

## Supporting Information

# Water Confinement in Small Polycyclic Aromatic Hydrocarbons

*Alon Zamir,<sup>1</sup> Estefania Rossich Molina,<sup>1</sup> Musahid Ahmed,<sup>2</sup> Tamar Stein<sup>\*1</sup>*

<sup>1</sup> Fritz Haber Research Center for Molecular Dynamics, Hebrew University of Jerusalem,  
Jerusalem 9190401, Israel

<sup>2</sup> Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California  
94720, USA

\*Corresponding author: [tamar.stein@mail.huji.ac.il](mailto:tamar.stein@mail.huji.ac.il)

The OH $\cdots\pi$  interactions lengths marked in the paper are the length of the perpendicular line from the hydrogen pointing toward the  $\pi$  cloud to the PAH. The CH $\cdots$ O interactions lengths marked in the paper are the distances between the water's oxygen atom and a hydrogen on the PAH, with a cutoff value of 3Å.

### Tilting angles' calculation:

All the angles reported in the manuscript are summarized in Table S2. We refer to two PAH molecules as tilted from one another if the angle between their planar structures exceeds an established cutoff value of 3°.

The equation of the angle between two planes is shown in equation (1):

$$(1) \quad \cos\theta = \frac{|\vec{n}_1 \cdot \vec{n}_2|}{|\vec{n}_1| \cdot |\vec{n}_2|}$$

Where  $\vec{n}_1 \wedge \vec{n}_2$  are the normal vectors of each PAH. Even though the molecules are mostly aromatic, their geometries slightly deviate from perfect planarity. To tackle this issue and apply equation (1), we first translated the coordinates of the entire system such that the first three atoms in the first PAH (as presented in the XYZ coordinates given in the SI) are on the XZ plane. Then, we make the assumption that  $\vec{n}_1$  is the vector normal to the plane that contains those atoms.

$$(2) \quad \vec{n}_1 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Next, we fit the second PAH to a plane in the following manner:

The plane equation is:

$$(3) \quad ax + bz + c = y$$

Given  $n$  sets of points, we could transform them by equation (3):

$$(4) \quad A \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} x_0 & z_0 & 1 \\ \vdots & \ddots & \vdots \\ x_n & z_n & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} y_0 \\ \vdots \\ y_n \end{pmatrix}$$

To find the coefficients, we use Moore-Penrose inversion:[1]

$$(5) \quad \begin{pmatrix} a \\ b \\ c \end{pmatrix} = A^+ \begin{pmatrix} y_0 \\ \vdots \\ y_n \end{pmatrix} = (A^T A)^{-1} A^T \begin{pmatrix} y_0 \\ \vdots \\ y_n \end{pmatrix}$$

Where  $A^+$  is the left pseudo-inversion matrix:

$$(6) \quad A^+ A = I_n$$

After obtaining the coefficients, we can define the second normal vector:

$$(7) \quad \vec{n}_2 = \begin{pmatrix} a \\ 1 \\ b \end{pmatrix}$$

Once the two normal vectors are determined, we can use equation (1) to calculate the angles between the PAHs.

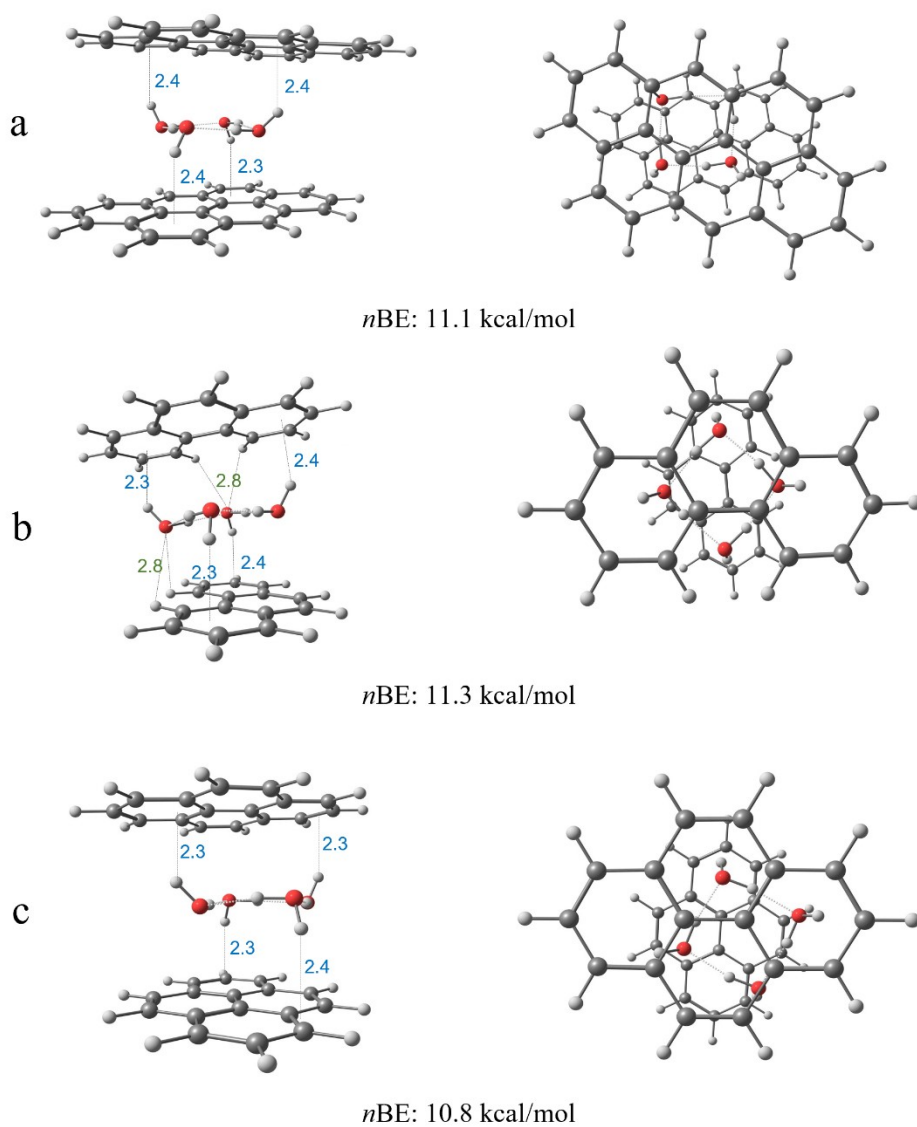


Figure S1: Four water clusters within the dimers of anthanthrene (parallel conformation) (a), phenanthrene (b) and pyrene (c). All reported bond lengths are in Å. The blue numbers mark the OH $\cdots\pi$  bond lengths, and the green numbers mark the CH $\cdots$ O bond lengths.

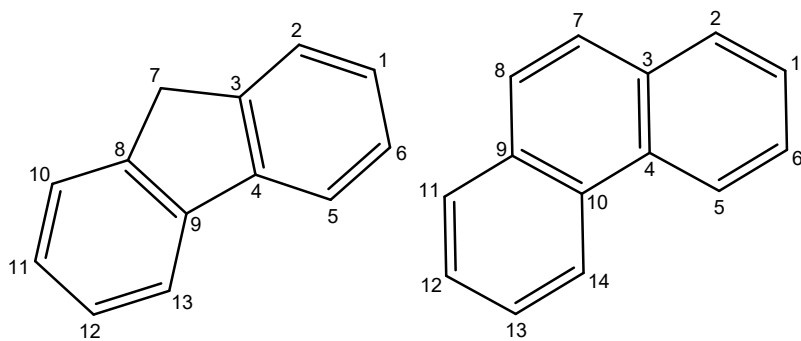


Figure S2: 2D structures of fluorene (right) and phenanthrene (left). The bay region is the concave area between carbons 13, 9, 4 and 5 in the fluorene, and between carbons 14, 10, 4 and 5 in the phenanthrene.

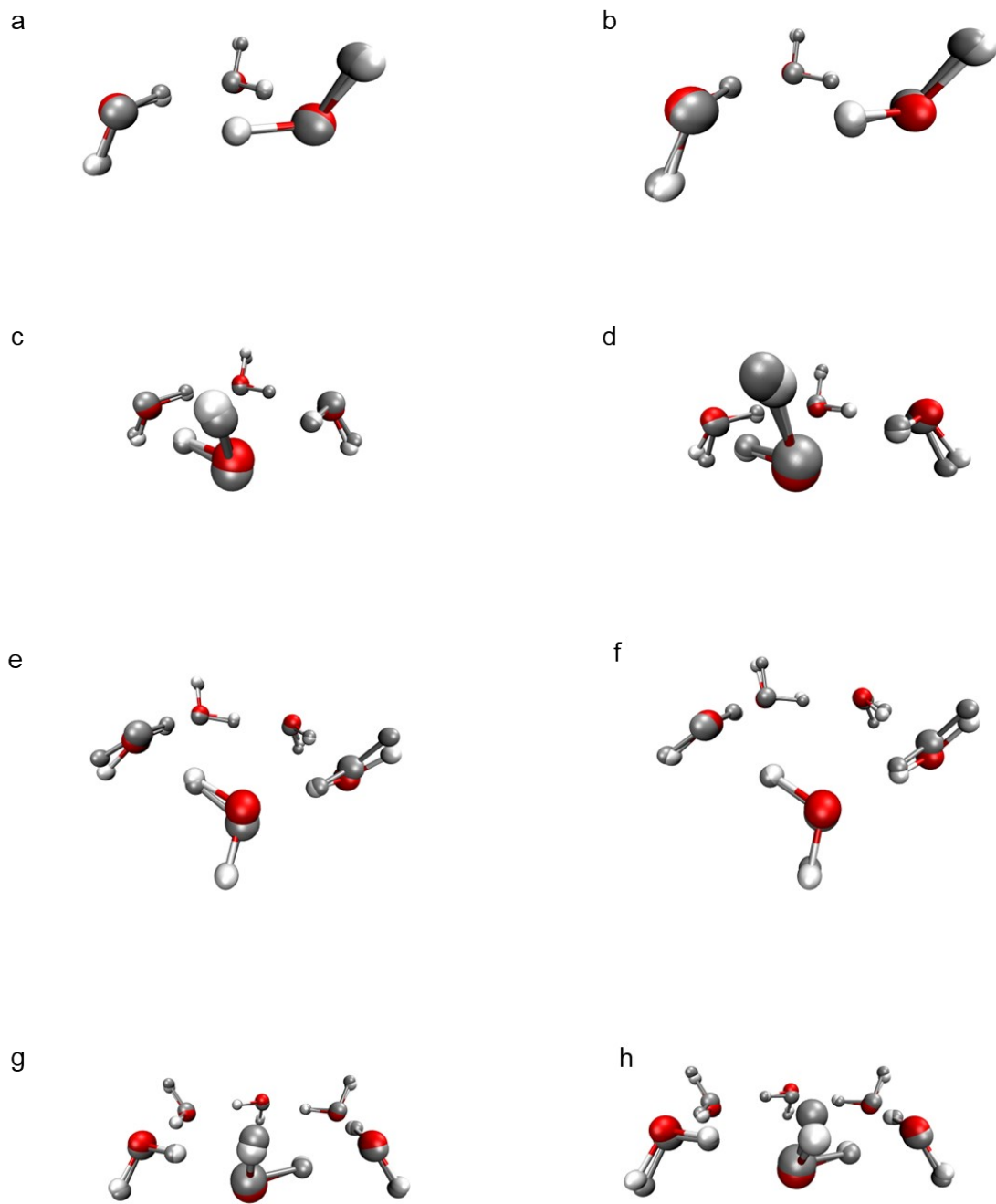


Figure S3: Overlap of isolated water cluster (colored in silver) and water cluster (colored in red and white) confined in the PAHs complexes of anthracene (a), fluorene (b), pyrene (c), anthanthrene (d, h), coronene(e,g) and phenanthrene(f), respectively.

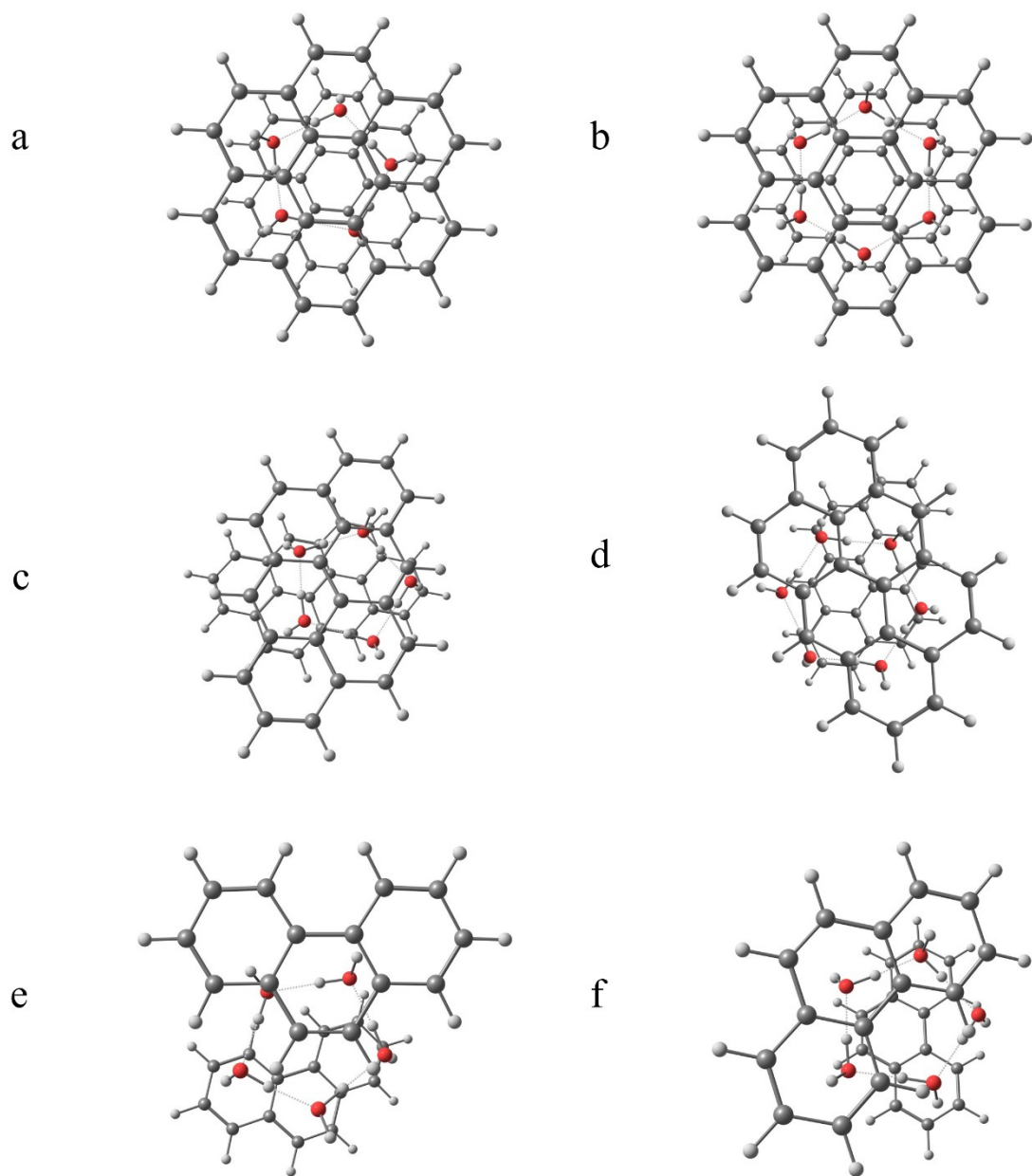


Figure S4: Top views of clusters of five and six water molecules confined within coronenes (a, b), anthanthrenes (c, d), and five water molecules with two conformers of phenanthrenes (e, f).

