**H-BEE Program User Manual**

H-BEE is a software utility for estimating the intermolecular hydrogen bond (HB) energy in molecular clusters using quantum chemical methods. H-BEE is a Linux-based code written in Python as a programming language. The current version of H-BEE is executed in serial mode. The current version of H-BEE uses the Gaussian programat the backend.

**Prerequisites**

1. Computer with Linux operating system.
2. Python (version 2.7).
3. Gaussian *ab initio* software package.
4. H-BEE driver python file.
5. A file containing the Cartesian coordinates (in Å) of the molecular cluster.

**Input section**

The program accepts the user-defined parameters through a file named “INPUT”. The sample INPUT file is as below. The XYZFile, HBMinDist, HBMaxDist, nproc, mem, and distTH are the keywords. The associated values need to be supplied by the user after “=”. It may be noted that the extension of the file should be xyz and it must contain the Cartesian coordinates (in Å) of the molecular cluster (closed shell) in standard XYZ format. See Appendix-I for a sample xyz file W12.xyz for W12 cluster.

[INPUT]

XYZFile= W12.xyz. # Name of the XYZ file

HBMinDist= 1.2 #Distance in Å

HBMaxDist= 2.5 #Distance in Å

nproc= 16 #No of cores to be used for calculation

mem= 120GB #The memory along with its unit (preferably in GB)

distTH = 2.5 #Distance in Å

The parameter HBMinDist and HBMaxDist respectively are the minimum and maximum distance to define the HB. The parameter distTH represents the distance cut-off to decide the neighbours while forming HB centric shell.

**Execution procedure**

To use the H-BEE program, the user has to move to a directory containing the INPUT and xyz files. To start the calculation user may take the following steps.

1. Call the H-BEE driver script with the Python command.
2. Provide the choice of the method (1/2/3) to be used for estimating HB energy. For more details about methods 1, 2 and 3, please refer to the main text of the paper.
3. Furnish the desired level of theory and basis set (as per Gaussian keyword) at which HB energy to execute.
4. In case the user goes with Method-1, then the program prompts for the availability of the whole cluster and used in subsequent calculation.
5. In case the user opts for Method-2, the program checks for the frag.list file containing information about the fragments. Please note, this file should be in a specific format (see Appendix-II) and must be available in the same folder. The name of the file should have the same input prefix as XYZ file with “-frag.list” as an extension. For example, if XYZ file name is “W12.xyz”, then the fragment-file name should be “W12-frag.list”. For details, see the discussion in the main text.

**Output section**

With all this information, the program calculates the HB energies and results are redirected to the output file. The name of the output file will be derived from XYZ file name. For example, if XYZ file name is “W12.xyz”, then the output file name is “W12-OUTPUT”.

The first few lines of output file enlist the input provided by the user such as Input file name, cartesian coordinates, level of theory, basis set, choice of the method, etc. This is followed by writing the total number of monomers (along with indices of atoms constituting the monomer) identified by the program. With this input, the individual HB energies and cooperativity contribution in kcal/mol are printed. At last, all HB energies available in the cluster are printed in tabular format along with the total elapsed time (in min). See Appendix-III for a sample output file associated with Method-I presenting the HB energies for the W12 cluster.

