

Correction      i-1,i

**Atom   C $\alpha$**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.06     | -0.08    | -0.13    | -0.05    | -0.11    | -0.09    | -0.01    | -0.05    | 0.11     | 0.12     | -0.04    | -0.02    | -0.16    | -0.09    | -0.21    | -0.12    | -0.08    | 0.16     | -0.16    | -0.08    | -0.46    |
| <b>R</b> | 0.11     | -0.17    | -0.09    | -0.24    | 0.2      | -0.06    | 0.11     | -0.06    | -0.2     | 0.01     | 0.04     | 0.03     | -0.26    | -0.41    | -0.03    | -0.17    | -0.02    | -0.53    | -0.69    | -0.08    | -0.17    |
| <b>N</b> | 0.19     | 0.22     | 0.48     | 0.38     | 0.43     | 0.36     | 0.41     | 0.2      | 1.43     | 0.03     | -0.04    | 0.21     | 0.42     | 0.08     | 0.54     | 0.48     | 0.45     | 0.47     | -0.59    | -0.2     | -0.18    |
| <b>D</b> | 0.46     | 0.17     | 0.39     | 0.43     | -0.22    | 0.15     | 0.32     | 0.22     | 0.22     | 0.58     | 0.05     | 0.37     | 0.05     | 0.67     | 0.5      | 0.31     | 0.64     | 1.09     | 0.57     | -0.03    | 0.05     |
| <b>C</b> | 0.52     | 0.7      | 1.25     | 0.95     | 0.54     | 0.61     | 0.36     | 0.42     | 1.09     | -0.69    | 0.54     | 0.89     | --       | 0.39     | 0.62     | 0.64     | 0.52     | --       | 0.88     | -0.07    | --       |
| <b>Q</b> | -0.33    | 0.02     | -0.01    | 0.13     | 1.47     | 0.05     | -0.14    | 0.02     | -0.12    | -0.24    | -0.03    | 0.11     | -0.06    | 0.2      | 0.16     | -0.19    | -0.03    | 0.82     | 0.13     | -0.08    | --       |
| <b>E</b> | -0.11    | -0.06    | -0.01    | 0.09     | 0.57     | -0.28    | 0.07     | 0.03     | -0.44    | 0.03     | -0.19    | 0.01     | -0.01    | 0.09     | 0.07     | 0.17     | 0.08     | 0        | 0        | -0.13    | 0.25     |
| <b>G</b> | -0.23    | -0.1     | -0.26    | 0.06     | 0.03     | -0.18    | -0.51    | -0.34    | -0.39    | -0.36    | -0.13    | -0.51    | -0.01    | -0.21    | 0.02     | 0.02     | 0.06     | -0.24    | -0.23    | -0.14    | 0.34     |
| <b>H</b> | 0.12     | 0.14     | 0.51     | 0.19     | 0.07     | 0.16     | 0.35     | -0.07    | 0.2      | 0.3      | 0.47     | 0.15     | -0.33    | 0.42     | 0.68     | -0.14    | 0.36     | -1.09    | 0.65     | 0.05     | --       |
| <b>I</b> | -0.56    | -0.25    | -0.09    | -0.71    | -0.37    | -0.47    | -0.07    | -0.03    | -0.22    | 0.29     | -0.19    | 0.01     | -0.54    | -0.3     | -0.29    | -0.57    | -0.84    | --       | -0.68    | -0.22    | -0.17    |
| <b>L</b> | 0.08     | 0.07     | -0.07    | -0.28    | -0.48    | 0.08     | -0.15    | 0.09     | -0.17    | 0.19     | 0.12     | -0.26    | -0.23    | -0.2     | -0.29    | -0.15    | -0.35    | -1       | -0.45    | 0.01     | 0.52     |
| <b>K</b> | -0.32    | -0.2     | -0.01    | 0.02     | 0.61     | 0.11     | -0.08    | -0.09    | -0.33    | -0.3     | -0.27    | 0.03     | 0.05     | -0.31    | -0.18    | -0.11    | 0.01     | -0.06    | -0.29    | 0.25     | 0.32     |
| <b>M</b> | 0.16     | 0.38     | -0.12    | -0.19    | --       | 0.14     | -0.07    | -0.13    | 0.53     | 0.09     | -0.27    | -0.15    | --       | -0.62    | -0.71    | -0.23    | -0.25    | --       | 0.74     | -0.05    | --       |
| <b>F</b> | -0.23    | -0.21    | 0.08     | -0.12    | -0.3     | 0.01     | 0.05     | 0.3      | 0.01     | -0.53    | 0.03     | -0.18    | -0.05    | -0.08    | -0.27    | -0.39    | -0.04    | --       | -0.19    | 0.18     | --       |
| <b>P</b> | 0.18     | 0.03     | -0.24    | 0.22     | -0.54    | 0.22     | 0.33     | -0.19    | 0.12     | 0.44     | 0.15     | 0.1      | 0.41     | 0.37     | -0.27    | 0.27     | -0.02    | 0.26     | 0.17     | 0.31     | -0.52    |
| <b>S</b> | 0.17     | 0.15     | 0.02     | 0.16     | 0.3      | -0.02    | 0.11     | -0.06    | 0.29     | 0.05     | 0.09     | 0.38     | 0.3      | -0.02    | 0.1      | 0.38     | 0.25     | -0.71    | 0.23     | 0.01     | 0.83     |
| <b>T</b> | 0.1      | 0.41     | 0.07     | 0.18     | -1.05    | 0.04     | 0.16     | -0.04    | -0.06    | 0.01     | 0.22     | 0.19     | 0.26     | 0.24     | 0.17     | 0.05     | 0.12     | 0.24     | 0.07     | 0.24     | 0        |
| <b>W</b> | -0.45    | -0.08    | 0.01     | -0.38    | -0.72    | -0.46    | -0.19    | 0.07     | 0.47     | 0.49     | 0.18     | 0.43     | --       | -1.55    | -0.04    | -0.68    | -0.2     | --       | --       | -0.28    | --       |
| <b>Y</b> | 0        | -0.46    | -0.28    | -0.65    | -0.79    | 0.3      | -0.2     | 0.36     | 0.18     | -0.35    | 0.25     | 0        | --       | -0.17    | 0.19     | -0.39    | -0.5     | -0.11    | -0.06    | 0.11     | --       |
| <b>V</b> | -0.2     | -0.2     | -0.23    | -0.27    | 0.17     | -0.2     | -0.42    | -0.14    | -0.6     | -0.5     | -0.26    | -0.51    | -0.3     | -0.12    | -0.21    | -0.29    | -0.27    | 0.09     | -0.47    | -0.16    | 0.1      |
| <b>X</b> | 1.26     | 0        | 0.39     | 0.03     | --       | 0.05     | 0.58     | -0.08    | 1.53     | --       | 0.69     | 0.19     | --       | --       | -0.38    | 0.85     | 0.41     | --       | --       | --       | -0.41    |

Correction      i-1,i

**Atom   C $\beta$**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.02    | -0.15    | -0.02    | -0.14    | 0.23     | -0.09    | 0        | ---      | -0.16    | 0.11     | 0.08     | 0.08     | 0.71     | -0.4     | -0.16    | -0.06    | 0.24     | -0.22    | -0.28    | 0.13     | 0.98     |
| <b>R</b> | -0.11    | 0.08     | 0.02     | 0.19     | 0.38     | 0.3      | -0.05    | ---      | 0.45     | 0.37     | 0.11     | -0.21    | 0.12     | 0.16     | 0.05     | 0.02     | -0.33    | 0.05     | -0.4     | 0.31     | -1.2     |
| <b>N</b> | -0.23    | -0.2     | -0.01    | -0.28    | -0.8     | 0.25     | 0        | ---      | -0.22    | -0.09    | 0.12     | -0.42    | 0.54     | -0.04    | -0.04    | -0.2     | 0.1      | -0.43    | 0.57     | -0.16    | 2.4      |
| <b>D</b> | -0.18    | -0.56    | -0.17    | 0.16     | -0.33    | -0.09    | -0.16    | ---      | -0.21    | 0.1      | -0.33    | -0.21    | -0.17    | -0.29    | -0.02    | -0.26    | 0.05     | 0.54     | 0.24     | -0.15    | -0.99    |
| <b>C</b> | -0.21    | -0.73    | -0.19    | -0.12    | -0.21    | -0.99    | -0.34    | ---      | -1.54    | 0.34     | -0.26    | -0.89    | ---      | -1.71    | -0.08    | -0.38    | -1.06    | ---      | -0.37    | -0.41    | ---      |
| <b>Q</b> | 0.28     | 0        | 0.1      | 0.02     | -1.46    | -0.05    | -0.05    | ---      | 0.23     | 0.01     | 0.28     | -0.07    | -0.05    | -0.18    | -0.02    | 0.01     | 0.28     | -0.03    | 0.62     | 0.14     | ---      |
| <b>E</b> | 0.23     | 0.14     | 0.17     | -0.01    | -0.91    | -0.1     | -0.05    | ---      | -0.34    | -0.22    | 0.11     | 0.11     | 0.1      | -0.23    | -0.01    | -0.3     | -0.16    | 0.58     | 0.23     | -0.04    | -1.79    |
| <b>G</b> | 0.2      | 0.49     | 0.32     | 0.08     | -0.9     | 0.29     | 0.42     | ---      | 0.16     | -0.21    | 0.12     | 0.59     | 0.31     | 0.22     | 0.16     | 0.14     | -0.52    | -0.02    | 0.39     | -0.14    | 0.04     |
| <b>H</b> | -0.1     | -0.15    | -0.06    | -0.49    | -0.77    | -0.3     | 0.28     | ---      | -0.26    | 0.02     | 0.6      | -0.44    | -0.11    | 0.48     | -0.09    | 0.08     | 0.17     | -0.06    | -1.5     | -0.1     | ---      |
| <b>I</b> | 0.14     | 0.17     | 0.06     | 0.14     | 0.5      | 0.51     | 0.33     | ---      | 0.52     | -0.36    | -0.14    | 0.35     | -0.27    | -0.05    | -0.04    | 0.5      | 0.01     | ---      | 0.49     | 0.32     | -0.82    |
| <b>L</b> | -0.05    | 0.05     | -0.15    | -0.03    | 0.71     | -0.2     | -0.19    | ---      | 0.21     | 0.1      | -0.18    | -0.03    | -0.46    | 0.27     | 0.03     | 0.18     | 0.68     | -0.01    | -0.21    | 0.05     | -0.65    |
| <b>K</b> | 0.16     | -0.02    | -0.09    | -0.14    | 0.08     | 0.06     | -0.01    | ---      | -0.06    | 0.05     | 0.11     | -0.1     | -0.15    | 0.22     | 0.04     | -0.06    | 0.16     | 0.16     | 0.09     | 0        | -0.01    |
| <b>M</b> | 0.05     | -0.13    | 0.27     | -2.02    | ---      | 0.32     | 0.19     | ---      | -0.2     | 0.23     | -0.16    | 0.2      | ---      | 0.7      | 0.03     | 0.13     | 0.08     | ---      | -0.47    | -0.03    | ---      |
| <b>F</b> | -0.28    | 0.05     | -0.41    | 0.25     | 0.69     | -0.26    | 0.24     | ---      | 0.46     | 0.62     | -0.12    | 0.02     | 1.26     | -0.1     | 0.02     | -0.04    | 0.39     | 0.01     | -0.23    | 0.05     | ---      |
| <b>P</b> | -0.33    | 0.14     | 0.07     | -0.28    | 2.04     | -0.12    | -0.32    | ---      | -0.12    | -0.09    | -0.03    | -0.33    | -0.54    | -0.2     | 0        | -0.12    | 0.01     | -1.14    | -0.3     | -0.04    | -0.28    |
| <b>S</b> | -0.06    | -0.13    | -0.02    | -0.02    | -1.64    | -0.26    | -0.1     | ---      | -0.25    | -0.23    | -0.21    | 0.09     | 0.13     | -0.11    | -0.13    | -0.11    | -0.43    | -0.32    | 0.13     | 0.13     | -0.89    |
| <b>T</b> | 0.07     | -0.59    | 0.22     | -0.05    | 1.36     | -0.11    | -0.17    | ---      | -0.44    | 0.34     | -0.04    | -0.35    | -0.14    | 0.18     | 0        | 0.02     | 0.09     | 0.28     | 0.46     | -0.09    | 0.2      |
| <b>W</b> | 0.15     | 0.59     | 0.37     | 0.28     | ---      | 0.69     | 0.28     | ---      | 0.81     | 0.08     | 0.26     | 0.01     | ---      | -0.33    | -0.56    | 0.3      | -0.55    | ---      | ---      | 0.25     | ---      |
| <b>Y</b> | 0        | -0.03    | -0.26    | 0.25     | 3.34     | -0.3     | 0.02     | ---      | 0.84     | 0.62     | 0        | 0.05     | ---      | 0.08     | 0.32     | 0.15     | -0.76    | 0.44     | -0.13    | 0.37     | ---      |
| <b>V</b> | 0.2      | 0.4      | -0.25    | 0.23     | 0.54     | 0.29     | 0.11     | ---      | 0.76     | -0.25    | -0.11    | 0.32     | -0.92    | 0.47     | 0.02     | 0.12     | 0.3      | -0.2     | 0.03     | -0.21    | 1.2      |
| <b>X</b> | -0.37    | 0.68     | -0.4     | -0.35    | ---      | -0.06    | 0.2      | ---      | ---      | ---      | ---      | 0.2      | ---      | ---      | 0.01     | -0.07    | -0.21    | ---      | ---      | ---      | 0.99     |

Correction      i-1,i

**Atom    C**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.18     | 0.37     | 0.09     | 0.1      | -0.41    | 0.2      | 0.36     | 0.3      | 0.34     | -0.37    | -0.05    | 0.18     | -0.22    | 0.16     | -0.29    | -0.01    | 0.08     | 0.02     | 0.47     | 0.08     | -0.73    |
| <b>R</b> | -0.04    | -0.12    | 0.03     | 0.14     | 0.04     | -0.01    | 0.02     | 0.08     | 0.2      | -0.13    | 0.19     | -0.04    | 0.29     | -0.03    | 0        | 0.15     | 0.12     | 0.18     | -0.06    | -0.09    | ---      |
| <b>N</b> | -0.21    | -0.17    | -0.21    | -0.22    | -0.31    | -0.03    | -0.05    | -0.07    | -0.14    | -0.16    | -0.2     | -0.16    | -0.25    | 0.04     | 0.26     | -0.2     | -0.12    | 0        | -0.02    | -0.16    | -0.22    |
| <b>D</b> | 0.33     | -1.1     | 0.15     | 0.02     | -0.16    | 0.03     | 0.18     | 0.18     | 0.02     | 0.23     | 0.05     | 0.29     | 0.43     | 0.28     | 0.3      | -0.01    | 0.45     | 0.2      | 0.2      | 0.08     | -0.3     |
| <b>C</b> | -0.91    | -0.09    | -0.14    | -0.02    | -0.6     | 0.03     | -0.94    | -1.16    | -0.75    | ---      | 0.18     | -0.1     | ---      | ---      | 0.37     | -0.14    | 0.55     | ---      | 0.09     | -0.17    | ---      |
| <b>Q</b> | -0.21    | 0.13     | -0.13    | -0.2     | -0.06    | 0.38     | -0.39    | 0.09     | 0.02     | -0.41    | 0.11     | -0.06    | -0.16    | -0.06    | -0.1     | 0.07     | -0.38    | 0.59     | 0.22     | 0.23     | ---      |
| <b>E</b> | 0.05     | 0.12     | -0.05    | 0.03     | 0.13     | 0.11     | 0.15     | 0.19     | -0.2     | 0.1      | -0.16    | 0        | 0.12     | 0.24     | -0.12    | 0.1      | 0.01     | 0.05     | 0.07     | 0.01     | ---      |
| <b>G</b> | -0.13    | -0.01    | 0.3      | -0.1     | -0.1     | 0.02     | -0.27    | -0.14    | -0.22    | -0.32    | -0.19    | -0.37    | -0.21    | -0.21    | 0.3      | -0.03    | -0.17    | -0.33    | 0.09     | -0.4     | 1.2      |
| <b>H</b> | -0.06    | -0.34    | -0.17    | -0.05    | -0.37    | -0.46    | -0.02    | -0.04    | -0.19    | -0.56    | 0.17     | -0.14    | -0.23    | 0.01     | 0.14     | 0.21     | -0.78    | 0.13     | -0.87    | -0.09    | ---      |
| <b>I</b> | -0.17    | -0.27    | 0.19     | -0.04    | -0.12    | -0.21    | -0.14    | -0.58    | 0.46     | 0.33     | 0.15     | 0.06     | 0.34     | -0.12    | 0.03     | -0.02    | 0.24     | ---      | 0.03     | 0.22     | ---      |
| <b>L</b> | -0.17    | 0.19     | -0.06    | 0.01     | -0.11    | -0.05    | 0.1      | -0.29    | 0.23     | 0.33     | 0.21     | -0.02    | 0.54     | -0.13    | -0.18    | 0.01     | 0.24     | 0.26     | -0.47    | 0.26     | ---      |
| <b>K</b> | -0.08    | 0.14     | 0.02     | 0.01     | 0.7      | -0.09    | -0.01    | 0.03     | -0.32    | 0.4      | -0.01    | 0.08     | -0.08    | -0.03    | -0.09    | 0.09     | -0.66    | -0.05    | 0.22     | 0.23     | -0.7     |
| <b>M</b> | -0.04    | 0.33     | -0.18    | -0.11    | ---      | 0.01     | 0.06     | 0.16     | 0.92     | 0.32     | -0.52    | 0.05     | ---      | -1.38    | -0.3     | -0.22    | 0.32     | ---      | 0.56     | 0.12     | ---      |
| <b>F</b> | -0.33    | 0.3      | -0.23    | 0.04     | -0.24    | -0.33    | -0.06    | -0.09    | 0.11     | -0.01    | -0.23    | -0.01    | -1.03    | 0.8      | -0.22    | -0.18    | 0.06     | ---      | -0.82    | -0.42    | ---      |
| <b>P</b> | 0.46     | 0.41     | 0.06     | 0.03     | 1.3      | 0.36     | 0.09     | 0.14     | 0.04     | 0.24     | 0.29     | 0.29     | 0.62     | 0.11     | -0.04    | 0.32     | -0.07    | -0.01    | 0.37     | 0.13     | ---      |
| <b>S</b> | 0.32     | 0.04     | -0.17    | -0.03    | 0.04     | 0        | 0.04     | -0.17    | 0.17     | 0.33     | 0.02     | 0.14     | -0.14    | -0.1     | 0.09     | -0.01    | 0.03     | -0.12    | -0.59    | 0.1      | ---      |
| <b>T</b> | -0.1     | 0.06     | -0.23    | 0.17     | 0.02     | -0.48    | 0.04     | 0.06     | -0.16    | -0.34    | 0.06     | -0.23    | 0.34     | 0.04     | -0.18    | -0.23    | -0.01    | 0.3      | -0.18    | 0.02     | 0.03     |
| <b>W</b> | -0.2     | ---      | -0.16    | -0.2     | ---      | -0.28    | 0.25     | -0.01    | ---      | -0.85    | 0.01     | 0.31     | ---      | ---      | 0.12     | -0.14    | 0.03     | ---      | ---      | -0.78    | ---      |
| <b>Y</b> | -0.26    | -0.16    | -0.04    | -0.12    | 0.56     | -0.15    | -0.11    | 0.18     | 0.94     | -0.29    | -0.28    | -0.03    | ---      | 0.07     | -0.3     | -0.15    | -0.22    | ---      | -0.32    | -0.3     | ---      |
| <b>V</b> | 0.07     | 0.19     | 0.1      | 0.04     | 0.01     | 0.25     | -0.24    | 0.33     | -0.22    | 0.1      | -0.07    | 0.03     | -0.19    | 0.14     | 0.1      | 0.09     | 0.06     | -0.59    | 0.15     | 0.19     | ---      |
| <b>X</b> | -1.11    | 0.05     | 0.31     | 0.42     | ---      | ---      | ---      | -0.24    | ---      | ---      | ---      | 0.17     | ---      | ---      | -0.52    | -0.29    | 0.7      | ---      | ---      | ---      | ---      |

