

**Supporting Information: Near dissociation states for  $\text{H}_2^+ - \text{He}$  on MRCI and FCI  
potential energy surfaces**

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TABLE S1: Grid for the diatomic potentials. All values in atomic units.

| Method | diatom         | $N$ | $r_{\min}$ | $r_{\max}$ |
|--------|----------------|-----|------------|------------|
| MRCI+Q | $\text{H}_2^+$ | 96  | 0.8        | 50.0       |
| FCI    | $\text{H}_2^+$ | 96  | 0.8        | 50.0       |
| MRCI+Q | $\text{HeH}^+$ | 102 | 0.7        | 50.0       |
| FCI    | $\text{HeH}^+$ | 102 | 0.7        | 50.0       |

TABLE S2: Grid for the triatomic potentials. All values in atomic units.

|            | MRCI+Q | FCI  |
|------------|--------|------|
| $N_R$      | 26     | 31   |
| $R_{\min}$ | 0.3    | 1.5  |
| $R_{\max}$ | 8.3    | 40.0 |
| $N_r$      | 27     | 16   |
| $r_{\min}$ | 0.9    | 0.9  |
| $r_{\max}$ | 4.5    | 3.9  |
| $N_\theta$ | 11     | 9    |

TABLE S3: Coefficients for the MRCI+Q/aug-cc-pV6Z diatomic potentials.

| Coefficients | $\text{H}_2^+$       | $\text{HeH}^+$      |
|--------------|----------------------|---------------------|
| $c_0$        | 1.0185817913777047   | 3.2233398865576910  |
| $\alpha$     | 1.6426016158795942   | 2.8140238576362075  |
| $c_1$        | -0.73688350635547695 | -3.3885062843889191 |
| $c_2$        | 5.1706704100481042   | 86.578369632144941  |
| $c_3$        | -83.346600494014567  | -2929.2064910602976 |
| $c_4$        | 874.72395010350556   | 73876.513409500127  |
| $c_5$        | -5621.3191308852929  | -1280675.3543930338 |
| $c_6$        | 23054.489047468251   | 14775779.204776313  |
| $c_7$        | -60955.753058022863  | -110729495.67500649 |
| $c_8$        | 100818.87103555651   | 512524888.74876255  |
| $c_9$        | -94989.664045708429  | -1315519328.5011687 |
| $c_{10}$     | 38921.331029687601   | 1401896260.3220801  |
| $\beta$      | 0.99809657513307815  | 2.1737434370604722  |

TABLE S4: Coefficients for the FCI/aug-cc-pV5Z diatomic potentials.

| Coefficients | $\text{H}_2^+$       | $\text{HeH}^+$      |
|--------------|----------------------|---------------------|
| $c_0$        | 1.0187329739360240   | 1.4607052781134291  |
| $\alpha$     | 1.6427288815351817   | 2.8820010945364949  |
| $c_1$        | -0.73635966940340725 | -3.4215724179324090 |
| $c_2$        | 5.1598925267102205   | 96.452411178877199  |
| $c_3$        | -83.517326447967520  | -3304.8226974189261 |
| $c_4$        | 881.03015485244248   | 89711.319427535549  |
| $c_5$        | -5696.2664864874414  | -1677314.4764108122 |
| $c_6$        | 23534.011016663684   | 21179550.008693457  |
| $c_7$        | -62775.390381188619  | -176458143.78657210 |
| $c_8$        | 104921.46142264079   | 928389438.74672687  |
| $c_9$        | -100077.26031466493  | -2792961078.7000194 |
| $c_{10}$     | 41598.163770554645   | 3667131828.9247351  |
| $\beta$      | 0.99821070143869606  | 2.1770149125762095  |

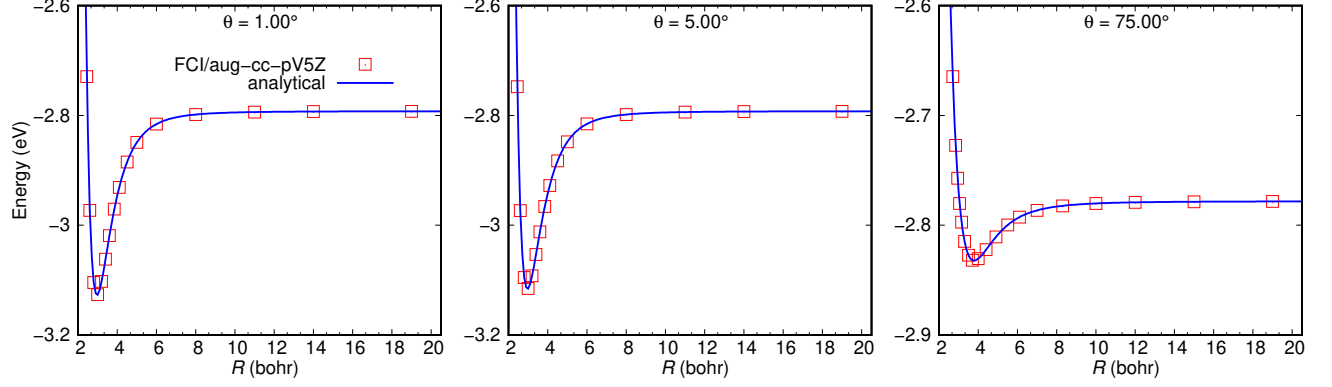


FIG. S1. The RKHS energies (solid lines) as a function of  $R$  along with the FCI/aug-cc-pV5Z energies for several Jacobi angles at fixed  $r = 2.01 a_0$  for  $\theta = 1.0^\circ, 9.0^\circ$  and  $r = 1.9$  for  $\theta = 75.0^\circ$ .

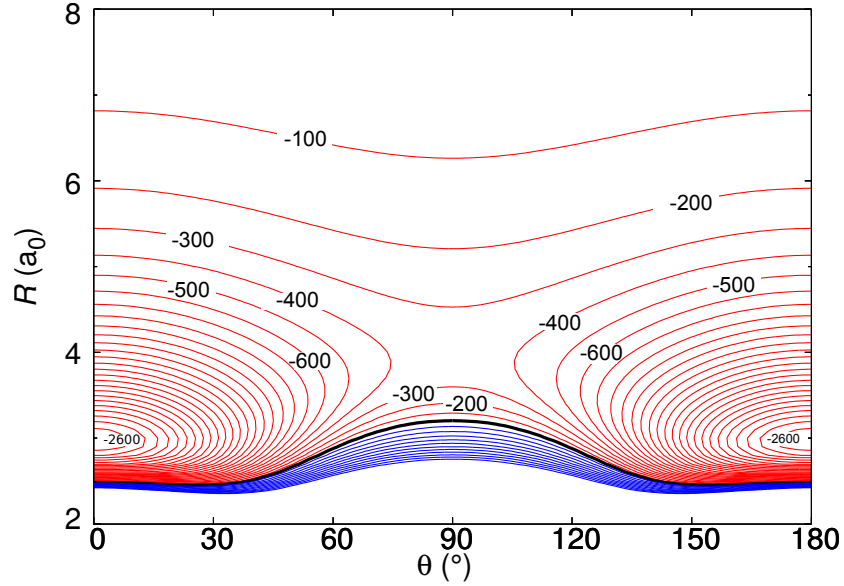


FIG. S2. Contour diagram for the MRCI+Q+LR PES for fixed  $r = 2.0 a_0$ . Energies are in  $\text{cm}^{-1}$  and the contour spacing is  $100 \text{ cm}^{-1}$ . The energy of  $r = 2.0 a_0$  and  $R = \infty$  is the zero of energy. The red and blue lines correspond to negative and positive energies, respectively. The black line is the zero of energy.