**Appendix-SI**

Sample xyz file for W12 cluster

36

H24O12

O 2.772110000 1.869460000 -0.353360000

H 2.900110000 1.480480000 0.533520000

H 1.846350000 2.175820000 -0.349560000

O 2.876610000 -0.246750000 -2.004630000

H 3.560310000 -0.166130000 -2.680920000

H 2.918350000 0.592620000 -1.471820000

O 2.772120000 -1.869460000 0.353320000

H 1.846360000 -2.175810000 0.349530000

H 2.900100000 -1.480480000 -0.533560000

O 2.876650000 0.246760000 2.004610000

H 3.560370000 0.166110000 2.680880000

H 2.918340000 -0.592620000 1.471800000

O -0.068530000 1.905110000 -0.398500000

H -0.991140000 2.225770000 -0.413500000

H -0.064550000 1.142850000 -1.024470000

O 0.068490000 -0.398510000 -1.905080000

H 0.991110000 -0.413520000 -2.225750000

H 0.064520000 -1.024480000 -1.142810000

O -0.068520000 -1.905090000 0.398520000

H -0.064540000 -1.142820000 1.024470000

H -0.991130000 -2.225780000 0.413460000

O 0.068540000 0.398510000 1.905100000

H 0.991160000 0.413500000 2.225750000

H 0.064550000 1.024490000 1.142850000

O -2.876650000 2.004660000 -0.246720000

H -3.560320000 2.680990000 -0.166220000

H -2.918410000 1.471930000 0.592690000

O -2.772130000 -0.353340000 -1.869420000

H -2.900120000 0.533530000 -1.480430000

H -1.846370000 -0.349530000 -2.175770000

O -2.876620000 -2.004650000 0.246730000

H -2.918380000 -1.471850000 -0.592650000

H -3.560330000 -2.680940000 0.166160000

O -2.772070000 0.353310000 1.869450000

H -2.900060000 -0.533560000 1.480450000

H -1.846310000 0.349490000 2.175800000

**Appendix-SII**

Sample frag.list file for W12 cluster with 3 fragments of size 24, 24 and 12 atoms, respectively.