Correction      i-1,i

**Atom    N**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -2.2     | -2.19    | -3.12    | -2.48    | -2.38    | -1.93    | -1.96    | -2.02    | -0.88    | -1.35    | -2.08    | -1.8     | -1.66    | -1.85    | --       | -2.06    | -1.91    | -2.03    | -1.28    | -2.34    | -3.47    |
| <b>R</b> | 0.12     | 0.8      | -0.77    | -0.66    | 0.15     | 0.11     | -0.68    | 0.13     | 0.61     | 1.24     | -0.41    | 0.09     | -0.33    | -0.05    | --       | -0.83    | -0.61    | 2.1      | -0.27    | 0.01     | 1.49     |
| <b>N</b> | -0.78    | -1.47    | -1.82    | -1.3     | -3.4     | -1.79    | -0.87    | -1.96    | -1.64    | -1.86    | -0.56    | -1.8     | -1.08    | 1.15     | --       | -1.45    | -0.55    | -0.54    | -1.62    | -1.49    | -0.55    |
| <b>D</b> | -0.41    | -0.91    | -1.32    | -0.65    | -1.74    | -1.05    | -0.55    | -1.3     | -1.88    | -0.65    | -0.09    | -0.58    | 0.13     | -0.08    | --       | -1.13    | -0.81    | 0.05     | 0.76     | -1.32    | -1.32    |
| <b>C</b> | 2.71     | 2.62     | 2.02     | 2.38     | 0.41     | 1.16     | 2.23     | 1.01     | 0.17     | 3.12     | 2.61     | 2.89     | --       | -0.75    | --       | 2.24     | 1.39     | --       | 3.39     | 3.97     | --       |
| <b>Q</b> | 0.46     | 0.01     | -0.27    | -0.41    | 0.79     | -0.1     | -0.16    | 0.15     | -1.74    | 0.39     | -0.07    | 0.05     | -0.62    | -0.58    | --       | -1.04    | -1.06    | 0.69     | -0.52    | -0.27    | -1.76    |
| <b>E</b> | -0.39    | -0.81    | -1.01    | -1.19    | 0.26     | -1.02    | -0.59    | 0.46     | -0.77    | 0.04     | 0.09     | -0.83    | -0.39    | -0.4     | --       | -0.44    | -0.5     | 0.75     | -0.53    | -0.03    | -0.76    |
| <b>G</b> | -0.72    | -1.25    | -0.02    | 0.25     | -1.39    | -0.99    | -0.62    | -1.33    | -1.17    | -1.17    | -1.49    | -1.36    | -0.77    | -0.91    | --       | -0.77    | -1.41    | -0.84    | -1.03    | -1.54    | -1.81    |
| <b>H</b> | -0.05    | 0.56     | 0.34     | -0.04    | -0.52    | -0.83    | -0.04    | -0.44    | 1.32     | -0.21    | -0.24    | 1.37     | 1.14     | 1.86     | --       | -0.23    | 0.4      | 2.29     | 0.8      | 1.2      | --       |
| <b>I</b> | 3.64     | 4.02     | 4.12     | 3.72     | 2.92     | 3.98     | 3.54     | 2.94     | 3.63     | 2.63     | 1.93     | 3.61     | 2.81     | 1.46     | --       | 3.44     | 2.58     | --       | 2.99     | 4.79     | 1.83     |
| <b>L</b> | -0.2     | 0.22     | 0        | 0        | -1.26    | -0.38    | -0.27    | -1.08    | 0.1      | -1.36    | -1.05    | -0.48    | -0.3     | -1.12    | --       | -0.25    | -0.3     | -2.18    | -1.28    | 0.24     | -1.91    |
| <b>K</b> | -0.12    | -0.72    | -0.86    | -0.87    | 0.74     | -0.56    | -0.3     | 0.32     | -1.02    | 0.66     | -0.16    | -0.2     | -0.01    | -0.52    | --       | -0.74    | -0.72    | -0.55    | -0.43    | 0.47     | 0.14     |
| <b>M</b> | -0.12    | 0.81     | 0.32     | 0.36     | --       | 1.01     | -0.55    | -0.59    | 0.33     | -1.65    | 0.52     | 0.71     | --       | -0.38    | --       | 1.05     | -0.12    | --       | 0.26     | 0.84     | --       |
| <b>F</b> | -0.3     | 0.05     | 1.96     | 0.62     | 2.24     | 1.12     | 0.59     | -0.34    | 0.99     | -1.42    | -0.49    | 0.43     | -1.09    | -1.69    | --       | 0.2      | 0.79     | --       | -0.43    | 0.88     | 0.52     |
| <b>P</b> | -1.19    | -1.02    | -2.26    | -2.62    | 0.17     | -0.94    | -1.5     | 0.6      | -1.52    | -0.21    | -0.37    | -1.38    | -1.23    | -1.39    | -0.65    | -1.72    | -1.5     | -2.31    | -1.02    | -1.41    | -1.91    |
| <b>S</b> | 0.97     | 1.32     | 0.55     | 1.11     | 1.22     | 0.78     | 1.06     | 1.32     | 1.21     | 0.34     | 0.96     | 1.11     | 1.88     | 0.88     | --       | 1.4      | 0.96     | -0.52    | 1.14     | 0.8      | 1.2      |
| <b>T</b> | 1.59     | 0.89     | 1.1      | 1.07     | 1.2      | 1.25     | 1.38     | 1.03     | 0.2      | 2.14     | 1.82     | 0.65     | 0.13     | 3.49     | --       | 1.23     | 1.37     | 1.96     | 1.99     | 2.06     | 2.28     |
| <b>W</b> | -1.09    | 0.89     | 1.7      | 1.04     | --       | 1.47     | 0.59     | -0.2     | 1.7      | 1.34     | 0.43     | 1.03     | --       | 1.76     | --       | 1.56     | 2.81     | --       | --       | 0.93     | 2.12     |
| <b>Y</b> | 0.14     | 0.6      | 2.2      | 0.51     | -0.17    | 0.49     | 0.45     | 0        | 0.99     | -0.84    | -0.06    | 1.02     | --       | -1.56    | --       | 0.04     | 0.53     | -1.06    | 1.56     | 0.5      | --       |
| <b>V</b> | 2.49     | 2.38     | 3.89     | 3.12     | 2.08     | 3.29     | 3.71     | 3.3      | 2.4      | 2.22     | 3.35     | 3        | 2.44     | 2.66     | --       | 2.74     | 2.77     | 2.41     | 4.87     | 3.33     | 5.81     |
| <b>X</b> | 0.58     | 0.45     | 1.88     | 0.25     | --       | 1.42     | 1.56     | 1.63     | --       | --       | 1.27     | -0.04    | --       | --       | --       | 2.12     | 2.04     | --       | --       | 1.18     | -0.2     |

Correction      i-1,i

**Atom    H**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.03    | -0.02    | -0.1     | -0.09    | -0.3     | -0.03    | -0.02    | -0.08    | 0.01     | -0.08    | -0.08    | 0.05     | 0.21     | 0.02     | --       | -0.02    | -0.12    | -0.14    | 0.07     | 0        | 0.03     |
| <b>R</b> | -0.06    | 0.05     | -0.09    | -0.03    | -0.01    | 0.03     | 0.02     | 0.02     | 0.05     | 0.12     | 0.03     | 0.01     | -0.13    | 0.01     | --       | -0.13    | 0.01     | 0.27     | 0.03     | 0.08     | 0.01     |
| <b>N</b> | -0.14    | -0.11    | -0.13    | 0.01     | -0.12    | -0.16    | 0.01     | 0.23     | -0.16    | -0.19    | -0.06    | -0.13    | -0.17    | 0        | --       | -0.14    | -0.1     | -0.12    | -0.14    | -0.11    | -0.14    |
| <b>D</b> | -0.06    | -0.05    | -0.03    | -0.03    | -0.06    | 0        | 0        | 0.02     | -0.08    | -0.12    | 0.02     | -0.06    | -0.08    | -0.02    | --       | -0.15    | -0.06    | -0.09    | 0.13     | -0.2     | -0.11    |
| <b>C</b> | 0.25     | 0.18     | 0.11     | 0.13     | 0.13     | 0.02     | 0.29     | -0.16    | 0.07     | 0.27     | 0.1      | 0.18     | --       | -0.34    | --       | 0.27     | 0.04     | --       | 0.32     | 0.18     | --       |
| <b>Q</b> | -0.09    | -0.09    | 0.05     | -0.02    | -0.05    | -0.11    | -0.03    | -0.01    | -0.02    | 0.01     | -0.12    | -0.02    | -0.09    | 0        | --       | -0.1     | -0.05    | 0.01     | -0.01    | 0.04     | -0.09    |
| <b>E</b> | -0.04    | -0.05    | -0.07    | -0.04    | 0.06     | -0.1     | -0.08    | 0.07     | -0.06    | 0.09     | 0.02     | 0.01     | -0.02    | -0.05    | --       | -0.02    | -0.02    | 0.07     | 0.05     | 0        | -0.12    |
| <b>G</b> | -0.1     | -0.19    | -0.18    | -0.12    | -0.2     | -0.12    | -0.21    | -0.18    | -0.33    | -0.24    | -0.18    | -0.22    | -0.13    | -0.17    | --       | -0.05    | -0.15    | -0.1     | -0.25    | -0.25    | -0.25    |
| <b>H</b> | -0.1     | 0.01     | 0.13     | -0.06    | -0.28    | 0.01     | 0.04     | -0.14    | 0.06     | 0.01     | -0.1     | -0.02    | 0.05     | 0.63     | --       | -0.01    | -0.08    | 0.14     | 0.02     | -0.11    | -0.46    |
| <b>I</b> | 0.2      | 0.2      | 0.27     | 0.14     | 0.29     | 0.2      | 0.15     | 0.12     | 0.27     | 0.12     | 0.14     | 0.21     | 0.23     | -0.03    | --       | 0.16     | 0.07     | -0.18    | 0.21     | 0.31     | -0.19    |
| <b>L</b> | 0.05     | 0.08     | -0.05    | -0.04    | 0.2      | -0.06    | -0.1     | -0.17    | 0.14     | -0.05    | -0.09    | 0.04     | -0.02    | -0.09    | --       | 0.04     | 0.1      | -0.41    | -0.04    | 0.1      | -0.16    |
| <b>K</b> | -0.05    | -0.1     | -0.01    | -0.06    | 0.05     | -0.13    | 0.03     | 0.05     | -0.16    | 0.03     | -0.08    | -0.03    | 0.01     | -0.08    | --       | -0.04    | -0.06    | 0.25     | -0.01    | 0.08     | -0.08    |
| <b>M</b> | 0.05     | -0.05    | 0.13     | -0.04    | --       | 0.18     | 0.02     | -0.1     | 0.17     | -0.1     | -0.01    | -0.01    | --       | -0.21    | --       | 0.17     | 0.25     | --       | 0.05     | 0.02     | --       |
| <b>F</b> | 0.14     | -0.08    | 0.17     | 0        | 0.07     | 0.1      | 0.06     | -0.03    | -0.02    | -0.09    | 0.05     | 0.14     | -0.41    | 0.08     | --       | -0.03    | 0.34     | -0.08    | 0.19     | -0.09    | -0.01    |
| <b>P</b> | 0.1      | 0.21     | 0.11     | 0.05     | 0.15     | 0.31     | 0.16     | 0.2      | 0.02     | 0.25     | 0.13     | 0.12     | 0.21     | -0.12    | --       | -0.04    | -0.1     | -0.43    | -0.15    | 0.08     | -0.11    |
| <b>S</b> | 0.03     | 0.1      | -0.2     | 0.07     | -0.01    | 0.01     | 0.06     | 0.05     | 0.18     | -0.11    | 0.04     | -0.06    | 0.01     | 0.09     | --       | 0.06     | -0.1     | -0.18    | -0.05    | -0.03    | 0.06     |
| <b>T</b> | 0.09     | 0.05     | -0.07    | 0.03     | 0.06     | 0.08     | 0.03     | -0.12    | -0.19    | 0.27     | 0.12     | 0.04     | -0.03    | 0.31     | --       | -0.03    | -0.09    | 0.38     | 0.16     | 0.07     | 0.24     |
| <b>W</b> | -0.18    | -0.27    | 0        | -0.21    | --       | -0.12    | 0.04     | -0.29    | -0.03    | 0.06     | -0.16    | 0.18     | --       | -0.47    | --       | 0.1      | 0.15     | --       | --       | 0.31     | -0.47    |
| <b>Y</b> | 0.07     | -0.03    | 0.06     | 0.08     | 0.16     | 0.05     | -0.07    | -0.17    | 0.06     | -0.03    | 0.05     | 0.04     | --       | -0.01    | --       | -0.05    | 0.22     | -0.02    | -0.12    | -0.07    | 0.52     |
| <b>V</b> | 0.12     | 0.15     | 0.37     | 0.14     | 0.15     | 0.08     | 0.11     | 0.1      | 0.25     | 0.2      | 0.25     | 0.11     | 0.18     | 0.26     | --       | 0.13     | 0.17     | 0.25     | 0.39     | 0.26     | 0.18     |
| <b>X</b> | 0.1      | 0.11     | 0.24     | 0.38     | --       | 0.09     | 0.32     | 0.13     | 0.26     | --       | 0.43     | 0.07     | --       | 0.41     | --       | 0.41     | 0.47     | --       | 0.6      | 0.44     | 0.55     |

Correction      i-1,i

**Atom   H $\alpha$**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.02     | -0.01    | 0        | -0.04    | -0.21    | 0.05     | 0        | ---      | -0.04    | 0.01     | -0.07    | -0.02    | 0.03     | -0.01    | -0.02    | -0.06    | -0.07    | 0.04     | -0.06    | -0.02    | 0.02     |
| <b>R</b> | 0        | -0.03    | 0.01     | 0.02     | -0.21    | 0.05     | -0.03    | ---      | 0        | -0.01    | 0.05     | -0.01    | 0.02     | 0.1      | 0.01     | 0.26     | -0.01    | 0.12     | 0.09     | 0        | 0.03     |
| <b>N</b> | -0.06    | -0.06    | -0.04    | -0.04    | -0.06    | -0.06    | -0.02    | ---      | -0.19    | 0        | -0.04    | -0.06    | -0.01    | 0        | -0.03    | 0.02     | -0.09    | -0.16    | -0.09    | -0.04    | -0.01    |
| <b>D</b> | -0.09    | -0.15    | -0.09    | -0.04    | 0.24     | -0.06    | -0.03    | ---      | -0.05    | -0.02    | -0.05    | -0.08    | -0.03    | -0.18    | -0.03    | -0.1     | -0.03    | -0.19    | -0.08    | -0.03    | -0.02    |
| <b>C</b> | -0.08    | -0.06    | -0.08    | -0.07    | 0.1      | -0.05    | -0.04    | ---      | 0.1      | 0.1      | 0.03     | -0.01    | ---      | -0.03    | 0.02     | -0.07    | -0.05    | ---      | -0.13    | 0.15     | ---      |
| <b>Q</b> | 0.01     | -0.02    | 0.04     | -0.06    | -0.25    | -0.03    | -0.06    | ---      | 0.03     | 0.04     | 0.02     | -0.03    | -0.02    | -0.06    | -0.01    | 0        | 0.07     | 0.09     | 0.04     | -0.02    | -0.01    |
| <b>E</b> | 0.04     | -0.01    | 0.01     | -0.02    | -0.1     | 0        | 0        | ---      | 0        | 0        | 0.04     | -0.03    | -0.04    | 0.03     | -0.04    | -0.06    | 0.01     | 0.01     | -0.01    | 0.19     | -0.14    |
| <b>G</b> | 0.06     | 0.09     | 0.06     | 0.03     | 0.04     | 0.06     | 0.05     | ---      | 0.11     | -0.06    | 0        | 0.11     | 0.09     | 0        | 0.04     | 0.02     | 0        | 0.05     | 0.03     | -0.03    | 0.06     |
| <b>H</b> | 0        | 0.03     | -0.06    | -0.07    | 0.02     | -0.06    | -0.06    | ---      | -0.07    | 0.02     | 0.02     | -0.04    | -0.06    | 0        | -0.05    | -0.02    | -0.08    | 0.06     | -0.15    | 0.02     | -0.03    |
| <b>I</b> | 0.09     | 0.09     | 0.04     | 0.07     | 0.17     | 0.08     | 0.03     | ---      | 0.11     | -0.04    | 0.01     | 0        | 0.05     | -0.03    | 0        | 0.05     | 0.13     | 0.06     | 0.19     | 0.06     | 0.01     |
| <b>L</b> | -0.04    | 0.01     | -0.02    | -0.03    | 0.02     | -0.04    | -0.03    | ---      | -0.06    | -0.05    | -0.01    | 0.03     | -0.12    | 0.03     | 0.06     | -0.05    | 0.02     | 0.01     | 0.04     | 0.01     | 0.04     |
| <b>K</b> | -0.01    | -0.05    | -0.05    | -0.01    | 0.1      | 0        | -0.01    | ---      | -0.04    | 0        | 0.01     | 0        | -0.03    | 0.04     | -0.04    | -0.01    | -0.03    | -0.01    | 0.06     | -0.09    | 0.03     |
| <b>M</b> | -0.01    | 0.04     | 0        | 0.01     | ---      | -0.02    | 0.06     | ---      | -0.08    | 0.03     | -0.02    | 0.06     | ---      | 0.03     | -0.03    | 0.03     | 0.08     | ---      | -0.13    | -0.08    | ---      |
| <b>F</b> | 0.02     | 0.04     | -0.01    | 0.01     | -0.09    | -0.09    | 0.02     | ---      | 0.04     | 0.01     | -0.05    | -0.02    | -0.11    | -0.06    | 0.06     | 0.03     | -0.02    | -0.03    | -0.07    | -0.09    | -0.12    |
| <b>P</b> | -0.08    | -0.01    | 0.02     | -0.04    | -0.11    | -0.07    | -0.07    | ---      | -0.05    | -0.1     | -0.02    | -0.05    | -0.05    | -0.03    | -0.02    | -0.12    | -0.1     | -0.14    | -0.02    | -0.05    | -0.09    |
| <b>S</b> | 0.07     | 0.03     | 0.05     | 0.04     | 0.07     | 0.03     | 0.04     | ---      | -0.02    | 0.09     | 0        | 0        | 0.02     | 0        | 0.03     | 0.02     | 0        | 0.06     | 0.02     | 0.09     | 0.06     |
| <b>T</b> | 0.01     | -0.06    | 0        | 0.04     | 0.01     | 0        | 0.01     | ---      | 0.02     | 0.05     | 0.01     | 0        | 0.1      | 0.01     | -0.01    | 0.03     | 0.04     | 0.04     | 0.05     | 0        | 0.02     |
| <b>W</b> | -0.11    | -0.1     | -0.11    | 0.01     | ---      | 0.18     | 0.1      | ---      | -0.24    | -0.08    | -0.01    | -0.05    | ---      | 0.16     | 0        | 0.02     | 0.07     | ---      | ---      | 0.08     | 0.24     |
| <b>Y</b> | 0.05     | 0.02     | -0.07    | 0.05     | 0.23     | -0.09    | 0        | ---      | 0.01     | 0.08     | -0.01    | -0.07    | ---      | -0.02    | -0.01    | 0.05     | 0.04     | 0.1      | -0.07    | -0.07    | -0.16    |
| <b>V</b> | 0.03     | 0.08     | 0.03     | 0.04     | -0.02    | 0.11     | 0.06     | ---      | 0.23     | 0.07     | 0.09     | 0.1      | 0.02     | 0.15     | 0.01     | 0.04     | 0.07     | -0.15    | 0.1      | 0        | -0.07    |
| <b>X</b> | -0.12    | 0.12     | 0.09     | 0.07     | ---      | -0.19    | 0.04     | ---      | -0.07    | 0.19     | -0.01    | 0.06     | ---      | 0.05     | 0.01     | -0.02    | 0.02     | ---      | -0.01    | 0        | -0.07    |