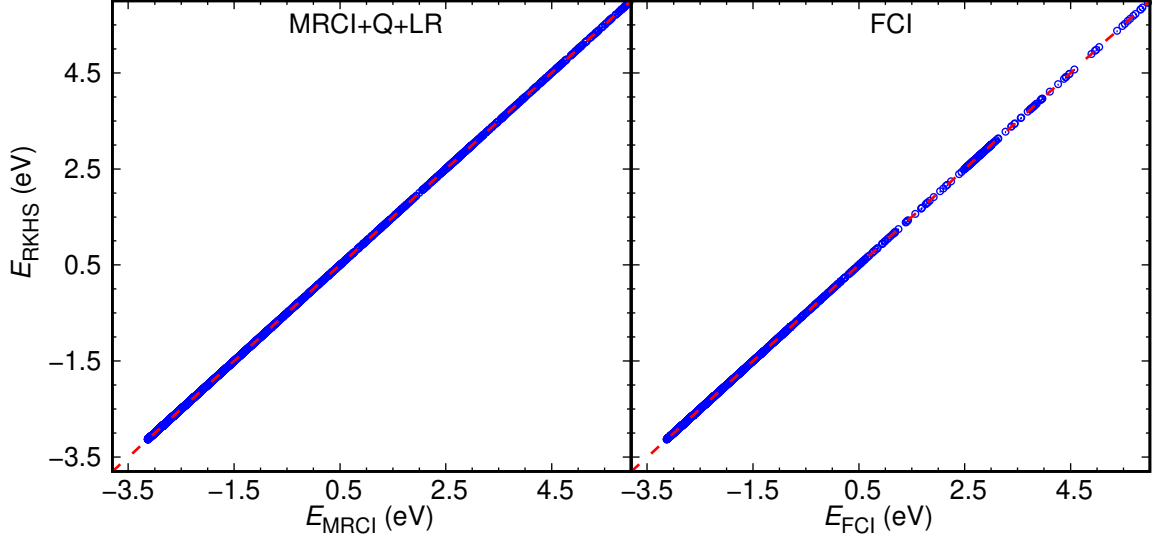


FIG. S3. Comparison between the reference MRCI/aug-cc-pv6Z and FCI/aug-cc-pv5Z *ab initio* on-grid energies and those obtained from the RKHS surfaces. The zero of energy is at  $E(\text{H}) + E(\text{He})$ , i.e for full dissociation.

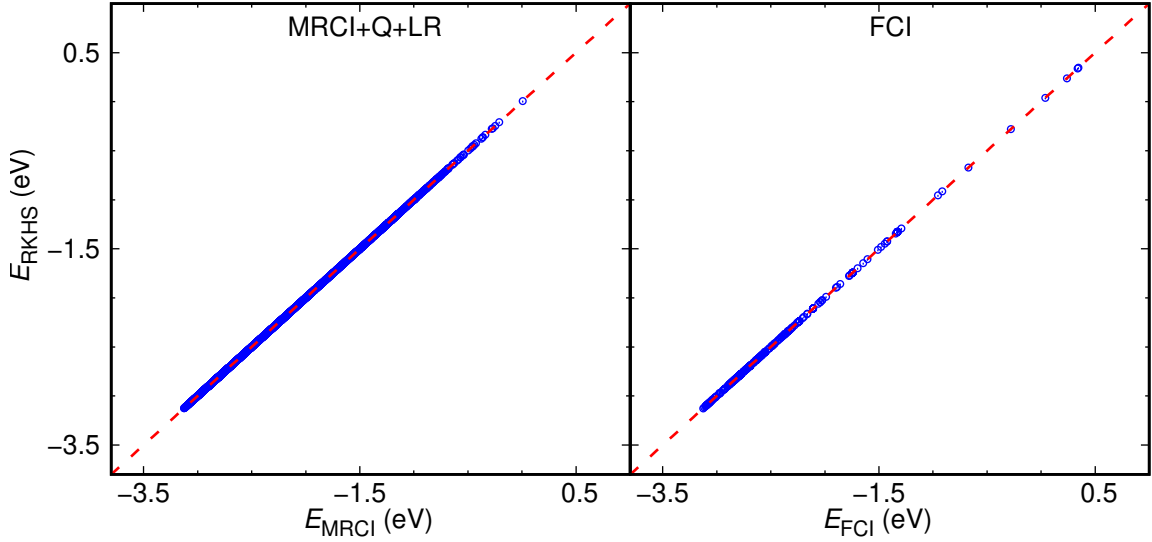


FIG. S4. Comparison between the reference MRCI/aug-cc-pv6Z (left) and FCI/aug-cc-pv5Z (right) *ab initio* off-grid energies and those obtained from the RKHS surfaces. 4912 and 468 off-grid energies for the MRCI/aug-cc-pV6Z and FCI/aug-cc-pV5Z, respectively. The zero of energy is at  $E(\text{H}) + E(\text{He})$ , i.e for full dissociation.