3

24

O 2.772110000 1.869460000 -0.353360000

H 2.900110000 1.480480000 0.533520000

H 1.846350000 2.175820000 -0.349560000

O 2.876610000 -0.246750000 -2.004630000

H 3.560310000 -0.166130000 -2.680920000

H 2.918350000 0.592620000 -1.471820000

O 2.772120000 -1.869460000 0.353320000

H 1.846360000 -2.175810000 0.349530000

H 2.900100000 -1.480480000 -0.533560000

O 2.876650000 0.246760000 2.004610000

H 3.560370000 0.166110000 2.680880000

H 2.918340000 -0.592620000 1.471800000

O -0.068530000 1.905110000 -0.398500000

H -0.991140000 2.225770000 -0.413500000

H -0.064550000 1.142850000 -1.024470000

O 0.068490000 -0.398510000 -1.905080000

H 0.991110000 -0.413520000 -2.225750000

H 0.064520000 -1.024480000 -1.142810000

O -0.068520000 -1.905090000 0.398520000

H -0.064540000 -1.142820000 1.024470000

H -0.991130000 -2.225780000 0.413460000

O 0.068540000 0.398510000 1.905100000

H 0.991160000 0.413500000 2.225750000

H 0.064550000 1.024490000 1.142850000

24

O -0.068530000 1.905110000 -0.398500000

H -0.991140000 2.225770000 -0.413500000

H -0.064550000 1.142850000 -1.024470000

O 0.068490000 -0.398510000 -1.905080000

H 0.991110000 -0.413520000 -2.225750000

H 0.064520000 -1.024480000 -1.142810000

O -0.068520000 -1.905090000 0.398520000

H -0.064540000 -1.142820000 1.024470000

H -0.991130000 -2.225780000 0.413460000

O 0.068540000 0.398510000 1.905100000

H 0.991160000 0.413500000 2.225750000

H 0.064550000 1.024490000 1.142850000

O -2.876650000 2.004660000 -0.246720000

H -3.560320000 2.680990000 -0.166220000

H -2.918410000 1.471930000 0.592690000

O -2.772130000 -0.353340000 -1.869420000

H -2.900120000 0.533530000 -1.480430000

H -1.846370000 -0.349530000 -2.175770000

O -2.876620000 -2.004650000 0.246730000

H -2.918380000 -1.471850000 -0.592650000

H -3.560330000 -2.680940000 0.166160000

O -2.772070000 0.353310000 1.869450000

H -2.900060000 -0.533560000 1.480450000

H -1.846310000 0.349490000 2.175800000

12

O -0.068530000 1.905110000 -0.398500000

H -0.991140000 2.225770000 -0.413500000

H -0.064550000 1.142850000 -1.024470000

O 0.068490000 -0.398510000 -1.905080000

H 0.991110000 -0.413520000 -2.225750000

H 0.064520000 -1.024480000 -1.142810000

O -0.068520000 -1.905090000 0.398520000

H -0.064540000 -1.142820000 1.024470000

H -0.991130000 -2.225780000 0.413460000

O 0.068540000 0.398510000 1.905100000

H 0.991160000 0.413500000 2.225750000

H 0.064550000 1.024490000 1.142850000

**Appendix-SIII**

Sample output file for W12 cluster

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* WELCOME TO THE HYDROGEN BOND ESTIMATION PROGRAM \*

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\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Input file name --> W12.xyz

Total number of atoms --> 36

Title card --> H24O12

Level of theory --> MP2/aug-cc-pVTZ

HB distance threshold (in Ang) --> [1.2, 2.5]

Method chosen for estimating HB strength --> ACT

Cartesian coordinates:

O 2.77211 1.86946 -0.35336

H 2.90011 1.48048 0.53352

H 1.84635 2.17582 -0.34956

O 2.87661 -0.24675 -2.00463

H 3.56031 -0.16613 -2.68092

H 2.91835 0.59262 -1.47182

O 2.77212 -1.86946 0.35332

H 1.84636 -2.17581 0.34953

H 2.9001 -1.48048 -0.53356

O 2.87665 0.24676 2.00461

H 3.56037 0.16611 2.68088

H 2.91834 -0.59262 1.4718

O -0.06853 1.90511 -0.3985

H -0.99114 2.22577 -0.4135

H -0.06455 1.14285 -1.02447

O 0.06849 -0.39851 -1.90508

H 0.99111 -0.41352 -2.22575

H 0.06452 -1.02448 -1.14281

O -0.06852 -1.90509 0.39852

H -0.06454 -1.14282 1.02447

H -0.99113 -2.22578 0.41346

O 0.06854 0.39851 1.9051

H 0.99116 0.4135 2.22575

H 0.06455 1.02449 1.14285

O -2.87665 2.00466 -0.24672

H -3.56032 2.68099 -0.16622

H -2.91841 1.47193 0.59269

O -2.77213 -0.35334 -1.86942

H -2.90012 0.53353 -1.48043

H -1.84637 -0.34953 -2.17577

O -2.87662 -2.00465 0.24673

H -2.91838 -1.47185 -0.59265

H -3.56033 -2.68094 0.16616

O -2.77207 0.35331 1.86945

H -2.90006 -0.53356 1.48045

H -1.84631 0.34949 2.1758

Total number of monomers: 12

Monomer no 1: 0,1,2,

Monomer no 2: 3,4,5,

Monomer no 3: 6,7,8,

Monomer no 4: 9,10,11,

Monomer no 5: 12,13,14,

Monomer no 6: 15,16,17,

Monomer no 7: 18,19,20,

Monomer no 8: 21,22,23,

Monomer no 9: 24,25,26,

Monomer no 10: 27,28,29,

Monomer no 11: 30,31,32,

Monomer no 12: 33,34,35,

Job Submission Time :: Tue Jul 18 00:11:14 2023

Calculating whole cluster energy at MP2/aug-cc-pVTZ

Hydrogen bond estimation at MP2/aug-cc-pVTZ is started

Weak Bond number 1 is between atom number 0 and 5 Distance 1.7 (Ang)

---HB energy in cluster--

E1= -839.78047 a.u.

E2= -839.77957 a.u.

E12= -763.43272 a.u.

Total -916.12732 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01634 a.u. (10.25 kcal/mol)

---HB energy in dimer--

E1= -76.32859 a.u.

E2= -76.32781 a.u.

E12= -152.66398 a.u.

HB Energy 0.00757 a.u. (4.75 kcal/mol)

Cooperativity = 5.5 kcal/mol

Weak Bond number 2 is between atom number 3 and 8 Distance 1.92 (Ang)

---HB energy in cluster--

E1= -839.77957 a.u.

E2= -839.78047 a.u.

E12= -763.42769 a.u.

