 -1.8448686230 -0.0904290109

8
```

```
1.20
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.5962709861 -0.9452131454 -0.4370732444
H -0.5962709861 -0.9452131454 -1.5281262444
H -1.6367282381 -0.9452128748 -0.1086651113
H -0.1482282157 -1.8842525041 -0.1086403960

8
1.25
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.6211156105 -0.9845970264 -0.4552846296
H -0.6211156105 -0.9845970264 -1.5463376296
H -1.6615728625 -0.9845967559 -0.1268764965
H -0.1730728401 -1.9236363851 -0.1268517812

8
1.30
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.6459602350 -1.0239809075 -0.4734960148
H -0.6459602350 -1.0239809075 -1.5645490148
H -1.6864174870 -1.0239806369 -0.1450878817
H -0.1979174645 -1.9630202662 -0.1450631664

8
1.35
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.6708048594 -1.0633647885 -0.4917073999
H -0.6708048594 -1.0633647885 -1.5827603999
H -1.7112621114 -1.0633645180 -0.1632992669
H -0.2227620889 -2.0024041473 -0.1632745516

8
1.40
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.6956494838 -1.1027486696 -0.5099187851
H -0.6956494838 -1.1027486696 -1.6009717851
H -1.7361067358 -1.1027483990 -0.1815106521
H -0.2476067134 -2.0417880283 -0.1814859368

8
1.45
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
```

```
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.7204941082 -1.1421325506 -0.5281301703
H -0.7204941082 -1.1421325506 -1.6191831703
H -1.7609513602 -1.1421322801 -0.1997220372
H -0.2724513378 -2.0811719094 -0.1996973220

8
1.50
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.7453387326 -1.1815164317 -0.5463415555
H -0.7453387326 -1.1815164317 -1.6373945555
H -1.7857959847 -1.1815161611 -0.2179334224
H -0.2972959622 -2.1205557904 -0.2179087071

8
1.55
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.7701833571 -1.2209003127 -0.5645529407
H -0.7701833571 -1.2209003127 -1.6556059407
H -1.8106406091 -1.2209000422 -0.2361448076
H -0.3221405866 -2.1599396715 -0.2361200923

8
1.60
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.7950279815 -1.2602841938 -0.5827643259
H -0.7950279815 -1.2602841938 -1.6738173259
H -1.8354852335 -1.2602839233 -0.2543561928
H -0.3469852111 -2.1993235525 -0.2543314775

8
1.65
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.8198726059 -1.2996680749 -0.6009757110
H -0.8198726059 -1.2996680749 -1.6920287110
H -1.8603298579 -1.2996678043 -0.2725675780
H -0.3718298355 -2.2387074336 -0.2725428627

8
1.70
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.8447172303 -1.3390519559 -0.6191870962
```

```
H -0.8447172303 -1.3390519559 -1.7102400962
H -1.8851744823 -1.3390516854 -0.2907789632
H -0.3966744599 -2.2780913146 -0.2907542479

8
1.75
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.8695618547 -1.3784358370 -0.6373984814
H -0.8695618547 -1.3784358370 -1.7284514814
H -1.9100191068 -1.3784355664 -0.3089903483
H -0.4215190843 -2.3174751957 -0.3089656331

8
1.80
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.8944064792 -1.4178197180 -0.6556098666
H -0.8944064792 -1.4178197180 -1.7466628666
H -1.9348637312 -1.4178194475 -0.3272017335
H -0.4463637087 -2.3568590768 -0.3271770182

8
1.85
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.9192511036 -1.4572035991 -0.6738212518
H -0.9192511036 -1.4572035991 -1.7648742518
H -1.9597083556 -1.4572033285 -0.3454131187
H -0.4712083332 -2.3962429578 -0.3453884034

8
1.90
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.9440957280 -1.4965874801 -0.6920326370
H -0.9440957280 -1.4965874801 -1.7830856370
H -1.9845529800 -1.4965872096 -0.3636245039
H -0.4960529576 -2.4356268389 -0.3635997886

8
1.95
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.9689403524 -1.5359713612 -0.7102440221
H -0.9689403524 -1.5359713612 -1.8012970221
H -2.0093976044 -1.5359710907 -0.3818358891
H -0.5208975820 -2.4750107199 -0.3818111738
```