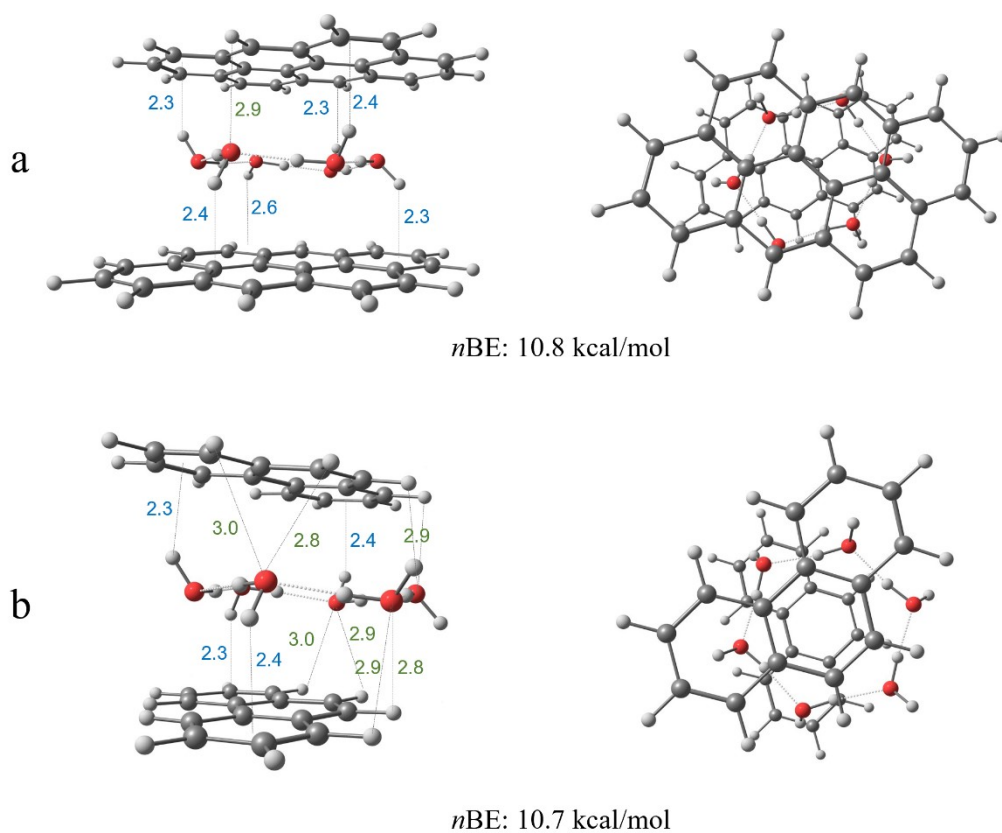


Figure S5: Six water clusters within the dimers of anthanthrene (parallel conformation) (a), phenanthrene (b). All reported bond lengths are in Å. The blue numbers mark the OH $\cdots$  $\pi$  bond lengths, and the green numbers mark the CH $\cdots$ O bond lengths.

Table S1: Root-mean square deviation (RMSD) between confined water clusters and their isolated counterparts. The small values indicate that bond lengths and angles do not change significantly.

| 3-water cluster             |      |
|-----------------------------|------|
| PAH dimer                   | RMSD |
| Phenanthrene                | 0.05 |
| Anthracene                  | 0.07 |
| Pyrene                      | 0.04 |
| Fluorene                    | 0.07 |
| 4-water cluster             |      |
| PAH dimer                   | RMSD |
| Phenanthrene                | 0.15 |
| Anthracene                  | 0.12 |
| Pyrene                      | 0.12 |
| Fluorene                    | 0.14 |
| Anthanthrene (SI)           | 0.15 |
| Anthanthrene (Paper)        | 0.13 |
| Coronene                    | 0.16 |
| 5-water cluster             |      |
| PAH dimer                   | RMSD |
| Phenanthrene (confined)     | 0.23 |
| Phenanthrene (non-confined) | 0.19 |
| Anthanthrene                | 0.26 |
| Coronene                    | 0.22 |
| 6-water cluster             |      |
| PAH dimer                   | RMSD |
| Phenanthrene                | 0.19 |
| Anthanthrene (SI)           | 0.24 |
| Anthanthrene (Paper)        | 0.15 |
| Coronene                    | 0.09 |



Table S2: Summary of the binding energies (BE), normalized BE (*n*BE), and the tilting angles of all structures presented in the paper and SI.

| Phenanthrene          |               |                        |                   |
|-----------------------|---------------|------------------------|-------------------|
| N° of water molecules | BE (kcal/mol) | <i>n</i> BE (kcal/mol) | Tilting Angle (°) |
| 3                     | -29.1         | 9.7                    | 6.7               |
| 4                     | -45.1         | 11.3                   | 11.2              |
| 5 (non-confined)      | -54.0         | 10.8                   | 10.7              |
| 5                     | -52.0         | 10.4                   | 11.3              |
| 6                     | -64.0         | 10.7                   | 5.2               |
| Anthanthrene          |               |                        |                   |
| 4 (SI)                | -44.4         | 11.1                   | 5.9               |
| 6 (SI)                | -64.6         | 10.8                   | 3.0               |
| 4 (Paper)             | -44.5         | 11.1                   | 2.2               |
| 5 (Paper)             | -57.5         | 11.5                   | 2.3               |
| 6 (Paper)             | -65.5         | 10.9                   | 2.1               |
| Anthracene            |               |                        |                   |
| 3                     | -27.7         | 9.2                    | 18.5              |
| 4                     | -44.5         | 11.1                   | 2.2               |
| 8                     | -91.5         | 11.4                   | 2.6               |
| 12                    | -136.6        | 11.4                   | 2.3               |
| Coronene              |               |                        |                   |
| 4                     | -45.7         | 11.4                   | 2.3               |
| 5                     | -57.4         | 11.5                   | 1.1               |
| 6                     | -68.2         | 11.4                   | 1.1               |
| Pyrene                |               |                        |                   |
| 3                     | -28.5         | 9.5                    | 7.6               |
| 4                     | -43.2         | 10.8                   | 3.9               |
| Fluorene              |               |                        |                   |
| 3                     | -32.0         | 10.7                   | 9.1               |
| 4                     | -49.1         | 12.3                   | 10.3              |

**Cartesian coordinates of the structures reported in the manuscript:**

**Phenanthrene dimer:**

**3w:**

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.000000000  | 0.000000000  | 0.000000000  |
| 6 | 0.000000000  | 0.000000000  | 1.382627727  |
| 6 | 1.215393286  | 0.000000000  | -0.713652504 |
| 6 | 2.410235159  | 0.010276709  | -0.021836787 |
| 6 | 1.211871532  | -0.003527300 | 2.114020117  |
| 6 | 1.249794036  | -0.004335753 | 3.577151269  |
| 6 | 2.430765523  | 0.013244172  | 1.393103158  |
| 6 | 3.686166219  | 0.051263392  | 2.105425817  |
| 6 | 3.722346596  | 0.075852028  | 3.458762153  |
| 6 | 2.504531229  | 0.044647050  | 4.234721704  |
| 1 | -0.953150493 | 0.037956236  | 1.910702763  |
| 1 | 3.362733288  | 0.022271823  | -0.561413532 |
| 1 | 4.612306807  | 0.067586888  | 1.522196938  |
| 1 | 4.676991782  | 0.112425738  | 3.992885224  |
| 6 | 2.555400329  | 0.054986456  | 5.649810965  |
| 1 | 3.533786465  | 0.097727850  | 6.139589306  |
| 1 | 1.449857744  | 0.009293988  | 7.497184866  |
| 6 | 1.397716109  | 0.006458314  | 6.404527103  |
| 6 | 0.146779389  | -0.048537053 | 5.753830408  |
| 1 | -0.774449450 | -0.081248328 | 6.342782115  |
| 6 | 0.078344794  | -0.051076301 | 4.372119747  |
| 1 | -0.901965804 | -0.067232927 | 3.894654327  |
| 1 | -0.950533160 | 0.005335152  | -0.541569421 |
| 1 | 1.210351885  | 0.000116168  | -1.807710853 |
| 6 | 2.548212618  | 6.079816104  | -0.783732123 |
| 6 | 1.364671928  | 5.955413889  | -0.081279246 |
| 6 | 3.767368377  | 6.258515500  | -0.098395543 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 6 | 3.773453029  | 6.302998187 | 1.281069664  |
| 6 | 1.341503511  | 6.002372393 | 1.335279039  |
| 6 | 0.107321832  | 5.870309902 | 2.112387124  |
| 6 | 2.571745466  | 6.175044524 | 2.020802771  |
| 6 | 2.593858658  | 6.191975889 | 3.466215725  |
| 6 | 1.456015629  | 6.037352695 | 4.184371844  |
| 6 | 0.179764290  | 5.878729213 | 3.526974105  |
| 1 | 0.436488925  | 5.812029148 | -0.638121810 |
| 1 | 4.712954437  | 6.433434175 | 1.827163645  |
| 1 | 3.558641304  | 6.311911727 | 3.968331276  |
| 1 | 1.479085330  | 6.008361792 | 5.276530183  |
| 6 | -1.001679272 | 5.731740830 | 4.294046414  |
| 1 | -0.914346640 | 5.705292644 | 5.383694169  |
| 1 | -3.140237801 | 5.497262005 | 4.283883665  |
| 6 | -2.233097622 | 5.606518386 | 3.682916211  |
| 6 | -2.313883361 | 5.610287550 | 2.272873929  |
| 1 | -3.285861043 | 5.513488480 | 1.780739128  |
| 6 | -1.167497695 | 5.731403167 | 1.507747811  |
| 1 | -1.260590476 | 5.726166555 | 0.419768906  |
| 1 | 2.537312925  | 6.035395438 | -1.876364426 |
| 1 | 4.701877113  | 6.356676254 | -0.657792971 |
| 8 | 0.829485448  | 3.208375526 | 5.170197172  |
| 1 | 1.037102582  | 2.371304824 | 5.614073363  |
| 1 | 1.442268687  | 3.210577333 | 4.397089482  |
| 8 | -0.818947095 | 2.579395046 | 3.021688227  |
| 8 | 1.917982784  | 2.948447486 | 2.676774881  |
| 1 | -1.329952836 | 3.366853240 | 2.782723934  |
| 1 | -0.463762881 | 2.798353445 | 3.913833816  |
| 1 | 2.171270592  | 3.689213382 | 2.108159480  |
| 1 | 0.973489552  | 2.780875491 | 2.463300632  |

**4w:**

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.000000000  | 0.000000000  | 0.000000000  |
| 6 | 0.000000000  | 0.000000000  | 1.382915237  |
| 6 | 1.218628939  | 0.000000000  | -0.712984939 |
| 6 | 2.413360919  | 0.003672410  | -0.019101309 |
| 6 | 1.212635061  | 0.013649352  | 2.115847975  |
| 6 | 1.248097037  | 0.024919695  | 3.578529700  |
| 6 | 2.433954864  | 0.017755273  | 1.397210703  |
| 6 | 3.689434752  | 0.031314519  | 2.109787459  |
| 6 | 3.722697389  | 0.039656669  | 3.462714842  |
| 6 | 2.503626044  | 0.035524606  | 4.236260233  |
| 1 | -0.953360502 | -0.041236413 | 1.910018465  |
| 1 | 3.366209167  | -0.000818778 | -0.557802459 |
| 1 | 4.615783865  | 0.023576123  | 1.527731857  |
| 1 | 4.676653379  | 0.039352969  | 3.998560324  |
| 6 | 2.553243418  | 0.035576883  | 5.652366554  |
| 1 | 3.531588855  | 0.037330348  | 6.143496072  |
| 1 | 1.443587311  | 0.035500363  | 7.496620802  |
| 6 | 1.393432802  | 0.034371443  | 6.403936119  |
| 6 | 0.141905994  | 0.031537207  | 5.751704241  |
| 1 | -0.779764656 | 0.024605969  | 6.340361388  |
| 6 | 0.073495711  | 0.025814329  | 4.371068836  |
| 1 | -0.905448034 | -0.013198307 | 3.892981231  |
| 1 | -0.949761476 | -0.011224063 | -0.542307808 |
| 1 | 1.215047056  | -0.005566458 | -1.806753298 |
| 6 | -2.120692155 | -5.376931227 | 4.637309701  |
| 6 | -0.756409484 | -5.568489855 | 4.522337450  |
| 6 | -2.950901397 | -5.459977485 | 3.498522297  |
| 6 | -2.390382194 | -5.734232036 | 2.265723502  |
| 6 | -0.158799657 | -5.855475439 | 3.269869568  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 1.281691224  | -6.057239943 | 3.112517369  |
| 6 | -0.994797066 | -5.938029558 | 2.128364685  |
| 6 | -0.419544837 | -6.207114891 | 0.831670104  |
| 6 | 0.915408111  | -6.373796162 | 0.683548234  |
| 6 | 1.804005809  | -6.306717958 | 1.819142543  |
| 1 | -0.131796398 | -5.458777687 | 5.408933186  |
| 1 | -3.020447013 | -5.796523697 | 1.372694948  |
| 1 | -1.088573996 | -6.254294922 | -0.032829505 |
| 1 | 1.349671473  | -6.556925628 | -0.303679740 |
| 6 | 3.198137732  | -6.492983820 | 1.649950293  |
| 1 | 3.584618480  | -6.677393344 | 0.642564654  |
| 1 | 5.131342983  | -6.600064185 | 2.590186618  |
| 6 | 4.057133522  | -6.449880918 | 2.731675727  |
| 6 | 3.538819646  | -6.209537031 | 4.022383724  |
| 1 | 4.213513285  | -6.168155168 | 4.882112137  |
| 6 | 2.182612577  | -6.014351738 | 4.205191968  |
| 1 | 1.811996890  | -5.796441693 | 5.206993540  |
| 1 | -2.556046756 | -5.149139429 | 5.614430273  |
| 1 | -4.029535019 | -5.304470292 | 3.592569670  |
| 8 | 1.167057338  | -3.109264063 | 4.749548435  |
| 8 | -0.838483195 | -2.614531806 | 2.953192007  |
| 1 | 1.343377793  | -2.318691738 | 5.281554150  |
| 1 | 1.895802847  | -3.109127300 | 4.071585088  |
| 1 | -1.499980269 | -3.309932331 | 3.087263021  |
| 1 | -0.179021412 | -2.780223851 | 3.675449267  |
| 8 | 0.925761757  | -3.137548432 | 0.912531814  |
| 8 | 2.939367102  | -3.108465719 | 2.718310229  |
| 1 | 0.919014616  | -2.325413921 | 0.383937829  |
| 1 | 0.202601465  | -2.985540473 | 1.569366662  |
| 1 | 3.353958797  | -3.980596928 | 2.636481581  |