Total -916.13235 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01131 a.u. (7.1 kcal/mol)

---HB energy in dimer--

E1= -76.32781 a.u.

E2= -76.32859 a.u.

E12= -152.66439 a.u.

HB Energy 0.00799 a.u. (5.01 kcal/mol)

Cooperativity = 2.09 kcal/mol

Weak Bond number 3 is between atom number 3 and 16 Distance 1.91 (Ang)

---HB energy in cluster--

E1= -839.77957 a.u.

E2= -839.77318 a.u.

E12= -763.42036 a.u.

Total -916.13238 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01128 a.u. (7.08 kcal/mol)

---HB energy in dimer--

E1= -76.32781 a.u.

E2= -76.3282 a.u.

E12= -152.6632 a.u.

HB Energy 0.00719 a.u. (4.51 kcal/mol)

Cooperativity = 2.57 kcal/mol

Weak Bond number 4 is between atom number 6 and 11 Distance 1.7 (Ang)

---HB energy in cluster--

E1= -839.78047 a.u.

E2= -839.77957 a.u.

E12= -763.43272 a.u.

Total -916.12732 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01634 a.u. (10.25 kcal/mol)

---HB energy in dimer--

E1= -76.32859 a.u.

E2= -76.32781 a.u.

E12= -152.66398 a.u.

HB Energy 0.00757 a.u. (4.75 kcal/mol)

Cooperativity = 5.5 kcal/mol

Weak Bond number 5 is between atom number 9 and 1 Distance 1.92 (Ang)

---HB energy in cluster--

E1= -839.78047 a.u.

E2= -839.77957 a.u.

E12= -763.42769 a.u.

Total -916.13235 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01131 a.u. (7.1 kcal/mol)

---HB energy in dimer--

E1= -76.32781 a.u.

E2= -76.32859 a.u.

E12= -152.66439 a.u.

HB Energy 0.00799 a.u. (5.01 kcal/mol)

Cooperativity = 2.09 kcal/mol

Weak Bond number 6 is between atom number 9 and 22 Distance 1.91 (Ang)

---HB energy in cluster--

E1= -839.77957 a.u.

E2= -839.77318 a.u.

E12= -763.42036 a.u.

Total -916.13238 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01128 a.u. (7.08 kcal/mol)

---HB energy in dimer--

E1= -76.32781 a.u.

E2= -76.3282 a.u.

E12= -152.6632 a.u.

HB Energy 0.00719 a.u. (4.51 kcal/mol)

Cooperativity = 2.57 kcal/mol

Weak Bond number 7 is between atom number 12 and 2 Distance 1.93 (Ang)

---HB energy in cluster--

E1= -839.78047 a.u.

E2= -839.77318 a.u.

E12= -763.42107 a.u.

Total -916.13258 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01108 a.u. (6.95 kcal/mol)

---HB energy in dimer--

E1= -76.3282 a.u.

E2= -76.32859 a.u.

E12= -152.66389 a.u.

HB Energy 0.0071 a.u. (4.46 kcal/mol)

Cooperativity = 2.49 kcal/mol

Weak Bond number 8 is between atom number 12 and 23 Distance 1.78 (Ang)

---HB energy in cluster--

E1= -839.77318 a.u.

E2= -839.77318 a.u.

E12= -763.41658 a.u.

Total -916.12978 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01389 a.u. (8.71 kcal/mol)

---HB energy in dimer--

E1= -76.3282 a.u.

E2= -76.3282 a.u.

E12= -152.664 a.u.

HB Energy 0.00761 a.u. (4.77 kcal/mol)

Cooperativity = 3.94 kcal/mol

Weak Bond number 9 is between atom number 15 and 14 Distance 1.78 (Ang)

---HB energy in cluster--

E1= -839.77318 a.u.

E2= -839.77318 a.u.

E12= -763.41658 a.u.

Total -916.12977 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01389 a.u. (8.71 kcal/mol)

---HB energy in dimer--

E1= -76.3282 a.u.

E2= -76.3282 a.u.

E12= -152.664 a.u.