Correction      i,i+1

**Atom   C $\alpha$**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.34     | 0.07     | 0.33     | 0.31     | 0.35     | 0.31     | 0.34     | 0.42     | -0.06    | -0.1     | 0.09     | 0.08     | 0.56     | 0.22     | -2.27    | 0.17     | 0.16     | -0.18    | -0.01    | -0.19    | 0.15     |
| <b>R</b> | 0.05     | 0.09     | 0.24     | 0.75     | -0.3     | 0.43     | 0.71     | 0.23     | 0.21     | 0.04     | 0.15     | -0.19    | 0.5      | 0.2      | -2.28    | 0.11     | 0.25     | -0.36    | 0.19     | 0.05     | -0.32    |
| <b>N</b> | -0.12    | 0.13     | 0.47     | 0.61     | 1.56     | -0.14    | 0.11     | 0.27     | 0.08     | 0.15     | 0        | 0.19     | 0.5      | 0.12     | -2.15    | 0.13     | 0.33     | -0.15    | -0.04    | 0.15     | 0.07     |
| <b>D</b> | -0.14    | -0.12    | 0.3      | 0.94     | 0.19     | 0.5      | 0.23     | 0.04     | 0.33     | 0.34     | 0.06     | 0.09     | 0.23     | -0.18    | -2.51    | 0.17     | 0.43     | 0.43     | 0.01     | 0.22     | 0.56     |
| <b>C</b> | -0.35    | 0.52     | 0.25     | 1.02     | --       | 0.64     | 0.22     | 0.63     | 0.49     | -0.24    | 0.13     | 0.74     | --       | 0.45     | -2.1     | 0.21     | -0.44    | --       | -0.16    | -1.11    | --       |
| <b>Q</b> | 0.07     | 0        | 0.44     | 0.47     | 0.04     | 0.22     | -0.04    | 0.35     | 1.04     | -0.06    | 0.11     | 0.28     | 0.34     | -0.01    | -2.21    | 0.6      | 0.02     | -0.67    | 0.38     | -0.29    | --       |
| <b>E</b> | -0.18    | 0.25     | 0.46     | 0.59     | 0.46     | 0.4      | 0.29     | 0.24     | 0.24     | -0.1     | -0.09    | 0.12     | 0.48     | -0.1     | -2.7     | 0.45     | 0.18     | -0.23    | -0.48    | -0.31    | 0.91     |
| <b>G</b> | -0.09    | 0.09     | 0.27     | 0.24     | 0.1      | 0        | -0.09    | 0.04     | -0.03    | 0.15     | 0.12     | 0.04     | 0        | 0.03     | -0.82    | 0.01     | -0.08    | 0.01     | -0.2     | 0.11     | -0.01    |
| <b>H</b> | -0.09    | 0.64     | 0.43     | 0.37     | 0.94     | 0.74     | 0.19     | 0.45     | -0.03    | 0.4      | 0.48     | 0.29     | 0.33     | -0.63    | -2.19    | 0.23     | 0.13     | -0.29    | 0.62     | -0.2     | --       |
| <b>I</b> | -0.14    | 0.41     | 0.11     | 0.22     | 0.44     | 0.74     | 0.53     | 1.07     | -0.6     | 0.34     | 0.67     | 0.35     | 0.4      | 1.09     | -2.54    | -0.01    | 0.14     | 0.89     | -0.01    | 0.1      | -0.34    |
| <b>L</b> | 0.14     | 0.18     | 0.15     | 0.26     | 0.72     | 0.1      | 0.36     | 0.48     | 0.4      | 0.28     | 0.64     | 0.01     | 0.65     | 0.27     | -2.35    | 0.12     | -0.01    | 0.89     | 0.26     | 0.43     | 0.68     |
| <b>K</b> | -0.05    | 0.16     | 0.66     | 0.72     | 0.47     | 0.67     | 0.23     | 0.44     | 0.59     | -0.52    | -0.11    | 0.17     | 0.11     | -0.01    | -2.72    | 0.09     | 0.2      | 0.28     | -0.18    | -0.18    | -0.35    |
| <b>M</b> | 0.24     | 0.59     | 0.2      | 0.42     | --       | 0.15     | 0.56     | -0.09    | -0.04    | 0.32     | 0.31     | 0.5      | 0.43     | 0.01     | -2.11    | -0.31    | 0.3      | --       | 1.38     | -0.03    | --       |
| <b>F</b> | -0.3     | -0.12    | 0.21     | -0.04    | 0.41     | 0.58     | 0.69     | 0.94     | 0.19     | -0.2     | 0.25     | -0.14    | 0.34     | 1.36     | -2.34    | -0.02    | -0.39    | --       | 0.24     | 0.41     | --       |
| <b>P</b> | -0.21    | 0.08     | 0.32     | 0.35     | -0.51    | 0.16     | 0.25     | 0.38     | 0.3      | -0.21    | -0.1     | -0.03    | 0.37     | -0.07    | -2.08    | 0.21     | 0.15     | 0.28     | 0.28     | -0.38    | -0.22    |
| <b>S</b> | -0.27    | 0.17     | 0.6      | 0.35     | 0.59     | 0.25     | 0.01     | 0.28     | 0.15     | 0        | -0.09    | 0.38     | 0.3      | -0.1     | -2.3     | 0.31     | 0.34     | 0.02     | 0.21     | -0.18    | -0.41    |
| <b>T</b> | -0.12    | 0.16     | 0.57     | 0.27     | 0.62     | 0.25     | -0.12    | 0.33     | 0.2      | -0.2     | 0.06     | 0.35     | -0.31    | 0.05     | -2.1     | 0.19     | 0.47     | 0.22     | 0.26     | 0.2      | -0.17    |
| <b>W</b> | -0.01    | 0.86     | -0.08    | 0.34     | --       | -0.27    | 1.02     | 0.05     | --       | -0.91    | -0.29    | -0.54    | --       | -1.06    | -2.4     | 0.7      | 1.36     | --       | --       | 0.13     | -0.85    |
| <b>Y</b> | 0.18     | 0.58     | 0.23     | 0.16     | 0.55     | -0.06    | 0.38     | 0.65     | -0.32    | -0.28    | 0.1      | 0.1      | 0.59     | 0.82     | -2.46    | 0.03     | -0.1     | -0.8     | 0.93     | 0.63     | --       |
| <b>V</b> | -0.06    | -0.09    | 0.43     | 0.29     | 1.34     | 0.14     | 0.07     | 1.29     | 0.59     | -0.09    | 0.56     | 0.04     | 0.88     | 0.15     | -2.64    | 0.06     | 0.17     | 0.24     | -1.31    | 0.09     | --       |
| <b>X</b> | 0.04     | 1.23     | 0.15     | -0.14    | --       | --       | -0.28    | 0.09     | 2.13     | --       | --       | 0.72     | --       | --       | -1.33    | 0.15     | 0.02     | --       | --       | --       | --       |

Correction      i,i+1

**Atom   C $\beta$**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.08    | 0.34     | 0.27     | -0.04    | 0        | 0.02     | 0.04     | -0.44    | -0.02    | 0.11     | 0.27     | 0.18     | -0.45    | 0.05     | -0.87    | 0.27     | 0.25     | -0.58    | -0.12    | 0.64     | 0.34     |
| <b>R</b> | 0.33     | -0.07    | 0.06     | -0.19    | 0.82     | -0.19    | 0.17     | -0.11    | 0.22     | 0.07     | -0.11    | -0.2     | -0.34    | 0.28     | -0.53    | -0.01    | 0.22     | 0.26     | 0.18     | 0.33     | -0.1     |
| <b>N</b> | 0.05     | 0        | -0.2     | 0.31     | 0.06     | 0.05     | 0.33     | -0.25    | -0.32    | -0.37    | -0.2     | -0.11    | 0.05     | 0.06     | 0.35     | 0.27     | -0.07    | 0.1      | -0.37    | 0.04     | 0.3      |
| <b>D</b> | 0.01     | 0.14     | -0.34    | 0.24     | -0.1     | -0.21    | -0.03    | -0.37    | -0.25    | 0.3      | -0.06    | -0.17    | -0.06    | -0.01    | 0.6      | 0.05     | -0.1     | 0.43     | 0.26     | -0.1     | 0.84     |
| <b>C</b> | 0        | 0.01     | 0.85     | 1.39     | ---      | -0.71    | 0.75     | 0.28     | 0.96     | -0.99    | 0        | -0.52    | ---      | 0.87     | -0.49    | -0.14    | -0.7     | ---      | -0.95    | 1.87     | ---      |
| <b>Q</b> | -0.37    | -0.04    | -0.04    | 0.23     | -0.03    | -0.2     | 0.06     | -0.34    | -0.88    | 0.24     | -0.13    | 0.16     | -0.09    | 0.1      | -0.23    | -0.1     | 0.46     | 0.11     | -0.21    | 0.91     | ---      |
| <b>E</b> | -0.1     | -0.05    | -0.06    | -0.1     | 0.36     | -0.22    | -0.12    | -0.28    | -0.1     | 0.43     | 0.18     | 0.2      | 0.01     | 0.22     | -0.14    | -0.07    | 0.18     | 0.64     | 0.06     | 0.2      | ---      |
| <b>G</b> | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      |
| <b>H</b> | -0.08    | 0.51     | 0.01     | -0.1     | 0.74     | -0.27    | 0.07     | -0.23    | -0.52    | 0.14     | -0.64    | 0.57     | -0.34    | -0.47    | 0.15     | 0.11     | 0.15     | 0.9      | 0.64     | 0.59     | ---      |
| <b>I</b> | 0.18     | -0.06    | 0.33     | 0.09     | 0.21     | -0.25    | -0.14    | -0.54    | 0.52     | 0.28     | -0.38    | -0.04    | -0.81    | 0.23     | 0.01     | -0.05    | 0.14     | -0.44    | 0.23     | 0.03     | 1.19     |
| <b>L</b> | -0.05    | 0.24     | 0.05     | 0.17     | 0.34     | -0.08    | 0.02     | -0.16    | 0.25     | 0        | -0.32    | -0.06    | 0.02     | 0.35     | -0.57    | 0.38     | 0.17     | -0.15    | 0.22     | -0.01    | 0.62     |
| <b>K</b> | 0.23     | -0.14    | 0.29     | -0.2     | 0.38     | -0.35    | 0.41     | -0.48    | -0.51    | 0.25     | -0.04    | -0.13    | -0.04    | 0.07     | 0.01     | 0.11     | 0.2      | 0.49     | 0.2      | 0.08     | 0.76     |
| <b>M</b> | -0.51    | -0.2     | 0.45     | 0.05     | ---      | -0.03    | 0.04     | -0.6     | 0.03     | 0.14     | -0.51    | -0.15    | 0.13     | -1.03    | -0.11    | 0.94     | 0.54     | ---      | -0.31    | -0.02    | ---      |
| <b>F</b> | -0.07    | 0.14     | 0.1      | 0.34     | 0.99     | -0.21    | 0.29     | -0.24    | -0.14    | -0.08    | 0.02     | 0.23     | -0.27    | 0.26     | -0.5     | -0.11    | 0.23     | ---      | -0.68    | 0.08     | ---      |
| <b>P</b> | 0.14     | 0.15     | 0.02     | -0.05    | 0.04     | 0.2      | 0.14     | -0.22    | 0.02     | 0.21     | 0.03     | 0.09     | 0.06     | -0.19    | -0.98    | 0.11     | 0.23     | -0.37    | -0.09    | 0.02     | 0.62     |
| <b>S</b> | 0.11     | 0.01     | -0.25    | -0.12    | 0.17     | -0.16    | 0.17     | 0.07     | -0.21    | 0.27     | -0.12    | 0.33     | -0.17    | 0.02     | -0.58    | 0.08     | 0.01     | 0.05     | 0.13     | 0.2      | -0.32    |
| <b>T</b> | -0.09    | 0.39     | -0.19    | 0.07     | -0.05    | -0.44    | 0.5      | -0.03    | 0.18     | 0.56     | -0.06    | 0.34     | 0.02     | 0.04     | -0.34    | 0.12     | -0.36    | -1.82    | 0.47     | -0.36    | -0.55    |
| <b>W</b> | -2.28    | -0.97    | 0.32     | -0.54    | ---      | 0.75     | 0.01     | -0.14    | ---      | 0.09     | 0.17     | 0.24     | ---      | -0.32    | -0.32    | 0.14     | 1.1      | ---      | ---      | 0.15     | 0.67     |
| <b>Y</b> | 0.01     | -0.38    | 0.11     | 0.28     | 0.43     | -0.3     | 0.11     | -0.23    | 0.07     | 0.65     | 0.12     | -0.23    | 0.91     | 0.07     | -0.73    | 0.03     | 0.4      | -0.5     | -0.24    | 0.47     | ---      |
| <b>V</b> | 0.15     | 0.17     | 0.03     | -0.02    | 0.25     | -0.22    | 0.05     | -0.64    | -0.25    | 0.14     | -0.15    | 0.11     | -0.41    | 0.1      | 0.06     | -0.07    | 0.21     | 0.16     | 0.81     | 0.21     | ---      |
| <b>X</b> | 0.15     | 0.83     | 0.6      | -0.28    | ---      | ---      | -0.7     | 0.62     | 0.51     | ---      | ---      | -0.13    | ---      | ---      | -0.32    | 0.8      | -0.64    | ---      | ---      | ---      | ---      |



Correction      i,i+1

**Atom    C**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.03    | -0.12    | 0.03     | -0.26    | -0.19    | 0.44     | 0.55     | 0.62     | -0.41    | -0.15    | -0.04    | 0.14     | -0.06    | -0.73    | -3.89    | 0.2      | 0.31     | -0.44    | -0.37    | -0.06    | -0.17    |
| <b>R</b> | -0.02    | 0.07     | -0.01    | 0.13     | -0.17    | 0.16     | 0.32     | -0.04    | 0.31     | -0.46    | -0.02    | 0.35     | 0.19     | 0.02     | -1.47    | 0.33     | 0.33     | -0.49    | 0.01     | -0.24    | ---      |
| <b>N</b> | 0.02     | -0.1     | -0.02    | 0.07     | 0.24     | -0.06    | 0.21     | 0.88     | -0.05    | -0.26    | -0.31    | -0.17    | -0.68    | -0.41    | -1.61    | 0.3      | 0.25     | 0.06     | -0.45    | 0        | -0.38    |
| <b>D</b> | -0.04    | 0.07     | -0.16    | -0.1     | -0.14    | 0.1      | 0.14     | 0.58     | 0.14     | -0.33    | -0.09    | 0.08     | 0.08     | -0.33    | -1.18    | 0.08     | 0.29     | -0.04    | -0.24    | -0.34    | -1.23    |
| <b>C</b> | 0.44     | 0.49     | 0.26     | 1.07     | ---      | -0.2     | -0.05    | 0.84     | 0.73     | ---      | -0.79    | 0.78     | ---      | -2.29    | -0.88    | -0.33    | -0.13    | ---      | ---      | 0.43     | ---      |
| <b>Q</b> | -0.21    | -0.11    | 0.23     | -0.06    | 0.29     | 0.35     | -0.04    | 0.58     | 0.13     | -0.17    | 0.03     | 0.28     | -0.22    | -0.43    | -1.99    | 0.45     | 0.07     | -0.32    | -0.28    | 0.02     | ---      |
| <b>E</b> | -0.33    | 0.17     | -0.11    | 0.01     | 0.09     | -0.08    | 0.29     | 0.55     | 0.07     | -0.11    | -0.09    | -0.04    | 0.14     | -0.29    | -1.88    | 0.46     | 0.13     | -0.46    | -0.42    | -0.27    | ---      |
| <b>G</b> | -0.07    | 0.05     | 0.16     | 0.01     | 0.29     | -0.74    | -0.23    | 0.61     | -0.06    | -0.01    | 0.29     | -0.13    | 0.36     | 0.14     | -2.83    | 0.34     | 0.29     | 0        | -0.01    | -0.06    | 0.58     |
| <b>H</b> | -0.31    | -0.01    | 0.17     | 0.23     | 0.48     | -0.21    | 0.04     | 0.97     | -0.67    | 1.55     | 0.25     | -0.15    | 0.34     | -0.56    | -0.99    | 0.06     | 0.28     | -0.52    | -0.23    | 0.2      | ---      |
| <b>I</b> | -0.16    | 0.25     | -0.21    | -0.64    | 0.62     | 0.21     | 0.08     | 1.16     | -0.23    | 0.21     | -0.03    | 0.03     | 0.61     | -0.51    | -1.34    | 0.05     | 0.05     | 1.09     | -0.1     | -0.08    | ---      |
| <b>L</b> | -0.16    | 0.15     | -0.12    | -0.12    | 0.62     | 0.01     | 0.27     | 0.99     | 0        | -0.13    | 0.12     | -0.18    | 0.44     | -0.53    | -1.88    | 0.21     | 0.07     | 0.07     | -0.06    | -0.04    | ---      |
| <b>K</b> | -0.24    | -0.14    | -0.1     | 0.06     | 0.02     | 0.17     | 0.15     | 0.68     | -0.3     | -0.36    | -0.1     | 0.29     | -0.14    | -0.2     | -2.83    | 0.1      | 0.35     | -0.07    | -0.27    | -0.22    | -0.19    |
| <b>M</b> | -0.04    | 0.36     | -0.41    | -0.28    | ---      | -0.07    | 0.33     | 0.86     | ---      | 0.28     | 0.35     | 0.17     | ---      | -0.56    | -1.66    | -0.19    | 0.19     | ---      | -0.32    | -0.47    | ---      |
| <b>F</b> | -0.44    | 0.07     | -0.05    | 0.12     | 0.55     | 0.04     | -0.06    | 1.13     | 0.13     | -0.59    | -0.59    | 0.08     | 0.95     | -0.4     | -1.36    | -0.11    | -0.05    | ---      | -0.48    | -0.02    | ---      |
| <b>P</b> | -0.12    | 0.18     | -0.27    | -0.13    | -0.03    | 0        | 0.18     | 0.6      | 0.14     | -0.22    | -0.37    | 0.04     | -0.22    | -0.19    | -0.45    | 0.32     | -0.25    | -0.12    | -0.36    | -0.24    | -0.08    |
| <b>S</b> | -0.11    | -0.03    | -0.13    | -0.37    | 0.13     | 0.24     | 0.05     | 0.49     | -0.35    | -0.1     | -0.06    | 0.24     | 0.22     | -0.58    | -1.21    | 0.2      | 0.14     | -0.53    | -0.21    | -0.26    | ---      |
| <b>T</b> | -0.02    | 0.03     | 0.1      | -0.66    | -0.2     | 0.09     | 0.27     | 0.86     | 0.1      | -0.21    | -0.16    | 0.16     | 0.2      | -0.31    | -1.6     | 0.16     | 0.23     | -0.2     | -0.19    | -0.19    | -0.17    |
| <b>W</b> | 0.48     | ---      | 0.34     | -0.64    | ---      | 0.08     | 0.62     | 0.34     | ---      | -1.15    | -0.19    | 0.26     | ---      | ---      | ---      | 0.42     | 0.1      | ---      | ---      | -0.4     | ---      |
| <b>Y</b> | -0.23    | -0.15    | -0.35    | -0.23    | 0.42     | -0.15    | 0.1      | 0.85     | -0.72    | -0.67    | 0.05     | -0.19    | ---      | -0.23    | -1.22    | 0.68     | -0.02    | ---      | 0.42     | 0.15     | ---      |
| <b>V</b> | -0.18    | 0.01     | -0.04    | -0.32    | 0.77     | -0.05    | 0.03     | 1.08     | -0.78    | -0.17    | -0.03    | -0.35    | -0.13    | -0.24    | -1.01    | 0.12     | 0.28     | -0.27    | -1.16    | 0.45     | ---      |
| <b>X</b> | -0.55    | ---      | ---      | -0.2     | ---      | ---      | 0.35     | -0.63    | ---      | ---      | ---      | 0.7      | ---      | ---      | ---      | 0.6      | 0.34     | ---      | ---      | ---      | ---      |