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|---|-------------|--------------|-------------|
| 1 | 2.273896066 | -3.100792298 | 1.982522762 |
|---|-------------|--------------|-------------|

**5w (non-confined):**

|   |             |             |             |
|---|-------------|-------------|-------------|
| 6 | 0.000000000 | 0.000000000 | 0.000000000 |
|---|-------------|-------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| 6 | 0.000000000 | 0.000000000 | 1.382402561 |
|---|-------------|-------------|-------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 6 | 1.218499693 | 0.000000000 | -0.712313736 |
|---|-------------|-------------|--------------|

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|---|-------------|--------------|--------------|
| 6 | 2.414386070 | -0.007137190 | -0.021114206 |
|---|-------------|--------------|--------------|

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|---|-------------|-------------|-------------|
| 6 | 1.212623242 | 0.001079956 | 2.117432126 |
|---|-------------|-------------|-------------|

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|---|-------------|-------------|-------------|
| 6 | 1.252752529 | 0.052725065 | 3.580820953 |
|---|-------------|-------------|-------------|

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|---|-------------|--------------|-------------|
| 6 | 2.431943493 | -0.008540530 | 1.396308244 |
|---|-------------|--------------|-------------|

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|---|-------------|-------------|-------------|
| 6 | 3.690966271 | 0.019486397 | 2.104252083 |
|---|-------------|-------------|-------------|

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|---|-------------|-------------|-------------|
| 6 | 3.727650674 | 0.078421066 | 3.456501880 |
|---|-------------|-------------|-------------|

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|---|-------------|-------------|-------------|
| 6 | 2.510918428 | 0.108000880 | 4.233569973 |
|---|-------------|-------------|-------------|

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|---|--------------|-------------|-------------|
| 1 | -0.958406635 | 0.004816874 | 1.906109599 |
|---|--------------|-------------|-------------|

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|---|-------------|-------------|--------------|
| 1 | 3.371671633 | 0.027741604 | -0.548610126 |
|---|-------------|-------------|--------------|

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|---|-------------|-------------|-------------|
| 1 | 4.611134342 | 0.031841049 | 1.516264769 |
|---|-------------|-------------|-------------|

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| 1 | 4.679873198 | 0.149873694 | 3.988024188 |
|---|-------------|-------------|-------------|

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|---|-------------|-------------|-------------|
| 6 | 2.567664391 | 0.235792012 | 5.642629379 |
|---|-------------|-------------|-------------|

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|---|-------------|-------------|-------------|
| 1 | 3.549308241 | 0.321194141 | 6.116926492 |
|---|-------------|-------------|-------------|

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|---|-------------|-------------|-------------|
| 1 | 1.466554833 | 0.396154911 | 7.482925473 |
|---|-------------|-------------|-------------|

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|---|-------------|-------------|-------------|
| 6 | 1.412443416 | 0.289094734 | 6.396004320 |
|---|-------------|-------------|-------------|

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|---|-------------|-------------|-------------|
| 6 | 0.158191634 | 0.213844097 | 5.755862422 |
|---|-------------|-------------|-------------|

|   |              |             |             |
|---|--------------|-------------|-------------|
| 1 | -0.760667359 | 0.253857739 | 6.347685818 |
|---|--------------|-------------|-------------|

|   |             |             |             |
|---|-------------|-------------|-------------|
| 6 | 0.082018016 | 0.100232956 | 4.380005142 |
|---|-------------|-------------|-------------|

|   |              |             |             |
|---|--------------|-------------|-------------|
| 1 | -0.902770490 | 0.052621530 | 3.910284261 |
|---|--------------|-------------|-------------|

|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | -0.949997736 | 0.002946953 | -0.542335365 |
|---|--------------|-------------|--------------|

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|---|-------------|-------------|--------------|
| 1 | 1.212710668 | 0.007506074 | -1.806137640 |
|---|-------------|-------------|--------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 6 | 5.215651495 | 4.957570121 | -1.484860154 |
|---|-------------|-------------|--------------|

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|---|-------------|-------------|--------------|
| 6 | 4.829122576 | 5.200795500 | -0.178132949 |
|---|-------------|-------------|--------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 6 | 6.573303733 | 4.735694677 | -1.797680913 |
|---|-------------|-------------|--------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 6 | 7.519346554 | 4.777956874 | -0.790970137 |
|---|-------------|-------------|--------------|

|   |             |             |              |
|---|-------------|-------------|--------------|
| 6 | 5.780117123 | 5.240431827 | 0.870717947  |
| 6 | 5.406363086 | 5.496368448 | 2.262851381  |
| 6 | 7.145513587 | 5.039994441 | 0.549023038  |
| 6 | 8.148550770 | 5.125162360 | 1.585646132  |
| 6 | 7.807624104 | 5.415866187 | 2.863721196  |
| 6 | 6.426623261 | 5.613076203 | 3.239887587  |
| 1 | 3.768387985 | 5.330385931 | 0.040056403  |
| 1 | 8.577860749 | 4.617703204 | -1.019652783 |
| 1 | 9.195561463 | 4.968650991 | 1.307334503  |
| 1 | 8.574295894 | 5.500929722 | 3.640621190  |
| 6 | 6.081373919 | 5.911990131 | 4.579762420  |
| 1 | 6.883022480 | 6.014914964 | 5.318766148  |
| 1 | 4.502850022 | 6.308727680 | 5.990695930  |
| 6 | 4.758415850 | 6.073646489 | 4.953187512  |
| 6 | 3.739254504 | 5.908757120 | 3.993318215  |
| 1 | 2.688935345 | 5.967204511 | 4.287666985  |
| 6 | 4.059615475 | 5.627187570 | 2.677711043  |
| 1 | 3.249497512 | 5.461703976 | 1.964914589  |
| 1 | 4.460601635 | 4.929568669 | -2.275771687 |
| 1 | 6.874267976 | 4.539054638 | -2.830636616 |
| 8 | 6.242221932 | 2.337135519 | 2.479987119  |
| 8 | 4.951742811 | 2.035092135 | 0.152346741  |
| 1 | 6.934326813 | 1.759401353 | 2.825656801  |
| 1 | 5.651778585 | 2.512922345 | 3.261484625  |
| 1 | 5.373005758 | 2.661636991 | -0.455321513 |
| 1 | 5.479964806 | 2.126033682 | 0.987477588  |
| 8 | 2.194857204 | 3.223345875 | 3.593224074  |
| 8 | 4.667271493 | 2.757427467 | 4.616457609  |
| 1 | 1.579852336 | 2.506023972 | 3.804957240  |
| 1 | 2.306609807 | 3.168851606 | 2.611469771  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| 1 | 4.896810759 | 3.633837113 | 4.962012317 |
| 1 | 3.746056681 | 2.892836243 | 4.268868943 |
| 1 | 1.912400477 | 2.588918193 | 0.450027447 |
| 8 | 2.559117442 | 3.170034663 | 0.878140538 |
| 1 | 3.425620248 | 2.757104333 | 0.626534318 |

**5w:**

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.000000000  | 0.000000000  | 0.000000000  |
| 6 | 0.000000000  | 0.000000000  | 1.382937130  |
| 6 | 1.219704504  | 0.000000000  | -0.711230429 |
| 6 | 2.412482959  | -0.005313949 | -0.013984760 |
| 6 | 1.210366025  | 0.002984213  | 2.122180289  |
| 6 | 1.246048003  | 0.035130781  | 3.585319815  |
| 6 | 2.429863175  | -0.013580447 | 1.402009233  |
| 6 | 3.686871473  | -0.037112686 | 2.111716054  |
| 6 | 3.717359405  | -0.027107829 | 3.465644556  |
| 6 | 2.500822654  | 0.027749521  | 4.242323583  |
| 1 | -0.960702193 | -0.016642095 | 1.904173936  |
| 1 | 3.368505968  | 0.007079140  | -0.545417375 |
| 1 | 4.609561677  | -0.036485877 | 1.526679069  |
| 1 | 4.673468123  | -0.052796310 | 3.999772245  |
| 6 | 2.552671633  | 0.087200740  | 5.654870067  |
| 1 | 3.531620996  | 0.082785387  | 6.145128019  |
| 1 | 1.452233149  | 0.217468150  | 7.496642212  |
| 6 | 1.398790465  | 0.160484749  | 6.406073030  |
| 6 | 0.147554343  | 0.164331763  | 5.758912278  |
| 1 | -0.772166230 | 0.219842322  | 6.347936375  |
| 6 | 0.075754139  | 0.097468408  | 4.380750213  |
| 1 | -0.910277108 | 0.092935865  | 3.909236780  |
| 1 | -0.949417130 | -0.006634358 | -0.543072963 |



|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | 1.217681033  | 0.000649799 | -1.805149970 |
| 6 | 4.273745999  | 5.627812695 | -0.620153992 |
| 6 | 3.353663988  | 5.753884112 | 0.405505735  |
| 6 | 5.656474435  | 5.706424881 | -0.351141991 |
| 6 | 6.086946242  | 5.926270009 | 0.943889541  |
| 6 | 3.771717821  | 5.972051824 | 1.740978795  |
| 6 | 2.824953098  | 6.111882398 | 2.848708117  |
| 6 | 5.160343775  | 6.075511549 | 2.004177555  |
| 6 | 5.619874075  | 6.350952201 | 3.345529536  |
| 6 | 4.741435041  | 6.535283974 | 4.359074751  |
| 6 | 3.317988508  | 6.424057279 | 4.140202516  |
| 1 | 2.293225796  | 5.650549594 | 0.174003920  |
| 1 | 7.156347274  | 5.997904006 | 1.166859221  |
| 1 | 6.697918250  | 6.422358458 | 3.519884754  |
| 1 | 5.094354784  | 6.761045192 | 5.370234275  |
| 6 | 2.408567005  | 6.612744972 | 5.208963865  |
| 1 | 2.804619477  | 6.868686019 | 6.197188707  |
| 1 | 0.351488285  | 6.627010526 | 5.847114570  |
| 6 | 1.045363635  | 6.476522704 | 5.014607229  |
| 6 | 0.556440336  | 6.116493637 | 3.741837928  |
| 1 | -0.511618350 | 5.943538724 | 3.590186833  |
| 6 | 1.429434321  | 5.940603208 | 2.683951660  |
| 1 | 1.027009901  | 5.621830812 | 1.720479389  |
| 1 | 3.924176241  | 5.456105154 | -1.642236593 |
| 1 | 6.381451153  | 5.599407389 | -1.163225036 |
| 8 | 4.272700440  | 3.206864466 | 3.651162525  |
| 8 | 4.168320323  | 2.692481941 | 1.014678709  |
| 1 | 4.666421359  | 2.486464033 | 4.161993346  |
| 1 | 3.347716404  | 3.249408948 | 4.020904852  |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | 4.643917701  | 3.445476060 | 0.632278814  |
| 1 | 4.243953991  | 2.845760365 | 1.994838506  |
| 8 | -0.027953405 | 3.116986516 | 2.778259295  |
| 8 | 1.841976963  | 3.225546736 | 4.756419066  |
| 1 | -0.515390071 | 2.285699258 | 2.713386828  |
| 1 | 0.547190446  | 3.115823037 | 1.968339352  |
| 1 | 1.681626989  | 4.124701194 | 5.080943441  |
| 1 | 1.134451805  | 3.108777420 | 4.074816385  |
| 1 | 1.294479562  | 2.428682932 | -0.007023377 |
| 8 | 1.536997813  | 3.160961216 | 0.579381251  |
| 1 | 2.502914815  | 2.994081019 | 0.753182887  |