HB Energy 0.00761 a.u. (4.77 kcal/mol)

Cooperativity = 3.94 kcal/mol

Weak Bond number 10 is between atom number 15 and 29 Distance 1.93 (Ang)

---HB energy in cluster--

E1= -839.77318 a.u.

E2= -839.78047 a.u.

E12= -763.42107 a.u.

Total -916.13258 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01108 a.u. (6.95 kcal/mol)

---HB energy in dimer--

E1= -76.3282 a.u.

E2= -76.32859 a.u.

E12= -152.66389 a.u.

HB Energy 0.0071 a.u. (4.46 kcal/mol)

Cooperativity = 2.49 kcal/mol

Weak Bond number 11 is between atom number 18 and 7 Distance 1.93 (Ang)

---HB energy in cluster--

E1= -839.78047 a.u.

E2= -839.77318 a.u.

E12= -763.42107 a.u.

Total -916.13258 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01108 a.u. (6.95 kcal/mol)

---HB energy in dimer--

E1= -76.3282 a.u.

E2= -76.32859 a.u.

E12= -152.66389 a.u.

HB Energy 0.0071 a.u. (4.46 kcal/mol)

Cooperativity = 2.49 kcal/mol

Weak Bond number 12 is between atom number 18 and 17 Distance 1.78 (Ang)

---HB energy in cluster--

E1= -839.77318 a.u.

E2= -839.77318 a.u.

E12= -763.41658 a.u.

Total -916.12977 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01389 a.u. (8.71 kcal/mol)

---HB energy in dimer--

E1= -76.3282 a.u.

E2= -76.3282 a.u.

E12= -152.664 a.u.

HB Energy 0.00761 a.u. (4.77 kcal/mol)

Cooperativity = 3.94 kcal/mol

Weak Bond number 13 is between atom number 21 and 19 Distance 1.78 (Ang)

---HB energy in cluster--

E1= -839.77318 a.u.

E2= -839.77318 a.u.

E12= -763.41658 a.u.

Total -916.12977 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01389 a.u. (8.71 kcal/mol)

---HB energy in dimer--

E1= -76.3282 a.u.

E2= -76.3282 a.u.

E12= -152.664 a.u.

HB Energy 0.00761 a.u. (4.77 kcal/mol)

Cooperativity = 3.94 kcal/mol

Weak Bond number 14 is between atom number 21 and 35 Distance 1.93 (Ang)

---HB energy in cluster--

E1= -839.77318 a.u.

E2= -839.78047 a.u.

E12= -763.42107 a.u.

Total -916.13258 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01108 a.u. (6.95 kcal/mol)

---HB energy in dimer--

E1= -76.3282 a.u.

E2= -76.32859 a.u.

E12= -152.66389 a.u.

HB Energy 0.0071 a.u. (4.46 kcal/mol)

Cooperativity = 2.49 kcal/mol

Weak Bond number 15 is between atom number 24 and 13 Distance 1.91 (Ang)

---HB energy in cluster--

E1= -839.77318 a.u.

E2= -839.77957 a.u.

E12= -763.42036 a.u.

Total -916.13238 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01128 a.u. (7.08 kcal/mol)

---HB energy in dimer--

E1= -76.32781 a.u.

E2= -76.3282 a.u.

E12= -152.6632 a.u.

HB Energy 0.00719 a.u. (4.51 kcal/mol)

Cooperativity = 2.57 kcal/mol

Weak Bond number 16 is between atom number 24 and 28 Distance 1.92 (Ang)

---HB energy in cluster--

E1= -839.77957 a.u.

E2= -839.78047 a.u.

E12= -763.42769 a.u.

Total -916.13235 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01131 a.u. (7.1 kcal/mol)

---HB energy in dimer--

E1= -76.32781 a.u.

E2= -76.32859 a.u.

E12= -152.66439 a.u.

HB Energy 0.00799 a.u. (5.01 kcal/mol)

Cooperativity = 2.09 kcal/mol

Weak Bond number 17 is between atom number 27 and 31 Distance 1.7 (Ang)

---HB energy in cluster--

E1= -839.78047 a.u.