```
8
2.00
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -0.9937849769 -1.5753552423 -0.7284554073
H -0.9937849769 -1.5753552423 -1.8195084073
H -2.0342422289 -1.5753549717 -0.4000472743
H -0.5457422064 -2.5143946010 -0.4000225590

8
2.10
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.0434742257 -1.6541230044 -0.7648781777
H -1.0434742257 -1.6541230044 -1.8559311777
H -2.0839314777 -1.6541227338 -0.4364700446
H -0.5954314553 -2.5931623631 -0.4364453293

8
2.20
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.0931634745 -1.7328907665 -0.8013009481
H -1.0931634745 -1.7328907665 -1.8923539481
H -2.1336207266 -1.7328904959 -0.4728928150
H -0.6451207041 -2.6719301252 -0.4728680997

8
2.30
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.1428527234 -1.8116585286 -0.8377237184
H -1.1428527234 -1.8116585286 -1.9287767184
H -2.1833099754 -1.8116582580 -0.5093155854
H -0.6948099530 -2.7506978873 -0.5092908701

8
2.40
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.1925419722 -1.8904262907 -0.8741464888
H -1.1925419722 -1.8904262907 -1.9651994888
H -2.2329992242 -1.8904260202 -0.5457383557
H -0.7444992018 -2.8294656494 -0.5457136404

8
2.50
```

```
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.2422312211 -1.9691940528 -0.9105692592
H -1.2422312211 -1.9691940528 -2.0016222592
H -2.2826884731 -1.9691937823 -0.5821611261
H -0.7941884506 -2.9082334115 -0.5821364108

8
2.60
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.2919204699 -2.0479618149 -0.9469920295
H -1.2919204699 -2.0479618149 -2.0380450295
H -2.3323777219 -2.0479615444 -0.6185838965
H -0.8438776995 -2.9870011737 -0.6185591812

8
2.70
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.3416097188 -2.1267295770 -0.9834147999
H -1.3416097188 -2.1267295770 -2.0744677999
H -2.3820669708 -2.1267293065 -0.6550066668
H -0.8935669483 -3.0657689358 -0.6549819515

8
2.80
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.3912989676 -2.2054973392 -1.0198375703
H -1.3912989676 -2.2054973392 -2.1108905703
H -2.4317562196 -2.2054970686 -0.6914294372
H -0.9432561972 -3.1445366979 -0.6914047219

8
2.90
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.4409882164 -2.2842651013 -1.0562603406
H -1.4409882164 -2.2842651013 -2.1473133406
H -2.4814454685 -2.2842648307 -0.7278522076
H -0.9929454460 -3.2233044600 -0.7278274923

8
3.10
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
```

```
H -0.4480430575 0.9390393681 -0.3284324300
C -1.5403667141 -2.4418006255 -1.1291058814
H -1.5403667141 -2.4418006255 -2.2201588814
H -2.5808239661 -2.4418003549 -0.8006977483
H -1.0923239437 -3.3808399842 -0.8006730330

8
3.30
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.6397452118 -2.5993361497 -1.2019514221
H -1.6397452118 -2.5993361497 -2.2930044221
H -2.6802024638 -2.5993358792 -0.8735432890
H -1.1917024414 -3.5383755085 -0.8735185737

8
3.50
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0910530000
H 1.0404571178 0.0000000000 -0.3284085581
H -0.4480430575 0.9390393681 -0.3284324300
C -1.7391237095 -2.7568716740 -1.2747969628
H -1.7391237095 -2.7568716740 -2.3658499628
H -2.7795809615 -2.7568714034 -0.9463888298
H -1.2910809391 -3.6959110327 -0.9463641145
```

- C_2H_4 (homolytic dissociation of the C=C bond):

```
6
0.70
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.5953070199 -0.0000000000 -0.3682520225
H -0.5953070199 0.0000000000 -1.4508300225
H -1.5639855575 -0.0000000000 0.1151103488

6
0.75
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.6378289498 -0.0000000000 -0.3945557384
H -0.6378289498 0.0000000000 -1.4771337384
H -1.6065074875 -0.0000000000 0.0888066329

6
0.80
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.6803508798 -0.0000000000 -0.4208594543
H -0.6803508798 0.0000000000 -1.5034374543
H -1.6490294174 -0.0000000000 0.0625029170