**6w:**

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.000000000  | 0.000000000  | 0.000000000  |
| 6 | 0.000000000  | 0.000000000  | 1.382075326  |
| 6 | 1.219335902  | 0.000000000  | -0.713865907 |
| 6 | 2.413964269  | 0.014155094  | -0.021013180 |
| 6 | 1.212115568  | -0.016257306 | 2.116046090  |
| 6 | 1.249741672  | -0.047293048 | 3.578393283  |
| 6 | 2.430666850  | 0.001234627  | 1.395467787  |
| 6 | 3.687273634  | 0.019744222  | 2.107598237  |
| 6 | 3.721900427  | -0.013082421 | 3.461464609  |
| 6 | 2.503693427  | -0.068207131 | 4.235729084  |
| 1 | -0.955312013 | 0.019392097  | 1.908424082  |
| 1 | 3.368211056  | 0.056374938  | -0.553054586 |
| 1 | 4.607227747  | 0.083016160  | 1.519732837  |
| 1 | 4.670998866  | 0.018815876  | 4.003794023  |
| 6 | 2.558285360  | -0.119494487 | 5.650430685  |
| 1 | 3.538332805  | -0.108204615 | 6.135089810  |
| 1 | 1.451779758  | -0.198894705 | 7.494370088  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 1.400802762  | -0.153390377 | 6.402498665  |
| 6 | 0.146686418  | -0.114295668 | 5.752670584  |
| 1 | -0.774537615 | -0.126519440 | 6.342490225  |
| 6 | 0.076902729  | -0.056010819 | 4.373186668  |
| 1 | -0.903324070 | -0.006724111 | 3.897016104  |
| 1 | -0.949850898 | 0.004277074  | -0.542527503 |
| 1 | 1.214907866  | 0.001383516  | -1.807935516 |
| 6 | 4.102600133  | 5.909080300  | -0.770418584 |
| 6 | 2.903584174  | 5.942569286  | -0.083670366 |
| 6 | 5.322660795  | 5.777781632  | -0.069980365 |
| 6 | 5.308814832  | 5.667197608  | 1.306696793  |
| 6 | 2.864476249  | 5.860538034  | 1.330385620  |
| 6 | 1.616083004  | 5.921339228  | 2.091132038  |
| 6 | 4.088774381  | 5.709206924  | 2.025700683  |
| 6 | 4.087806595  | 5.582850893  | 3.464571252  |
| 6 | 2.931786789  | 5.639315359  | 4.168531485  |
| 6 | 1.663810174  | 5.827616706  | 3.503051032  |
| 1 | 1.974808272  | 6.024980541  | -0.649826961 |
| 1 | 6.237684825  | 5.522595793  | 1.865088770  |
| 1 | 5.046450987  | 5.419789947  | 3.964915243  |
| 1 | 2.924736499  | 5.522716865  | 5.255711207  |
| 6 | 0.466268094  | 5.897352695  | 4.256579956  |
| 1 | 0.526575548  | 5.791448630  | 5.343150700  |
| 1 | -1.672912361 | 6.126184760  | 4.221514709  |
| 6 | -0.753267792 | 6.067050143  | 3.631974625  |
| 6 | -0.808443277 | 6.149410139  | 2.222528956  |
| 1 | -1.772665992 | 6.270668077  | 1.720260710  |
| 6 | 0.350063147  | 6.069884187  | 1.472457443  |
| 1 | 0.277558771  | 6.115711853  | 0.384903358  |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | 4.104945013  | 5.980769159 | -1.861946330 |
| 1 | 6.269772313  | 5.752092010 | -0.617121010 |
| 8 | 1.462274420  | 3.114798826 | 0.560020389  |
| 1 | 2.441582812  | 2.986560941 | 0.640350862  |
| 1 | 1.192006500  | 2.343221186 | 0.039271871  |
| 8 | 5.601591527  | 2.852049362 | 2.897916317  |
| 1 | 6.217562208  | 2.109834191 | 2.966468019  |
| 1 | 5.060635139  | 2.781255797 | 3.727224676  |
| 8 | 0.141864618  | 2.878340528 | 2.901329692  |
| 1 | 0.671411879  | 2.932360626 | 2.062388954  |
| 1 | -0.367093032 | 3.703109030 | 2.885541601  |
| 8 | 4.229654789  | 2.601852503 | 5.208243513  |
| 1 | 4.473621819  | 3.266482264 | 5.866865525  |
| 1 | 3.243746840  | 2.729025170 | 5.113039815  |
| 8 | 1.584334043  | 3.001957486 | 5.169887672  |
| 1 | 1.116283560  | 2.978932095 | 4.290881506  |
| 1 | 1.205166630  | 2.238481737 | 5.631631953  |
| 8 | 4.153723924  | 2.681879977 | 0.574338006  |
| 1 | 4.610978343  | 2.725527000 | 1.449458372  |
| 1 | 4.507652452  | 3.455792565 | 0.110259043  |

**Anthanthrene:**

**4w (paper):**

|   |             |             |              |
|---|-------------|-------------|--------------|
| 6 | 0.000000000 | 0.000000000 | 0.000000000  |
| 6 | 0.000000000 | 0.000000000 | 1.429542347  |
| 6 | 1.281781182 | 0.000000000 | 2.124321734  |
| 6 | 2.453134667 | 0.001253256 | 1.446243770  |
| 6 | 1.232064254 | 0.008849553 | -0.719253898 |
| 6 | 1.223431570 | 0.027783905 | -2.126723491 |
| 6 | 2.488602241 | 0.004391422 | -0.009664710 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 3.671351732  | 0.020798428  | -0.713818006 |
| 6 | 2.455234525  | 0.053317177  | -2.845627671 |
| 6 | 2.454551162  | 0.093652765  | -4.274629424 |
| 6 | 3.689264005  | 0.049942639  | -2.137999441 |
| 6 | 4.899616560  | 0.091407483  | -2.872152025 |
| 6 | 4.885876243  | 0.135933608  | -4.253691049 |
| 6 | 3.666075955  | 0.137426069  | -4.956684441 |
| 1 | 1.273380896  | -0.001913492 | 3.219109218  |
| 1 | 3.406841226  | 0.001533973  | 1.983466013  |
| 1 | 4.624017849  | 0.030329036  | -0.174216504 |
| 1 | 5.848550982  | 0.094013156  | -2.327198166 |
| 1 | 5.827889971  | 0.171024043  | -4.808424594 |
| 1 | 3.665273037  | 0.172032174  | -6.050764907 |
| 6 | -0.033195498 | 0.029061698  | -2.836328229 |
| 6 | 0.001604800  | 0.066497758  | -4.291794731 |
| 1 | -0.952205403 | 0.073221299  | -4.828713413 |
| 6 | 1.172757727  | 0.098609683  | -4.969431199 |
| 1 | 1.180874625  | 0.128358140  | -6.063807043 |
| 6 | -1.215934310 | 0.014100411  | -2.132210978 |
| 1 | -2.168702139 | 0.030451839  | -2.671324303 |
| 6 | -1.233998255 | 0.003896802  | -0.707653883 |
| 6 | -2.444650414 | 0.011947264  | 0.026817281  |
| 1 | -3.393318104 | 0.021756097  | -0.518341202 |
| 6 | -2.431566169 | 0.015842887  | 1.409043275  |
| 1 | -3.373937443 | 0.025380635  | 1.964146499  |
| 6 | -1.211967945 | 0.009901468  | 2.112203241  |
| 1 | -1.211509697 | 0.013605038  | 3.206809665  |
| 6 | 1.387631326  | 6.174031354  | -0.652839576 |
| 6 | 2.676566866  | 6.180622059  | -0.034386262 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 6 | 3.856858035  | 6.184711133 | -0.888518796 |
| 6 | 3.752597323  | 6.153071005 | -2.238315301 |
| 6 | 1.270544512  | 6.138345098 | -2.073446718 |
| 6 | -0.002193027 | 6.127964121 | -2.676874642 |
| 6 | 2.454438402  | 6.108580323 | -2.897977695 |
| 6 | 2.330804706  | 6.038151042 | -4.267200488 |
| 6 | -0.118062476 | 6.055480202 | -4.095445820 |
| 6 | -1.406297440 | 6.031305454 | -4.712202477 |
| 6 | 1.053987576  | 5.998842723 | -4.899607590 |
| 6 | 0.915791797  | 5.913633078 | -6.306951526 |
| 6 | -0.336905594 | 5.884531469 | -6.891908881 |
| 6 | -1.497510487 | 5.944928219 | -6.097723287 |
| 1 | 4.840030082  | 6.215351009 | -0.407553980 |
| 1 | 4.649044873  | 6.155709121 | -2.866888712 |
| 1 | 3.230058621  | 6.008100516 | -4.891833797 |
| 1 | 1.817354808  | 5.869510947 | -6.925945746 |
| 1 | -0.430108623 | 5.816901751 | -7.979605462 |
| 1 | -2.484650655 | 5.924635813 | -6.570195498 |
| 6 | -1.186578256 | 6.186240689 | -1.854538926 |
| 6 | -2.484754445 | 6.175448455 | -2.516255989 |
| 1 | -3.381492599 | 6.224975315 | -1.890546255 |
| 6 | -2.586363748 | 6.098150156 | -3.861726804 |
| 1 | -3.568897743 | 6.084987694 | -4.344065265 |
| 6 | -1.061388023 | 6.222673088 | -0.479651359 |
| 1 | -1.960414143 | 6.260478776 | 0.145650626  |
| 6 | 0.215991091  | 6.203965351 | 0.154705453  |
| 6 | 0.355433876  | 6.214321969 | 1.564688222  |
| 1 | -0.545828189 | 6.228787136 | 2.185208955  |
| 6 | 1.606806532  | 6.202576244 | 2.148186548  |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | 1.700695734  | 6.206436948 | 3.237780806  |
| 6 | 2.767185670  | 6.190224559 | 1.351866861  |
| 1 | 3.754251697  | 6.190305835 | 1.824866750  |
| 8 | 0.972830668  | 3.153641666 | -3.305514377 |
| 8 | -0.702907398 | 3.001215441 | -1.191339538 |
| 1 | 1.029366901  | 2.432711091 | -3.948614856 |
| 1 | 1.804397387  | 3.082855207 | -2.768167569 |
| 1 | -1.116252603 | 3.876973484 | -1.198353208 |
| 1 | -0.181362278 | 2.992835157 | -2.035377879 |
| 8 | 1.361068806  | 3.130791970 | 0.549759262  |
| 8 | 3.031548774  | 3.017952265 | -1.566887921 |
| 1 | 1.321317430  | 2.364946903 | 1.140294767  |
| 1 | 0.538213827  | 3.061006758 | -0.001433075 |
| 1 | 3.514658924  | 3.856589297 | -1.533202520 |
| 1 | 2.507627323  | 3.015712222 | -0.723987580 |

**5w (paper):**

|   |             |             |              |
|---|-------------|-------------|--------------|
| 6 | 0.000000000 | 0.000000000 | 0.000000000  |
| 6 | 0.000000000 | 0.000000000 | 1.430234684  |
| 6 | 1.281420953 | 0.000000000 | 2.126252283  |
| 6 | 2.451884666 | 0.007013509 | 1.447544876  |
| 6 | 1.231220954 | 0.009526334 | -0.720499334 |
| 6 | 1.224361655 | 0.025759469 | -2.128296888 |
| 6 | 2.485616881 | 0.013562293 | -0.008216185 |
| 6 | 3.669639723 | 0.042570039 | -0.708693611 |
| 6 | 2.456171754 | 0.044808711 | -2.845105789 |
| 6 | 2.455807683 | 0.060683361 | -4.274160288 |
| 6 | 3.688332093 | 0.055432660 | -2.133732884 |
| 6 | 4.904100684 | 0.080182273 | -2.864436839 |
| 6 | 4.890790333 | 0.094134395 | -4.248326865 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 3.668998732  | 0.086884542  | -4.953064944 |
| 1 | 1.272339680  | -0.005395347 | 3.220895203  |
| 1 | 3.406907143  | 0.014093856  | 1.981925365  |
| 1 | 4.619444154  | 0.089971207  | -0.169109565 |
| 1 | 5.850585729  | 0.091840388  | -2.315648170 |
| 1 | 5.833507174  | 0.110305089  | -4.803276343 |
| 1 | 3.671460168  | 0.099638374  | -6.047427025 |
| 6 | -0.028357101 | 0.021072115  | -2.843091002 |
| 6 | 0.008533257  | 0.022717401  | -4.298100790 |
| 1 | -0.944807981 | 0.012133965  | -4.835277109 |
| 6 | 1.178255792  | 0.042371897  | -4.971102852 |
| 1 | 1.190994035  | 0.049222231  | -6.065320512 |
| 6 | -1.213963531 | 0.006995509  | -2.138685691 |
| 1 | -2.166295805 | -0.000039483 | -2.679859157 |
| 6 | -1.235346825 | -0.000275796 | -0.710366747 |
| 6 | -2.447782431 | 0.003856884  | 0.026267690  |
| 1 | -3.397576330 | 0.004811183  | -0.517416671 |
| 6 | -2.432243560 | 0.007918003  | 1.408287295  |
| 1 | -3.374400894 | 0.012648687  | 1.963681969  |
| 6 | -1.212148147 | 0.005784462  | 2.111733942  |
| 1 | -1.212552571 | 0.008269190  | 3.206159079  |
| 6 | 2.656046118  | 6.045988484  | 1.251854660  |
| 6 | 3.975711780  | 6.063991052  | 1.797621139  |
| 6 | 5.106895174  | 6.136476445  | 0.880886342  |
| 6 | 4.927523872  | 6.175978375  | -0.460387022 |
| 6 | 2.459925475  | 6.086985640  | -0.160050547 |
| 6 | 1.157007667  | 6.052565123  | -0.690958160 |
| 6 | 3.594563127  | 6.145009243  | -1.048193459 |
| 6 | 3.399644354  | 6.154520729  | -2.411258723 |



|   |              |             |              |
|---|--------------|-------------|--------------|
| 6 | 0.963666233  | 6.072864750 | -2.103158345 |
| 6 | -0.357737351 | 6.033582943 | -2.648768719 |
| 6 | 2.090299062  | 6.120117049 | -2.971995419 |
| 6 | 1.878074051  | 6.122620313 | -4.375071601 |
| 6 | 0.594534298  | 6.083400052 | -4.890497919 |
| 6 | -0.522601088 | 6.037896956 | -4.029790200 |
| 1 | 6.114855399  | 6.162198698 | 1.307925639  |
| 1 | 5.785827785  | 6.229797201 | -1.137854071 |
| 1 | 4.261300665  | 6.155187096 | -3.084797929 |
| 1 | 2.745954550  | 6.150769712 | -5.040710742 |
| 1 | 0.440839334  | 6.088813605 | -5.973808562 |
| 1 | -1.532995992 | 6.007873708 | -4.449679626 |
| 6 | 0.020205582  | 5.986751216 | 0.194020705  |
| 6 | -1.310509091 | 5.971787730 | -0.395222678 |
| 1 | -2.170034881 | 5.935586086 | 0.281441924  |
| 6 | -1.488947746 | 5.994669924 | -1.733052689 |
| 1 | -2.495755053 | 5.977819402 | -2.162039267 |
| 6 | 0.220873723  | 5.946250748 | 1.555392799  |
| 1 | -0.641444850 | 5.892506540 | 2.228741662  |
| 6 | 1.530969287  | 5.968112851 | 2.118983052  |
| 6 | 1.749014156  | 5.914035330 | 3.517673888  |
| 1 | 0.884248703  | 5.855246397 | 4.186148177  |
| 6 | 3.031928597  | 5.931605567 | 4.034295333  |
| 1 | 3.185326847  | 5.887927236 | 5.116446623  |
| 6 | 4.145974126  | 6.006069997 | 3.177394635  |
| 1 | 5.157775507  | 6.018694219 | 3.594911371  |
| 8 | 3.973079155  | 3.243984721 | -3.133044095 |
| 8 | 1.316849461  | 2.969100196 | -3.551896854 |
| 1 | 4.397265350  | 2.439981680 | -3.468490588 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | 4.108363872  | 3.177473289 | -2.151145222 |
| 1 | 1.091788640  | 3.741986284 | -4.091101831 |
| 1 | 2.292669234  | 3.070688744 | -3.397692066 |
| 8 | 1.881069802  | 3.099254662 | 0.661714650  |
| 8 | 4.325683970  | 2.970689736 | -0.452068814 |
| 1 | 1.647021433  | 2.404290757 | 1.292599071  |
| 1 | 1.143563284  | 3.092105059 | -0.004845243 |
| 1 | 4.719219061  | 3.776583737 | -0.084543452 |
| 1 | 3.416991481  | 2.961636757 | -0.047534944 |
| 1 | -0.642484948 | 2.384413085 | -1.274787677 |
| 8 | -0.005192424 | 3.110711596 | -1.233345805 |
| 1 | 0.477061882  | 3.058138540 | -2.101682196 |