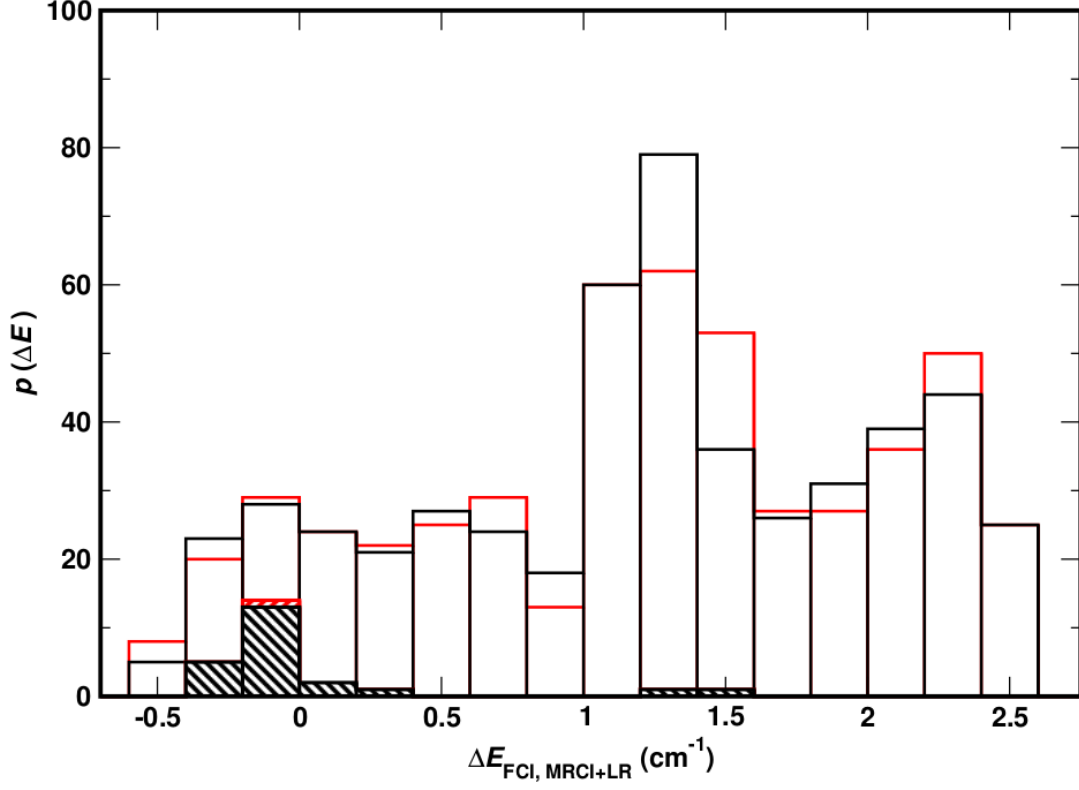


FIG. S5. The distribution of the energy difference  $\Delta E$  on the FCI and MRCI+LR PESs for all bound states (i.e.  $J = 0$  to 21, for  $e-$  and  $f-$ parity *ortho* and *para*  $\text{H}_2^+-\text{He}$ ). Bound state calculations with DVR3D (black) and CCVM (red) are reported separately. Open boxes for all bound states and fill boxes for near-dissociative states, i.e. within  $10 \text{ cm}^{-1}$  of dissociation. The average difference between FCI and MRCI+Q+LR is  $1.21 \text{ cm}^{-1}$  for both bound state methods.

TABLE S5: All bound energy levels from DVR3D and CCVM calculations for  $e-$  and  $f-$ parity, *ortho* (o) and *para* (p)  $\text{H}_2^+-\text{He}$  in  $\text{cm}^{-1}$ , using the FCI and MRCI+Q+LR PES (MRCI). The zero of energy is that of  $\text{H}_2^+(v=0, j=0)$ .

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 0   | e      | 1   | -1795.1567 | -1793.7632 | -1795.3328 | -1793.9067 |
| o   | 0   | e      | 2   | -1063.7471 | -1062.6727 | -1063.3612 | -1062.2742 |
| o   | 0   | e      | 3   | -660.1392  | -657.6932  | -660.2838  | -657.8235  |
| o   | 0   | e      | 4   | -538.7132  | -538.1281  | -538.1236  | -537.5470  |
| o   | 0   | e      | 5   | -254.8020  | -254.3251  | -254.6102  | -254.1331  |
| o   | 0   | e      | 6   | -190.6043  | -190.0415  | -190.4699  | -189.9211  |
| o   | 0   | e      | 7   | -48.1814   | -48.5279   | -47.9117   | -48.2657   |
| o   | 0   | e      | 8   | 19.2177    | 19.0868    | 18.5291    | 18.4236    |
| o   | 0   | e      | 9   | 40.3210    | 40.0360    | 39.8955    | 39.5748    |
| o   | 0   | e      | 10  | 55.8761    | 55.8602    | 55.6889    | 55.6620    |
| o   | 1   | e      | 1   | -1786.9898 | -1785.5973 | -1787.1676 | -1785.7423 |
| o   | 1   | e      | 2   | -1156.0232 | -1153.7813 | -1156.1818 | -1153.9126 |
| o   | 1   | e      | 3   | -1056.3771 | -1055.3035 | -1055.9973 | -1054.9108 |
| o   | 1   | e      | 4   | -652.4661  | -650.0284  | -652.6083  | -650.1564  |
| o   | 1   | e      | 5   | -566.0520  | -564.6730  | -565.9535  | -564.5672  |
| o   | 1   | e      | 6   | -531.6576  | -531.0451  | -531.0936  | -530.4897  |
| o   | 1   | e      | 7   | -264.3738  | -263.2100  | -264.3214  | -263.1671  |
| o   | 1   | e      | 8   | -249.3284  | -248.8408  | -249.1223  | -248.6344  |
| o   | 1   | e      | 9   | -186.9282  | -186.1513  | -186.8255  | -186.0576  |
| o   | 1   | e      | 10  | -175.7091  | -174.2152  | -175.7432  | -174.2595  |
| o   | 1   | e      | 11  | -69.2871   | -68.9712   | -69.1863   | -68.8806   |
| o   | 1   | e      | 12  | -44.7877   | -45.1411   | -44.5115   | -44.8730   |
| o   | 1   | e      | 13  | -27.7742   | -27.0299   | -27.8145   | -27.0795   |
| o   | 1   | e      | 14  | 23.0413    | 22.8241    | 22.5508    | 22.3559    |
| o   | 1   | e      | 15  | 30.9127    | 30.5164    | 30.8918    | 30.4832    |



| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 1   | e      | 16  | 43.6677    | 43.4379    | 43.1988    | 42.9343    |
| o   | 1   | e      | 17  | 54.5821    | 54.5753    | 54.5141    | 54.4935    |
| o   | 1   | e      | 18  | 57.2725    | 57.2317    | 56.9590    | 56.9161    |
| o   | 1   | f      | 1   | -1155.9068 | -1153.4648 | -1155.8671 | -1153.5957 |
| o   | 1   | f      | 2   | -565.3280  | -563.7240  | -565.0456  | -563.6327  |
| o   | 1   | f      | 3   | -264.2372  | -262.8397  | -263.9824  | -262.7923  |
| o   | 1   | f      | 4   | -177.7497  | -175.8616  | -177.6001  | -175.9153  |
| o   | 1   | f      | 5   | -69.2720   | -68.7581   | -68.9665   | -68.6609   |
| o   | 1   | f      | 6   | -28.4535   | -27.5094   | -28.2910   | -27.5540   |
| o   | 1   | f      | 7   | 30.1113    | 29.9118    | 30.3342    | 29.9213    |
| o   | 1   | f      | 8   | 54.4640    | 54.6476    | 54.6289    | 54.6006    |
| o   | 2   | e      | 1   | -1770.6650 | -1769.2743 | -1770.8461 | -1769.4226 |
| o   | 2   | e      | 2   | -1140.2714 | -1138.0381 | -1140.4328 | -1138.1719 |
| o   | 2   | e      | 3   | -1041.6441 | -1040.5717 | -1041.2764 | -1040.1910 |
| o   | 2   | e      | 4   | -637.1448  | -634.7245  | -637.2830  | -634.8481  |
| o   | 2   | e      | 5   | -557.3420  | -555.7147  | -557.2793  | -555.6344  |
| o   | 2   | e      | 6   | -541.3563  | -538.7918  | -541.4221  | -538.8453  |
| o   | 2   | e      | 7   | -517.4518  | -516.7724  | -516.9418  | -516.2723  |
| o   | 2   | e      | 8   | -253.2841  | -252.2489  | -253.2366  | -252.2108  |
| o   | 2   | e      | 9   | -238.2869  | -237.7936  | -238.0550  | -237.5618  |
| o   | 2   | e      | 10  | -177.7376  | -176.8303  | -177.6672  | -176.7689  |
| o   | 2   | e      | 11  | -160.9265  | -159.4781  | -160.9730  | -159.5339  |
| o   | 2   | e      | 12  | -129.0765  | -127.7549  | -129.0885  | -127.7639  |
| o   | 2   | e      | 13  | -60.8852   | -60.6194   | -60.7985   | -60.5431   |
| o   | 2   | e      | 14  | -38.1052   | -38.4707   | -37.8218   | -38.1967   |
| o   | 2   | e      | 15  | -16.2651   | -15.5362   | -16.3163   | -15.5962   |
| o   | 2   | e      | 16  | 29.2257    | 28.9067    | 29.0301    | 28.7185    |
| o   | 2   | e      | 17  | 36.8861    | 36.4658    | 36.8443    | 36.4166    |
| o   | 2   | e      | 18  | 49.7546    | 49.6466    | 49.3446    | 49.2128    |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 2   | e      | 19  | 56.9232    | 56.9159    | 56.6388    | 56.6233    |
| o   | 2   | e      | 20  | 59.1856    | 59.1620    | 58.2724    | 58.2708    |
| o   | 2   | f      | 1   | 139.3222   | -1137.0820 | -1139.4823 | -1137.2146 |
| o   | 2   | f      | 2   | 555.4666   | -553.6852  | -555.4432  | -553.6438  |
| o   | 2   | f      | 3   | 540.3615   | -537.8587  | -540.4319  | -537.9191  |
| o   | 2   | f      | 4   | 252.0531   | -250.9242  | -251.9933  | -250.8740  |
| o   | 2   | f      | 5   | 164.7003   | -162.9638  | -164.7550  | -163.0232  |
| o   | 2   | f      | 6   | 129.1048   | -127.7836  | -129.1167  | -127.7924  |
| o   | 2   | f      | 7   | -60.2646   | -60.0011   | -60.1577   | -59.9049   |
| o   | 2   | f      | 8   | -17.6055   | -16.8608   | -17.6396   | -16.9030   |
| o   | 2   | f      | 9   | 34.9327    | 34.5617    | 34.9539    | 34.5675    |
| o   | 2   | f      | 10  | 56.4390    | 56.4365    | 56.3285    | 56.3143    |
| o   | 3   | e      | 1   | 746.1992   | -1744.8124 | -1746.3862 | -1744.9654 |
| o   | 3   | e      | 2   | 116.6904   | -1114.4702 | -1116.8561 | -1114.6083 |
| o   | 3   | e      | 3   | 019.5579   | -1018.4905 | -1019.2123 | -1018.1278 |
| o   | 3   | e      | 4   | 614.2254   | -611.8344  | -614.3605  | -611.9526  |
| o   | 3   | e      | 5   | 540.9512   | -539.3824  | -540.8797  | -539.2946  |
| o   | 3   | e      | 6   | 516.6202   | -514.1562  | -516.6592  | -514.1774  |
| o   | 3   | e      | 7   | 495.8888   | -495.0796  | -495.4694  | -494.6700  |
| o   | 3   | e      | 8   | 237.3570   | -236.4672  | -237.3158  | -236.4336  |
| o   | 3   | e      | 9   | 221.7092   | -221.2521  | -221.4532  | -220.9932  |
| o   | 3   | e      | 10  | 162.4168   | -161.4340  | -162.3956  | -161.4212  |
| o   | 3   | e      | 11  | 139.8134   | -138.3285  | -139.8837  | -138.4064  |
| o   | 3   | e      | 12  | 111.6749   | -110.3976  | -111.6955  | -110.4156  |
| o   | 3   | e      | 13  | -48.6143   | -48.4085   | -48.5513   | -48.3555   |
| o   | 3   | e      | 14  | -29.6395   | -28.6943   | -29.6833   | -28.4228   |
| o   | 3   | e      | 15  | -28.3078   | -27.3409   | -28.0281   | -27.3808   |
| o   | 3   | e      | 16  | 0.4480     | 1.0877     | 0.3795     | 1.0112     |