Correction      i,i+1

**Atom    N**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.41     | 0.51     | -0.12    | -0.19    | -1.29    | -0.07    | -0.36    | 0.54     | -0.24    | -0.79    | -0.7     | -0.61    | -0.08    | -0.96    | 1.69     | -0.09    | -0.25    | -0.49    | -0.16    | -0.03    | -1.28    |
| <b>R</b> | -0.34    | 0.14     | 0.26     | -0.6     | -0.48    | -0.07    | 0.32     | 0.46     | -0.47    | -0.23    | -0.94    | -0.12    | -0.58    | 0.08     | 1.07     | -0.02    | 0.03     | 0.16     | -0.45    | 0.28     | -1.7     |
| <b>N</b> | -0.69    | -0.57    | 0.69     | 0.16     | -0.59    | -0.52    | -0.26    | 0.88     | -0.65    | -0.43    | -0.37    | -0.3     | -0.17    | -0.23    | 1.05     | -0.07    | 0.54     | -0.94    | -1.03    | -0.31    | 0.28     |
| <b>D</b> | -0.07    | -0.16    | -0.49    | 0.61     | -0.5     | -0.9     | 0.25     | -0.64    | -0.36    | 0.07     | -0.25    | 0.24     | 0.33     | 0.02     | 1.4      | 0.29     | -0.66    | 0.4      | 0.12     | -0.4     | 1.06     |
| <b>C</b> | 0.34     | 0.84     | -0.59    | -0.26    | 1.04     | -0.75    | 0.34     | -1.66    | -3.61    | -0.56    | -0.6     | 1.15     | ---      | -1.24    | 3.99     | -0.67    | -1.66    | ---      | -0.03    | 0.37     | ---      |
| <b>Q</b> | 0.36     | -0.79    | -0.13    | 0.08     | -1.78    | -0.23    | -0.21    | 0.48     | -0.64    | 0.19     | -0.3     | 0.17     | -0.57    | -0.47    | 0.98     | -0.16    | 0.46     | 0.33     | 0.01     | -0.64    | 0.1      |
| <b>E</b> | -0.03    | -0.18    | 0.17     | 0.2      | -0.76    | -0.79    | -0.1     | 0.78     | 0.08     | -0.4     | -0.61    | -0.1     | -0.23    | -0.53    | 1.47     | 0.41     | -0.55    | -0.66    | -0.36    | -1       | 0.26     |
| <b>G</b> | 0.24     | -0.34    | 0.28     | 1.22     | 0.16     | 0.24     | 0.22     | 0.49     | -0.72    | -1.27    | -0.96    | -0.52    | -0.09    | -1.35    | 0.01     | 0.89     | 0.18     | 0.28     | -0.32    | -0.23    | 0.26     |
| <b>H</b> | -0.9     | 0.26     | -0.13    | -0.51    | 1.18     | -0.77    | -0.46    | 0.46     | 1.13     | -0.8     | -1.96    | 0.01     | 0.15     | -0.05    | 1.48     | 0.07     | -0.08    | -1.43    | -0.61    | -0.61    | ---      |
| <b>I</b> | -0.18    | 0.29     | 0.62     | 0.04     | -1.55    | -1.65    | 0.65     | -0.31    | 0.63     | -0.18    | -0.12    | 0.06     | 0.45     | -0.9     | 1.11     | -0.82    | 0.37     | -1.58    | -1.33    | 0.57     | -3.76    |
| <b>L</b> | 0.31     | -0.15    | -0.19    | 0.29     | -0.81    | -0.73    | 0.09     | -0.42    | 0.05     | -0.24    | -0.68    | -0.35    | 0.7      | -0.42    | 0.82     | 0.11     | 0.35     | 0.12     | -0.09    | 0.11     | -1.67    |
| <b>K</b> | -0.46    | -0.05    | 0.37     | 0.47     | 0.23     | -1.28    | 0.29     | 0.42     | -0.79    | -0.53    | -1.33    | 0.41     | -1.18    | -0.8     | 1.42     | 0.19     | -0.56    | -1.24    | -0.28    | 0.32     | 0.02     |
| <b>M</b> | -0.41    | -0.05    | -0.19    | -0.28    | ---      | 0.19     | -0.16    | -0.81    | -1.53    | -1.22    | -1.71    | -0.14    | -0.39    | -0.41    | 2.63     | 0.54     | -0.24    | ---      | -1.31    | 0.73     | ---      |
| <b>F</b> | -0.33    | -1.67    | 0.06     | -0.35    | 2.95     | -0.61    | 0.34     | 0.24     | 0.55     | -1.06    | -1.16    | 0.06     | -0.34    | 0.87     | 0.89     | 0.07     | -0.15    | ---      | 1.11     | -0.14    | ---      |
| <b>P</b> | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | 0.18     | ---      | ---      | ---      | ---      | ---      | ---      |
| <b>S</b> | -0.06    | -0.02    | 0        | -0.04    | -0.19    | -0.14    | 0.17     | 0.03     | -0.75    | -0.76    | -0.19    | 0.27     | -1.01    | -0.45    | 1.3      | -0.29    | -0.11    | 0.25     | 0.4      | -0.09    | -1.33    |
| <b>T</b> | 0.05     | 0.03     | -0.55    | -0.75    | 1.86     | -0.73    | 0.28     | -1.07    | -0.91    | -0.23    | 0.35     | 0.01     | -0.59    | 0.54     | 1.93     | 0.08     | 0.13     | 0.82     | -0.28    | -0.08    | -1.1     |
| <b>W</b> | -2.07    | -0.14    | 0.99     | -1.51    | ---      | -0.48    | 0.35     | 1.78     | ---      | -0.63    | -2.53    | 1.34     | ---      | -2.02    | 3.59     | 0.86     | 2.67     | ---      | ---      | -1.57    | -5.11    |
| <b>Y</b> | -0.21    | -0.22    | 0        | 0        | -2.13    | -1.06    | 1.25     | 0.23     | 0.94     | -1.34    | 0.46     | 1.04     | -2.37    | -1.45    | 0.65     | 0.05     | -0.19    | -3.52    | -0.57    | 0.29     | ---      |
| <b>V</b> | -0.78    | -0.13    | -0.01    | -0.54    | 1.1      | -0.09    | -0.17    | -0.04    | -0.08    | -0.94    | 0.54     | 0.57     | 1.3      | -0.78    | 1.3      | -0.24    | 0.22     | -1.34    | -1.82    | -0.36    | 0.48     |
| <b>X</b> | 1.15     | 0.05     | 0.31     | 1.18     | ---      | -2.83    | -1.31    | -1.14    | -2.62    | ---      | -1.26    | -1.79    | ---      | ---      | 2.04     | 0.45     | 1.32     | ---      | ---      | 0.18     | -2.84    |

Correction      i,i+1

**Atom    H**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.03     | 0.06     | 0.08     | 0.09     | -0.14    | -0.1     | 0        | 0.13     | -0.03    | -0.09    | -0.05    | -0.12    | 0.08     | -0.06    | -0.13    | -0.04    | 0.04     | -0.45    | 0.11     | -0.01    | 0.03     |
| <b>R</b> | 0        | 0        | 0.05     | -0.15    | 0.09     | 0.03     | 0.03     | 0.1      | -0.01    | -0.1     | -0.1     | 0.05     | 0.02     | 0.06     | -0.07    | 0.02     | 0.04     | -0.14    | -0.07    | 0.07     | 0        |
| <b>N</b> | -0.08    | -0.02    | 0.08     | 0.09     | 0.46     | -0.06    | -0.08    | 0.16     | -0.06    | -0.1     | -0.04    | 0.01     | 0.19     | -0.06    | -0.09    | 0.02     | 0.04     | -0.84    | 0.02     | 0.02     | -0.05    |
| <b>D</b> | -0.05    | -0.03    | -0.03    | 0.12     | 0.06     | 0.05     | 0.05     | 0.04     | 0.02     | -0.09    | -0.05    | -0.01    | -0.02    | -0.06    | -0.15    | 0.05     | 0.05     | -0.13    | 0.02     | 0.06     | 0.13     |
| <b>C</b> | -0.17    | 0.11     | -0.02    | -0.07    | 0.16     | -0.21    | -0.01    | 0.16     | -0.16    | 0.01     | -0.02    | 0.04     | --       | -0.09    | 0.05     | -0.03    | -0.19    | --       | 0.24     | 0.12     | --       |
| <b>Q</b> | 0.09     | -0.14    | -0.09    | 0.01     | 0.03     | 0.04     | 0.06     | 0.07     | 0.09     | 0.02     | -0.1     | 0.02     | -0.1     | 0.02     | -0.07    | 0.01     | 0.12     | -0.15    | 0.01     | -0.1     | 0.14     |
| <b>E</b> | -0.02    | 0        | 0.1      | 0.14     | 0.25     | -0.06    | 0.02     | 0.09     | -0.06    | -0.05    | -0.02    | -0.04    | -0.05    | -0.11    | -0.17    | 0.05     | 0.02     | 0.01     | -0.07    | -0.14    | 0.03     |
| <b>G</b> | -0.02    | 0        | 0        | 0.36     | 0.09     | 0.16     | 0.02     | 0.01     | -0.11    | -0.12    | -0.14    | 0.02     | 0.01     | -0.24    | -0.23    | 0.03     | 0.05     | 0.06     | -0.03    | -0.07    | 0        |
| <b>H</b> | -0.28    | 0.01     | 0.02     | 0.05     | 0.04     | -0.2     | -0.16    | 0.06     | 0.08     | -0.02    | -0.05    | 0.1      | 0.2      | -0.05    | -0.06    | 0.15     | 0.12     | -0.16    | -0.06    | -0.07    | 0.08     |
| <b>I</b> | 0.03     | -0.05    | 0.08     | 0.02     | 0.35     | -0.12    | 0.01     | 0.09     | -0.33    | -0.01    | 0.09     | 0.02     | 0.07     | -0.09    | -0.17    | 0.08     | 0.03     | 0.12     | -0.05    | 0.15     | -0.1     |
| <b>L</b> | -0.05    | -0.02    | -0.09    | 0.04     | 0.13     | -0.04    | 0        | 0.16     | 0.23     | 0.03     | -0.05    | -0.04    | 0.21     | -0.07    | -0.12    | 0.03     | -0.01    | -0.04    | -0.05    | -0.01    | 0.33     |
| <b>K</b> | -0.07    | -0.04    | -0.02    | 0.04     | 0.39     | 0.03     | 0.1      | 0.07     | -0.12    | -0.08    | -0.09    | 0.07     | 0.04     | -0.04    | -0.14    | 0.02     | 0.03     | 0.01     | -0.13    | -0.01    | 0.02     |
| <b>M</b> | -0.02    | 0        | -0.1     | 0.06     | --       | -0.14    | 0.07     | 0.12     | -0.23    | -0.28    | 0.01     | -0.03    | -0.18    | -0.21    | -0.18    | 0.12     | 0.08     | --       | 0.03     | 0.17     | --       |
| <b>F</b> | 0.04     | -0.09    | -0.07    | -0.04    | 0.26     | 0.01     | -0.09    | 0.38     | -0.11    | -0.23    | -0.22    | -0.01    | 0.21     | -0.04    | -0.09    | 0.03     | -0.11    | --       | 0.07     | 0.01     | 0.16     |
| <b>P</b> | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       |
| <b>S</b> | 0.02     | 0.02     | 0.02     | 0.04     | 0.24     | 0.07     | 0.03     | 0.03     | -0.11    | -0.14    | -0.05    | 0.01     | -0.06    | -0.1     | -0.14    | 0.02     | 0.12     | 0.02     | 0        | -0.03    | -0.1     |
| <b>T</b> | 0.02     | -0.05    | 0.04     | -0.02    | 0.4      | -0.11    | 0.2      | 0.02     | -0.03    | -0.06    | 0.05     | -0.08    | -0.09    | -0.09    | -0.07    | 0.04     | 0.06     | -0.05    | -0.02    | -0.1     | -0.23    |
| <b>W</b> | -0.19    | 0.03     | 0.24     | -0.21    | --       | -0.08    | 0.41     | 0.28     | --       | 0.04     | -0.12    | 0.22     | --       | -0.49    | -0.01    | 0.03     | 0.24     | -0.17    | -0.77    | -0.26    | -0.67    |
| <b>Y</b> | -0.03    | -0.08    | 0.01     | -0.01    | 0.3      | -0.34    | 0.19     | 0.09     | -0.06    | 0.02     | 0.01     | 0.09     | -0.33    | -0.17    | -0.18    | 0.1      | 0.17     | -0.54    | -0.13    | 0.07     | 0.1      |
| <b>V</b> | -0.1     | -0.03    | 0.08     | 0.03     | 0.3      | 0.03     | 0.01     | 0.11     | 0.05     | -0.11    | -0.03    | -0.07    | 0.2      | 0.03     | -0.1     | -0.03    | 0.04     | 0.1      | 0.01     | -0.1     | 0.1      |
| <b>X</b> | -0.19    | 0.22     | 0.04     | -0.05    | --       | -0.25    | -0.07    | -0.32    | -0.21    | -0.21    | -0.01    | 0.07     | -0.29    | 0.05     | 0.27     | 0.03     | 0.09     | --       | -0.06    | -0.01    | 0.05     |

Correction      i,i+1

**Atom   H $\alpha$**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.05    | 0.02     | -0.12    | -0.05    | 0.04     | -0.03    | -0.04    | -0.11    | 0.01     | 0.07     | 0.01     | 0        | -0.08    | -0.05    | 0.17     | 0.01     | 0.11     | -0.04    | -0.06    | 0.12     | 0.13     |
| <b>R</b> | -0.02    | 0.04     | -0.1     | -0.14    | 0.17     | -0.03    | -0.1     | -0.04    | -0.05    | -0.03    | 0.03     | -0.01    | -0.12    | -0.01    | 0.22     | -0.05    | 0.06     | 0.08     | -0.05    | 0.09     | 0.1      |
| <b>N</b> | -0.02    | -0.06    | -0.09    | -0.06    | 0.01     | 0.01     | -0.03    | -0.06    | -0.07    | -0.05    | -0.01    | -0.06    | -0.02    | 0        | 0.26     | 0.04     | 0.07     | -0.03    | -0.03    | 0.02     | 0        |
| <b>D</b> | -0.03    | -0.01    | -0.1     | -0.07    | 0.03     | -0.1     | -0.03    | -0.03    | -0.1     | 0.06     | 0        | -0.05    | -0.07    | 0.04     | 0.21     | 0.01     | 0.02     | 0.01     | 0.05     | 0.04     | 0.04     |
| <b>C</b> | 0.18     | -0.09    | -0.1     | -0.07    | 0.01     | -0.11    | 0.04     | 0.19     | -0.08    | 0.24     | 0.01     | 0.02     | --       | -0.18    | -0.03    | -0.02    | -0.23    | --       | -0.08    | 0.13     | --       |
| <b>Q</b> | -0.01    | -0.03    | -0.11    | -0.03    | 0.08     | -0.04    | -0.04    | -0.07    | -0.14    | -0.07    | -0.03    | -0.09    | -0.06    | -0.02    | 0.32     | -0.01    | 0.06     | 0.13     | -0.05    | 0.07     | -0.04    |
| <b>E</b> | 0.01     | -0.01    | -0.1     | -0.05    | 0.04     | -0.05    | -0.03    | -0.08    | -0.12    | 0.05     | -0.01    | -0.02    | -0.03    | -0.01    | 0.35     | -0.02    | 0.04     | 0.06     | 0.08     | 0.04     | 0.04     |
| <b>G</b> | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       |
| <b>H</b> | -0.09    | -0.05    | -0.04    | -0.04    | 0.05     | -0.16    | -0.03    | -0.06    | -0.07    | 0.05     | -0.09    | -0.1     | -0.02    | 0.11     | 0.12     | 0.07     | 0.19     | 0.03     | -0.03    | 0.12     | 0.26     |
| <b>I</b> | 0        | -0.02    | 0.01     | -0.07    | 0.18     | -0.12    | -0.08    | -0.13    | -0.08    | -0.03    | -0.12    | -0.07    | -0.08    | -0.17    | 0.15     | 0.13     | 0.14     | -0.18    | 0.19     | -0.01    | 0.17     |
| <b>L</b> | -0.03    | 0.05     | -0.06    | -0.07    | 0.09     | -0.01    | -0.07    | -0.06    | -0.04    | 0        | -0.03    | -0.01    | -0.08    | -0.14    | 0.19     | 0.07     | 0.08     | -0.23    | -0.11    | -0.01    | 0.06     |
| <b>K</b> | 0        | -0.04    | -0.06    | -0.11    | 0.05     | -0.08    | 0.01     | -0.11    | -0.07    | 0.14     | 0.01     | -0.04    | -0.02    | -0.01    | 0.24     | 0.04     | 0.07     | -0.01    | -0.04    | 0.07     | 0        |
| <b>M</b> | -0.05    | -0.1     | -0.06    | -0.06    | --       | 0        | -0.07    | -0.05    | -0.01    | -0.14    | -0.11    | -0.05    | -0.08    | 0        | 0.12     | 0.1      | 0.13     | --       | -0.2     | 0.12     | --       |
| <b>F</b> | -0.1     | 0.01     | -0.13    | 0        | -0.06    | -0.12    | -0.01    | -0.07    | 0        | 0.03     | -0.02    | -0.03    | 0.16     | -0.15    | 0.12     | 0.07     | 0.24     | -0.27    | -0.07    | -0.08    | 0.15     |
| <b>P</b> | -0.01    | 0.01     | -0.05    | -0.04    | 0.08     | 0        | -0.03    | -0.07    | -0.07    | 0.07     | -0.01    | -0.03    | -0.02    | -0.03    | 0.2      | -0.01    | 0.04     | -0.12    | -0.03    | 0.08     | 0.1      |
| <b>S</b> | -0.04    | -0.02    | -0.12    | -0.1     | 0.03     | -0.06    | 0.1      | -0.05    | -0.12    | 0.02     | -0.02    | -0.01    | -0.03    | 0        | 0.26     | -0.02    | 0.03     | 0.02     | -0.01    | 0.06     | 0.05     |
| <b>T</b> | 0.02     | -0.05    | -0.11    | -0.05    | 0.07     | -0.06    | -0.01    | -0.07    | -0.07    | 0.04     | 0.01     | -0.06    | 0.03     | -0.03    | 0.21     | 0        | 0.04     | -0.03    | -0.04    | 0.07     | -0.03    |
| <b>W</b> | -0.06    | -0.27    | -0.09    | -0.14    | --       | 0.13     | 0.04     | -0.11    | --       | 0.28     | -0.04    | 0.02     | --       | -0.01    | 0.02     | 0.06     | 0.13     | -0.03    | -0.31    | 0.05     | 0.24     |
| <b>Y</b> | 0.03     | -0.07    | -0.06    | -0.03    | 0.09     | -0.01    | -0.08    | -0.09    | -0.02    | 0.12     | 0.07     | -0.05    | -0.04    | -0.15    | 0.21     | -0.02    | 0.09     | -0.19    | -0.12    | 0.11     | 0        |
| <b>V</b> | -0.06    | 0.03     | -0.12    | -0.09    | -0.01    | -0.04    | 0        | -0.26    | -0.09    | -0.01    | -0.06    | -0.03    | -0.09    | -0.06    | 0.23     | 0        | 0.35     | 0.03     | 0.18     | 0.03     | -0.14    |
| <b>X</b> | -0.21    | -0.04    | -0.02    | 0.02     | --       | 0.02     | -0.2     | 0.02     | -0.12    | 0.21     | -0.07    | -0.11    | 0.03     | 0.07     | 0.11     | -0.03    | 0.12     | --       | 0.24     | -0.05    | 0.04     |