**6w (paper):**

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 0.000000000 | 0.000000000  | 0.000000000  |
| 6 | 0.000000000 | 0.000000000  | 1.428464545  |
| 6 | 1.280761913 | 0.000000000  | 2.124413765  |
| 6 | 2.452779796 | 0.001447605  | 1.447360553  |
| 6 | 1.231184840 | 0.018566970  | -0.718979126 |
| 6 | 1.223818855 | 0.048302984  | -2.126254077 |
| 6 | 2.486984949 | 0.016197089  | -0.008829661 |
| 6 | 3.671040951 | 0.051013113  | -0.709692002 |
| 6 | 2.456343149 | 0.088024547  | -2.844553867 |
| 6 | 2.456810004 | 0.129268465  | -4.272789532 |
| 6 | 3.689888483 | 0.087791467  | -2.134193550 |
| 6 | 4.903659016 | 0.121068844  | -2.866802061 |
| 6 | 4.889179054 | 0.156652433  | -4.250729709 |
| 6 | 3.667617331 | 0.169947074  | -4.953877755 |
| 1 | 1.271120083 | -0.007455271 | 3.219218184  |
| 1 | 3.407249653 | -0.001049942 | 1.983306909  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 4.621977389  | 0.084087094  | -0.170249603 |
| 1 | 5.850996047  | 0.118855159  | -2.319040542 |
| 1 | 5.831954246  | 0.175503173  | -4.806346923 |
| 1 | 3.665650121  | 0.214518752  | -6.046836139 |
| 6 | -0.030225884 | 0.032264596  | -2.839175341 |
| 6 | 0.009008258  | 0.059283793  | -4.295970121 |
| 1 | -0.943453426 | 0.035508144  | -4.837260602 |
| 6 | 1.178582202  | 0.123444561  | -4.969452982 |
| 1 | 1.191827549  | 0.170113258  | -6.062021294 |
| 6 | -1.213540920 | 0.002305310  | -2.134412299 |
| 1 | -2.167081379 | -0.010039070 | -2.674012558 |
| 6 | -1.233243286 | -0.002038768 | -0.709013117 |
| 6 | -2.444188569 | -0.004224540 | 0.025322047  |
| 1 | -3.393654351 | -0.006311032 | -0.519065035 |
| 6 | -2.431072051 | 0.001903211  | 1.407891122  |
| 1 | -3.373817115 | 0.003989336  | 1.962534731  |
| 6 | -1.211915064 | 0.004032032  | 2.111363910  |
| 1 | -1.211993937 | 0.008007934  | 3.205889897  |
| 6 | 0.839095064  | 6.091077526  | 0.377018144  |
| 6 | 1.732457586  | 6.052995918  | 1.491587350  |
| 6 | 3.165605012  | 6.077649772  | 1.237568167  |
| 6 | 3.656852390  | 6.117069942  | -0.020093971 |
| 6 | 1.351036664  | 6.128002258  | -0.953397491 |
| 6 | 0.467598082  | 6.165169182  | -2.049990168 |
| 6 | 2.776254119  | 6.126874061  | -1.180270420 |
| 6 | 3.263018174  | 6.153503359  | -2.467823146 |
| 6 | 0.982252704  | 6.213179155  | -3.378946429 |
| 6 | 0.090802678  | 6.268823823  | -4.494683869 |
| 6 | 2.388536390  | 6.204189150  | -3.592630796 |

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|---|--------------|-------------|--------------|
| 6 | 2.883763307  | 6.259232988 | -4.920681572 |
| 6 | 2.010306195  | 6.325413769 | -5.992350373 |
| 6 | 0.615353416  | 6.325127061 | -5.781356037 |
| 1 | 3.839240163  | 6.072190753 | 2.100363943  |
| 1 | 4.737044367  | 6.159924643 | -0.199026607 |
| 1 | 4.341925046  | 6.116263200 | -2.645655343 |
| 1 | 3.965580969  | 6.239442016 | -5.081322296 |
| 1 | 2.401508232  | 6.375045513 | -7.013019191 |
| 1 | -0.065373779 | 6.372799521 | -6.637077359 |
| 6 | -0.957231717 | 6.176640234 | -1.825974536 |
| 6 | -1.836125527 | 6.235196951 | -2.985115243 |
| 1 | -2.916429251 | 6.243767653 | -2.809848304 |
| 6 | -1.342210282 | 6.277522533 | -4.240920238 |
| 1 | -2.015635983 | 6.319442273 | -5.102543384 |
| 6 | -1.443261666 | 6.139695088 | -0.534592748 |
| 1 | -2.525281790 | 6.155007010 | -0.362272843 |
| 6 | -0.567730848 | 6.090282629 | 0.593269865  |
| 6 | -1.055898134 | 6.034623010 | 1.924295651  |
| 1 | -2.137296239 | 6.028491877 | 2.092737386  |
| 6 | -0.180127533 | 5.990333257 | 2.991896153  |
| 1 | -0.568717736 | 5.948244975 | 4.013513122  |
| 6 | 1.212549092  | 6.004233053 | 2.778451571  |
| 1 | 1.895820330  | 5.973899982 | 3.632879343  |
| 8 | -0.269371575 | 3.249877328 | -3.526218198 |
| 1 | 0.616027253  | 3.216749814 | -3.979680930 |
| 1 | -0.724504094 | 2.478982098 | -3.890988904 |
| 8 | 4.292123106  | 3.371915826 | -3.393839508 |
| 1 | 4.774710122  | 2.564869261 | -3.628119231 |
| 1 | 4.222794412  | 3.298464588 | -2.406690384 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 8 | -0.301278421 | 3.021172930 | -0.859126831 |
| 1 | -0.229363848 | 3.081478878 | -1.847806145 |
| 1 | -0.868727816 | 3.771696151 | -0.631370148 |
| 8 | 4.314511726  | 3.034606091 | -0.706951166 |
| 1 | 4.706012612  | 3.788342514 | -0.244656434 |
| 1 | 3.408897062  | 2.987455402 | -0.292923908 |
| 8 | 1.959624405  | 3.103774975 | 0.539480001  |
| 1 | 1.136442415  | 3.099597270 | -0.020380765 |
| 1 | 1.800434299  | 2.397012756 | 1.181703887  |
| 8 | 2.039603953  | 3.141589616 | -4.870948076 |
| 1 | 2.828628470  | 3.207053756 | -4.272023228 |
| 1 | 2.074396757  | 3.973981236 | -5.365509262 |

**4w (SI):**

|   |             |              |              |
|---|-------------|--------------|--------------|
| 6 | 0.000000000 | 0.000000000  | 0.000000000  |
| 6 | 0.000000000 | 0.000000000  | 1.429677130  |
| 6 | 1.281883519 | 0.000000000  | 2.123893587  |
| 6 | 2.453219612 | -0.000506326 | 1.445313235  |
| 6 | 1.231706626 | 0.009910287  | -0.719789060 |
| 6 | 1.223453373 | 0.031601055  | -2.127234151 |
| 6 | 2.488441814 | 0.003474879  | -0.010728923 |
| 6 | 3.671015867 | 0.018496240  | -0.715419333 |
| 6 | 2.454562945 | 0.058412792  | -2.846696615 |
| 6 | 2.453244490 | 0.112948498  | -4.274242845 |
| 6 | 3.688852184 | 0.052498843  | -2.139514700 |
| 6 | 4.898563743 | 0.100853327  | -2.873515737 |
| 6 | 4.884196569 | 0.159319657  | -4.254815580 |
| 6 | 3.664308663 | 0.165827221  | -4.956737850 |
| 1 | 1.274021460 | -0.001839130 | 3.218670019  |
| 1 | 3.407034419 | -0.001760903 | 1.982494952  |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | 4.623958164  | 0.021595343 | -0.175672127 |
| 1 | 5.848181744  | 0.100013966 | -2.329460558 |
| 1 | 5.825940721  | 0.202553131 | -4.809356206 |
| 1 | 3.662747777  | 0.213273050 | -6.050277136 |
| 6 | -0.033802399 | 0.034126273 | -2.835897197 |
| 6 | 0.000189250  | 0.076257700 | -4.291795475 |
| 1 | -0.953886441 | 0.078058018 | -4.828534635 |
| 6 | 1.171783085  | 0.119872175 | -4.968540791 |
| 1 | 1.179804797  | 0.156748455 | -6.062681792 |
| 6 | -1.216591935 | 0.017115331 | -2.131351278 |
| 1 | -2.169777713 | 0.033020715 | -2.669881504 |
| 6 | -1.234378621 | 0.003966082 | -0.706990792 |
| 6 | -2.444927540 | 0.011714640 | 0.027615119  |
| 1 | -3.393655097 | 0.022439012 | -0.517340351 |
| 6 | -2.431612796 | 0.015540705 | 1.409574884  |
| 1 | -3.373904138 | 0.025071040 | 1.964790743  |
| 6 | -1.211748805 | 0.010212389 | 2.112480911  |
| 1 | -1.211119682 | 0.013693080 | 3.207086695  |
| 6 | 0.651156264  | 6.136764200 | -0.236034780 |
| 6 | 0.286271292  | 6.039309435 | 1.142290185  |
| 6 | 1.341969590  | 5.900021048 | 2.134508825  |
| 6 | 2.641603722  | 5.836923515 | 1.775827882  |
| 6 | 2.020651481  | 6.065056707 | -0.622310798 |
| 6 | 2.372148827  | 6.136565225 | -1.983962460 |
| 6 | 3.046431944  | 5.903113354 | 0.379305570  |
| 6 | 4.366491010  | 5.815359796 | -0.006550794 |
| 6 | 3.741707252  | 6.037561329 | -2.374264715 |
| 6 | 4.100906543  | 6.072228743 | -3.757948949 |
| 6 | 4.750852993  | 5.877079709 | -1.380786857 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 6 | 6.104327047  | 5.766118150 | -1.791747750 |
| 6 | 6.437700855  | 5.809219866 | -3.132376035 |
| 6 | 5.440215566  | 5.959796114 | -4.115209795 |
| 1 | 1.050966696  | 5.841331540 | 3.187880728  |
| 1 | 3.425212280  | 5.727160912 | 2.531904659  |
| 1 | 5.146264240  | 5.690658405 | 0.752481474  |
| 1 | 6.880806816  | 5.643904173 | -1.030273175 |
| 1 | 7.484737671  | 5.721357396 | -3.436314735 |
| 1 | 5.716352103  | 5.983776946 | -5.173914517 |
| 6 | 1.345225760  | 6.277174818 | -2.985389536 |
| 6 | 1.744423349  | 6.298112558 | -4.384078854 |
| 1 | 0.956878299  | 6.381275782 | -5.138572947 |
| 6 | 3.041781195  | 6.207251217 | -4.748516484 |
| 1 | 3.326257289  | 6.219912056 | -5.805259889 |
| 6 | 0.025781114  | 6.358044944 | -2.601526622 |
| 1 | -0.754431961 | 6.448328858 | -3.364090987 |
| 6 | -0.356291089 | 6.288781859 | -1.230533799 |
| 6 | -1.716965782 | 6.339903125 | -0.825792743 |
| 1 | -2.492957255 | 6.463068573 | -1.588073988 |
| 6 | -2.056182624 | 6.229341494 | 0.510741374  |
| 1 | -3.107637681 | 6.262211755 | 0.810579774  |
| 6 | -1.057881684 | 6.081739909 | 1.494368322  |
| 1 | -1.339880399 | 5.999306083 | 2.548522920  |
| 8 | 0.702381193  | 3.245478947 | -3.333618692 |
| 8 | -0.833107554 | 3.049313611 | -1.082115552 |
| 1 | 0.717632625  | 2.450897410 | -3.887687124 |
| 1 | 1.567332945  | 3.207833838 | -2.849884826 |
| 1 | -1.261058300 | 3.913542087 | -0.989672079 |
| 1 | -0.366597396 | 3.105819142 | -1.955233551 |

|   |             |             |              |
|---|-------------|-------------|--------------|
| 8 | 1.365532299 | 3.097668977 | 0.488042581  |
| 8 | 2.872827226 | 2.959973952 | -1.744517094 |
| 1 | 1.364292907 | 2.340064740 | 1.090308750  |
| 1 | 0.497412709 | 3.041968169 | 0.009583901  |
| 1 | 3.575052349 | 3.623202939 | -1.694585321 |
| 1 | 2.428607898 | 2.996423035 | -0.858792792 |