E2= -839.77957 a.u.

E12= -763.43272 a.u.

Total -916.12732 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01634 a.u. (10.25 kcal/mol)

---HB energy in dimer--

E1= -76.32859 a.u.

E2= -76.32781 a.u.

E12= -152.66398 a.u.

HB Energy 0.00757 a.u. (4.75 kcal/mol)

Cooperativity = 5.5 kcal/mol

Weak Bond number 18 is between atom number 30 and 20 Distance 1.91 (Ang)

---HB energy in cluster--

E1= -839.77318 a.u.

E2= -839.77957 a.u.

E12= -763.42036 a.u.

Total -916.13238 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01128 a.u. (7.08 kcal/mol)

---HB energy in dimer--

E1= -76.32781 a.u.

E2= -76.3282 a.u.

E12= -152.6632 a.u.

HB Energy 0.00719 a.u. (4.51 kcal/mol)

Cooperativity = 2.57 kcal/mol

Weak Bond number 19 is between atom number 30 and 34 Distance 1.92 (Ang)

---HB energy in cluster--

E1= -839.77957 a.u.

E2= -839.78047 a.u.

E12= -763.42769 a.u.

Total -916.13235 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01131 a.u. (7.1 kcal/mol)

---HB energy in dimer--

E1= -76.32781 a.u.

E2= -76.32859 a.u.

E12= -152.66439 a.u.

HB Energy 0.00799 a.u. (5.01 kcal/mol)

Cooperativity = 2.09 kcal/mol

Weak Bond number 20 is between atom number 33 and 26 Distance 1.7 (Ang)

---HB energy in cluster--

E1= -839.77957 a.u.

E2= -839.78047 a.u.

E12= -763.43272 a.u.

Total -916.12732 a.u.

Cluster energy (ACT) -916.14366 a.u.

HB Energy 0.01634 a.u. (10.25 kcal/mol)

---HB energy in dimer--

E1= -76.32859 a.u.

E2= -76.32781 a.u.

E12= -152.66398 a.u.

HB Energy 0.00757 a.u. (4.75 kcal/mol)

Cooperativity = 5.5 kcal/mol

Job completion Time :: Wed Jul 19 13:42:12 2023

Total Elapsed Time :: 2250.97 Minutes

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SUMMARY

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| Sr No. | Atm indices |Distance (Ang) | HB Energy (kcal/mol) |Cooperativity (kcal/mol) |

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| 1 | [1, 6] | 1.70 | 10.25 | 5.50 |

| 2 | [4, 9] | 1.92 | 7.10 | 2.09 |

| 3 | [4, 17] | 1.91 | 7.08 | 2.57 |

| 4 | [7, 12] | 1.70 | 10.25 | 5.50 |

| 5 | [10, 2] | 1.92 | 7.10 | 2.09 |

| 6 | [10, 23] | 1.91 | 7.08 | 2.57 |

| 7 | [13, 3] | 1.93 | 6.95 | 2.49 |

| 8 | [13, 24] | 1.78 | 8.71 | 3.94 |

| 9 | [16, 15] | 1.78 | 8.71 | 3.94 |

| 10 | [16, 30] | 1.93 | 6.95 | 2.49 |

| 11 | [19, 8] | 1.93 | 6.95 | 2.49 |

| 12 | [19, 18] | 1.78 | 8.71 | 3.94 |

| 13 | [22, 20] | 1.78 | 8.71 | 3.94 |

| 14 | [22, 36] | 1.93 | 6.95 | 2.49 |

| 15 | [25, 14] | 1.91 | 7.08 | 2.57 |

| 16 | [25, 29] | 1.92 | 7.10 | 2.09 |

| 17 | [28, 32] | 1.70 | 10.25 | 5.50 |

| 18 | [31, 21] | 1.91 | 7.08 | 2.57 |

| 19 | [31, 35] | 1.92 | 7.10 | 2.09 |

| 20 | [34, 27] | 1.70 | 10.25 | 5.50 |

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