6
0.85
```

```
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.7228728098 -0.0000000000 -0.4471631702
H -0.7228728098 0.0000000000 -1.5297411702
H -1.6915513474 -0.0000000000 0.0361992011

6
0.90
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.7653947398 -0.0000000000 -0.4734668861
H -0.7653947398 0.0000000000 -1.5560448861
H -1.7340732774 -0.0000000000 0.0098954852

6
0.95
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.8079166698 -0.0000000000 -0.4997706020
H -0.8079166698 0.0000000000 -1.5823486020
H -1.7765952074 -0.0000000000 -0.0164082307

6
1.00
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.8504385998 -0.0000000000 -0.5260743179
H -0.8504385998 0.0000000000 -1.6086523179
H -1.8191171374 -0.0000000000 -0.0427119466

6
1.05
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.8929605298 -0.0000000000 -0.5523780338
H -0.8929605298 0.0000000000 -1.6349560338
H -1.8616390674 -0.0000000000 -0.0690156625

6
1.10
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.9354824598 -0.0000000000 -0.5786817497
H -0.9354824598 -0.0000000000 -1.6612597497
H -1.9041609974 -0.0000000000 -0.0953193784

6
1.15
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -0.9780043898 -0.0000000000 -0.6049854656
```

```
H -0.9780043898 -0.0000000000 -1.6875634656
H -1.9466829274 -0.0000000000 -0.1216230943

6
1.20
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.0205263198 -0.0000000000 -0.6312891815
H -1.0205263198 -0.0000000000 -1.7138671815
H -1.9892048574 -0.0000000000 -0.1479268102

6
1.25
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.0630482497 -0.0000000000 -0.6575928974
H -1.0630482497 -0.0000000000 -1.7401708974
H -2.0317267874 -0.0000000000 -0.1742305261

6
1.30
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.1055701797 -0.0000000000 -0.6838966133
H -1.1055701797 -0.0000000000 -1.7664746133
H -2.0742487173 -0.0000000000 -0.2005342420

6
1.35
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.1480921097 -0.0000000000 -0.7102003292
H -1.1480921097 -0.0000000000 -1.7927783292
H -2.1167706473 -0.0000000000 -0.2268379579

6
1.40
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.1906140397 -0.0000000000 -0.7365040451
H -1.1906140397 -0.0000000000 -1.8190820451
H -2.1592925773 -0.0000000000 -0.2531416737

6
1.45
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.2331359697 -0.0000000000 -0.7628077610
H -1.2331359697 -0.0000000000 -1.8453857610
H -2.2018145073 -0.0000000000 -0.2794453896

6
```

```
1.50
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.2756578997 -0.0000000000 -0.7891114769
H -1.2756578997 -0.0000000000 -1.8716894769
H -2.2443364373 -0.0000000000 -0.3057491055

6
1.55
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.3181798297 -0.0000000000 -0.8154151928
H -1.3181798297 -0.0000000000 -1.8979931928
H -2.2868583673 -0.0000000000 -0.3320528214

6
1.60
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.3607017597 -0.0000000000 -0.8417189087
H -1.3607017597 -0.0000000000 -1.9242969087
H -2.3293802973 -0.0000000000 -0.3583565373

6
1.65
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.4032236897 -0.0000000000 -0.8680226246
H -1.4032236897 -0.0000000000 -1.9506006246
H -2.3719022273 -0.0000000000 -0.3846602532

6
1.70
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.4457456197 -0.0000000000 -0.8943263405
H -1.4457456197 -0.0000000000 -1.9769043405
H -2.4144241573 -0.0000000000 -0.4109639691

6
1.75
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.4882675496 -0.0000000000 -0.9206300564
H -1.4882675496 -0.0000000000 -2.0032080564
H -2.4569460872 -0.0000000000 -0.4372676850

6
1.80
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
```

```
C -1.5307894796 -0.0000000000 -0.9469337723
H -1.5307894796 -0.0000000000 -2.0295117723
H -2.4994680172 -0.0000000000 -0.4635714009

6
1.85
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.5733114096 -0.0000000000 -0.9732374882
H -1.5733114096 -0.0000000000 -2.0558154882
H -2.5419899472 -0.0000000000 -0.4898751168