Correction      i-2,i

**Atom   Cα**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.39     | 0.14     | 0.25     | 0.26     | 0.18     | 0.22     | 0.42     | 0.1      | 0.7      | 0.39     | 0.08     | 0.27     | 0.4      | 0.06     | 0.53     | 0.15     | 0.16     | -0.85    | -0.13    | 0.59     | -0.1     |
| <b>R</b> | 0.57     | 0.38     | 0.16     | -0.03    | 0.82     | 0.35     | 0.36     | 0.32     | 0.64     | 0.47     | 0.27     | 0.57     | 0.85     | 0.29     | 0.45     | 0.1      | 0.38     | 0.57     | 0.05     | 0.16     | 0.31     |
| <b>N</b> | 0.34     | 0.5      | 0.16     | 0.21     | 0.67     | 0.15     | 0.46     | 0.12     | 0.33     | 0.57     | 0.49     | 0.22     | 0.03     | 0.41     | 0.45     | 0.48     | 0.23     | 0.75     | -0.1     | 0.27     | 0.21     |
| <b>D</b> | 0.29     | 0.77     | 0.14     | 0.28     | -0.18    | 0.19     | 0.33     | 0.16     | -0.04    | 0.89     | 0.59     | 0.27     | 0.4      | 0.6      | 0.25     | 0.92     | 1.29     | 1.11     | 0.19     | 0.39     | 0.33     |
| <b>C</b> | 0.57     | 1.06     | 0.53     | 1.03     | 1.55     | 0.28     | 1.01     | -0.01    | 1.11     | 0.95     | 1.39     | 0.81     | --       | 0.46     | 0.64     | 0.48     | 1.09     | -0.54    | 1.09     | 2.16     | --       |
| <b>Q</b> | 0.16     | 0.3      | 0.36     | 0.23     | 0.04     | 0.48     | 0.6      | 0.21     | -0.28    | 0.32     | 0.4      | 0.01     | 0        | 0.21     | 0.41     | 0.11     | 0.43     | 0.39     | 0.58     | 0.04     | 0.6      |
| <b>E</b> | 0.43     | 0.22     | 0.17     | 0.4      | 0.49     | 0.41     | 0.28     | 0.18     | -0.01    | 0.62     | 0.31     | 0.27     | 0.59     | 0.27     | 0.17     | 0.31     | 0.25     | -0.46    | 0.41     | 0.68     | 0.56     |
| <b>G</b> | 0.28     | 0.1      | 0        | 0.26     | 0.48     | 0.06     | 0.25     | 0.12     | -0.2     | 0.42     | 0.19     | 0.02     | -0.06    | 0.56     | 0.19     | 0.14     | 0.19     | 0.55     | 0.38     | 0.27     | 0.04     |
| <b>H</b> | 0.41     | 0.5      | 0.33     | 0.44     | --       | 0.59     | 0.7      | 0.07     | 0.22     | 0.29     | 0.27     | 0.49     | 0        | 0.53     | 0.27     | 0.49     | 0.11     | --       | -0.79    | 0.8      | 0.04     |
| <b>I</b> | 0.4      | 0.86     | 0.39     | 0.45     | 1.07     | 0.24     | 0.97     | 0.14     | 0.48     | 0.42     | 0.36     | 1.16     | 0.34     | 0.83     | 0.6      | 0.23     | 0.7      | 0.66     | 0.44     | 0.14     | 0.55     |
| <b>L</b> | 0.37     | 0.46     | 0.26     | 0.28     | 0.21     | 0.26     | 0.6      | 0.19     | 0.27     | -0.05    | 0.31     | 0.74     | 0.29     | 0        | 0.72     | 0.46     | 0.19     | -0.2     | -0.22    | 0.48     | -0.06    |
| <b>K</b> | 0.41     | 0.22     | 0.31     | 0.39     | 0.6      | 0.31     | 0.39     | 0.12     | 0.17     | 0.56     | 0.25     | 0.27     | 0.11     | -0.14    | 0.35     | 0.35     | 0.27     | 0.06     | 0.09     | 0.67     | --       |
| <b>M</b> | 0.65     | 0.29     | 0.41     | 0.23     | 0.11     | 0.68     | 0.15     | 0.43     | 0.17     | 0.51     | 0.11     | 0.54     | -0.21    | 0.58     | 0.24     | 0.16     | 0.42     | --       | 0.09     | 0.32     | 0.22     |
| <b>F</b> | 0.26     | 0.11     | 0.13     | 0.1      | -0.1     | 0.27     | 0.57     | 0.21     | 1.03     | 0.41     | 0.37     | 0.57     | -0.34    | 0.57     | 0.67     | -0.14    | 0.42     | --       | -0.01    | 0.12     | 0.15     |
| <b>P</b> | 0.25     | -0.1     | 0.02     | 0.04     | 0.9      | -0.01    | 0.23     | -0.03    | 0.61     | 0.35     | 0.23     | -0.12    | -0.28    | 0.25     | 0.38     | 0.3      | -0.01    | -0.14    | 0.33     | 0.69     | --       |
| <b>S</b> | 0.39     | 0.35     | -0.17    | 0.27     | 0.07     | 0.24     | 0.51     | 0.23     | 0.52     | 0.23     | 0.41     | 0.37     | -0.03    | -0.09    | 0.26     | 0.34     | 0.22     | 0.27     | 0.64     | 0.4      | 0.21     |
| <b>T</b> | 0.41     | 0        | 0.19     | 0.2      | 0.25     | 0.27     | 0.38     | 0.2      | -0.19    | 0.12     | 0.42     | 0.4      | -0.2     | 0.13     | 0.29     | 0.24     | 0.2      | 0.33     | 0.49     | 0.36     | 0.49     |
| <b>W</b> | 0.38     | 0.16     | 0.32     | 0.34     | 0.07     | -0.13    | 0.87     | 0.1      | -0.15    | 1.07     | 0.76     | 0.76     | --       | 0.51     | 0.03     | 0.49     | 0.09     | --       | 0.56     | 1.59     | --       |
| <b>Y</b> | 0.55     | -0.21    | 0.08     | 0.36     | 0.11     | 0.66     | 0.94     | 0.04     | 0.11     | 0.67     | 0.49     | 0.71     | -0.27    | 0.49     | 0.26     | 0.68     | 0.4      | -0.09    | -0.15    | 0.69     | -0.15    |
| <b>V</b> | 0.47     | 0.52     | 0.16     | 0.32     | 0.72     | 0.25     | 0.6      | 0.12     | 0.53     | -0.01    | 0.07     | 0.52     | -0.33    | 0.69     | 0.51     | 0.3      | 0.21     | 0.22     | 0.17     | 0.33     | 0.57     |
| <b>X</b> | --       | 0.04     | 0.2      | 0.04     | --       | 0.27     | --       | 0.66     | 0.17     | 0.23     | 0.23     | 0.34     | -0.2     | 0        | 0.11     | 0.23     | 1.01     | 0.22     | --       | --       | 0.22     |

Correction i-2,i

Atom Cβ

|   | A     | R     | N     | D     | C     | Q     | E     | G   | H     | I     | L     | K     | M     | F     | P     | S     | T     | W     | Y     | V     | X     |
|---|-------|-------|-------|-------|-------|-------|-------|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| A | -0.53 | -0.17 | -0.4  | -0.27 | 1.26  | -0.06 | -0.44 | --- | -0.34 | -0.25 | -0.25 | -0.2  | -0.79 | -0.14 | -0.06 | -0.09 | 0.06  | -0.31 | -0.44 | -0.43 | -0.18 |
| R | -0.41 | -0.13 | -0.3  | -0.58 | 0.19  | -0.45 | -0.24 | --- | 0.59  | -0.12 | -0.39 | -0.08 | -0.46 | -0.03 | -0.02 | -0.16 | -0.04 | 0.23  | -0.84 | -0.15 | 0.2   |
| N | -0.46 | -0.22 | -0.16 | -0.49 | 0.81  | -0.11 | -0.49 | --- | -0.52 | -0.3  | -0.42 | -0.13 | -1.24 | -0.63 | 0.12  | -0.25 | 0.02  | -0.72 | -0.89 | -0.07 | 0     |
| D | -0.18 | -0.11 | -0.33 | -0.27 | 1.42  | -0.4  | -0.23 | --- | -0.5  | -0.4  | -0.24 | -0.31 | -0.41 | -0.77 | 0.03  | -0.36 | -0.5  | 0.02  | -0.33 | -0.24 | -0.18 |
| C | 0.6   | -0.36 | 0.22  | -0.15 | -1.32 | -0.52 | -0.28 | --- | 0.31  | -1.03 | -0.28 | 0.41  | ---   | -0.41 | -0.64 | -0.34 | 0.04  | -1.31 | -1    | 0.01  | ---   |
| Q | -0.41 | -0.31 | -0.44 | -0.46 | 0.11  | -0.38 | -0.54 | --- | 0.18  | -0.35 | -0.31 | 0.01  | 0.16  | -0.33 | -0.06 | -0.06 | -0.06 | -1.17 | -0.44 | -0.46 | -0.18 |
| E | -0.23 | -0.4  | -0.39 | -0.28 | 0.62  | -0.5  | -0.34 | --- | -0.2  | -0.38 | -0.17 | -0.53 | -0.46 | -0.45 | 0.12  | -0.26 | -0.56 | -0.36 | -0.61 | -0.14 | -0.48 |
| G | -0.07 | -0.11 | -0.14 | 0.06  | -0.21 | -0.07 | -0.25 | --- | 0.02  | -0.16 | -0.25 | -0.01 | -0.28 | -0.35 | -0.04 | -0.1  | -0.24 | -0.17 | -0.09 | -0.15 | ---   |
| H | -0.08 | -0.74 | -0.68 | -0.25 | ---   | -0.59 | -0.47 | --- | -0.42 | -0.11 | -0.3  | -0.06 | -0.43 | -0.8  | -0.12 | 0.24  | -0.14 | ---   | -1.45 | -0.47 | ---   |
| I | -0.53 | -0.31 | -0.17 | -0.27 | 0.49  | -0.65 | -0.27 | --- | 0.11  | -0.16 | -0.12 | -0.48 | -0.36 | 0.43  | 0.05  | -0.15 | -0.57 | -0.22 | -0.32 | -0.19 | ---   |
| L | -0.09 | -0.49 | -0.39 | -0.43 | 0.52  | -0.25 | -0.49 | --- | -0.16 | 0.09  | -0.29 | -0.22 | 0.14  | -0.44 | -0.09 | -0.2  | -0.13 | -0.46 | -0.44 | -0.4  | ---   |
| K | -0.19 | -0.52 | -0.34 | -0.45 | -0.25 | -0.46 | -0.29 | --- | -0.49 | -0.32 | -0.17 | -0.34 | 0.84  | -0.47 | -0.12 | -0.22 | -0.54 | -0.01 | -0.17 | -0.1  | -0.18 |
| M | -0.45 | -0.02 | -0.4  | -0.34 | -0.93 | -0.34 | -0.19 | --- | -0.57 | -0.33 | -0.55 | 0.04  | 0.03  | -0.4  | -0.33 | -0.25 | -0.21 | ---   | -0.12 | -0.07 | ---   |
| F | -0.07 | 0.19  | 0.09  | -0.43 | 0.7   | -0.62 | -0.26 | --- | -0.57 | 0.26  | -0.15 | -0.13 | -0.42 | -0.48 | -0.22 | -0.13 | 0.18  | -0.72 | 0.04  | -0.18 | ---   |
| P | -0.2  | 0.04  | -0.52 | -0.37 | 0.59  | 0.22  | -0.23 | --- | -0.17 | -0.36 | -0.34 | -0.46 | 0.16  | -0.56 | 0.05  | -0.3  | 0.13  | -0.69 | -0.52 | -0.3  | 0.27  |
| S | -0.35 | -0.21 | -0.36 | -1.28 | 0.59  | -0.44 | -0.29 | --- | -0.19 | -0.33 | -0.27 | -0.11 | 0.23  | -0.21 | 0.04  | -0.29 | -0.04 | -0.4  | -0.43 | -0.24 | -0.34 |
| T | -0.12 | 0.1   | -0.06 | -0.11 | -0.47 | -0.08 | -0.17 | --- | 0.06  | -0.5  | -0.12 | 0.07  | -0.24 | -0.51 | 0.04  | -0.04 | 0.05  | -0.08 | -0.3  | -0.34 | -0.17 |
| W | -0.03 | -0.01 | 0.02  | -0.54 | 1.38  | 0.2   | -0.4  | --- | 0.71  | 0.32  | -0.62 | -0.43 | ---   | -0.35 | -0.17 | -0.42 | 0.17  | ---   | ---   | -0.7  | ---   |
| Y | -0.52 | -0.42 | -0.46 | -0.47 | -0.12 | -0.42 | -0.58 | --- | -0.1  | -0.6  | -0.22 | -0.12 | -0.41 | -0.67 | -0.02 | -0.13 | -1.25 | 0.43  | -0.9  | -0.55 | ---   |
| V | -0.13 | -0.16 | -0.37 | -0.06 | 0.75  | -0.31 | -0.1  | --- | -0.44 | 0.28  | -0.07 | 0.02  | -0.09 | -0.16 | -0.16 | -0.11 | -0.39 | -0.51 | -0.14 | -0.23 | 0.27  |
| X | ---   | ---   | -0.09 | -0.18 | ---   | -0.08 | -0.14 | --- | ---   | -0.56 | -0.07 | -0.37 | ---   | 0.21  | -0.7  | 0.24  | 0.13  | ---   | 0.19  | -0.17 | ---   |

Correction      i-2,i

**Atom    C**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.34     | 0.09     | 0.18     | 0.26     | 0.75     | 0.13     | 0.12     | 0.2      | 0.1      | 0.43     | -0.17    | 0.22     | 0.55     | 0.46     | 0.26     | 0.04     | 0.53     | -0.19    | 0.16     | 0.51     | 0.87     |
| <b>R</b> | 0.24     | 0.18     | 0.14     | 0.19     | 0.58     | -0.04    | 0.32     | 0.28     | 0.23     | 0.31     | 0.28     | 0.38     | 1        | -0.1     | 0.26     | 0.24     | 0.33     | 0.62     | 0.05     | 0.41     | 0.23     |
| <b>N</b> | 0.41     | 0.29     | 0.41     | 0.23     | 0.08     | 0.01     | 0.33     | 0.02     | -0.1     | 0.2      | 0.06     | 0.18     | 0.56     | 0.45     | 0.26     | -0.12    | 0.16     | -0.11    | 0.33     | 0.21     | 0.08     |
| <b>D</b> | 0.31     | 0.22     | 0.36     | 0.42     | -0.04    | 0.3      | 0.38     | 0.29     | -0.07    | 0.19     | 0.31     | 0.32     | 0.7      | -0.06    | 0.24     | 0.34     | 0.71     | 0.54     | -0.01    | 0.15     | 0.59     |
| <b>C</b> | 0.39     | 0.35     | 0.32     | 0.28     | 0.76     | 0.69     | 0.64     | -1.85    | 0.48     | 0.07     | 0.42     | 0.68     | ---      | 0.12     | 0.29     | 0.92     | 0        | -0.53    | 0.61     | 0.89     | ---      |
| <b>Q</b> | 0.11     | -0.02    | 0.08     | 0.16     | -1.02    | 0.15     | 0.18     | 0.13     | -0.52    | -0.03    | 0.16     | -0.14    | 0.62     | -0.02    | 0.06     | -0.03    | -0.71    | 0.5      | 0.43     | 0.1      | 0.66     |
| <b>E</b> | 0.35     | 0.01     | 0.15     | 0.27     | 0.75     | -0.1     | 0.28     | 0.12     | 0.21     | 0.4      | 0        | 0.02     | 0.76     | 0.45     | 0.21     | 0.28     | 0.42     | -0.15    | 0.14     | 0.18     | 0.42     |
| <b>G</b> | 0.27     | 0.15     | 0.33     | 0.08     | 0.51     | 0.17     | 0.23     | 0.04     | 0.28     | 0.22     | 0.06     | 0.1      | 0.46     | 0.3      | 0.13     | 0.2      | 0.4      | -0.18    | 0.42     | 0.22     | -0.41    |
| <b>H</b> | 0.23     | 0.05     | -0.1     | 0.23     | ---      | 0.16     | 0.14     | 0.14     | -0.11    | 0.34     | 0.18     | 0.23     | 0.83     | 0.45     | 0.19     | 0.09     | 0.08     | ---      | ---      | 0.37     | ---      |
| <b>I</b> | 0.23     | 0.32     | 0.22     | 0.36     | 0.41     | 0.16     | 0.56     | 0.18     | 0.35     | -0.08    | 0.34     | 0.27     | 0.61     | 0.32     | 0.12     | 0.04     | 0.39     | ---      | 0.72     | -0.02    | ---      |
| <b>L</b> | 0.34     | 0.12     | 0.09     | 0.32     | 0.24     | 0.04     | 0.34     | 0.19     | -0.04    | -0.11    | 0.31     | 0.43     | 0.62     | 0.32     | 0.54     | -0.04    | 0.15     | -0.58    | 0.73     | 0.51     | ---      |
| <b>K</b> | 0.43     | -1.04    | 0.21     | 0.17     | 0.26     | -0.18    | 0.2      | 0.18     | 0.19     | 0.33     | 0.26     | 0.21     | 0.08     | -0.05    | 0.25     | 0.08     | 0.28     | 0.36     | -0.02    | 0.02     | 0.24     |
| <b>M</b> | 0.58     | 0.09     | -0.12    | 0.04     | ---      | 0.26     | 0.22     | 0.28     | -0.61    | 0.57     | 0        | 0.21     | ---      | 0.3      | 0.43     | -0.17    | -0.26    | ---      | 0.15     | 0.5      | ---      |
| <b>F</b> | 0.27     | 0.59     | 0.13     | 0.24     | 0.59     | 0.18     | 0.25     | 0.16     | 0.1      | 0.54     | 0.17     | 0.06     | 0        | 0.06     | 0.51     | 0.17     | 0.11     | ---      | 0.14     | 0.12     | ---      |
| <b>P</b> | 0.4      | 0.03     | 0.01     | 0.09     | 1.16     | -0.04    | 0.27     | 0.2      | 0.24     | 0.18     | 0.14     | -0.22    | 0.76     | -0.09    | 0.15     | 0.11     | 0.14     | -0.25    | 0.05     | 0.07     | 0.29     |
| <b>S</b> | 0.29     | 0.1      | -0.05    | 0.2      | 0.32     | -0.05    | 0.41     | 0.65     | 0.48     | 0.33     | 0.24     | 0.21     | 0.69     | 0.39     | 0.27     | 0.19     | 0.06     | 0.48     | 0.21     | 0.24     | -0.53    |
| <b>T</b> | 0.42     | 0.1      | 0.29     | 0.23     | 1.03     | 0.06     | 0.21     | -0.37    | 0.5      | 0.22     | 0.06     | 0.23     | 0.45     | -0.08    | -0.02    | 0.14     | 0.38     | 0.53     | 0.31     | 0.13     | -0.05    |
| <b>W</b> | 0.83     | 0.05     | 0.74     | 0.17     | ---      | 0.33     | 0.2      | -0.35    | ---      | 0.77     | 1.04     | -0.16    | ---      | ---      | 0.25     | 0.21     | 0.14     | ---      | ---      | 1.2      | ---      |
| <b>Y</b> | 0.76     | 0.04     | -0.03    | 0.41     | ---      | 0.15     | 0.57     | 0.09     | -0.07    | 0.2      | -0.05    | 0.36     | 1.2      | 0.81     | 0.4      | 0.17     | 0.49     | -0.51    | 0.66     | 0.2      | ---      |
| <b>V</b> | 0.26     | 0.34     | 0.28     | 0.52     | 0.82     | 0.19     | 0.33     | 0.13     | 0.74     | 0.31     | 0.25     | 0.36     | 0.32     | 0.27     | 0.44     | 0.17     | 0.22     | 0.67     | -0.13    | 0.11     | 0.41     |
| <b>X</b> | ---      | ---      | ---      | -0.82    | ---      | ---      | -0.12    | 0.13     | ---      | ---      | -0.19    | -0.87    | ---      | -0.7     | -0.6     | 0.32     | 0.1      | ---      | -0.28    | -0.23    | ---      |

