

## CCSD(T)/aVQZ

|                     | $R_e / \text{cm}^{-1}$ | $D_e / \text{cm}^{-1}$ | $D_0 / \text{cm}^{-1}$ | $\omega_e / \text{cm}^{-1}$ | $\omega_e x_e / \text{cm}^{-1}$ | $B_e / \text{cm}^{-1}$ | $\alpha / \text{cm}^{-1}$ | $D_e^{\text{Morse}}/D_e$ | $k / \text{N m}^{-1}$ |
|---------------------|------------------------|------------------------|------------------------|-----------------------------|---------------------------------|------------------------|---------------------------|--------------------------|-----------------------|
| B <sup>+</sup> - He | 2.777                  | 176.9                  | 129.4                  | 103.6                       | 17.3                            | 0.745                  | 0.128                     | 0.877                    | 1.86                  |
| B <sup>+</sup> - Ne | 2.710                  | 387.7                  | 341.3                  | 96.1                        | 6.65                            | 0.323                  | 0.0227                    | 0.895                    | 3.86                  |
| B <sup>+</sup> - Ar | 2.457                  | 2283.3                 | 2184.9                 | 199.0                       | 4.35                            | 0.324                  | 0.00803                   | 0.997                    | 20.1                  |
| B <sup>+</sup> - Kr | 2.435                  | 3954.6                 | 3831.7                 | 247.7                       | 3.69                            | 0.292                  | 0.00509                   | 1.05                     | 35.2                  |
| B <sup>+</sup> - Xe | 2.526                  | 6414.0                 | 6268.2                 | 293.1                       | 2.91                            | 0.260                  | 0.00313                   | 1.15                     | 51.4                  |
| B <sup>+</sup> - Rn | 2.566                  | 7962.2                 | 7806.9                 | 311.9                       | 2.63                            | 0.244                  | 0.00243                   | 1.16                     | 60.1                  |

## CCSD(T)/aV5Z

|                     | $R_e / \text{cm}^{-1}$ | $D_e / \text{cm}^{-1}$ | $D_0 / \text{cm}^{-1}$ | $\omega_e / \text{cm}^{-1}$ | $\omega_e x_e / \text{cm}^{-1}$ | $B_e / \text{cm}^{-1}$ | $\alpha / \text{cm}^{-1}$ | $D_e^{\text{Morse}}/D_e$ | $k / \text{N m}^{-1}$ |
|---------------------|------------------------|------------------------|------------------------|-----------------------------|---------------------------------|------------------------|---------------------------|--------------------------|-----------------------|
| B <sup>+</sup> - He | 2.769                  | 180.6                  | 132.4                  | 105.0                       | 17.3                            | 0.7490                 | 0.128                     | 0.883                    | 1.91                  |
| B <sup>+</sup> - Ne | 2.684                  | 405.9                  | 357.5                  | 100.1                       | 6.83                            | 0.3296                 | 0.0231                    | 0.904                    | 4.19                  |
| B <sup>+</sup> - Ar | 2.445                  | 2334.7                 | 2235.2                 | 201.2                       | 4.41                            | 0.3267                 | 0.00818                   | 0.983                    | 20.6                  |
| B <sup>+</sup> - Kr | 2.429                  | 4005.0                 | 3881.0                 | 249.9                       | 3.70                            | 0.2936                 | 0.00515                   | 1.05                     | 35.8                  |
| B <sup>+</sup> - Xe | 2.521                  | 6464.9                 | 6318.3                 | 294.7                       | 2.91                            | 0.2610                 | 0.00311                   | 1.15                     | 52.0                  |
| B <sup>+</sup> - Rn | 2.561                  | 7997.0                 | 7841.1                 | 313.2                       | 2.64                            | 0.2450                 | 0.00259                   | 1.16                     | 60.6                  |

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|---------------------|------------------------|------------------------|------------------------|-----------------------------|---------------------------------|------------------------|---------------------------|--------------------------|-----------------------|
| B <sup>+</sup> - He | 2.762                  | 184.5                  | 135.6                  | 106.4                       | 17.3                            | 0.7528                 | 0.126                     | 0.888                    | 1.96                  |
| B <sup>+</sup> - Ne | 2.660                  | 426.4                  | 375.9                  | 104.5                       | 7.01                            | 0.3356                 | 0.0224                    | 0.914                    | 4.57                  |
| B <sup>+</sup> - Ar | 2.433                  | 2390.1                 | 2289.4                 | 203.6                       | 4.49                            | 0.3299                 | 0.00795                   | 0.966                    | 21.1                  |
| B <sup>+</sup> - Kr | 2.423                  | 4058.5                 | 3933.3                 | 252.2                       | 3.70                            | 0.2950                 | 0.00510                   | 1.06                     | 36.5                  |
| B <sup>+</sup> - Xe | 2.516                  | 6519.1                 | 6371.6                 | 296.4                       | 2.907                           | 0.2621                 | 0.00301                   | 1.16                     | 52.6                  |
| B <sup>+</sup> - Rn | 2.556                  | 8034.2                 | 7877.5                 | 314.6                       | 2.643                           | 0.2460                 | 0.00267                   | 1.17                     | 61.2                  |