6
1.90
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.6158333396 -0.0000000000 -0.9995412040
H -1.6158333396 -0.0000000000 -2.0821192040
H -2.5845118772 -0.0000000000 -0.5161788327

6
1.95
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.6583552696 -0.0000000000 -1.0258449199
H -1.6583552696 -0.0000000000 -2.1084229199
H -2.6270338072 -0.0000000000 -0.5424825486

6
2.00
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.7008771996 -0.0000000000 -1.0521486358
H -1.7008771996 -0.0000000000 -2.1347266358
H -2.6695557372 -0.0000000000 -0.5687862645

6
2.10
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.7859210596 -0.0000000000 -1.1047560676
H -1.7859210596 -0.0000000000 -2.1873340676
H -2.7545995972 -0.0000000000 -0.6213936963

6
2.20
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.8709649196 -0.0000000000 -1.1573634994
H -1.8709649196 -0.0000000000 -2.2399414994
H -2.8396434572 -0.0000000000 -0.6740011281
```

```
6
2.30
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -1.9560087795 -0.0000000000 -1.2099709312
H -1.9560087795 -0.0000000000 -2.2925489312
H -2.9246873171 -0.0000000000 -0.7266085599

6
2.40
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -2.0410526395 -0.0000000000 -1.2625783630
H -2.0410526395 -0.0000000000 -2.3451563630
H -3.0097311771 -0.0000000000 -0.7792159917

6
2.50
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -2.1260964995 -0.0000000000 -1.3151857948
H -2.1260964995 -0.0000000000 -2.3977637948
H -3.0947750371 -0.0000000000 -0.8318234235

6
2.60
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -2.2111403595 -0.0000000000 -1.3677932266
H -2.2111403595 -0.0000000000 -2.4503712266
H -3.1798188971 -0.0000000000 -0.8844308552

6
2.70
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -2.2961842195 -0.0000000000 -1.4204006584
H -2.2961842195 -0.0000000000 -2.5029786584
H -3.2648627571 -0.0000000000 -0.9370382870

6
2.80
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -2.3812280794 -0.0000000000 -1.4730080902
H -2.3812280794 -0.0000000000 -2.5555860902
H -3.3499066170 -0.0000000000 -0.9896457188

6
2.90
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
```

```
H 0.9686785376 0.0000000000 -0.4833623713
C -2.4662719394 -0.0000000000 -1.5256155220
H -2.4662719394 -0.0000000000 -2.6081935220
H -3.4349504770 -0.0000000000 -1.0422531506

6
3.00
C 0.0000000000 0.0000000000 0.0000000000
H 0.0000000000 0.0000000000 1.0825780000
H 0.9686785376 0.0000000000 -0.4833623713
C -2.5513157994 -0.0000000000 -1.5782229538
H -2.5513157994 -0.0000000000 -2.6608009538
H -3.5199943370 -0.0000000000 -1.0948605824
```

- C_6H_6 (equilibrium):

```
12

C -3.8911621157 2.9164322674 0.0000000000
C -5.1281752268 2.2636966566 0.0000000000
C -2.7073785257 2.1715134604 0.0000000000
C -5.1813003426 0.8660536064 0.0000000000
C -3.9975158364 0.1211344628 0.0000000000
C -2.7605034790 0.7738692909 0.0000000000
H -3.8495188396 4.0083664589 0.0000000000
H -6.0530178846 2.8456856838 0.0000000000
H -6.1477228423 0.3560586120 0.0000000000
H -4.0391599137 -0.9707997725 0.0000000000
H -1.8356597322 0.1918821717 0.0000000000
H -1.7409552615 2.6815071015 0.0000000000
```

- $C_{10}H_8$ (equilibrium):

```
18

C -3.8065064212 2.7402100514 0.0000000000
C -5.1022043185 2.1620117099 0.0000000000
C -2.6865516991 1.9359860131 0.0000000000
C -5.2517046941 0.7913602999 0.0000000000
C -4.1165855241 -0.0673270294 0.0000000000
C -2.8057244680 0.5176448014 0.0000000000
H -3.7002161940 3.8274429418 0.0000000000
H -5.9823335447 2.8091095384 0.0000000000
H -6.2491460334 0.3438655268 0.0000000000
H -1.6871692277 2.3791247930 0.0000000000
C -1.6706053179 -0.3410425170 0.0000000000
C -1.8201056893 -1.7116939382 0.0000000000
C -3.1158035635 -2.2898922779 0.0000000000
C -4.2357582979 -1.4856682258 0.0000000000
H -0.6731639745 0.1064522329 0.0000000000
H -0.9399764406 -2.3587917349 0.0000000000
H -5.2351407700 -1.9288070172 0.0000000000
H -3.2220938216 -3.3771251681 0.0000000000
```

- $C_{14}H_{10}$ (equilibrium):