Correction      i-2,i

**Atom    N**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.76    | -0.84    | -1.15    | -1.93    | -0.94    | -0.59    | -1.03    | -0.41    | -0.9     | -0.84    | -1.17    | -0.91    | -1.24    | -1.31    | --       | -0.99    | -1.14    | -3.62    | -1.51    | 0.42     | -0.23    |
| <b>R</b> | 0.44     | 0.26     | 0.2      | -0.65    | -1.39    | -0.7     | -0.57    | 0.44     | -0.13    | -0.52    | 0.21     | -0.24    | -0.02    | -0.34    | --       | -0.03    | -0.84    | -3.27    | -0.26    | 0.22     | -0.18    |
| <b>N</b> | -1.26    | -0.99    | -0.93    | -1.55    | -1       | -0.95    | -1.01    | 0.18     | -1.14    | -0.53    | -1.8     | -1.51    | -1.96    | -1.3     | --       | -0.82    | -0.28    | -2.34    | -2.32    | -0.79    | -0.36    |
| <b>D</b> | -1.18    | -1.39    | -1.69    | -1.41    | -0.63    | -1.2     | -1.35    | -0.47    | -1.65    | -0.61    | -1.6     | -1.38    | -0.86    | -0.86    | --       | -0.4     | -1.06    | 0        | -1.29    | -0.21    | -0.64    |
| <b>C</b> | -0.84    | 0.35     | 0.45     | -0.71    | 0.97     | -1.35    | -0.69    | -0.37    | 0.12     | -0.19    | -0.72    | -0.23    | --       | 1.14     | --       | -1.19    | -0.12    | -2.15    | 0.85     | -0.08    | --       |
| <b>Q</b> | -0.02    | -0.22    | -0.56    | -0.05    | -0.74    | -0.57    | -0.51    | 0.13     | -1.2     | -0.91    | -0.68    | -0.63    | 0.41     | -1.72    | --       | -0.18    | -0.17    | -1.89    | -1.4     | -0.4     | -0.25    |
| <b>E</b> | -0.5     | -0.45    | 0.06     | 0.29     | -1.21    | -0.44    | -0.28    | -0.22    | 0.22     | -0.77    | -0.92    | -0.91    | -0.82    | -1.15    | --       | -0.6     | -0.31    | 0.45     | -0.5     | -0.24    | -0.36    |
| <b>G</b> | -0.77    | -0.06    | -0.03    | -0.24    | 0.02     | -0.45    | -0.25    | 0.14     | -0.52    | -0.89    | -0.44    | -0.38    | -0.46    | -0.96    | -1.5     | 0.14     | -0.3     | -0.74    | -1.05    | -0.29    | 0.03     |
| <b>H</b> | 0.37     | -0.67    | -0.5     | -0.59    | --       | -0.7     | 0.23     | 0.01     | 0.45     | -2.9     | -0.56    | -0.3     | -1.05    | -0.42    | --       | 0.38     | -1.59    | --       | 1.82     | -0.98    | --       |
| <b>I</b> | -0.15    | -0.43    | -0.51    | -0.72    | -0.72    | -1.12    | -0.64    | 0.05     | 1.35     | 0.99     | 0.14     | -0.58    | 0.87     | 1.71     | --       | -0.76    | -0.7     | 0.59     | 0.92     | -0.56    | --       |
| <b>L</b> | -0.86    | -0.98    | -1.35    | -1.05    | -0.29    | -0.68    | -0.9     | 0.34     | -0.52    | -0.71    | -1.09    | -0.82    | -1.47    | -0.43    | --       | -0.92    | -1.16    | -2.44    | -0.44    | -0.95    | -0.43    |
| <b>K</b> | -0.04    | -0.24    | -0.49    | -0.41    | -1.18    | -0.43    | -0.14    | 0.41     | -0.92    | 0.09     | -0.26    | -0.56    | 0.28     | 0.29     | --       | 0.1      | -0.89    | -0.28    | -0.03    | -0.68    | -0.5     |
| <b>M</b> | 0.48     | 0.61     | 0        | -1.15    | -2.77    | -0.12    | -0.46    | 0.94     | -1.69    | 0.22     | -0.3     | -0.07    | 0.27     | 1.14     | --       | -0.08    | -0.37    | --       | -1.28    | -0.03    | --       |
| <b>F</b> | -0.48    | -2.05    | -1.31    | -1.16    | 2.28     | -0.6     | -1.04    | -0.27    | 0.12     | 0.89     | -0.3     | -0.99    | -1.85    | 0.11     | --       | -1.64    | -1.29    | --       | 0.73     | -0.56    | --       |
| <b>P</b> | -0.86    | -1.13    | -0.76    | -2.01    | -1.11    | -1.63    | -0.91    | 0.23     | -2.92    | -0.45    | -0.76    | -1.22    | -1.02    | -1.06    | 3.1      | -1       | -1.91    | -2.31    | -0.65    | -0.65    | --       |
| <b>S</b> | -0.82    | -0.43    | -0.83    | -1.19    | 0.52     | -1.22    | -0.89    | 0.43     | -1.3     | -1.13    | -1.58    | -1.31    | -0.03    | -1.41    | --       | -1.11    | -0.66    | -0.49    | -1.46    | -0.74    | -0.77    |
| <b>T</b> | -0.67    | -0.91    | -0.5     | -1.02    | 0.26     | -0.36    | -0.23    | 0.46     | -1.08    | -0.29    | -0.39    | -0.92    | -0.06    | -1.14    | --       | -0.82    | -0.44    | 0.66     | -0.36    | -0.4     | -0.78    |
| <b>W</b> | -1.57    | -0.14    | -1.87    | -0.89    | 0.97     | -1.69    | -0.31    | 0.39     | -1.23    | 0.26     | -1.27    | -0.43    | --       | -0.99    | --       | -0.75    | -1.7     | --       | 1.9      | -0.14    | --       |
| <b>Y</b> | -0.41    | -0.62    | -1.88    | -0.56    | 2.53     | -0.14    | -0.14    | -0.54    | -0.69    | -0.91    | 0.41     | -0.31    | -1.48    | 0.92     | --       | -0.11    | -2.01    | -0.96    | 1.28     | -0.1     | -0.29    |
| <b>V</b> | -0.44    | -0.14    | -0.04    | -0.23    | 1.56     | -0.53    | 0.02     | -0.05    | -0.07    | -0.02    | 1.17     | -0.26    | 1.01     | 1.04     | --       | -0.31    | -0.72    | 0.02     | 0.91     | -0.41    | 0.65     |
| <b>X</b> | -0.58    | -0.93    | -0.16    | -0.39    | --       | -0.13    | -0.36    | 0.59     | -0.21    | -0.44    | -0.96    | 0.55     | --       | -0.34    | --       | -0.68    | 0.9      | --       | -0.17    | -1.06    | -0.78    |



Correction      i-2,i

**Atom    H**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.18    | -0.12    | 0.01     | -0.14    | -0.26    | -0.16    | -0.03    | 0.02     | -0.11    | -0.04    | -0.18    | -0.09    | -0.28    | -0.25    | --       | -0.21    | -0.17    | -0.61    | -0.25    | -0.15    | 0.01     |
| <b>R</b> | 0.04     | 0.06     | 0.09     | 0.01     | 0.09     | -0.09    | 0.18     | 0.08     | 0.05     | -0.01    | 0.07     | -0.03    | -0.08    | -0.01    | --       | -0.02    | -0.13    | -0.43    | -0.09    | -0.01    | -0.09    |
| <b>N</b> | -0.07    | 0.01     | 0.09     | 0.05     | -0.23    | -0.09    | -0.07    | 0.11     | -0.06    | -0.07    | -0.09    | -0.02    | -0.17    | -0.22    | --       | -0.02    | 0.06     | -0.4     | -0.16    | -0.05    | -0.07    |
| <b>D</b> | -0.06    | -0.06    | 0.07     | -0.01    | 0.01     | 0.03     | 0.04     | 0.09     | 0.05     | -0.08    | -0.1     | 0        | 0.09     | -0.04    | --       | 0.05     | 0.07     | -0.11    | 0        | -0.19    | 0.05     |
| <b>C</b> | 0.13     | 0.31     | 0.11     | 0.21     | 0.36     | -0.05    | 0.07     | 0.24     | 0.28     | 0.18     | 0.18     | 0.36     | --       | 0.58     | --       | 0.11     | 0.01     | -0.33    | 0.43     | 0.23     | --       |
| <b>Q</b> | -0.01    | 0.01     | -0.01    | 0.04     | -0.35    | -0.02    | 0.09     | -0.03    | 0.08     | -0.16    | -0.06    | 0.04     | -0.16    | -0.18    | --       | -0.06    | -0.04    | -0.28    | -0.13    | -0.07    | -0.08    |
| <b>E</b> | -0.15    | -0.04    | 0.05     | 0.07     | -0.06    | 0.01     | 0.02     | -0.02    | 0        | -0.03    | -0.16    | -0.02    | -0.11    | -0.12    | --       | -0.1     | -0.1     | -0.07    | -0.14    | -0.02    | -0.04    |
| <b>G</b> | 0.11     | 0.08     | 0.17     | 0.13     | -0.01    | 0.15     | 0.19     | 0.35     | 0.05     | 0.02     | 0.1      | 0.11     | 0.14     | 0        | --       | 0.11     | 0.09     | 0.05     | 0.04     | -0.02    | 0.07     |
| <b>H</b> | 0.16     | 0.02     | 0.43     | 0.36     | -0.03    | 0.14     | 0.28     | 0.13     | 0.09     | -0.2     | 0.09     | 0.07     | 0.22     | 0.19     | --       | 0.22     | -0.22    | --       | 0.07     | 0.09     | -0.37    |
| <b>I</b> | 0.07     | -0.01    | 0.02     | 0.02     | -0.09    | 0.01     | 0.14     | 0.49     | 0.03     | 0.14     | 0.07     | -0.01    | 0.1      | 0.5      | --       | -0.06    | -0.04    | 0.12     | 0.05     | 0.08     | 0.36     |
| <b>L</b> | -0.05    | -0.05    | 0.02     | -0.05    | 0.06     | -0.04    | 0.01     | 0.12     | 0.04     | -0.12    | -0.03    | -0.06    | -0.31    | -0.11    | --       | -0.18    | -0.19    | -0.23    | -0.11    | -0.04    | -0.05    |
| <b>K</b> | -0.06    | -0.05    | 0.09     | 0.09     | -0.17    | -0.06    | 0.12     | 0.11     | 0.04     | -0.07    | -0.02    | -0.08    | -0.13    | -0.06    | --       | -0.01    | -0.09    | 0.02     | -0.01    | -0.17    | -0.04    |
| <b>M</b> | 0.09     | 0.12     | 0.15     | -0.12    | -0.11    | 0        | 0.08     | 0.24     | -0.35    | 0.09     | 0.11     | 0.07     | 0.03     | -0.15    | --       | 0.06     | -0.1     | --       | 0.03     | -0.03    | --       |
| <b>F</b> | -0.09    | -0.04    | 0.05     | 0.04     | -0.07    | 0.1      | 0.15     | 0.09     | 0.1      | 0.11     | -0.06    | -0.15    | -0.03    | 0.09     | --       | -0.15    | -0.13    | -0.26    | -0.02    | 0.04     | -0.08    |
| <b>P</b> | -0.2     | -0.07    | 0.04     | -0.18    | -0.22    | -0.17    | 0        | 0.14     | -0.28    | -0.2     | -0.23    | 0        | -0.26    | -0.22    | --       | -0.15    | -0.34    | -0.39    | -0.3     | -0.27    | --       |
| <b>S</b> | -0.06    | -0.07    | 0.07     | -0.04    | -0.28    | -0.1     | -0.02    | 0.04     | 0.06     | -0.09    | -0.18    | -0.07    | 0        | -0.22    | --       | -0.09    | -0.08    | -0.2     | -0.17    | -0.12    | -0.04    |
| <b>T</b> | 0.01     | -0.05    | 0.08     | 0.02     | -0.37    | 0.02     | 0.1      | 0.14     | -0.14    | 0.13     | -0.05    | 0.04     | 0.02     | -0.07    | --       | 0        | -0.02    | 0.19     | 0.1      | 0        | -0.01    |
| <b>W</b> | -0.07    | -0.3     | -0.24    | 0.08     | 0.59     | -0.24    | 0.13     | -0.05    | -0.09    | 0.33     | -0.4     | -0.04    | --       | -0.33    | --       | 0.12     | -0.2     | --       | 0.19     | 0.14     | --       |
| <b>Y</b> | 0        | -0.16    | -0.13    | 0.02     | 0.3      | -0.06    | 0.06     | -0.16    | 0.1      | 0.15     | 0.18     | 0.04     | -0.2     | 0.02     | --       | -0.03    | 0.13     | -0.24    | 0.01     | -0.14    | 0.2      |
| <b>V</b> | 0.03     | 0.06     | 0.09     | 0.06     | 0.13     | -0.1     | 0.07     | 0.15     | 0.24     | -0.01    | 0.22     | 0.01     | 0.07     | 0.31     | --       | -0.01    | -0.16    | -0.14    | 0.2      | 0.04     | -0.29    |
| <b>X</b> | -0.05    | -0.04    | 0.03     | -0.17    | --       | -0.22    | -0.01    | 0.13     | -0.3     | -0.23    | 0.21     | 0.01     | -0.08    | -0.34    | --       | 0.07     | 0.07     | --       | -0.35    | -0.12    | -0.23    |

Correction      i-2,i

**Atom   H $\alpha$**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.1     | -0.08    | -0.05    | -0.07    | -0.04    | -0.08    | -0.08    | ---      | -0.15    | -0.03    | 0        | -0.05    | -0.08    | -0.09    | -0.08    | -0.04    | -0.05    | 0        | -0.04    | -0.11    | 0        |
| <b>R</b> | -0.06    | -0.02    | -0.04    | -0.03    | -0.02    | -0.09    | -0.05    | ---      | -0.06    | -0.04    | -0.04    | -0.12    | 0.09     | -0.02    | -0.03    | -0.05    | -0.08    | 0.03     | -0.14    | -0.04    | -0.06    |
| <b>N</b> | -0.04    | -0.1     | -0.03    | -0.04    | -0.09    | 0.02     | -0.06    | ---      | -0.12    | -0.13    | -0.08    | -0.04    | 0.01     | -0.14    | -0.09    | -0.07    | -0.03    | -0.11    | -0.17    | -0.04    | -0.03    |
| <b>D</b> | -0.02    | -0.11    | 0.02     | 0        | -0.09    | -0.05    | -0.04    | ---      | 0        | -0.17    | -0.07    | 0.02     | 0.09     | -0.08    | -0.03    | -0.11    | -0.1     | -0.11    | -0.05    | 0.21     | 0.03     |
| <b>C</b> | -0.01    | -0.14    | 0.02     | 0.1      | -0.2     | 0.05     | -0.04    | ---      | 0        | -0.17    | -0.06    | 0.04     | ---      | -0.19    | -0.11    | -0.06    | -0.08    | -0.23    | -0.15    | -0.23    | ---      |
| <b>Q</b> | -0.01    | -0.07    | -0.04    | -0.05    | -0.21    | -0.09    | -0.1     | ---      | 0.09     | -0.05    | -0.09    | 0        | -0.16    | 0.01     | -0.03    | -0.09    | -0.06    | -0.2     | -0.13    | 0        | -0.04    |
| <b>E</b> | -0.02    | -0.04    | -0.07    | -0.05    | -0.12    | -0.07    | -0.06    | ---      | -0.01    | -0.07    | -0.09    | -0.06    | -0.12    | 0.02     | -0.05    | -0.07    | -0.03    | -0.02    | -0.13    | -0.09    | -0.07    |
| <b>G</b> | 0.01     | 0.02     | 0.01     | 0        | -0.08    | 0        | -0.02    | ---      | 0.03     | -0.07    | -0.04    | 0.02     | 0.03     | -0.03    | -0.01    | -0.01    | 0.01     | -0.1     | -0.07    | -0.03    | ---      |
| <b>H</b> | -0.04    | -0.06    | -0.09    | -0.03    | -0.22    | -0.12    | -0.09    | ---      | -0.04    | -0.03    | -0.04    | -0.05    | 0.06     | -0.14    | -0.03    | -0.06    | 0.03     | ---      | 0.03     | -0.13    | -0.33    |
| <b>I</b> | -0.07    | -0.12    | -0.03    | -0.06    | 0.17     | -0.17    | -0.11    | ---      | -0.11    | -0.06    | -0.03    | -0.11    | 0.05     | -0.19    | -0.04    | 0        | -0.08    | -0.11    | -0.07    | -0.04    | 0.17     |
| <b>L</b> | -0.06    | -0.09    | -0.1     | -0.1     | -0.01    | -0.04    | -0.11    | ---      | -0.09    | -0.05    | -0.06    | -0.1     | -0.06    | 0.01     | -0.07    | -0.09    | -0.07    | -0.1     | -0.05    | -0.1     | -0.05    |
| <b>K</b> | -0.08    | -0.08    | -0.05    | -0.04    | -0.17    | -0.07    | -0.07    | ---      | -0.13    | -0.15    | -0.06    | -0.05    | 0.03     | -0.11    | -0.06    | 0.09     | -0.07    | 0.02     | -0.1     | -0.09    | -0.13    |
| <b>M</b> | -0.06    | -0.04    | -0.05    | -0.04    | 0.11     | -0.07    | -0.05    | ---      | 0.03     | -0.06    | -0.09    | -0.06    | 0.07     | -0.08    | -0.08    | -0.07    | -0.07    | ---      | -0.12    | -0.07    | ---      |
| <b>F</b> | -0.04    | 0        | -0.04    | -0.04    | -0.01    | -0.13    | -0.1     | ---      | -0.17    | -0.08    | -0.04    | -0.1     | 0.12     | -0.06    | -0.06    | -0.07    | 0.02     | -0.2     | 0.06     | -0.1     | -0.08    |
| <b>P</b> | -0.02    | -0.05    | -0.03    | -0.03    | -0.04    | 0.02     | -0.06    | ---      | -0.06    | -0.06    | -0.07    | -0.04    | 0        | -0.12    | -0.02    | -0.08    | -0.05    | -0.08    | -0.2     | -0.12    | -0.01    |
| <b>S</b> | -0.04    | -0.07    | 0.01     | -0.04    | -0.07    | -0.07    | -0.06    | ---      | -0.01    | -0.05    | -0.08    | -0.05    | 0.02     | 0        | 0.02     | -0.06    | -0.02    | 0.03     | -0.12    | -0.06    | -0.13    |
| <b>T</b> | -0.03    | -0.03    | -0.01    | -0.03    | 0.08     | -0.01    | -0.02    | ---      | 0.01     | -0.05    | -0.05    | -0.07    | 0.05     | 0        | -0.02    | -0.02    | 0.01     | -0.05    | -0.08    | -0.09    | -0.13    |
| <b>W</b> | -0.11    | -0.1     | -0.04    | -0.1     | -0.27    | 0.03     | -0.13    | ---      | 0.07     | -0.14    | -0.05    | -0.23    | ---      | -0.09    | -0.09    | -0.2     | 0.02     | ---      | 0.02     | -0.19    | ---      |
| <b>Y</b> | -0.2     | -0.03    | -0.03    | -0.07    | 0.01     | -0.09    | -0.12    | ---      | -0.08    | -0.17    | -0.03    | -0.07    | 0.13     | -0.12    | 0.01     | -0.13    | -0.07    | -0.08    | -0.1     | -0.21    | -0.13    |
| <b>V</b> | -0.04    | -0.14    | -0.07    | -0.07    | -0.07    | -0.04    | -0.08    | ---      | -0.02    | 0.07     | 0.01     | -0.05    | 0.1      | -0.16    | -0.07    | -0.07    | -0.08    | -0.07    | 0.14     | -0.05    | -0.2     |
| <b>X</b> | -0.01    | -0.01    | -0.06    | 0.02     | ---      | -0.08    | -0.19    | ---      | -0.04    | 0.04     | -0.16    | -0.09    | -0.01    | -0.12    | -0.1     | -0.11    | -0.07    | ---      | -0.18    | 0.11     | -0.07    |