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|---------------------|------------------------|------------------------|------------------------|-----------------------------|---------------------------------|------------------------|---------------------------|--------------------------|-----------------------|
| B <sup>+</sup> - He | 3.078                  | 89.8                   | 59.9                   | 67.0                        | 14.6                            | 0.6062                 | 0.144                     | 0.856                    | 0.777                 |
| B <sup>+</sup> - Ne | 3.083                  | 166.2                  | 138.8                  | 57.8                        | 6.09                            | 0.2498                 | 0.0267                    | 0.825                    | 1.40                  |
| B <sup>+</sup> - Ar | 2.833                  | 989.7                  | 930.5                  | 120.3                       | 3.97                            | 0.2433                 | 0.00876                   | 0.921                    | 7.36                  |
| B <sup>+</sup> - Kr | 2.726                  | 1862.0                 | 1784.5                 | 156.8                       | 3.44                            | 0.2331                 | 0.00572                   | 0.959                    | 14.1                  |
| B <sup>+</sup> - Xe | 2.740                  | 3430.3                 | 3328.2                 | 205.7                       | 2.98                            | 0.2210                 | 0.00366                   | 1.03                     | 25.3                  |
| B <sup>+</sup> - Rn | 2.748                  | 4491.3                 | 4377.3                 | 229.4                       | 2.78                            | 0.2128                 | 0.00298                   | 1.05                     | 32.5                  |

## HF/aV5Z

|                     | $R_e / \text{cm}^{-1}$ | $D_e / \text{cm}^{-1}$ | $D_0 / \text{cm}^{-1}$ | $\omega_e / \text{cm}^{-1}$ | $\omega_e x_e / \text{cm}^{-1}$ | $B_e / \text{cm}^{-1}$ | $\alpha / \text{cm}^{-1}$ | $D_e^{\text{Morse}}/D_e$ | $k / \text{N m}^{-1}$ |
|---------------------|------------------------|------------------------|------------------------|-----------------------------|---------------------------------|------------------------|---------------------------|--------------------------|-----------------------|
| B <sup>+</sup> - He | 3.073                  | 90.7                   | 60.5                   | 67.8                        | 14.8                            | 0.6081                 | 0.144                     | 0.857                    | 0.796                 |
| B <sup>+</sup> - Ne | 3.062                  | 168.1                  | 140.0                  | 59.3                        | 6.42                            | 0.2532                 | 0.0272                    | 0.815                    | 1.47                  |
| B <sup>+</sup> - Ar | 2.830                  | 1001.2                 | 941.9                  | 120.5                       | 3.94                            | 0.2439                 | 0.00866                   | 0.919                    | 7.38                  |
| B <sup>+</sup> - Kr | 2.725                  | 1866.4                 | 1788.8                 | 156.9                       | 3.45                            | 0.2333                 | 0.00571                   | 0.955                    | 14.1                  |
| B <sup>+</sup> - Xe | 2.739                  | 3436.9                 | 3334.7                 | 205.8                       | 2.98                            | 0.2211                 | 0.00374                   | 1.03                     | 25.4                  |
| B <sup>+</sup> - Rn | 2.747                  | 4497.7                 | 4383.6                 | 229.6                       | 2.78                            | 0.2130                 | 0.00310                   | 1.05                     | 32.6                  |

## HF/BSE

|                     | $R_e / \text{cm}^{-1}$ | $D_e / \text{cm}^{-1}$ | $D_0 / \text{cm}^{-1}$ | $\omega_e / \text{cm}^{-1}$ | $\omega_e x_e / \text{cm}^{-1}$ | $B_e / \text{cm}^{-1}$ | $\alpha / \text{cm}^{-1}$ | $D_e^{\text{Morse}}/D_e$ | $k / \text{N m}^{-1}$ |
|---------------------|------------------------|------------------------|------------------------|-----------------------------|---------------------------------|------------------------|---------------------------|--------------------------|-----------------------|
| B <sup>+</sup> - He | 3.069                  | 91.7                   | 61.1                   | 68.6                        | 15.0                            | 0.6097                 | 0.143                     | 0.858                    | 0.815                 |
| B <sup>+</sup> - Ne | 3.040                  | 170.5                  | 141.6                  | 61.1                        | 6.75                            | 0.2569                 | 0.0277                    | 0.810                    | 1.56                  |
| B <sup>+</sup> - Ar | 2.827                  | 1013.3                 | 954.0                  | 120.6                       | 3.91                            | 0.2444                 | 0.00849                   | 0.918                    | 7.40                  |
| B <sup>+</sup> - Kr | 2.724                  | 1871.1                 | 1793.4                 | 157.1                       | 3.47                            | 0.2334                 | 0.00569                   | 0.952                    | 14.2                  |
| B <sup>+</sup> - Xe | 2.738                  | 3443.9                 | 3341.6                 | 206.0                       | 2.99                            | 0.2213                 | 0.00381                   | 1.03                     | 25.4                  |
| B <sup>+</sup> - Rn | 2.746                  | 4504.4                 | 4390.2                 | 229.8                       | 2.79                            | 0.2131                 | 0.00320                   | 1.05                     | 32.6                  |