```
24
```

```
C -3.7556315581 2.6112555868 0.0000000000
C -5.0741805824 2.0624481954 0.0000000000
C -2.6595064353 1.7858612869 0.0000000000
C -5.2611764360 0.7031123841 0.0000000000
C -4.1451003122 -0.1944397790 0.0000000000
C -2.8094219214 0.3615105854 0.0000000000
H -3.6256857478 3.6958434344 0.0000000000
H -5.9352494969 2.7345949559 0.0000000000
H -6.2696259154 0.2814170995 0.0000000000
H -1.6494864374 2.2037151947 0.0000000000
C -1.7085867067 -0.5080714468 0.0000000000
C -1.8676188582 -1.9018877193 0.0000000000
C -3.2032972505 -2.4578381031 0.0000000000
C -4.3041324813 -1.5882560623 0.0000000000
H -0.6986375215 -0.0880866392 0.0000000000
H -5.3140816855 -2.0082408723 0.0000000000
C -0.7515427437 -2.7994398605 0.0000000000
C -0.9385385757 -4.1587756790 0.0000000000
C -2.2570875773 -4.7075830880 0.0000000000
C -3.3532127187 -3.8821888041 0.0000000000
H 0.2569067239 -2.3777445801 0.0000000000
H -0.0774696428 -4.8309224170 0.0000000000
H -2.3870333981 -5.7921709369 0.0000000000
H -4.3632327211 -4.3000427356 0.0000000000
```

- $C_{18}H_{12}$ (equilibrium):

```
30

C -3.7300512201 2.5369337722 0.0000000000
C -5.0553203053 1.9925504158 0.0000000000
C -2.6390730934 1.7095474779 0.0000000000
C -5.2499123874 0.6372128302 0.0000000000
C -4.1370899172 -0.2705475355 0.0000000000
C -2.7927573695 0.2816813726 0.0000000000
H -3.5968632706 3.6211009189 0.0000000000
H -5.9121107620 2.6701001331 0.0000000000
H -6.2604215479 0.2205776453 0.0000000000
H -1.6272995167 2.1230283561 0.0000000000
C -1.6996961004 -0.5852144736 0.0000000000
C -1.8602134096 -1.9886502383 0.0000000000
C -3.2049573685 -2.5410458091 0.0000000000
C -4.3054528750 -1.6554446233 0.0000000000
H -0.6879795084 -0.1699403000 0.0000000000
H -5.3172185099 -2.0705977112 0.0000000000
C -0.7597180200 -2.8742513779 0.0000000000
C -0.9280808317 -4.2591483864 0.0000000000
C -2.2724132926 -4.8113774830 0.0000000000
C -3.3654747239 -3.9444816696 0.0000000000
H 0.2520475009 -2.4590983278 0.0000000000
H -4.3771914286 -4.3597558884 0.0000000000
C 0.1847416819 -5.1669086576 0.0000000000
C -0.0098501898 -6.5222462302 0.0000000000
C -2.4260974708 -6.2392436298 0.0000000000
C -1.3351191795 -7.0666298006 0.0000000000
H 1.1952507791 -4.7502734792 0.0000000000
H 0.8469403893 -7.1997957905 0.0000000000
```

```
H -3.4378710921 -6.6527245493 0.0000000000
H -1.4683069603 -8.1507969610 0.0000000000
```

- $C_{22}H_{14}$ (equilibrium):