**6w (SI):**

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.000000000  | 0.000000000  | 0.000000000  |
| 6 | 0.000000000  | 0.000000000  | 1.428509755  |
| 6 | 1.278821365  | 0.000000000  | 2.125599486  |
| 6 | 2.451250444  | 0.022908531  | 1.450028903  |
| 6 | 1.230546683  | 0.030465157  | -0.719031724 |
| 6 | 1.225573182  | 0.043851005  | -2.127952515 |
| 6 | 2.484964707  | 0.054792129  | -0.005862144 |
| 6 | 3.669154554  | 0.102309949  | -0.706089982 |
| 6 | 2.457677113  | 0.083356026  | -2.843588787 |
| 6 | 2.459513899  | 0.092367755  | -4.272778098 |
| 6 | 3.688999785  | 0.112291833  | -2.130965960 |
| 6 | 4.904701789  | 0.158200274  | -2.860999319 |
| 6 | 4.893278361  | 0.174129418  | -4.244569760 |
| 6 | 3.672791706  | 0.140722113  | -4.951118729 |
| 1 | 1.267421482  | -0.026758821 | 3.220249710  |
| 1 | 3.406917916  | 0.014734123  | 1.984699677  |
| 1 | 4.618127114  | 0.161599637  | -0.165855660 |
| 1 | 5.850471092  | 0.189558355  | -2.311794999 |
| 1 | 5.836235902  | 0.211605970  | -4.797825618 |
| 1 | 3.676358058  | 0.149347898  | -6.045595747 |
| 6 | -0.026187856 | 0.004888801  | -2.843147492 |
| 6 | 0.013159637  | -0.006860491 | -4.298369887 |



|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | -0.938425323 | -0.051420664 | -4.837773370 |
| 6 | 1.183427001  | 0.039785068  | -4.970837912 |
| 1 | 1.196904366  | 0.033587001  | -6.065315799 |
| 6 | -1.211397619 | -0.030951820 | -2.136979098 |
| 1 | -2.163911380 | -0.079164999 | -2.678338193 |
| 6 | -1.232911591 | -0.016167068 | -0.709838033 |
| 6 | -2.444703536 | -0.015942953 | 0.024951258  |
| 1 | -3.394726861 | -0.024094990 | -0.518658864 |
| 6 | -2.430100012 | -0.003798690 | 1.406497030  |
| 1 | -3.372717448 | -0.001801757 | 1.961397737  |
| 6 | -1.210741064 | -0.001697754 | 2.109887352  |
| 1 | -1.211328183 | 0.000497221  | 3.204391517  |
| 6 | 0.750435727  | 6.099991307  | 0.385682019  |
| 6 | 0.266835629  | 6.063853924  | 1.730064006  |
| 6 | 1.231796083  | 6.107916074  | 2.819366615  |
| 6 | 2.559017423  | 6.178957808  | 2.581900654  |
| 6 | 2.150848046  | 6.174413284  | 0.128740547  |
| 6 | 2.621537859  | 6.206209873  | -1.197613385 |
| 6 | 3.086032059  | 6.215801413  | 1.225972974  |
| 6 | 4.437075909  | 6.294376188  | 0.966636678  |
| 6 | 4.022868931  | 6.277941683  | -1.457267282 |
| 6 | 4.505540273  | 6.298951749  | -2.801255492 |
| 6 | 4.941587556  | 6.326054670  | -0.369195420 |
| 6 | 6.331798817  | 6.381573782  | -0.650153840 |
| 6 | 6.784354875  | 6.392577567  | -1.956455799 |
| 6 | 5.874945193  | 6.354093288  | -3.030983667 |
| 1 | 0.849997182  | 6.082443677  | 3.844918033  |
| 1 | 3.273269225  | 6.210685191  | 3.410474563  |
| 1 | 5.148086154  | 6.330172146  | 1.799328928  |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | 7.040516314  | 6.416608895 | 0.183271326  |
| 1 | 7.858313100  | 6.433858719 | -2.160139578 |
| 1 | 6.245765338  | 6.362469929 | -4.060492254 |
| 6 | 1.684998491  | 6.157299288 | -2.294533856 |
| 6 | 2.212439818  | 6.197707745 | -3.650954601 |
| 1 | 1.496098080  | 6.173783005 | -4.478589115 |
| 6 | 3.539579903  | 6.260331280 | -3.889677508 |
| 1 | 3.922706504  | 6.277205463 | -4.914437058 |
| 6 | 0.335210876  | 6.076617219 | -2.035016584 |
| 1 | -0.377752572 | 6.006779848 | -2.862006547 |
| 6 | -0.166791404 | 6.053646368 | -0.700889247 |
| 6 | -1.555779375 | 5.972943903 | -0.426808069 |
| 1 | -2.255293445 | 5.907780776 | -1.264474755 |
| 6 | -2.012753649 | 5.948084194 | 0.877799425  |
| 1 | -3.086281897 | 5.886049315 | 1.079234286  |
| 6 | -1.104713378 | 5.991734849 | 1.957103799  |
| 1 | -1.478019436 | 5.968798535 | 2.986039190  |
| 8 | -0.467634326 | 2.983463335 | 0.353498713  |
| 1 | 0.504027962  | 3.061173184 | 0.546040129  |
| 1 | -0.862233317 | 3.668890159 | 0.912269512  |
| 8 | 4.345446535  | 3.079814735 | -0.360915940 |
| 1 | 4.852616185  | 3.892774721 | -0.221308402 |
| 1 | 4.139767864  | 3.111672736 | -1.333673324 |
| 8 | -1.038444845 | 3.276496077 | -2.226544216 |
| 1 | -0.815752263 | 3.235924198 | -1.253839358 |
| 1 | -1.432999916 | 2.404978761 | -2.378517694 |
| 8 | 3.833814828  | 3.253492566 | -2.990281023 |
| 1 | 4.167050916  | 2.466273005 | -3.445338847 |
| 1 | 2.862189690  | 3.236626402 | -3.179528918 |

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|---|-------------|-------------|--------------|
| 8 | 1.230896313 | 3.054366865 | -3.644090384 |
| 1 | 0.438416430 | 3.157358424 | -3.052738925 |
| 1 | 0.986009425 | 3.545498968 | -4.439259161 |
| 8 | 2.086338405 | 3.209991854 | 1.110148412  |
| 1 | 2.879740335 | 3.198396757 | 0.512861830  |
| 1 | 2.216776515 | 2.427605336 | 1.665081545  |

**Anthracene:**

**3w:**

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.000000000  | 0.000000000  | 0.000000000  |
| 6 | 0.000000000  | 0.000000000  | 1.365709529  |
| 6 | 1.236191749  | 0.000000000  | 2.092926901  |
| 6 | 2.428876577  | 0.002479440  | 1.427808638  |
| 6 | 1.234338368  | -0.001390220 | -0.739650798 |
| 6 | 1.266268653  | -0.022341341 | -2.141393102 |
| 6 | 2.473243911  | 0.003577180  | -0.010826259 |
| 6 | 3.684103449  | -0.018449549 | -0.716656716 |
| 6 | 2.476519115  | -0.036941333 | -2.845715196 |
| 6 | 2.523348049  | -0.057418287 | -4.282875851 |
| 6 | 3.712725620  | -0.037220652 | -2.115777184 |
| 6 | 4.950932822  | -0.069632803 | -2.846355072 |
| 6 | 4.952496127  | -0.084346811 | -4.209806268 |
| 6 | 3.718152773  | -0.076412210 | -4.940109646 |
| 1 | -0.942024739 | -0.001531237 | -0.557448174 |
| 1 | -0.945468805 | -0.000251366 | 1.915575426  |
| 1 | 1.215820491  | -0.001776821 | 3.186444587  |
| 1 | 3.375733624  | 0.000345131  | 1.976990412  |
| 1 | 0.322346610  | -0.027206990 | -2.697406038 |
| 1 | 4.628528885  | -0.054006397 | -0.165508043 |
| 1 | 1.578887294  | -0.058788085 | -4.836205664 |

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| 1 | 5.885754739 | -0.104072417 | -2.280070107 |
| 1 | 5.898891157 | -0.110194810 | -4.757682077 |
| 1 | 3.743188661 | -0.093372030 | -6.033640695 |
| 6 | 7.839971156 | -6.550292726 | -1.746690942 |
| 6 | 8.459190345 | -6.242712316 | -0.569356674 |
| 6 | 7.694343138 | -5.796346691 | 0.559138923  |
| 6 | 6.336292661 | -5.678303592 | 0.471854703  |
| 6 | 6.413276489 | -6.428406727 | -1.885339425 |
| 6 | 5.755553643 | -6.708527263 | -3.089994906 |
| 6 | 5.646307598 | -5.988551460 | -0.753304229 |
| 6 | 4.258759585 | -5.842282362 | -0.875644297 |
| 6 | 4.368052145 | -6.559763774 | -3.214708426 |
| 6 | 3.680836954 | -6.808124144 | -4.454976249 |
| 6 | 3.604054933 | -6.115878800 | -2.082495652 |
| 6 | 2.184618888 | -5.927135592 | -2.229558254 |
| 6 | 1.571283656 | -6.169416649 | -3.425254421 |
| 6 | 2.331735677 | -6.619531433 | -4.556259951 |
| 1 | 8.420803127 | -6.887942729 | -2.610697405 |
| 1 | 9.545260609 | -6.334428430 | -0.477937479 |
| 1 | 8.208168109 | -5.552888875 | 1.493356181  |
| 1 | 5.746499843 | -5.340010419 | 1.329892139  |
| 1 | 6.338788881 | -7.040553697 | -3.955612058 |
| 1 | 3.674319835 | -5.469011084 | -0.029444973 |
| 1 | 4.264342792 | -7.145101884 | -5.317495567 |
| 1 | 1.625829175 | -5.545802401 | -1.371295426 |
| 1 | 0.494231257 | -6.011990727 | -3.531978388 |
| 1 | 1.821962506 | -6.805739725 | -5.506089525 |
| 8 | 2.592297286 | -3.221359669 | -0.580121786 |
| 8 | 3.658873994 | -3.079530408 | -3.164529132 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 1 | 3.539564094 | -2.976947688 | -0.468422082 |
| 1 | 2.116453708 | -2.425275855 | -0.300641162 |
| 1 | 3.602125365 | -3.935963706 | -3.612012629 |
| 1 | 3.009190637 | -3.158114967 | -2.433304287 |
| 8 | 5.290370041 | -2.670206663 | -0.988339213 |
| 1 | 5.875512860 | -3.425552976 | -0.830654482 |
| 1 | 4.950350657 | -2.820384000 | -1.902619809 |

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| 6 | 0.000000000  | 0.000000000  | 1.365776963  |
| 6 | 1.238972533  | 0.000000000  | 2.091510725  |
| 6 | 2.431909531  | -0.003091434 | 1.424015740  |
| 6 | 1.233714940  | -0.001438461 | -0.739201161 |
| 6 | 1.255587653  | -0.039586368 | -2.137346353 |
| 6 | 2.473046472  | -0.007578963 | -0.014353133 |
| 6 | 3.681138862  | -0.056831734 | -0.718171364 |
| 6 | 2.463852306  | -0.087862905 | -2.841222473 |
| 6 | 2.503082468  | -0.164853881 | -4.277416339 |
| 6 | 3.702789558  | -0.099666571 | -2.116349677 |
| 6 | 4.934314129  | -0.196811282 | -2.852625346 |
| 6 | 4.932756077  | -0.270243686 | -4.216484658 |
| 6 | 3.694146232  | -0.252180315 | -4.942764986 |
| 1 | -0.940657179 | -0.011937955 | -0.558979258 |
| 1 | -0.944498553 | -0.004884451 | 1.917254781  |
| 1 | 1.220421510  | -0.001216539 | 3.185228197  |
| 1 | 3.379238038  | -0.012754737 | 1.971972838  |
| 1 | 0.311336988  | -0.076237934 | -2.687971401 |
| 1 | 4.623558787  | -0.106966524 | -0.165451542 |
| 1 | 1.555514278  | -0.161812363 | -4.825001949 |

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| 1 | 5.873839528  | -0.222862337 | -2.292298864 |
| 1 | 5.875323185  | -0.349007205 | -4.765667397 |
| 1 | 3.711141736  | -0.314555670 | -6.034745295 |
| 6 | -0.501342578 | -6.110803219 | -1.304418406 |
| 6 | -1.176230149 | -6.090498836 | -2.493070849 |
| 6 | -0.459790669 | -6.137804923 | -3.736488290 |
| 6 | 0.904364603  | -6.206478548 | -3.745150329 |
| 6 | 0.935595878  | -6.179436225 | -1.272665963 |
| 6 | 1.649017219  | -6.158972204 | -0.069266602 |
| 6 | 1.650810757  | -6.232138666 | -2.516206038 |
| 6 | 3.049507603  | -6.265359826 | -2.503227092 |
| 6 | 3.047673456  | -6.188975000 | -0.056512727 |
| 6 | 3.796374143  | -6.121473768 | 1.169640675  |
| 6 | 3.763010718  | -6.244720615 | -1.299996591 |
| 6 | 5.201831495  | -6.238454743 | -1.270405829 |
| 6 | 5.878525988  | -6.175873752 | -0.084399077 |
| 6 | 5.162232263  | -6.114979484 | 1.158716096  |
| 1 | -1.041685644 | -6.065055028 | -0.353781740 |
| 1 | -2.268571933 | -6.033650893 | -2.504730711 |
| 1 | -1.016464174 | -6.112822027 | -4.677614466 |
| 1 | 1.456775600  | -6.230893666 | -4.689425572 |
| 1 | 1.105448291  | -6.075022264 | 0.876083042  |
| 1 | 3.595138810  | -6.264171822 | -3.451113164 |
| 1 | 3.244545782  | -6.062558019 | 2.112734300  |
| 1 | 5.742239538  | -6.273979104 | -2.221301625 |
| 1 | 6.972301381  | -6.166709681 | -0.074551241 |
| 1 | 5.720799638  | -6.057306476 | 2.097275383  |
| 8 | 1.557822980  | -3.149997426 | 0.362589698  |
| 8 | 0.677577944  | -3.025063607 | -2.226730942 |

|   |             |              |              |
|---|-------------|--------------|--------------|
| 1 | 1.433402501 | -2.339475898 | 0.878235541  |
| 1 | 2.522545894 | -3.137130176 | 0.136225094  |
| 1 | 0.130050680 | -3.814173193 | -2.351920174 |
| 1 | 0.894677036 | -3.041516609 | -1.259986878 |
| 8 | 3.258130966 | -3.289329924 | -3.107051055 |
| 8 | 4.147402052 | -3.054468449 | -0.528735987 |
| 1 | 3.416919194 | -2.512502290 | -3.663578405 |
| 1 | 2.294900784 | -3.224203950 | -2.884069639 |
| 1 | 4.648383875 | -3.864900084 | -0.354260611 |
| 1 | 3.929514076 | -3.116721017 | -1.493396221 |

**8w:**

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|---|--------------|--------------|--------------|
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| 6 | 0.000000000  | 0.000000000  | 1.366135473  |
| 6 | 1.238987313  | 0.000000000  | 2.092933887  |
| 6 | 2.431899036  | -0.010568250 | 1.426074856  |
| 6 | 3.680322515  | -0.093229279 | -0.716514764 |
| 6 | 2.473085971  | -0.019880649 | -0.012242002 |
| 6 | 1.234467528  | -0.002215974 | -0.737950555 |
| 6 | 1.256468638  | -0.026733297 | -2.136945848 |
| 6 | 2.503378865  | -0.159384937 | -4.278427045 |
| 6 | 2.464238592  | -0.091606461 | -2.841386183 |
| 6 | 3.701404191  | -0.141334060 | -2.115035204 |
| 6 | 4.929980391  | -0.283891213 | -2.848912080 |
| 6 | 4.927512222  | -0.356536081 | -4.212946998 |
| 6 | 3.691653347  | -0.287827330 | -4.941768446 |
| 1 | -0.944907151 | -0.003277833 | 1.916974018  |
| 1 | -0.939805578 | -0.012293223 | -0.559858494 |
| 1 | 1.219752378  | 0.003735322  | 3.186661086  |
| 1 | 3.378707374  | -0.023345294 | 1.974912406  |