| o   | 3   | e      | 17  | 36.9032    | 36.5421    | 36.8878    | 36.5234    |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 3   | e      | 18  | 44.9410    | 44.5130    | 44.9380    | 44.4973    |
| o   | 3   | e      | 19  | 55.5880    | 55.5770    | 55.4434    | 55.4216    |
| o   | 3   | f      | 1   | 114.7727   | -1112.5383 | -1114.9357 | -1112.6735 |
| o   | 3   | f      | 2   | 537.4321   | -535.6310  | -537.4179  | -535.6006  |
| o   | 3   | f      | 3   | 514.0733   | -511.6189  | -514.1462  | -511.6795  |
| o   | 3   | f      | 4   | 234.4370   | -233.4051  | -234.3742  | -233.3524  |
| o   | 3   | f      | 5   | 145.1540   | -143.3639  | -145.2173  | -143.4310  |
| o   | 3   | f      | 6   | 111.8198   | -110.5442  | -111.8399  | -110.5617  |
| o   | 3   | f      | 7   | -47.4665   | -47.2688   | -47.3632   | -47.1765   |
| o   | 3   | f      | 8   | -29.6378   | -27.3421   | -29.6818   | -27.3825   |
| o   | 3   | f      | 9   | -1.7765    | -1.0725    | -1.8056    | -1.1087    |
| o   | 3   | f      | 10  | 41.7827    | 41.4734    | 41.7976    | 41.4729    |
| o   | 4   | e      | 1   | -1713.6215 | -1712.2384 | -1713.8150 | -1712.3977 |
| o   | 4   | e      | 2   | -1085.3377 | -1083.1359 | -1085.5099 | -1083.2803 |
| o   | 4   | e      | 3   | -990.1450  | -989.0786  | -989.8239  | -988.7402  |
| o   | 4   | e      | 4   | -583.7937  | -581.4420  | -583.9254  | -581.5562  |
| o   | 4   | e      | 5   | -517.8296  | -516.3664  | -517.7529  | -516.2752  |
| o   | 4   | e      | 6   | -485.6063  | -483.3000  | -485.6049  | -483.2746  |
| o   | 4   | e      | 7   | -466.6638  | -465.6226  | -466.3657  | -465.3387  |
| o   | 4   | e      | 8   | -216.8848  | -216.1171  | -216.8498  | -216.0881  |
| o   | 4   | e      | 9   | -200.0454  | -199.6724  | -199.7703  | -199.3986  |
| o   | 4   | e      | 10  | -140.8270  | -139.8171  | -140.8779  | -139.8747  |
| o   | 4   | e      | 11  | -112.1289  | -110.5610  | -112.2321  | -110.6703  |
| o   | 4   | e      | 12  | -88.6270   | -87.4017   | -88.6600   | -87.4326   |
| o   | 4   | e      | 13  | -32.6719   | -32.5266   | -32.6432   | -32.5074   |
| o   | 4   | e      | 14  | -15.6217   | -16.0210   | -15.3586   | -15.7680   |
| o   | 4   | e      | 15  | -0.4856    | 1.7209     | -0.5304    | 1.6795     |
| o   | 4   | e      | 16  | 20.7175    | 21.0952    | 20.6360    | 21.0072    |
| o   | 4   | e      | 17  | 45.9709    | 45.6105    | 46.0219    | 45.6523    |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 4   | e      | 18  | 54.3754    | 54.0835    | 54.3747    | 54.0665    |
| o   | 4   | f      | 1   | -1082.0973 | -1079.8707 | -1082.2640 | -1080.0094 |
| o   | 4   | f      | 2   | -512.0117  | -510.2382  | -512.0047  | -510.2162  |
| o   | 4   | f      | 3   | -480.5780  | -478.1346  | -480.6601  | -478.2027  |
| o   | 4   | f      | 4   | -211.5633  | -210.6444  | -211.4995  | -210.5912  |
| o   | 4   | f      | 5   | -118.7145  | -116.8834  | -118.7874  | -116.9592  |
| o   | 4   | f      | 6   | -89.0727   | -87.8501   | -89.1049   | -87.8802   |
| o   | 4   | f      | 7   | -31.0142   | -30.8839   | -30.9189   | -30.7998   |
| o   | 4   | f      | 8   | -0.4857    | 1.7205     | -0.5302    | 1.6793     |
| o   | 4   | f      | 9   | 18.4858    | 19.0399    | 18.4686    | 19.0165    |
| o   | 4   | f      | 10  | 50.7116    | 50.5470    | 50.7177    | 50.5378    |
| o   | 5   | e      | 1   | -1672.9671 | -1671.5886 | -1673.1685 | -1671.7557 |
| o   | 5   | e      | 2   | -1046.2925 | -1044.1152 | -1046.4749 | -1044.2695 |
| o   | 5   | e      | 3   | -953.4240  | -952.3572  | -953.1348  | -952.0505  |
| o   | 5   | e      | 4   | -545.9660  | -543.6687  | -546.1009  | -543.7852  |
| o   | 5   | e      | 5   | -488.3004  | -486.9574  | -488.2432  | -486.8887  |
| o   | 5   | e      | 6   | -448.4808  | -446.4055  | -448.4368  | -446.3358  |
| o   | 5   | e      | 7   | -429.4606  | -428.1031  | -429.3026  | -427.9588  |
| o   | 5   | e      | 8   | -191.8566  | -191.1840  | -191.8381  | -191.1693  |
| o   | 5   | e      | 9   | -173.9936  | -173.7302  | -173.7344  | -173.4777  |
| o   | 5   | e      | 10  | -113.2100  | -112.2307  | -113.3529  | -112.3778  |
| o   | 5   | e      | 11  | -77.5370   | -75.8753   | -77.6898   | -76.0327   |
| o   | 5   | e      | 12  | -60.0243   | -58.8556   | -60.0797   | -58.9100   |
| o   | 5   | e      | 13  | -13.1595   | -13.0714   | -13.1826   | -13.1026   |
| o   | 5   | e      | 14  | -0.2589    | -0.6713    | -0.0448    | -0.4701    |
| o   | 5   | e      | 15  | 35.3405    | 37.4275    | 35.2899    | 37.3794    |
| o   | 5   | e      | 16  | 40.7105    | 40.6264    | 40.6545    | 40.5654    |
| o   | 5   | e      | 17  | 55.5065    | 55.2199    | 55.5180    | 55.2194    |