```
36

C -3.7758622606 2.4710863314 0.0000000000
C -5.0913309955 1.8975036778 0.0000000000
C -2.6680320871 1.6688409455 0.0000000000
C -5.2574547020 0.5398415010 0.0000000000
C -4.1249665797 -0.3463298191 0.0000000000
C -2.7895311313 0.2359525520 0.0000000000
H -3.6668437420 3.5579411802 0.0000000000
H -5.9618621715 2.5572792757 0.0000000000
H -6.2588673602 0.1018649818 0.0000000000
H -1.6654884998 2.1042054820 0.0000000000
C -1.6799929637 -0.6036438116 0.0000000000
C -1.8073807046 -2.0151259214 0.0000000000
C -3.1443789259 -2.5980681177 0.0000000000
C -4.2650998786 -1.7306536718 0.0000000000
H -0.6775427403 -0.1665856983 0.0000000000
H -5.2677947949 -2.1671427448 0.0000000000
C -0.6919663176 -2.8689909202 0.0000000000
C -0.8257194716 -4.2673418967 0.0000000000
C -2.1627176878 -4.8502841484 0.0000000000
C -3.2781321339 -3.9964191134 0.0000000000
H 0.3105009622 -2.4323000433 0.0000000000
H -4.2805994698 -4.4331100221 0.0000000000
C 0.2950014519 -5.1347562910 0.0000000000
C 0.1548682201 -6.5190801417 0.0000000000
C -2.2901054092 -6.2617662577 0.0000000000
C -1.1805671685 -7.1013626089 0.0000000000
H 1.2976963388 -4.6982672741 0.0000000000
H -3.2925556755 -6.6988243997 0.0000000000
C 1.2873563677 -7.4052513999 0.0000000000
C -1.3020661670 -8.5342509896 0.0000000000
C -0.1942359232 -9.3364963304 0.0000000000
C 1.1212327454 -8.7629135847 0.0000000000
H 2.2887690213 -6.9672749235 0.0000000000
H 1.9917639975 -9.4226890851 0.0000000000
H -2.3046097790 -8.9696155267 0.0000000000
H -0.3032543641 -10.4233511856 0.0000000000
```

- $C_{26}H_{16}$ (equilibrium):

```
42

C -3.7676382299 2.4456173446 0.0000000000
C -5.0849317567 1.8730603925 0.0000000000
C -2.6610710858 1.6429033206 0.0000000000
C -5.2530017965 0.5163921070 0.0000000000
C -4.1213029597 -0.3723940732 0.0000000000
C -2.7834410764 0.2090915450 0.0000000000
H -3.6578731917 3.5323892694 0.0000000000
H -5.9543802057 2.5342497115 0.0000000000
H -6.2549610632 0.0796896932 0.0000000000
```

```
H -1.6580811418 2.0772133613 0.0000000000
C -1.6757935006 -0.6298706862 0.0000000000
C -1.8032408646 -2.0437493060 0.0000000000
C -3.1433498322 -2.6261780746 0.0000000000
C -4.2638344300 -1.7545676552 0.0000000000
H -0.6729094393 -0.1938549063 0.0000000000
H -5.2670767210 -2.1897492068 0.0000000000
C -0.6906629862 -2.8949303161 0.0000000000
C -0.8231124860 -4.2982133483 0.0000000000
C -2.1643214197 -4.8811050293 0.0000000000
C -3.2804247970 -4.0202974942 0.0000000000
H 0.3121849330 -2.4592207294 0.0000000000
H -4.2834619259 -4.4555677446 0.0000000000
C 0.2929910230 -5.1590209878 0.0000000000
C 0.1559158347 -6.5531404376 0.0000000000
C -2.2967708749 -6.2843880094 0.0000000000
C -1.1841932276 -7.1355690526 0.0000000000
H 1.2960283958 -4.7237507096 0.0000000000
H -3.2996186490 -6.7200973355 0.0000000000
C 1.2764004279 -7.4247510886 0.0000000000
C -1.3116407216 -8.5494476255 0.0000000000
C -0.2039934177 -9.3884100259 0.0000000000
C 1.1338686249 -8.8069246640 0.0000000000
H 2.2796429638 -6.9895697241 0.0000000000
H -2.3145247813 -8.9854630322 0.0000000000
C 2.2655673254 -9.6957111309 0.0000000000
C 2.0974969731 -11.0523793511 0.0000000000
C 0.7802032851 -11.6249360186 0.0000000000
C -0.3263636649 -10.8222217629 0.0000000000
H 3.2675267886 -9.2590090323 0.0000000000
H 2.9669452935 -11.7135688281 0.0000000000
H 0.6704380957 -12.7117079324 0.0000000000
H -1.3293537172 -11.2565314257 0.0000000000
```