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|---|--------------|--------------|--------------|
| 1 | 4.622907636  | -0.157755791 | -0.164511111 |
| 1 | 0.310618719  | -0.039520165 | -2.686994524 |
| 1 | 1.558103033  | -0.117993864 | -4.828513146 |
| 1 | 5.866182783  | -0.347452355 | -2.286546840 |
| 1 | 5.867264987  | -0.471640071 | -4.760451415 |
| 1 | 3.708806692  | -0.342940240 | -6.034143245 |
| 1 | 2.931177047  | -5.065447177 | -3.362736489 |
| 1 | 3.318654481  | -6.125531012 | -2.329752722 |
| 1 | 3.102609936  | -5.963805446 | -0.111393491 |
| 1 | 4.511805013  | -6.627476509 | -0.255151353 |
| 1 | 1.523351036  | -4.898748260 | 0.733648864  |
| 1 | 1.042890786  | -5.975589501 | -0.241784859 |
| 1 | 1.263784842  | -5.945717565 | -2.465163054 |
| 1 | -0.193660266 | -6.484266547 | -2.282906960 |
| 8 | 4.158845284  | -3.162233189 | -0.750102315 |
| 8 | 1.616910959  | -3.105247116 | 0.414604126  |
| 8 | 0.454884751  | -3.035797140 | -1.965879927 |
| 8 | 2.989788835  | -3.257895782 | -3.124177915 |
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| 8 | 1.593725740  | -5.863546869 | 0.564599838  |
| 8 | 0.409599908  | -5.798550082 | -1.958930339 |
| 6 | -0.672579288 | -8.789322004 | -0.423911647 |
| 6 | -1.650483813 | -8.726084700 | -1.375119835 |
| 6 | -1.311693848 | -8.783399030 | -2.769447489 |
| 6 | -0.006458796 | -8.897237820 | -3.160868968 |
| 6 | 2.398430193  | -9.019170022 | -2.566174646 |
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| 6 | 0.712007656  | -8.908894985 | -0.794321283 |



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| 6 | 1.732430657  | -8.933679216 | 0.163340893  |
| 6 | 4.140695280  | -8.976387263 | 0.755888223  |
| 6 | 3.078366490  | -8.995741204 | -0.214659284 |
| 6 | 3.419126810  | -9.034220707 | -1.608807229 |
| 6 | 4.808077052  | -9.042003080 | -1.982167096 |
| 6 | 5.789748351  | -9.015183862 | -1.033098798 |
| 6 | 5.450024052  | -8.983591647 | 0.361852547  |
| 1 | -2.699458771 | -8.628193559 | -1.081674905 |
| 1 | -0.923458730 | -8.736779208 | 0.639878171  |
| 1 | -2.107941904 | -8.734506323 | -3.518022132 |
| 1 | 0.257969112  | -8.934064314 | -4.222279408 |
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| 1 | 1.474919571  | -8.858352936 | 1.223930408  |
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| 1 | 6.249180615  | -8.964992510 | 1.108679384  |
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| 1 | 3.348858200  | -3.001456929 | -0.217345944 |
| 1 | 1.288977407  | -2.387938508 | 0.977253776  |
| 1 | 1.114774102  | -3.008139057 | -0.449420710 |
| 1 | 0.212580631  | -3.983992794 | -2.045251550 |
| 1 | 1.279298890  | -2.983562992 | -2.498863585 |
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| 1 | 3.500312002  | -3.157593004 | -2.265182198 |

**12w:**

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| 6 | 0.000000000 | 0.000000000 | 1.366023424 |
| 6 | 1.239113387 | 0.000000000 | 2.092617886 |

|   |              |              |              |
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| 6 | 3.680609398  | -0.092126999 | -0.717156328 |
| 6 | 2.473264899  | -0.019621721 | -0.012812698 |
| 6 | 1.234392007  | -0.002645094 | -0.738259237 |
| 6 | 1.256276647  | -0.027465900 | -2.137307957 |
| 6 | 2.503169151  | -0.154926691 | -4.279078111 |
| 6 | 2.464051766  | -0.089876014 | -2.841935622 |
| 6 | 3.701542248  | -0.137991572 | -2.115742011 |
| 6 | 4.930665785  | -0.274577063 | -2.850037347 |
| 6 | 4.928192331  | -0.342983089 | -4.214389609 |
| 6 | 3.691857335  | -0.277096665 | -4.942924133 |
| 1 | -0.944728664 | -0.003565452 | 1.917011613  |
| 1 | -0.940007651 | -0.011428237 | -0.559550289 |
| 1 | 1.220052985  | 0.004125902  | 3.186336191  |
| 1 | 3.379128924  | -0.021253743 | 1.974559764  |
| 1 | 4.623340080  | -0.155689309 | -0.165357028 |
| 1 | 0.310435776  | -0.039606142 | -2.687381290 |
| 1 | 1.557784116  | -0.115547910 | -4.829091221 |
| 1 | 5.867195116  | -0.336068173 | -2.288002185 |
| 1 | 5.868306835  | -0.452442582 | -4.762409096 |
| 1 | 3.709083977  | -0.329386282 | -6.035418326 |
| 1 | 2.908839011  | -7.802475766 | -3.340023000 |
| 1 | 3.300617195  | -8.810897193 | -2.251723237 |
| 1 | 3.123831464  | -8.684277201 | -0.027427061 |
| 1 | 4.521427806  | -9.364381194 | -0.202396942 |
| 1 | 1.499808724  | -7.640897343 | 0.893194386  |
| 1 | 1.035653588  | -8.681212556 | -0.134698425 |
| 1 | 1.215490685  | -8.679616360 | -2.362672305 |
| 1 | -0.223379765 | -9.254704170 | -2.152646926 |

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| 8 | 2.735568478  | -8.722206232  | -3.050966664 |
| 8 | 3.984686346  | -8.630975235  | -0.539514863 |
| 8 | 1.607465215  | -8.585934367  | 0.658922209  |
| 8 | 0.361822548  | -8.541582773  | -1.854753488 |
| 8 | 4.048186679  | -5.912652618  | -0.549337135 |
| 8 | 1.545872912  | -5.825144445  | 0.500714971  |
| 8 | 0.492122561  | -5.828148199  | -2.001382776 |
| 8 | 2.993044795  | -5.970279268  | -3.050986484 |
| 6 | -0.648028208 | -11.537738628 | -0.264987639 |
| 6 | -1.648727715 | -11.483745760 | -1.192755997 |
| 6 | -1.342624709 | -11.540146746 | -2.594732428 |
| 6 | -0.046101966 | -11.643620177 | -3.017102095 |
| 6 | 2.373386835  | -11.745316834 | -2.479314825 |
| 6 | 1.036267522  | -11.694512808 | -2.069686230 |
| 6 | 0.728301638  | -11.647133722 | -0.668060109 |
| 6 | 1.771114053  | -11.664976322 | 0.265317829  |
| 6 | 4.193073654  | -11.695862482 | 0.801151756  |
| 6 | 3.108196920  | -11.719134212 | -0.144281518 |
| 6 | 3.416445884  | -11.753924703 | -1.546184392 |
| 6 | 4.796242857  | -11.753222039 | -1.952160532 |
| 6 | 5.799854332  | -11.722911982 | -1.026383029 |
| 6 | 5.492857786  | -11.695713368 | 0.376259491  |
| 1 | -2.691186872 | -11.394074324 | -0.874659373 |
| 1 | -0.874023563 | -11.485920325 | 0.804366320  |
| 1 | -2.156848718 | -11.499097335 | -3.324170916 |
| 1 | 0.193108699  | -11.679381473 | -4.084520470 |
| 1 | 2.609075311  | -11.734967552 | -3.547534852 |
| 1 | 1.538017320  | -11.592852475 | 1.331759148  |
| 1 | 3.953888354  | -11.668583592 | 1.868840256  |

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| 1 | 5.023253399 | -11.764039935 | -3.022510249 |
| 1 | 6.845472662 | -11.716064632 | -1.346703524 |
| 1 | 6.309197175 | -11.674543656 | 1.104161642  |
| 1 | 4.322162877 | -6.850541700  | -0.448631294 |
| 1 | 3.174389426 | -5.883395190  | -0.080569485 |
| 1 | 1.491040951 | -4.885692906  | 0.782045068  |
| 1 | 1.081145813 | -5.820440869  | -0.375651351 |
| 1 | 0.151269343 | -6.747974152  | -2.049420081 |
| 1 | 1.364630522 | -5.888104137  | -2.469409826 |
| 1 | 3.110220672 | -5.053196013  | -3.382521574 |
| 1 | 3.458281396 | -5.949750205  | -2.175122440 |
| 1 | 1.330824039 | -3.020354665  | -2.495494359 |
| 8 | 0.518561345 | -3.060861503  | -1.943878548 |
| 8 | 3.055281474 | -3.255326242  | -3.148394778 |
| 8 | 4.213543850 | -3.161838529  | -0.757304633 |
| 8 | 1.670996485 | -3.110062552  | 0.449834066  |
| 1 | 0.222312419 | -3.987759543  | -2.055247180 |
| 1 | 3.400435359 | -2.558774533  | -3.727041802 |
| 1 | 3.561391948 | -3.155258214  | -2.288063274 |
| 1 | 3.405678877 | -3.035278324  | -0.212198762 |
| 1 | 1.378905405 | -2.361065589  | 0.990980619  |
| 1 | 1.175140602 | -3.015798011  | -0.417331617 |
| 1 | 4.445022527 | -4.099647375  | -0.594179662 |

**Coronene:**

**4w:**

|   |             |             |             |
|---|-------------|-------------|-------------|
| 6 | 0.000000000 | 0.000000000 | 0.000000000 |
| 6 | 0.000000000 | 0.000000000 | 1.431458463 |
| 6 | 1.236946125 | 0.000000000 | 2.113304994 |
| 6 | 2.463788517 | 0.004779446 | 1.373583786 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 2.438909075  | 0.002833939  | -0.037538994 |
| 6 | 1.174660673  | -0.001397602 | -0.706465597 |
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| 1 | -2.166124802 | -0.019868820 | 1.655465977  |
| 1 | -2.117340388 | -0.071916044 | 4.129289206  |
| 6 | 0.105373101  | -0.141358631 | 5.695116682  |
| 6 | 1.301924504  | -0.198228087 | 6.356436406  |
| 6 | 2.539377820  | -0.170570290 | 5.641340719  |
| 1 | -0.835834137 | -0.166520312 | 6.253203246  |
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| 6 | 4.977247772  | -0.223399591 | 5.602510118  |

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| 1 | 3.816492505  | -0.322819119 | 7.399552339  |
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| 6 | -1.457821613 | -5.976544638 | 2.090417998  |
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| 1 | -1.819860207 | -5.921576415 | -0.018634797 |

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| 6 | 0.000000000 | 0.000000000  | 1.428897290  |
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| 6 | 2.434240516 | 0.005649361  | -0.032952699 |
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| 6 | 3.712794379  | -0.013185115 | 2.073411173  |
| 6 | 3.737097545  | -0.029954179 | 3.504661208  |
| 6 | 2.509809334  | -0.029235029 | 4.240909578  |
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| 6 | -1.254492548 | -6.145966112 | 3.286342888  |
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| 6 | 0.000000000 | 0.000000000 | 1.429257129  |
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| 6 | 2.433200158 | 0.015508490 | -0.030979182 |

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| 6 | 3.712556926  | 0.038301434  | 2.074677460  |
| 6 | 3.736801485  | 0.063723170  | 3.506301140  |
| 6 | 2.508598796  | 0.056548063  | 4.243476954  |
| 6 | 4.971316169  | 0.124231597  | 4.187634405  |
| 6 | 6.183793326  | 0.151243576  | 3.431009384  |
| 6 | 6.160772349  | 0.127033014  | 2.064825686  |
| 6 | 4.923793212  | 0.075134474  | 1.350697907  |
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| 1 | 7.136311543  | 0.191706075  | 3.968293170  |
| 1 | 7.094747902  | 0.148335372  | 1.494851970  |
| 6 | -1.212781273 | 0.014262240  | 2.188254570  |
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| 1 | -2.167461591 | 0.016363428  | 1.652184053  |
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| 6 | 1.290387253  | 0.126114283  | 6.367569202  |
| 6 | 2.528650727  | 0.112497927  | 5.653542512  |
| 1 | -0.846668451 | 0.103976415  | 6.261030757  |
| 1 | 1.316048256  | 0.162140119  | 7.461005733  |
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| 1 | 5.926833930  | 0.220355435  | 6.142874386  |

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| 1 | 5.751243760  | -3.684798363 | 2.895801837 |
| 8 | -0.099014400 | -3.087407014 | 2.907077229 |
| 1 | 0.416708436  | -3.087161568 | 2.055140702 |
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**Pyrene:**

**3w:**

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| 6 | 0.000000000  | 0.000000000  | 1.355376495  |
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| 6 | 1.239774412  | -0.020400564 | -0.748916234 |
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| 6 | 1.256760316  | -0.020560684 | -2.151628380 |
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| 6 | 3.680940565  | -0.070141079 | -2.153974274 |
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| 6 | 2.473014170  | 0.056587021  | 4.202915931  |
| 6 | 3.704689624  | 0.004294778  | 2.108977812  |
| 6 | 4.942949509  | -0.010583511 | 1.356193664  |
| 6 | 4.942415491  | -0.038847806 | 0.000897221  |
| 6 | 3.684050912  | 0.038741725  | 3.510581360  |
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| 1 | -0.942350064 | 0.019841588  | 1.911728901  |
| 1 | 0.314885875  | 0.051042163  | 4.059588481  |
| 1 | 5.886116242  | 0.002621362  | 1.911257950  |
| 1 | 5.885040341  | -0.049034925 | -0.555187215 |
| 1 | 2.473029691  | 0.086808608  | 5.296065106  |
| 1 | 4.631404175  | 0.054259416  | 4.057959846  |
| 1 | 0.308695132  | 0.028195434  | -2.692867825 |
| 1 | 2.465378637  | -0.062249007 | -3.938747142 |
| 1 | 4.627252895  | -0.091408171 | -2.703516315 |
| 6 | 2.613479011  | 6.289799689  | -2.316790627 |
| 6 | 1.391904346  | 6.152853262  | -2.885940449 |
| 6 | 0.204847301  | 5.975210216  | -2.075716639 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 6 | 0.337765553  | 5.960219837 | -0.659279805 |
| 6 | 2.779315763  | 6.280671387 | -0.878961615 |
| 6 | 1.630466383  | 6.125404249 | -0.058039277 |
| 6 | 4.037476814  | 6.416159948 | -0.274150074 |
| 6 | 4.162312668  | 6.404864328 | 1.114408956  |
| 6 | 3.035176341  | 6.260594737 | 1.924650560  |
| 6 | 1.762176624  | 6.115934592 | 1.357084705  |
| 6 | -1.066619403 | 5.802987340 | -2.646165561 |
| 6 | -2.188733620 | 5.615835674 | -1.836550788 |
| 6 | -0.810482356 | 5.778659284 | 0.161599921  |
| 6 | -0.646140440 | 5.784007854 | 1.600712670  |
| 6 | 0.573488707  | 5.947925515 | 2.166318450  |
| 6 | -2.063561957 | 5.603166412 | -0.445086761 |
| 1 | 3.506548166  | 6.401865087 | -2.939016687 |
| 1 | 1.279480546  | 6.155684504 | -3.974572337 |
| 1 | -1.169067356 | 5.813620773 | -3.735862601 |
| 1 | -1.536525517 | 5.649967583 | 2.222998298  |
| 1 | 0.685782439  | 5.947096536 | 3.255106849  |
| 1 | -3.172740995 | 5.479739720 | -2.294834627 |
| 1 | -2.947293997 | 5.459615694 | 0.184583392  |
| 1 | 4.923894091  | 6.527634063 | -0.906225217 |
| 1 | 5.150271796  | 6.511741583 | 1.571905811  |
| 1 | 3.138484901  | 6.253629292 | 3.014244318  |
| 8 | -0.317542170 | 2.674815945 | -1.481501990 |
| 8 | 2.432676121  | 3.136019520 | -1.695443128 |
| 1 | -0.000253737 | 2.778722801 | -0.553524852 |
| 1 | -0.885249623 | 3.448328557 | -1.618786494 |
| 1 | 2.821866852  | 2.277855703 | -1.920689919 |
| 1 | 1.481728137  | 3.013665132 | -1.912941446 |

|   |             |             |             |
|---|-------------|-------------|-------------|
| 8 | 1.212558832 | 3.114915403 | 0.754005506 |
| 1 | 1.515591735 | 2.398192247 | 1.328809497 |
| 1 | 1.901817005 | 3.178551092 | 0.053232614 |