Correction      i,i+2

**Atom   C $\alpha$**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.24     | 0.33     | 0.53     | 0.21     | 0.53     | 0.57     | 0.52     | 0.51     | 0.49     | 0.04     | 0.58     | 0.44     | 0.18     | 0.31     | -0.23    | 0.51     | 0.48     | -0.14    | 0.58     | 0.07     | 0.32     |
| <b>R</b> | 0.39     | 0.55     | 0.39     | 0.01     | 0.99     | 0.85     | 0.04     | 0.19     | 0.79     | 0.36     | 0.25     | 0.59     | -0.12    | 0.18     | -0.05    | 0.25     | 0.69     | 0.6      | 0.11     | 0.12     | 0.19     |
| <b>N</b> | -0.12    | 0.39     | -0.01    | -0.29    | 1.1      | 0.46     | -0.05    | 0.41     | 0.07     | 0.31     | 0.37     | 0.13     | 0.01     | 0.25     | 0.14     | 0.01     | 0.28     | 0.38     | 0.24     | 0.19     | -0.06    |
| <b>D</b> | 0        | 0.02     | -0.29    | 0.09     | 1.36     | 0.07     | 0.1      | 0.49     | 0.68     | 0.64     | 0.66     | 0.07     | 0.65     | 0.53     | 0.15     | -0.23    | 0.34     | 1.3      | 0.38     | 0.71     | 0.72     |
| <b>C</b> | 0.2      | 0.2      | 0.79     | 0.42     | 0.87     | 0.47     | 0.75     | 0.45     | 0.66     | 0.86     | 0.54     | 0.95     | --       | 1.86     | -0.51    | 0.13     | 0.41     | 0.65     | 0.69     | -0.03    | --       |
| <b>Q</b> | 0.21     | 0.35     | 0.54     | 0.25     | 0.95     | 0.26     | 0.07     | 0.15     | 0.45     | 0.34     | 0.21     | 0.2      | 0.73     | 0.82     | -0.12    | 0.18     | -0.01    | -0.23    | 0.2      | 0.49     | 0.33     |
| <b>E</b> | 0.73     | 0.41     | -0.08    | 0.45     | 1.14     | 0.3      | 0.53     | 0.65     | 0.27     | 0.4      | 0.54     | 0.46     | 0.61     | 0.54     | -0.15    | 0.35     | 0.63     | 0.65     | 0.55     | 0.43     | 0.65     |
| <b>G</b> | 0.17     | 0.18     | 0.08     | 0.39     | -0.03    | 0.2      | 0.11     | 0.11     | 0.04     | 0.14     | 0.22     | 0.19     | 0.05     | 0.09     | -0.13    | 0.02     | 0.22     | 0.04     | 0.22     | 0.06     | 0.33     |
| <b>H</b> | 0.59     | 0.65     | 0.15     | -0.44    | 0.84     | 0.2      | 0.01     | -0.21    | 0.31     | 0.08     | 0.66     | 0.45     | -0.55    | 0.42     | 0.08     | 0.18     | 0.76     | --       | 0.32     | 0.24     | --       |
| <b>I</b> | 0.78     | 0.64     | 0.46     | 0.79     | 1.25     | 0.68     | 0.23     | 0.57     | 0.52     | -0.14    | 0.75     | 0.38     | 0.83     | -0.41    | -0.3     | 0.52     | 0.1      | -0.1     | 0.36     | -0.12    | --       |
| <b>L</b> | 0.12     | 0.19     | 0.15     | 0.34     | 0.62     | 0.86     | 0.3      | 0.28     | 0.38     | 0.27     | 0.14     | 0.53     | 0.28     | 0.3      | -0.14    | 0.54     | 0.49     | 0.27     | 0.42     | 0.06     | --       |
| <b>K</b> | 0.44     | 0.71     | 0.38     | 0.38     | 0.9      | 0.56     | 0.29     | 0.32     | 0.67     | 0.34     | 0.36     | 0.44     | 1.01     | 0.11     | -0.07    | 0.42     | 0.22     | 0.36     | 0.01     | 0.45     | -0.05    |
| <b>M</b> | 0.11     | 0.05     | 0.36     | 0.42     | 0.43     | 0.22     | 0.21     | 0.35     | -0.35    | -0.08    | -0.05    | 0.2      | 0.62     | 0.1      | -0.3     | 0.13     | -0.06    | --       | 0.34     | 0.09     | --       |
| <b>F</b> | 0.06     | 0.2      | 0.71     | 0.58     | 0.15     | 1.09     | 0.33     | 0.08     | 0.41     | -0.48    | -0.1     | 0.67     | 1.44     | 0.37     | 0.41     | 0.33     | 0.18     | 0.62     | -0.36    | -0.59    | --       |
| <b>P</b> | 0.58     | 0.22     | 0.38     | 0.47     | 0.92     | 0.63     | 0.15     | 0.58     | 0.38     | 0.49     | 0.56     | 0.27     | 0.32     | 0.46     | 0.01     | 0.14     | 0.43     | 0.5      | 0.42     | 0.18     | 0.49     |
| <b>S</b> | 0.15     | 0.3      | 0.1      | 0.06     | 1.38     | 0.16     | -0.25    | 0.48     | 0.24     | 0.63     | 0.43     | 0.4      | 0.8      | 0.42     | 0.42     | 0.16     | 0.11     | 0.6      | 0.72     | 0.41     | 0.78     |
| <b>T</b> | 0.2      | 0.68     | 0.24     | -0.13    | 1.38     | -0.03    | -0.26    | 0.72     | 0.58     | 0.76     | 0.74     | 0.2      | 0.75     | 0.95     | 0.18     | 0.34     | 0.08     | 0.99     | 1.02     | 0.48     | 0.99     |
| <b>W</b> | 0.09     | -0.27    | 1.08     | 0.17     | 2.12     | 1.58     | 0.83     | -0.74    | 2.28     | 0.2      | -0.6     | -0.06    | --       | -1.07    | 0.07     | -0.23    | -0.42    | --       | --       | -0.49    | --       |
| <b>Y</b> | 0.38     | 0.49     | -0.55    | 0.67     | 0.07     | 0.71     | 0.6      | 0.12     | -0.42    | 0.01     | 0.39     | 0.53     | 0.83     | 0.12     | 0.41     | 0.09     | -0.16    | -0.91    | 0.03     | -0.82    | --       |
| <b>V</b> | 0.3      | 0.24     | 0.69     | 0.99     | 0.54     | 0.98     | 0.6      | 0.48     | 0.37     | 0.01     | 0.25     | 0.92     | -0.17    | 0.02     | -0.1     | 0.39     | 0.55     | -0.16    | 0.23     | -0.19    | 0.85     |
| <b>X</b> | -0.06    | --       | 0.15     | 0.1      | --       | 0.35     | 0.07     | 0        | --       | 0.17     | 0.74     | -0.08    | --       | 0.29     | 0.11     | 0.26     | 0.26     | --       | 0.63     | 0.17     | --       |

Correction      i,i+2

**Atom   Cβ**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.45    | 0.14     | -0.21    | -0.28    | -0.53    | -0.5     | -0.48    | -0.43    | -0.37    | 0.16     | -0.24    | -0.43    | -0.54    | -0.01    | -0.06    | -0.5     | -0.19    | 0.3      | -0.28    | 0.24     | -0.51    |
| <b>R</b> | -0.34    | -0.68    | -0.37    | 0.13     | -0.61    | -0.58    | 0.09     | -0.04    | 0.28     | -0.19    | -0.31    | -0.39    | -0.49    | -0.32    | -0.32    | -0.28    | -0.32    | -1.11    | -0.05    | 0        | 0.2      |
| <b>N</b> | -0.6     | -0.29    | 0.01     | -0.08    | 0.08     | -0.5     | -0.3     | -0.27    | -0.04    | -0.12    | -0.17    | -0.61    | 0.24     | -0.22    | -0.55    | -0.33    | -0.41    | -0.22    | -0.14    | -0.54    | -0.91    |
| <b>D</b> | -0.25    | -0.1     | -0.45    | -0.39    | -0.26    | -0.38    | -0.32    | -0.35    | -0.29    | -0.01    | -0.23    | -0.44    | -0.33    | -0.37    | -0.48    | -0.3     | -0.32    | 0.25     | -0.24    | -0.2     | -0.51    |
| <b>C</b> | 0.77     | 0.95     | 0.32     | 0.18     | 0.14     | 0.43     | -0.41    | 1.29     | 0.54     | -1.17    | 0.7      | 1.42     | ---      | -0.08    | -0.52    | -0.2     | 1.18     | -0.84    | 0.82     | 0.9      | ---      |
| <b>Q</b> | -0.47    | -0.32    | -0.61    | -0.26    | -0.38    | -0.31    | -0.3     | -0.3     | -0.43    | -0.23    | -0.35    | -0.31    | -0.84    | -0.63    | -0.02    | -0.62    | -0.29    | 0.06     | 0.41     | -0.14    | -0.88    |
| <b>E</b> | -0.42    | -0.42    | -0.08    | -0.17    | 0.05     | -0.51    | -0.38    | -0.34    | -0.35    | -0.5     | -0.12    | -0.5     | -0.3     | -0.31    | -0.13    | -0.45    | -0.46    | -0.58    | -0.47    | -0.24    | -0.48    |
| <b>G</b> | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      |
| <b>H</b> | -0.41    | -0.05    | 0.27     | -0.2     | -1.1     | 0.17     | -0.02    | 0.08     | -0.47    | 0.13     | 0.04     | -0.18    | -0.19    | -0.23    | -0.91    | -0.05    | -0.88    | ---      | -0.2     | 0.36     | ---      |
| <b>I</b> | -0.82    | -0.06    | -0.39    | -0.34    | 0.16     | -0.57    | -0.34    | -0.34    | -0.51    | 0.15     | -0.13    | -0.36    | -0.29    | 0.58     | -0.08    | -0.32    | 0.11     | ---      | -0.23    | 0.03     | ---      |
| <b>L</b> | -0.33    | -0.45    | -0.45    | -0.52    | -0.71    | -0.1     | -0.31    | -0.45    | -0.52    | 0.31     | 0.08     | -0.42    | -0.15    | -0.1     | -0.19    | -0.31    | -0.39    | -0.37    | 0.08     | 0.36     | ---      |
| <b>K</b> | -0.43    | -0.51    | -0.3     | -0.31    | -0.23    | -0.5     | -0.08    | 0.07     | -0.33    | -0.14    | 0        | -0.32    | -0.64    | -0.43    | -0.34    | -0.17    | -0.14    | -0.42    | 0.2      | 0.01     | -0.62    |
| <b>M</b> | 0.21     | 0.92     | -0.31    | -0.29    | 0.01     | -0.5     | -0.4     | -0.17    | -0.64    | -0.13    | -0.17    | -0.28    | -0.08    | -0.19    | -0.65    | -0.4     | -0.75    | ---      | -0.06    | 0.3      | ---      |
| <b>F</b> | -0.47    | -0.17    | -0.48    | -0.29    | -1.19    | -0.49    | -0.47    | -0.84    | -1.17    | -0.15    | -0.34    | -0.53    | -1.24    | -0.01    | -0.53    | -0.24    | -0.4     | -0.58    | 0.65     | 0.19     | ---      |
| <b>P</b> | -0.04    | 0.06     | 0.04     | 0.05     | 0.02     | -0.01    | -0.02    | -0.05    | -0.04    | 0        | 0.01     | -0.04    | -0.07    | -0.15    | -0.2     | 0.05     | 0        | -0.13    | -0.01    | -0.16    | 0.27     |
| <b>S</b> | -0.06    | -0.18    | -0.19    | -0.17    | -0.36    | -0.2     | 0.06     | -0.27    | -0.23    | -0.17    | -0.35    | -0.13    | -0.47    | -0.01    | -0.35    | -0.12    | -0.13    | -0.39    | -0.37    | -0.28    | -0.34    |
| <b>T</b> | -0.12    | -0.15    | -0.24    | 0.06     | -0.47    | 0.1      | 0.23     | -0.44    | -0.51    | -0.32    | -0.57    | -0.02    | -0.09    | -0.17    | -0.24    | -0.35    | -0.01    | -0.27    | -1.18    | -0.59    | -2.44    |
| <b>W</b> | -0.04    | -0.76    | -0.18    | -0.47    | -0.02    | -0.66    | -1.43    | -0.76    | 1.58     | -1.44    | 0.29     | -0.6     | ---      | 0.37     | -0.21    | -0.26    | -0.25    | ---      | ---      | 0.05     | ---      |
| <b>Y</b> | -0.55    | -0.94    | -0.96    | -0.29    | -1.36    | -0.79    | -0.24    | -0.47    | -0.53    | -0.61    | -0.43    | -0.81    | -0.14    | -0.34    | -0.27    | -0.21    | -0.12    | 0.25     | -0.45    | -0.14    | ---      |
| <b>V</b> | -0.27    | -0.05    | -0.31    | -0.6     | -0.14    | -0.45    | -0.45    | -0.27    | -0.52    | -0.21    | -0.08    | -0.36    | 0.24     | -0.23    | -0.03    | -0.35    | -0.2     | -0.04    | -0.22    | 0        | 0.27     |
| <b>X</b> | ---      | ---      | -0.99    | -0.18    | ---      | -0.58    | -0.44    | -0.46    | ---      | -0.56    | -0.4     | -1.37    | ---      | 0.51     | -0.7     | 0.64     | -0.32    | ---      | 0.19     | 0.22     | ---      |

Correction      i,i+2

**Atom    C**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | 0.41     | 0.14     | 0.26     | 0.39     | -0.15    | 0.63     | 0.44     | 0.43     | 0.23     | 0.01     | 0.32     | 0.39     | 1.28     | 0.32     | -1.33    | 0.61     | 0.36     | 0.67     | 0.23     | -0.09    | -0.1     |
| <b>R</b> | 0.04     | 0.37     | 0.41     | -0.66    | 0.12     | 0.48     | 0.16     | 0.35     | 0.33     | -0.05    | -0.21    | 0.3      | 0.23     | -0.33    | -0.14    | 0.24     | 0.34     | 0.12     | -0.54    | -0.05    | 0.26     |
| <b>N</b> | 0.25     | 0.3      | 0.44     | 0.31     | 0.32     | 0.29     | 0.34     | 0.37     | 0.36     | -0.29    | -0.01    | 0.15     | 0.39     | 0.32     | -0.39    | 0.29     | 0.16     | 0.38     | 0.05     | -0.13    | 1.07     |
| <b>D</b> | 0.23     | 0.32     | 0.47     | 0.42     | 0.49     | 0.3      | 0.2      | 0.64     | 0.21     | -0.07    | 0.4      | 0.35     | 0.27     | -0.06    | -0.29    | 0.28     | 0.12     | 0.26     | 0.09     | 0.08     | 0.57     |
| <b>C</b> | 0.68     | 0.28     | 0.46     | 0.49     | 1.16     | 1.29     | 0.13     | 0.53     | 1.93     | 0.36     | 0.26     | 0.65     | ---      | 0.49     | -0.2     | 0.51     | 0.99     | -0.2     | 0.58     | 1.22     | ---      |
| <b>Q</b> | 0.07     | 0.03     | 0.38     | -0.1     | 0.74     | 0.05     | 0.18     | 0.13     | 0.12     | 0.01     | 0.15     | 0.02     | -0.01    | 0.07     | -0.09    | -0.05    | -0.23    | 0        | -0.03    | 0.17     | -0.05    |
| <b>E</b> | 0.47     | 0.2      | 0.42     | 0.28     | 0.56     | 0.25     | 0.48     | 0.57     | 0.33     | 0.13     | 0.18     | 0.15     | 0.6      | -0.06    | -0.26    | 0.34     | 0.56     | 0.05     | 0.14     | 0.23     | 0.22     |
| <b>G</b> | 0.26     | -0.41    | 0.47     | 0.39     | 0.19     | 0.41     | 0.29     | 0.29     | 0.28     | -0.17    | -0.25    | 0.34     | 0.25     | 0.25     | -0.21    | -0.05    | 0.33     | 0.42     | -0.12    | -0.1     | 0.43     |
| <b>H</b> | 0.11     | 0.33     | 0.56     | 0.22     | ---      | 0.63     | 0.11     | 0.67     | -0.3     | 0.25     | 0.16     | 0.33     | 0.11     | 0.04     | -0.55    | 0.22     | 0.32     | ---      | 0.01     | -0.12    | ---      |
| <b>I</b> | 0.54     | 0.06     | 0.54     | 0.51     | 0.3      | 0.52     | 0.18     | 0.42     | 0.07     | -0.45    | -0.22    | 0.64     | 0.29     | -0.56    | -0.4     | 0.34     | 0.2      | ---      | 0.1      | 0.08     | ---      |
| <b>L</b> | 0.28     | 0.15     | 0.23     | 0.45     | 0.21     | 0.53     | 0.25     | 0.22     | 0.59     | -0.5     | -0.15    | 0.35     | -0.33    | 0.13     | -0.23    | 0.06     | 0.37     | -0.18    | 0.45     | -0.19    | ---      |
| <b>K</b> | -0.92    | 0.33     | 0.28     | 0.37     | 0.4      | 0.5      | 0.22     | 0.3      | 0.57     | -0.01    | 0.18     | 0.21     | 0.05     | 0.22     | -0.33    | 0.45     | 0.06     | -0.43    | -0.1     | 0        | 0.01     |
| <b>M</b> | 0.6      | 0.14     | 0.67     | 0.67     | -0.1     | 0.43     | 0.42     | 0        | 0.94     | -0.74    | 0.27     | 0.68     | -0.02    | 0.17     | 0.18     | 1.2      | 0.42     | ---      | 0.47     | -0.2     | ---      |
| <b>F</b> | 0.58     | 0.45     | 0.28     | 0.38     | 0.08     | 0.94     | 0.33     | 0.91     | 0.61     | -0.32    | -0.55    | 0.31     | -0.33    | 0.16     | -0.54    | -0.02    | 0.14     | 0.27     | -0.21    | -0.31    | ---      |
| <b>P</b> | 0.44     | 0.41     | 0.47     | 0.56     | 0.11     | -0.21    | 0.43     | 0.39     | 0.41     | -0.18    | 0.17     | 0.23     | 0.35     | -0.07    | -0.3     | 0.61     | 0.11     | 0.24     | 0.14     | 0.03     | -0.32    |
| <b>S</b> | 0.23     | 0.25     | 0.03     | 0.31     | 0.49     | 0.19     | -0.02    | 0.36     | 0.14     | 0.03     | 0.12     | 0.36     | 0.3      | 0.15     | -0.26    | 0.19     | 0.03     | -0.07    | 0.31     | -0.05    | -0.18    |
| <b>T</b> | 0.29     | 0.42     | 0.2      | -0.14    | 0.36     | 0.23     | 0.45     | 0.42     | 0.53     | 0.02     | 0.17     | 0.66     | 0.1      | 0.05     | -0.11    | 0.44     | 0.4      | 0.08     | 0.12     | -0.12    | 0.44     |
| <b>W</b> | 0.28     | 0.15     | 0.89     | 0.35     | ---      | 0.81     | 0.55     | -0.15    | 0.49     | -0.83    | -0.11    | 0.59     | ---      | -0.8     | -0.2     | -0.22    | 0.1      | ---      | ---      | 0.27     | ---      |
| <b>Y</b> | 0.51     | 0.54     | 0.34     | 0.59     | ---      | 0.4      | 0.16     | 0.29     | -0.17    | 0.01     | -0.03    | 0.37     | 0.99     | 0.04     | -0.17    | 0.72     | 0.15     | -0.29    | 0.03     | -0.01    | ---      |
| <b>V</b> | 0.12     | 0.25     | 0.31     | 0.66     | 0.24     | 0.28     | 0.5      | 0.57     | 0.01     | -0.19    | -0.05    | 0.38     | 0.19     | -0.06    | -0.26    | 0.28     | 0.2      | 0.23     | 0        | -0.15    | -0.16    |
| <b>X</b> | ---      | ---      | ---      | 0.19     | ---      | ---      | -0.42    | -0.51    | ---      | ---      | -0.16    | 0.35     | ---      | -1.44    | 0.01     | 0.97     | 0.61     | ---      | -0.09    | -0.66    | ---      |