| o   | 5   | f      | 1   | -1041.3455 | -1039.1287 | -1041.5171 | -1039.2719 |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 5   | f      | 2   | -479.4488  | -477.7225  | -479.4520  | -477.7116  |
| o   | 5   | f      | 3   | -439.7929  | -437.3517  | -439.8871  | -437.4305  |
| o   | 5   | f      | 4   | -183.8249  | -183.0232  | -183.7660  | -182.9753  |
| o   | 5   | f      | 5   | -85.3406   | -83.5124   | -85.4221   | -83.5960   |
| o   | 5   | f      | 6   | -61.0697   | -59.8972   | -61.1301   | -59.9564   |
| o   | 5   | f      | 7   | -11.1566   | -11.0850   | -11.0753   | -11.0152   |
| o   | 5   | f      | 8   | 35.3263    | 37.3994    | 35.2794    | 37.3553    |
| o   | 5   | f      | 9   | 40.6802    | 40.8595    | 40.6822    | 40.8541    |
| o   | 6   | e      | 1   | -1624.2818 | -1622.9089 | -1624.4923 | -1623.0847 |
| o   | 6   | e      | 2   | -999.6579  | -997.5123  | -999.8573  | -997.6835  |
| o   | 6   | e      | 3   | -909.4215  | -908.3524  | -909.1702  | -908.0831  |
| o   | 6   | e      | 4   | -500.9106  | -498.6890  | -501.0626  | -498.8211  |
| o   | 6   | e      | 5   | -452.6194  | -451.3956  | -452.6219  | -451.3897  |
| o   | 6   | e      | 6   | -405.2982  | -403.4527  | -405.2359  | -403.3702  |
| o   | 6   | e      | 7   | -384.1933  | -382.5218  | -384.1644  | -382.4986  |
| o   | 6   | e      | 8   | -162.2267  | -161.6416  | -162.2261  | -161.6416  |
| o   | 6   | e      | 9   | -144.0906  | -143.9203  | -143.9110  | -143.7529  |
| o   | 6   | e      | 10  | -80.2280   | -79.3342   | -80.4695   | -79.5773   |
| o   | 6   | e      | 11  | -35.9887   | -34.2869   | -36.2191   | -34.5191   |
| o   | 6   | e      | 12  | -26.0048   | -24.8945   | -26.0839   | -24.9747   |
| o   | 6   | e      | 13  | 9.8977     | 9.9345     | 9.8250     | 9.8592     |
| o   | 6   | e      | 14  | 17.6004    | 17.1964    | 17.7097    | 17.2862    |
| o   | 6   | e      | 15  | 55.9592    | 55.6103    | 55.9853    | 55.6260    |
| o   | 6   | f      | 1   | -992.5800  | -990.3749  | -992.7575  | -990.5237  |
| o   | 6   | f      | 2   | -439.9244  | -438.2572  | -439.9441  | -438.2632  |
| o   | 6   | f      | 3   | -391.7431  | -389.3036  | -391.8532  | -389.3973  |
| o   | 6   | f      | 4   | -151.5839  | -150.8949  | -151.5372  | -150.8593  |
| o   | 6   | f      | 5   | -45.4746   | -43.7665   | -45.5574   | -43.8511   |
| o   | 6   | f      | 6   | -27.9696   | -26.8052   | -28.0677   | -26.9022   |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 6   | f      | 7   | 12.0288    | 12.0658    | 12.0901    | 12.1160    |
| o   | 7   | e      | 1   | -1567.6204 | -1566.2541 | -1567.8414 | -1566.4400 |
| o   | 7   | e      | 2   | -945.5651  | -943.4588  | -945.7937  | -943.6603  |
| o   | 7   | e      | 3   | -858.1611  | -857.0861  | -857.9544  | -856.8607  |
| o   | 7   | e      | 4   | -448.8730  | -446.7622  | -449.0682  | -446.9342  |
| o   | 7   | e      | 5   | -410.9804  | -409.8523  | -411.1120  | -409.9840  |
| o   | 7   | e      | 6   | -355.8919  | -354.2128  | -355.8510  | -354.1584  |
| o   | 7   | e      | 7   | -331.0639  | -329.1483  | -331.1412  | -329.2230  |
| o   | 7   | e      | 8   | -128.1155  | -127.6363  | -128.1281  | -127.6448  |
| o   | 7   | e      | 9   | -110.4851  | -110.3598  | -110.4777  | -110.3725  |
| o   | 7   | e      | 10  | -42.8309   | -42.0637   | -43.1758   | -42.4089   |
| o   | 7   | e      | 11  | 10.8994    | 12.1774    | 10.6460    | 11.9612    |
| o   | 7   | e      | 12  | 13.3644    | 14.5894    | 13.1879    | 14.3806    |
| o   | 7   | e      | 13  | 35.9485    | 35.7146    | 36.0581    | 35.8310    |
| o   | 7   | e      | 14  | 39.2843    | 39.3321    | 38.9474    | 38.9564    |
| o   | 7   | f      | 1   | -935.8766  | -933.6843  | -936.0620  | -933.8415  |
| o   | 7   | f      | 2   | -393.6232  | -392.0217  | -393.6683  | -392.0556  |
| o   | 7   | f      | 3   | -336.5044  | -334.0699  | -336.6360  | -334.1849  |
| o   | 7   | f      | 4   | -115.1570  | -114.5708  | -115.1308  | -114.5572  |
| o   | 7   | f      | 5   | -1.5438    | -0.3402    | -1.6030    | -0.4049    |
| o   | 7   | f      | 6   | 11.1023    | 12.4827    | 10.9391    | 12.3239    |
| o   | 7   | f      | 7   | 38.9194    | 39.0065    | 38.9521    | 39.0264    |
| o   | 8   | e      | 1   | -1503.0477 | -1501.6888 | -1503.2807 | -1501.8862 |
| o   | 8   | e      | 2   | -884.1731  | -882.1193  | -884.4559  | -882.3741  |
| o   | 8   | e      | 3   | -799.6614  | -798.5745  | -799.5066  | -798.4006  |
| o   | 8   | e      | 4   | -390.2388  | -388.3172  | -390.5444  | -388.5872  |
| o   | 8   | e      | 5   | -363.4263  | -362.3346  | -363.8231  | -362.7437  |
| o   | 8   | e      | 6   | -300.0590  | -298.4784  | -300.0699  | -298.4801  |