**4w:**

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.000000000  | 0.000000000  | 0.000000000  |
| 6 | 0.000000000  | 0.000000000  | 1.354548105  |
| 6 | 1.237400118  | 0.000000000  | 2.105989145  |
| 6 | 2.468617695  | -0.000553998 | 1.396908211  |
| 6 | 1.238708295  | 0.011662941  | -0.749758904 |
| 6 | 2.470000393  | 0.017137808  | -0.037812566 |
| 6 | 1.261176087  | 0.014989731  | -2.152757589 |
| 6 | 2.474871993  | 0.032698978  | -2.845190942 |
| 6 | 3.685403466  | 0.054724411  | -2.149542910 |
| 6 | 3.701817036  | 0.041876256  | -0.746968501 |
| 6 | 1.256396480  | -0.002749303 | 3.508157604  |
| 6 | 2.465925620  | -0.014392393 | 4.203027267  |
| 6 | 3.700481050  | -0.017688440 | 2.107794907  |
| 6 | 4.940360140  | 0.004473214  | 1.357274600  |
| 6 | 4.940521734  | 0.048277409  | 0.003426677  |
| 6 | 3.678953666  | -0.026936554 | 3.512174608  |
| 1 | -0.941881739 | -0.002261229 | -0.557473090 |
| 1 | -0.942391805 | -0.001656736 | 1.911002980  |
| 1 | 0.308594281  | 0.004777162  | 4.055357919  |
| 1 | 5.883118101  | 0.007768866  | 1.913440681  |
| 1 | 5.880255114  | 0.100356445  | -0.552683857 |
| 1 | 2.464557367  | -0.017190724 | 5.296828740  |
| 1 | 4.626050298  | -0.044943083 | 4.061275736  |
| 1 | 0.314659344  | 0.003758505  | -2.702400895 |
| 1 | 2.476169595  | 0.032606031  | -3.939307206 |



|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | 4.634219925  | 0.081801844 | -2.693621902 |
| 6 | 2.826461609  | 6.119996701 | -2.993501267 |
| 6 | 1.478579387  | 6.024705419 | -2.902505565 |
| 6 | 0.811444299  | 6.009847748 | -1.617659765 |
| 6 | 1.597005499  | 6.102938868 | -0.437294342 |
| 6 | 3.654374701  | 6.199472245 | -1.808305354 |
| 6 | 3.026646667  | 6.185136490 | -0.532177994 |
| 6 | 5.052266603  | 6.293213326 | -1.880167314 |
| 6 | 5.821889682  | 6.365966291 | -0.715964753 |
| 6 | 5.210053036  | 6.337356449 | 0.539035255  |
| 6 | 3.813801382  | 6.251655995 | 0.649504731  |
| 6 | -0.583204511 | 5.911236477 | -1.504093526 |
| 6 | -1.196609569 | 5.914441611 | -0.251317889 |
| 6 | 0.968346699  | 6.113638561 | 0.838345734  |
| 6 | 1.796864592  | 6.187280120 | 2.024752744  |
| 6 | 3.147495574  | 6.236657935 | 1.935170880  |
| 6 | -0.431036731 | 6.020653238 | 0.911389285  |
| 1 | 3.319666708  | 6.130896809 | -3.970414627 |
| 1 | 0.863267763  | 5.956538844 | -3.804996741 |
| 1 | -1.188786352 | 5.832092822 | -2.412320447 |
| 1 | 1.304602831  | 6.176659559 | 3.002245637  |
| 1 | 3.765541079  | 6.254859090 | 2.836647387  |
| 1 | -2.285404057 | 5.838114318 | -0.179025964 |
| 1 | -0.916869460 | 6.031281478 | 1.892515380  |
| 1 | 5.537237104  | 6.309552869 | -2.861247341 |
| 1 | 6.910957354  | 6.442043410 | -0.788400798 |
| 1 | 5.815047911  | 6.382192658 | 1.449590232  |
| 8 | 4.918819274  | 3.108353704 | -0.479219320 |
| 8 | 3.804619903  | 3.222296559 | 2.012307367  |

|   |             |             |              |
|---|-------------|-------------|--------------|
| 8 | 1.354398694 | 2.958083542 | 0.888051498  |
| 8 | 2.439807227 | 3.156273285 | -1.561489784 |
| 1 | 4.613591060 | 3.091145509 | 0.463646847  |
| 1 | 5.305000000 | 3.993000000 | -0.570000000 |
| 1 | 2.862919524 | 3.218883562 | 1.699603122  |
| 1 | 3.856895536 | 2.408004130 | 2.533959522  |
| 1 | 1.661455865 | 3.001923957 | -0.055929756 |
| 1 | 0.685819839 | 3.655796430 | 0.939926871  |
| 1 | 3.386080112 | 3.141034685 | -1.263258403 |
| 1 | 2.349927118 | 2.348808438 | -2.088612712 |

**Fluorene:**

**3w:**

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.000000000  | 0.000000000  | 0.000000000  |
| 6 | 0.000000000  | 0.000000000  | 1.400828248  |
| 6 | 1.201771859  | 0.000000000  | 2.112097857  |
| 6 | 1.202996007  | 0.008201906  | -0.713124471 |
| 6 | 2.403247528  | 0.008047255  | -0.007683799 |
| 6 | 2.400961730  | -0.006006071 | 1.397590835  |
| 6 | 3.820852450  | 0.057007255  | -0.532788694 |
| 6 | 4.644612251  | 0.021962155  | 0.736048683  |
| 6 | 3.802070780  | -0.003407994 | 1.863301302  |
| 6 | 4.334612907  | -0.021303865 | 3.153773311  |
| 6 | 5.724165170  | -0.026340921 | 3.307252491  |
| 6 | 6.028858341  | 0.030111652  | 0.892671045  |
| 6 | 6.566604838  | -0.000245199 | 2.186010197  |
| 1 | -0.951501563 | -0.001378451 | -0.540243260 |
| 1 | -0.951253557 | 0.003113411  | 1.941428130  |
| 1 | 1.204472961  | 0.023207201  | 3.204930168  |
| 1 | 1.198056494  | 0.020920196  | -1.807577974 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 3.990781922  | 1.002097485  | -1.073700504 |
| 1 | 4.053940582  | -0.785116405 | -1.206710884 |
| 1 | 3.677555070  | -0.013625870 | 4.027190113  |
| 1 | 6.160446110  | -0.044852763 | 4.310397945  |
| 1 | 6.690047711  | 0.056114591  | 0.020682470  |
| 1 | 7.652175809  | -0.005837411 | 2.323420457  |
| 6 | 3.826820438  | 6.354032378  | -1.558870677 |
| 6 | 2.440115239  | 6.163999090  | -1.500555661 |
| 6 | 1.793102442  | 6.021441314  | -0.269559020 |
| 6 | 4.590978705  | 6.404549648  | -0.387606995 |
| 6 | 3.952540241  | 6.261945520  | 0.842732754  |
| 6 | 2.558262307  | 6.069810518  | 0.898788844  |
| 6 | 4.545606178  | 6.235953288  | 2.234347796  |
| 6 | 3.330311494  | 6.003576198  | 3.104485215  |
| 6 | 2.170125634  | 5.903878876  | 2.313554003  |
| 6 | 0.924560570  | 5.652412440  | 2.894494150  |
| 6 | 0.851535689  | 5.496239874  | 4.282450239  |
| 6 | 3.252380299  | 5.846759087  | 4.486451625  |
| 6 | 2.006733609  | 5.592192167  | 5.071206385  |
| 1 | 4.316850929  | 6.459898964  | -2.530946386 |
| 1 | 1.860156022  | 6.123661167  | -2.426924550 |
| 1 | 0.711182033  | 5.863692137  | -0.227088148 |
| 1 | 5.674952994  | 6.545038600  | -0.440025379 |
| 1 | 5.059679665  | 7.180512428  | 2.482972664  |
| 1 | 5.263527645  | 5.405943604  | 2.347374735  |
| 1 | 0.023842065  | 5.569405097  | 2.278849501  |
| 1 | -0.113152424 | 5.293724161  | 4.756845125  |
| 1 | 4.151844512  | 5.907880064  | 5.106491172  |
| 1 | 1.932623434  | 5.460165228  | 6.154414219  |

|   |             |             |             |
|---|-------------|-------------|-------------|
| 8 | 5.273079776 | 3.184657371 | 2.446873308 |
| 8 | 3.369557832 | 2.961049124 | 0.448453932 |
| 1 | 4.439649673 | 3.005595493 | 2.943750574 |
| 1 | 5.737769561 | 2.333504391 | 2.474814122 |
| 1 | 3.174512104 | 3.806583831 | 0.018671299 |
| 1 | 4.205892792 | 3.124762836 | 0.939576663 |
| 8 | 2.670555215 | 2.670627589 | 3.155289789 |
| 1 | 2.142484062 | 3.417535393 | 3.475272224 |
| 1 | 2.583981974 | 2.716013181 | 2.177221730 |

**4w:**

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 0.000000000  | 0.000000000  | 0.000000000  |
| 6 | 0.000000000  | 0.000000000  | 1.402874844  |
| 6 | 1.201786237  | 0.000000000  | 2.115078136  |
| 6 | 1.205226719  | 0.000124641  | -0.713274476 |
| 6 | 2.406395517  | -0.006028836 | -0.006499737 |
| 6 | 2.401738707  | -0.005387258 | 1.400692477  |
| 6 | 3.825343113  | 0.016771188  | -0.530285787 |
| 6 | 4.644586757  | -0.002287760 | 0.741420245  |
| 6 | 3.801863040  | -0.000518303 | 1.868136298  |
| 6 | 4.329606903  | 0.015425625  | 3.160901682  |
| 6 | 5.718257969  | 0.022342102  | 3.315818493  |
| 6 | 6.029081906  | 0.013402140  | 0.900341595  |
| 6 | 6.562283768  | 0.021551283  | 2.194935873  |
| 1 | -0.951109477 | 0.001219103  | -0.540833554 |
| 1 | -0.951429751 | 0.006645993  | 1.942755814  |
| 1 | 1.203403024  | 0.033002353  | 3.207421352  |
| 1 | 1.200663070  | 0.007530079  | -1.807676240 |
| 1 | 4.011346906  | 0.948668202  | -1.089670660 |
| 1 | 4.045280436  | -0.844298004 | -1.184173664 |

|   |              |             |              |
|---|--------------|-------------|--------------|
| 1 | 3.670068535  | 0.050329559 | 4.031471131  |
| 1 | 6.153241394  | 0.036034153 | 4.319504909  |
| 1 | 6.691611370  | 0.022763005 | 0.029316746  |
| 1 | 7.647342330  | 0.030255610 | 2.335036974  |
| 6 | 4.067545106  | 6.459191523 | -1.416621518 |
| 6 | 2.684303686  | 6.225722668 | -1.409557284 |
| 6 | 2.002899800  | 6.021186265 | -0.207407412 |
| 6 | 4.792210769  | 6.489435754 | -0.218536586 |
| 6 | 4.115482141  | 6.289767620 | 0.983666244  |
| 6 | 2.727518035  | 6.057869541 | 0.985777841  |
| 6 | 4.659856777  | 6.248525162 | 2.394500116  |
| 6 | 3.415923922  | 5.999751784 | 3.218792187  |
| 6 | 2.290220835  | 5.875632878 | 2.383874041  |
| 6 | 1.026023902  | 5.613060298 | 2.916043716  |
| 6 | 0.898736739  | 5.480868627 | 4.301300609  |
| 6 | 3.286231903  | 5.857224030 | 4.598857633  |
| 6 | 2.019424121  | 5.600791225 | 5.136978208  |
| 1 | 4.584778956  | 6.616472877 | -2.367825299 |
| 1 | 2.136562314  | 6.198301695 | -2.356064722 |
| 1 | 0.931555244  | 5.806324850 | -0.203040083 |
| 1 | 5.872552327  | 6.664314314 | -0.229693760 |
| 1 | 5.169521500  | 7.185869381 | 2.675581256  |
| 1 | 5.365291249  | 5.408586974 | 2.507700875  |
| 1 | 0.160774944  | 5.485997363 | 2.260767399  |
| 1 | -0.082030888 | 5.273590202 | 4.739464630  |
| 1 | 4.158755423  | 5.941404275 | 5.254085721  |
| 1 | 1.901106756  | 5.490440567 | 6.219057008  |
| 8 | 1.293702513  | 3.133871998 | 0.889322097  |
| 8 | 2.531156561  | 2.657208873 | 3.285844738  |

|   |             |             |              |
|---|-------------|-------------|--------------|
| 1 | 0.838101500 | 2.332401375 | 0.588495026  |
| 1 | 2.130536149 | 3.140078448 | 0.359980685  |
| 1 | 2.262577116 | 3.382812764 | 3.870601244  |
| 1 | 1.989983841 | 2.809766711 | 2.469139257  |
| 8 | 4.934334521 | 3.144550637 | 2.119165137  |
| 8 | 3.751401316 | 3.133148774 | -0.328700691 |
| 1 | 5.457331179 | 2.339729234 | 2.258273552  |
| 1 | 4.103183004 | 2.973587934 | 2.635879994  |
| 1 | 3.909680977 | 4.008249740 | -0.715685682 |
| 1 | 4.279135464 | 3.145462902 | 0.511181094  |

1. Horn, R.A. and C.R. Johnson, *Matrix Analysis*. 1985, Cambridge: Cambridge University Press.