Correction      i,i+2

**Atom    N**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.3     | -0.39    | -1.27    | 0.03     | 1.1      | -0.24    | -0.36    | -0.37    | -1.23    | -0.66    | -0.9     | -1.21    | -0.74    | -1.36    | -0.52    | -0.15    | -0.5     | -1.56    | -1.57    | -1.11    | -1.23    |
| <b>R</b> | -0.4     | -0.2     | -0.16    | -0.53    | 2.38     | -1       | -0.59    | -0.57    | -1.16    | -0.62    | -1.23    | -0.82    | -0.06    | -0.67    | -1.55    | -0.59    | -0.95    | -0.93    | -1.03    | -1.03    | -0.18    |
| <b>N</b> | -0.44    | -0.86    | -1.02    | -0.9     | -0.54    | 0.24     | -0.28    | -0.48    | -0.51    | -1.31    | -1.06    | -0.35    | -0.83    | -1.05    | -1.4     | -0.66    | -1       | -1.79    | -2.15    | -0.53    | -0.36    |
| <b>D</b> | -1.06    | -0.88    | -0.46    | -0.51    | -0.27    | -0.58    | -0.37    | -0.66    | -1.78    | -0.75    | -1.18    | -0.56    | -0.2     | -1.56    | -1.92    | -1.03    | -1.42    | -0.94    | -1.49    | -0.98    | -0.64    |
| <b>C</b> | -0.04    | 0.3      | 0.59     | -0.31    | 0.85     | -1.31    | 0.59     | -1.02    | -0.87    | -0.17    | -1.18    | -0.46    | --       | -0.04    | -0.77    | -0.85    | 0.48     | -1.06    | 1.32     | -0.21    | --       |
| <b>Q</b> | -1.03    | -0.89    | -0.88    | -0.8     | -1.82    | -0.52    | -0.97    | -0.43    | -0.63    | -0.89    | -1.15    | -1.15    | -0.72    | -1.03    | -1.12    | -1.18    | -0.69    | -1.68    | -1.1     | -0.91    | -0.25    |
| <b>E</b> | -0.3     | -0.81    | -0.58    | -0.6     | 0.62     | -0.88    | -0.77    | -0.42    | -0.95    | -1.54    | -0.8     | -0.88    | 0.03     | -0.96    | -0.98    | -0.47    | -1.05    | -0.91    | -0.72    | -0.71    | -1.36    |
| <b>G</b> | -0.27    | 0.32     | 0.15     | 0.33     | 0.84     | 0.32     | 0.25     | -0.25    | -0.31    | 0.64     | -0.63    | 0.58     | -0.25    | 0.23     | -0.38    | 0.04     | 0.1      | -1.05    | -0.66    | -0.14    | 0.03     |
| <b>H</b> | -1.07    | 0.48     | -0.36    | 0.38     | --       | -1.43    | -0.61    | -0.31    | 0.21     | -1.56    | -0.38    | -1.08    | -2.31    | -1.14    | -2       | -0.52    | -2.18    | --       | -1.53    | -1.1     | --       |
| <b>I</b> | -0.47    | -0.81    | -0.59    | -0.43    | -0.5     | -0.88    | 0.03     | -0.41    | 0.02     | -0.54    | -0.93    | -0.85    | -0.17    | -1.33    | -0.78    | 0.07     | -0.89    | 0.24     | -0.35    | -0.58    | --       |
| <b>L</b> | -0.78    | -0.73    | -0.41    | -0.7     | 0.42     | -1.5     | -0.62    | -0.87    | -0.64    | -1.23    | -1.02    | -0.99    | -1.77    | -1.86    | -0.66    | 0.04     | -0.09    | -0.35    | -1.4     | -0.95    | -1.43    |
| <b>K</b> | -1.15    | -0.65    | -0.83    | -0.57    | 1.15     | -1.1     | -0.74    | -0.77    | -0.33    | -1.42    | -0.79    | -1.09    | -1.43    | -0.92    | -1.65    | -0.43    | -1.07    | -2.54    | -1.29    | -1.03    | -1.5     |
| <b>M</b> | -1.02    | -0.79    | -0.28    | -0.37    | -0.37    | -0.58    | 0.65     | -0.07    | -0.41    | 0.01     | -0.15    | 0        | 0.29     | -0.66    | -2.07    | -0.18    | -0.54    | --       | -3.95    | -0.63    | --       |
| <b>F</b> | -0.33    | -0.9     | -0.33    | -0.5     | 1.41     | -0.2     | -0.64    | -0.51    | 0.24     | -1.04    | -1.79    | -0.98    | -0.75    | -0.44    | -0.46    | -0.1     | 0.44     | -0.43    | -2.51    | -0.29    | --       |
| <b>P</b> | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | 2.2      | --       | --       | --       | --       | --       | --       |
| <b>S</b> | 0.07     | -0.9     | -0.78    | -0.52    | 0.44     | -0.11    | -0.5     | -0.72    | 0.05     | -0.69    | -1.11    | -0.62    | -1.07    | -1.02    | -0.88    | -0.65    | -1.02    | -0.77    | 0.26     | -0.73    | -0.77    |
| <b>T</b> | -0.69    | -1.1     | -0.54    | -1.2     | -0.01    | -2.04    | -1.23    | -0.83    | -1.91    | -0.84    | -0.58    | -1.5     | -0.4     | -0.1     | -0.65    | -0.35    | -0.62    | -0.82    | 0.24     | 0        | -0.78    |
| <b>W</b> | -1.48    | -1.61    | -1.35    | -0.2     | 4.12     | 1.97     | -0.14    | -2.14    | -0.04    | -1.87    | -1.43    | -0.47    | --       | 1.65     | -1.84    | -0.24    | -2.96    | --       | --       | -1.59    | --       |
| <b>Y</b> | -0.06    | -1.32    | -0.36    | -0.14    | 1.45     | -0.65    | -0.15    | 0.3      | -1.8     | -1.04    | -0.75    | -0.84    | -0.19    | -1.21    | -0.33    | -1.18    | -1.29    | -2.27    | -1.1     | -0.39    | -0.29    |
| <b>V</b> | -0.66    | -0.27    | -0.39    | -0.27    | 0.11     | -0.39    | -0.24    | -0.26    | 0.39     | -1.76    | -0.23    | -0.22    | 0.11     | -1.61    | -0.29    | -0.52    | -0.94    | -2.01    | -0.36    | -0.48    | 0.65     |
| <b>X</b> | -0.58    | -0.93    | -0.16    | -0.39    | --       | -0.13    | -0.36    | 0.59     | -0.21    | -0.44    | -0.96    | 0.55     | --       | -0.34    | 0.27     | -0.68    | 0.9      | --       | -0.17    | -0.06    | -0.78    |

Correction      i,i+2

**Atom    H**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.02    | 0.03     | -0.06    | 0.08     | 0.14     | 0.01     | 0.01     | 0.09     | -0.23    | -0.01    | -0.04    | -0.09    | -0.25    | -0.08    | -0.17    | 0.1      | 0.03     | -0.32    | -0.18    | -0.09    | 0.01     |
| <b>R</b> | -0.04    | 0.06     | 0.01     | -0.07    | 0.27     | 0.04     | 0.04     | 0.06     | -0.03    | 0.05     | -0.01    | 0.02     | -0.05    | 0.01     | -0.11    | 0.01     | 0        | 0.15     | 0        | -0.11    | -0.09    |
| <b>N</b> | -0.1     | 0.09     | 0.1      | 0        | 0.12     | 0.17     | 0.05     | 0.12     | 0.17     | 0.07     | 0.09     | 0.1      | 0.18     | 0.14     | 0        | 0.09     | 0.17     | -0.07    | -0.03    | 0.19     | -0.07    |
| <b>D</b> | 0.06     | 0.01     | -0.01    | 0        | 0.18     | 0.08     | 0.02     | 0.12     | -0.04    | 0.08     | 0.05     | 0.07     | 0.17     | 0        | -0.03    | -0.07    | -0.08    | 0.04     | 0.02     | 0.07     | 0.05     |
| <b>C</b> | 0.03     | 0.03     | 0.04     | -0.15    | -0.09    | -0.3     | -0.12    | -0.11    | -0.11    | 0.04     | -0.2     | -0.04    | --       | -0.23    | -0.15    | 0.14     | -0.07    | -0.1     | -0.13    | -0.14    | --       |
| <b>Q</b> | -0.12    | -0.04    | 0.02     | 0.06     | -0.04    | -0.02    | -0.04    | 0.05     | 0.08     | 0.07     | -0.06    | -0.05    | -0.05    | -0.02    | -0.04    | 0.01     | -0.02    | 0.01     | -0.16    | 0.01     | -0.08    |
| <b>E</b> | 0.12     | 0.11     | 0.09     | 0.17     | 0.23     | 0.16     | 0.13     | 0.16     | 0.02     | 0        | 0.08     | 0.04     | 0.07     | -0.01    | -0.05    | 0.09     | 0.05     | 0.11     | 0.11     | 0.09     | -0.04    |
| <b>G</b> | 0.05     | 0.15     | 0.11     | 0.04     | 0.18     | 0.15     | 0.13     | 0.03     | 0.04     | 0.34     | 0.13     | 0.14     | 0.22     | 0.12     | 0.08     | 0.08     | 0.15     | -0.04    | 0.09     | 0.38     | 0.07     |
| <b>H</b> | -0.09    | -0.03    | 0.02     | 0.08     | 0        | 0.1      | 0.01     | 0.01     | 0.1      | -0.06    | 0.08     | 0.1      | 0.01     | -0.13    | 0.14     | -0.04    | 0.04     | 0.05     | -0.15    | 0.16     | -0.37    |
| <b>I</b> | 0.06     | -0.09    | -0.01    | 0.04     | 0.19     | 0.07     | -0.02    | 0.09     | 0.04     | -0.04    | -0.05    | -0.11    | 0.04     | -0.47    | -0.12    | -0.11    | 0.01     | 0.01     | 0.1      | 0.04     | 0.36     |
| <b>L</b> | -0.04    | -0.03    | 0.07     | 0.05     | -0.15    | -0.04    | -0.08    | 0.04     | 0.04     | -0.1     | -0.13    | -0.01    | -0.04    | -0.03    | 0.01     | -0.03    | 0.01     | -0.13    | -0.15    | -0.06    | -0.05    |
| <b>K</b> | -0.03    | 0.04     | 0.04     | 0.07     | 0.2      | 0.05     | 0.06     | 0.1      | 0        | -0.02    | 0.01     | -0.1     | -0.07    | -0.1     | -0.03    | 0.07     | -0.02    | -0.14    | -0.08    | -0.03    | -0.04    |
| <b>M</b> | -0.07    | -0.08    | -0.17    | -0.13    | 0.35     | -0.21    | 0.04     | -0.14    | -0.02    | -0.2     | -0.03    | -0.02    | 0        | -0.08    | -0.06    | 0.11     | 0.07     | --       | -0.24    | -0.07    | --       |
| <b>F</b> | -0.09    | -0.07    | 0.14     | 0.05     | 0.22     | 0.05     | -0.07    | 0.03     | 0.14     | -0.26    | -0.19    | -0.07    | -0.06    | 0.07     | -0.1     | 0.18     | 0.04     | 0.06     | -0.13    | -0.13    | -0.08    |
| <b>P</b> | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       | --       |
| <b>S</b> | -0.01    | -0.06    | -0.03    | 0.01     | 0.33     | 0.1      | -0.02    | -0.01    | -0.06    | -0.08    | -0.01    | -0.04    | 0.02     | -0.12    | -0.03    | -0.01    | -0.09    | -0.04    | 0.03     | -0.13    | -0.04    |
| <b>T</b> | 0.06     | -0.14    | -0.13    | -0.04    | 0.11     | -0.15    | -0.04    | -0.06    | -0.17    | -0.17    | -0.1     | -0.12    | 0        | -0.13    | -0.15    | 0.03     | -0.04    | -0.19    | -0.03    | -0.09    | -0.01    |
| <b>W</b> | -0.14    | -0.27    | -0.23    | 0.21     | 0.49     | 0.31     | -0.03    | -0.4     | -0.26    | -0.28    | -0.23    | -0.06    | --       | 0.16     | -0.25    | -0.03    | -0.31    | -0.61    | -0.15    | -0.3     | --       |
| <b>Y</b> | -0.17    | 0.01     | -0.13    | 0.11     | 0.09     | 0.04     | -0.01    | -0.02    | -0.14    | -0.14    | -0.09    | -0.01    | -0.28    | -0.19    | 0.03     | -0.03    | -0.03    | -0.55    | -0.1     | -0.05    | 0.2      |
| <b>V</b> | -0.08    | -0.11    | -0.06    | 0.03     | 0.1      | -0.02    | 0.02     | 0.06     | 0.07     | -0.18    | -0.08    | -0.03    | 0.1      | -0.07    | -0.18    | -0.05    | -0.08    | -0.21    | -0.04    | -0.14    | -0.29    |
| <b>X</b> | -0.05    | -0.04    | 0.03     | -0.17    | --       | -0.22    | -0.01    | 0.13     | -0.3     | -0.23    | 0.21     | 0.01     | -0.08    | -0.34    | -0.14    | 0.07     | 0.07     | --       | -0.35    | -0.12    | -0.23    |

Correction      i,i+2

**Atom   H $\alpha$**

|          | <b>A</b> | <b>R</b> | <b>N</b> | <b>D</b> | <b>C</b> | <b>Q</b> | <b>E</b> | <b>G</b> | <b>H</b> | <b>I</b> | <b>L</b> | <b>K</b> | <b>M</b> | <b>F</b> | <b>P</b> | <b>S</b> | <b>T</b> | <b>W</b> | <b>Y</b> | <b>V</b> | <b>X</b> |
|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
| <b>A</b> | -0.07    | 0.05     | -0.07    | -0.08    | -0.15    | -0.12    | -0.07    | -0.06    | -0.08    | 0.01     | -0.05    | -0.08    | -0.04    | -0.04    | 0        | -0.03    | -0.04    | -0.05    | -0.04    | -0.03    | 0        |
| <b>R</b> | -0.06    | -0.1     | -0.11    | -0.02    | -0.06    | -0.12    | -0.03    | 0        | -0.05    | -0.09    | -0.03    | -0.03    | 0        | -0.17    | -0.07    | -0.05    | -0.09    | -0.18    | -0.14    | -0.02    | -0.06    |
| <b>N</b> | -0.01    | -0.01    | -0.03    | 0.04     | -0.15    | -0.07    | 0.03     | -0.01    | 0.01     | -0.07    | -0.03    | -0.1     | -0.01    | -0.02    | -0.04    | -0.02    | -0.05    | -0.11    | -0.1     | -0.06    | -0.03    |
| <b>D</b> | -0.04    | -0.04    | -0.06    | -0.05    | -0.1     | -0.03    | -0.02    | -0.03    | -0.05    | -0.01    | -0.03    | -0.07    | -0.04    | -0.06    | -0.04    | 0.01     | -0.08    | -0.05    | -0.07    | -0.03    | 0.03     |
| <b>C</b> | 0.13     | -0.07    | -0.24    | -0.15    | -0.1     | -0.01    | -0.06    | -0.02    | 0.09     | -0.24    | -0.13    | -0.12    | ---      | -0.18    | 0.07     | 0.15     | -0.08    | -0.11    | -0.2     | -0.26    | ---      |
| <b>Q</b> | -0.09    | -0.07    | -0.16    | -0.09    | -0.1     | -0.04    | -0.03    | -0.02    | -0.03    | -0.03    | -0.02    | -0.05    | -0.13    | -0.16    | -0.01    | -0.03    | -0.05    | 0        | -0.05    | 0.01     | -0.04    |
| <b>E</b> | -0.08    | -0.06    | -0.01    | -0.09    | -0.05    | -0.08    | -0.06    | -0.05    | -0.1     | -0.06    | -0.05    | -0.06    | -0.11    | -0.12    | -0.02    | -0.05    | -0.1     | -0.09    | -0.1     | -0.04    | -0.07    |
| <b>G</b> | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      | ---      |
| <b>H</b> | -0.09    | -0.08    | -0.09    | -0.07    | -0.3     | 0.08     | 0.06     | 0        | -0.11    | -0.05    | -0.04    | -0.07    | 0.07     | -0.1     | -0.02    | -0.05    | -0.01    | -0.08    | -0.07    | 0.07     | -0.33    |
| <b>I</b> | -0.1     | -0.12    | -0.07    | -0.09    | -0.15    | -0.14    | -0.03    | -0.07    | -0.18    | 0.03     | -0.08    | -0.11    | -0.1     | -0.04    | 0        | -0.11    | 0.03     | -0.13    | -0.13    | 0.02     | 0.17     |
| <b>L</b> | -0.04    | -0.09    | -0.05    | -0.05    | -0.03    | -0.07    | -0.06    | -0.03    | -0.06    | -0.01    | -0.02    | -0.07    | -0.04    | -0.13    | -0.06    | -0.05    | -0.11    | -0.03    | -0.05    | 0.04     | -0.05    |
| <b>K</b> | -0.06    | -0.1     | -0.09    | -0.09    | -0.09    | -0.14    | -0.03    | 0.01     | -0.1     | -0.03    | -0.02    | -0.06    | -0.07    | -0.06    | -0.04    | -0.04    | -0.01    | -0.11    | -0.04    | -0.03    | -0.13    |
| <b>M</b> | -0.16    | 0.02     | -0.05    | -0.1     | 0.26     | 0        | -0.05    | -0.03    | 0.11     | -0.04    | -0.03    | 0.02     | -0.11    | 0.03     | 0.01     | -0.03    | 0.1      | ---      | -0.04    | -0.01    | ---      |
| <b>F</b> | -0.04    | -0.01    | -0.15    | -0.03    | -0.14    | -0.18    | -0.02    | -0.08    | -0.16    | 0.09     | -0.04    | -0.15    | -0.21    | -0.06    | -0.1     | -0.03    | -0.06    | -0.28    | 0.01     | 0.02     | -0.08    |
| <b>P</b> | -0.09    | -0.04    | -0.05    | -0.07    | -0.07    | -0.09    | -0.05    | -0.03    | -0.06    | 0.01     | -0.02    | -0.03    | 0.01     | -0.07    | -0.03    | 0        | -0.04    | -0.07    | -0.03    | -0.03    | -0.01    |
| <b>S</b> | -0.04    | -0.1     | -0.05    | -0.05    | -0.14    | -0.05    | -0.01    | -0.06    | -0.1     | -0.04    | 0.1      | -0.07    | -0.09    | -0.01    | -0.08    | -0.04    | -0.04    | -0.07    | -0.1     | -0.07    | -0.13    |
| <b>T</b> | 0.01     | -0.05    | -0.03    | -0.02    | -0.24    | -0.01    | 0.02     | -0.09    | -0.14    | -0.05    | -0.06    | 0.01     | -0.04    | -0.12    | -0.08    | -0.05    | 0.02     | -0.2     | -0.11    | -0.06    | -0.13    |
| <b>W</b> | -0.12    | -0.06    | -0.19    | 0.02     | -0.2     | -0.23    | -0.16    | -0.1     | -0.1     | -0.17    | 0.02     | 0.04     | ---      | -0.03    | -0.04    | -0.15    | 0.07     | -0.08    | 0.09     | 0.08     | ---      |
| <b>Y</b> | -0.11    | -0.13    | -0.06    | -0.1     | -0.18    | -0.16    | -0.13    | -0.09    | -0.01    | -0.04    | -0.11    | -0.09    | 0.01     | -0.07    | -0.08    | -0.02    | -0.04    | -0.12    | -0.15    | 0.02     | -0.13    |
| <b>V</b> | -0.07    | -0.04    | -0.11    | -0.2     | -0.1     | -0.12    | -0.11    | -0.05    | -0.1     | -0.04    | -0.02    | -0.11    | -0.08    | -0.02    | -0.06    | -0.08    | -0.06    | -0.12    | -0.11    | 0.32     | -0.2     |
| <b>X</b> | -0.01    | -0.01    | -0.06    | 0.02     | ---      | -0.08    | -0.19    | -0.12    | -0.04    | 0.04     | -0.16    | -0.09    | -0.01    | -0.12    | -0.1     | -0.11    | -0.07    | ---      | -0.18    | 0.11     | -0.07    |