| o   | 8   | e      | 7   | -270.3484  | -268.2677  | -270.5540  | -268.4646  |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 8   | e      | 8   | -90.0081   | -89.6800   | -90.0127   | -89.6747   |
| o   | 8   | e      | 9   | -72.9295   | -72.7911   | -73.2276   | -73.1136   |
| o   | 8   | e      | 10  | -2.2095    | -1.6176    | -2.6983    | -2.1025    |
| o   | 8   | e      | 11  | 51.1076    | 51.1344    | 51.0256    | 51.0550    |
| o   | 8   | e      | 12  | 56.6101    | 56.9385    | 56.3904    | 56.7232    |
| o   | 8   | f      | 1   | -871.3245  | -869.1492  | -871.5213  | -869.3164  |
| o   | 8   | f      | 2   | -340.7447  | -339.2200  | -340.8341  | -339.2967  |
| o   | 8   | f      | 3   | -274.1857  | -271.7633  | -274.3558  | -271.9163  |
| o   | 8   | f      | 4   | -74.8522   | -74.3656   | -74.8583   | -74.3827   |
| o   | 8   | f      | 5   | 39.2080    | 39.6492    | 39.1558    | 39.5857    |
| o   | 9   | e      | 1   | -1430.6382 | -1429.2875 | -1430.8852 | -1429.4986 |
| o   | 9   | e      | 2   | -815.6793  | -813.6903  | -816.0584  | -814.0418  |
| o   | 9   | e      | 3   | -733.9299  | -732.8231  | -733.8371  | -732.7108  |
| o   | 9   | e      | 4   | -326.2806  | -324.7805  | -326.5207  | -324.9581  |
| o   | 9   | e      | 5   | -309.3565  | -308.0815  | -310.3422  | -309.1092  |
| o   | 9   | e      | 6   | -237.6805  | -236.1484  | -237.7629  | -236.2233  |
| o   | 9   | e      | 7   | -202.3919  | -200.2098  | -202.7129  | -200.5177  |
| o   | 9   | e      | 8   | -48.9250   | -48.7919   | -48.8680   | -48.7272   |
| o   | 9   | e      | 9   | -30.8462   | -30.6475   | -31.6123   | -31.4351   |
| o   | 9   | e      | 10  | 39.3835    | 39.6961    | 38.8858    | 39.2048    |
| o   | 9   | f      | 1   | -799.0312  | -796.8741  | -799.2422  | -797.0550  |
| o   | 9   | f      | 2   | -281.5350  | -280.0931  | -281.6835  | -280.2287  |
| o   | 9   | f      | 3   | -204.9543  | -202.5534  | -205.1775  | -202.7589  |
| o   | 9   | f      | 4   | -31.0556   | -30.6663   | -31.1030   | -30.7242   |
| o   | 10  | e      | 1   | -1350.4761 | -1349.1343 | -1350.7409 | -1349.3629 |
| o   | 10  | e      | 2   | -740.3013  | -738.3926  | -740.8643  | -738.9295  |
| o   | 10  | e      | 3   | -660.9611  | -659.8237  | -660.9438  | -659.7868  |
| o   | 10  | e      | 4   | -260.8401  | -260.0968  | -260.8683  | -260.1190  |
| o   | 10  | e      | 5   | -245.4741  | -243.6986  | -247.5271  | -245.7409  |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 10  | e      | 6   | -168.7289  | -167.2100  | -168.9012  | -167.3766  |
| o   | 10  | e      | 7   | -127.4583  | -125.2220  | -127.9104  | -125.6595  |
| o   | 10  | e      | 8   | -6.0023    | -6.0529    | -5.9376    | -5.9911    |
| o   | 10  | e      | 9   | 16.1354    | 16.3716    | 14.8284    | 15.0546    |
| o   | 10  | f      | 1   | -719.1130  | -716.9760  | -719.3481  | -717.1809  |
| o   | 10  | f      | 2   | -216.2559  | -214.9037  | -216.5030  | -215.1385  |
| o   | 10  | f      | 3   | -129.0195  | -126.6502  | -129.3216  | -126.9357  |
| o   | 10  | f      | 4   | 15.6765    | 15.9619    | 15.5749    | 15.8500    |
| o   | 11  | e      | 1   | -1262.6767 | -1261.3449 | -1262.9448 | -1261.5763 |
| o   | 11  | e      | 2   | -658.8037  | -656.9979  | -659.1889  | -657.3550  |
| o   | 11  | e      | 3   | -580.7891  | -579.6097  | -580.8132  | -579.6132  |
| o   | 11  | e      | 4   | -196.5935  | -196.1791  | -196.5529  | -196.1374  |
| o   | 11  | e      | 5   | -172.1815  | -170.3586  | -173.2863  | -171.4489  |
| o   | 11  | e      | 6   | -93.3707   | -91.8494   | -93.5607   | -92.0304   |
| o   | 11  | e      | 7   | -46.1749   | -43.9271   | -46.4655   | -44.2000   |
| o   | 11  | e      | 8   | 37.7768    | 37.5902    | 37.9437    | 37.7480    |
| o   | 11  | f      | 1   | -631.7572  | -629.6438  | -631.9812  | -629.8367  |
| o   | 11  | f      | 2   | -145.4933  | -144.2397  | -145.6397  | -144.3744  |
| o   | 11  | f      | 3   | -46.8659   | -44.5473   | -47.0835   | -44.7459   |
| o   | 12  | e      | 1   | -1167.3192 | -1165.9982 | -1167.6061 | -1166.2479 |
| o   | 12  | e      | 2   | -570.8360  | -569.1503  | -571.3966  | -569.6836  |
| o   | 12  | e      | 3   | -493.3133  | -492.0779  | -493.4302  | -492.1746  |
| o   | 12  | e      | 4   | -129.5925  | -129.3066  | -129.8373  | -129.5459  |
| o   | 12  | e      | 5   | -90.7462   | -89.1006   | -92.4048   | -90.7492   |
| o   | 12  | e      | 6   | -11.7334   | -10.2055   | -12.0204   | -10.4858   |
| o   | 12  | e      | 7   | 41.6331    | 43.8562    | 41.2143    | 43.4554    |
| o   | 12  | f      | 1   | -537.0590  | -534.9714  | -537.3052  | -535.1862  |
| o   | 12  | f      | 2   | -69.3031   | -68.1596   | -69.5283   | -68.3736   |
| o   | 12  | f      | 3   | 41.4141    | 43.6637    | 41.1253    | 43.3933    |



| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| o   | 13  | e      | 1   | -1064.5293 | -1063.2198 | -1064.8471 | -1063.5000 |
| o   | 13  | e      | 2   | -477.0168  | -475.4694  | -477.8862  | -476.3124  |
| o   | 13  | e      | 3   | -398.5395  | -397.2364  | -398.8007  | -397.4797  |
| o   | 13  | e      | 4   | -59.1220   | -58.9456   | -59.7471   | -59.5620   |
| o   | 13  | e      | 5   | -4.6681    | -3.2424    | -7.1159    | -5.6813    |
| o   | 13  | f      | 1   | -435.2213  | -433.1624  | -435.5084  | -433.4183  |
| o   | 13  | f      | 2   | 11.6097    | 12.6276    | 11.2553    | 12.2837    |
| o   | 14  | e      | 1   | -954.4943  | -953.1976  | -954.8042  | -953.4693  |
| o   | 14  | e      | 2   | -378.5088  | -377.1159  | -379.0680  | -377.6469  |
| o   | 14  | e      | 3   | -296.7142  | -295.3452  | -296.9874  | -295.5975  |
| o   | 14  | e      | 4   | 13.6474    | 13.7187    | 13.3700    | 13.4468    |
| o   | 14  | f      | 1   | -326.5530  | -324.5282  | -326.8090  | -324.7518  |
| o   | 15  | e      | 1   | -837.2827  | -835.9977  | -837.6304  | -836.3087  |
| o   | 15  | e      | 2   | -274.4768  | -273.2405  | -275.3434  | -274.0819  |
| o   | 15  | e      | 3   | -187.6883  | -186.2518  | -188.1490  | -186.6951  |
| o   | 15  | f      | 1   | -211.1674  | -209.1802  | -211.4621  | -209.4427  |
| o   | 16  | e      | 1   | -713.0808  | -711.8117  | -713.4964  | -712.1891  |
| o   | 16  | e      | 2   | -165.7499  | -164.6763  | -167.1046  | -166.0040  |
| o   | 16  | e      | 3   | -71.7692   | -70.2764   | -72.5696   | -71.0656   |
| o   | 16  | f      | 1   | -89.4000   | -87.4563   | -89.7708   | -87.7954   |
| o   | 17  | e      | 1   | -582.0521  | -580.7982  | -582.5945  | -581.3031  |
| o   | 17  | e      | 2   | -52.6909   | -51.7802   | -54.7654   | -53.8244   |
| o   | 17  | e      | 3   | 50.8555    | 52.3881    | 49.3175    | 50.8505    |
| o   | 17  | f      | 1   | 38.4136    | 40.3062    | 37.8960    | 39.8191    |
| o   | 18  | e      | 1   | -444.3786  | -443.1407  | -445.1424  | -443.8686  |
| o   | 19  | e      | 1   | -300.2620  | -299.0414  | -301.3889  | -300.1350  |
| o   | 20  | e      | 1   | -149.7211  | -148.5150  | -151.6224  | -150.3913  |
| o   | 21  | e      | 1   | 6.7592     | 7.9412     | 3.8163     | 5.0204     |
| p   | 0   | e      | 1   | -1795.1575 | -1793.7639 | -1795.3352 | -1793.9091 |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| p   | 0   | e      | 2   | -1063.7827 | -1062.7083 | -1063.3984 | -1062.3114 |
| p   | 0   | e      | 3   | -662.1132  | -659.6723  | -662.2749  | -659.8206  |
| p   | 0   | e      | 4   | -539.4297  | -538.8389  | -538.8525  | -538.2706  |
| p   | 0   | e      | 5   | -301.4467  | -300.6517  | -301.4014  | -300.6175  |
| p   | 0   | e      | 6   | -214.4946  | -214.3129  | -214.1766  | -214.0097  |
| p   | 0   | e      | 7   | -109.9271  | -109.8684  | -109.8808  | -109.8289  |
| p   | 0   | e      | 8   | -60.6972   | -60.7249   | -60.7455   | -60.7929   |
| p   | 0   | e      | 9   | -15.7192   | -16.0670   | -15.6409   | -16.0053   |
| p   | 0   | e      | 10  | -1.1368    | -1.1504    | -1.5090    | -1.5265    |
| p   | 1   | e      | 1   | -1786.9905 | -1785.5980 | -1787.1699 | -1785.7447 |
| p   | 1   | e      | 2   | -1155.9897 | -1153.7480 | -1156.1568 | -1153.8879 |
| p   | 1   | e      | 3   | -1056.4101 | -1055.3364 | -1056.0319 | -1054.9454 |
| p   | 1   | e      | 4   | -654.3137  | -651.8816  | -654.4730  | -652.0275  |
| p   | 1   | e      | 5   | -563.9041  | -562.5239  | -563.8107  | -562.4224  |
| p   | 1   | e      | 6   | -532.1888  | -531.5656  | -531.6393  | -531.0251  |
| p   | 1   | e      | 7   | -295.9271  | -295.1356  | -295.8749  | -295.0942  |
| p   | 1   | e      | 8   | -213.8730  | -212.6546  | -213.8144  | -212.5940  |
| p   | 1   | e      | 9   | -210.1857  | -209.9754  | -209.8876  | -209.6923  |
| p   | 1   | e      | 10  | -156.4334  | -154.5125  | -156.5453  | -154.6271  |
| p   | 1   | e      | 11  | -105.5803  | -105.5427  | -105.5159  | -105.4853  |
| p   | 1   | e      | 12  | -57.0345   | -57.0589   | -57.0950   | -57.1386   |
| p   | 1   | e      | 13  | -14.0353   | -14.3679   | -13.9650   | -14.3146   |
| p   | 1   | e      | 14  | -0.4303    | -0.4477    | -0.9542    | -0.9691    |
| p   | 1   | f      | 1   | -1155.8701 | -1153.4283 | -1155.8380 | -1153.5668 |
| p   | 1   | f      | 2   | -562.8482  | -561.2379  | -562.5708  | -561.1507  |
| p   | 1   | f      | 3   | -213.9034  | -212.4739  | -213.6404  | -212.4074  |
| p   | 1   | f      | 4   | -156.8473  | -154.6979  | -156.7529  | -154.8036  |
| p   | 2   | e      | 1   | -1770.6656 | -1769.2750 | -1770.8484 | -1769.4250 |
| p   | 2   | e      | 2   | -1140.2456 | -1138.0124 | -1140.4174 | -1138.1568 |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| p   | 2   | e      | 3   | -1041.6720 | -1040.5995 | -1041.3059 | -1040.2204 |
| p   | 2   | e      | 4   | -638.7466  | -636.3328  | -638.9022  | -636.4746  |
| p   | 2   | e      | 5   | -556.0217  | -554.3278  | -555.9838  | -554.2686  |
| p   | 2   | e      | 6   | -542.2887  | -539.7977  | -542.3536  | -539.8546  |
| p   | 2   | e      | 7   | -517.6946  | -517.0010  | -517.2002  | -516.5167  |
| p   | 2   | e      | 8   | -284.8796  | -284.0997  | -284.8154  | -284.0460  |
| p   | 2   | e      | 9   | -202.5942  | -201.5499  | -202.5247  | -201.4285  |
| p   | 2   | e      | 10  | -201.3838  | -201.0364  | -201.1450  | -200.8627  |
| p   | 2   | e      | 11  | -178.4708  | -177.3169  | -178.4829  | -177.3364  |
| p   | 2   | e      | 12  | -141.5481  | -139.6510  | -141.6852  | -139.7908  |
| p   | 2   | e      | 13  | -97.0685   | -97.0736   | -96.9718   | -96.9846   |
| p   | 2   | e      | 14  | -49.6789   | -49.7004   | -49.7621   | -49.8017   |
| p   | 2   | e      | 15  | -10.7659   | -11.0578   | -10.7122   | -11.0214   |
| p   | 2   | e      | 16  | 0.8949     | 0.8811     | -0.0607    | -0.0614    |
| p   | 2   | f      | 1   | -1139.2873 | -1137.0473 | -1139.4552 | -1137.1878 |
| p   | 2   | f      | 2   | -553.7206  | -551.7982  | -553.7281  | -551.7824  |
| p   | 2   | f      | 3   | -540.8119  | -538.4484  | -540.8711  | -538.5027  |
| p   | 2   | f      | 4   | -202.0169  | -200.8526  | -201.9473  | -200.7820  |
| p   | 2   | f      | 5   | -178.5053  | -177.3466  | -178.5158  | -177.3643  |
| p   | 2   | f      | 6   | -141.9751  | -139.9961  | -142.0884  | -140.1105  |
| p   | 3   | e      | 1   | -1746.1998 | -1744.8130 | -1746.3885 | -1744.9677 |
| p   | 3   | e      | 2   | -1116.6749 | -1114.4549 | -1116.8539 | -1114.6063 |
| p   | 3   | e      | 3   | -1019.5787 | -1018.5112 | -1019.2346 | -1018.1502 |
| p   | 3   | e      | 4   | -615.4751  | -613.0921  | -615.6299  | -613.2306  |
| p   | 3   | e      | 5   | -540.0044  | -538.4192  | -539.9576  | -538.3553  |
| p   | 3   | e      | 6   | -517.7668  | -515.3157  | -517.8192  | -515.3527  |
| p   | 3   | e      | 7   | -495.8879  | -495.0750  | -495.4796  | -494.6758  |
| p   | 3   | e      | 8   | -268.3268  | -267.5780  | -268.2512  | -267.5089  |
| p   | 3   | e      | 9   | -187.9933  | -187.6534  | -187.7801  | -187.4556  |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| p   | 3   | e      | 10  | -185.8049  | -184.8122  | -185.7869  | -184.7907  |
| p   | 3   | e      | 11  | -161.5033  | -160.3553  | -161.5289  | -160.3885  |
| p   | 3   | e      | 12  | -119.8175  | -117.9565  | -119.9861  | -118.1274  |
| p   | 3   | e      | 13  | -84.7585   | -84.8310   | -84.6283   | -84.7059   |
| p   | 3   | e      | 14  | -38.6301   | -38.6611   | -38.7404   | -38.7866   |
| p   | 3   | e      | 15  | -6.1093    | -6.3201    | -6.0817    | -6.3105    |
| p   | 3   | f      | 1   | -1114.7404 | -1112.5063 | -1114.9114 | -1112.6495 |
| p   | 3   | f      | 2   | -535.4256  | -533.5448  | -535.4327  | -533.5329  |
| p   | 3   | f      | 3   | -514.7125  | -512.3361  | -514.7835  | -512.3976  |
| p   | 3   | f      | 4   | -184.6875  | -183.6222  | -184.6116  | -183.5464  |
| p   | 3   | f      | 5   | -161.5924  | -160.4312  | -161.6092  | -160.4550  |
| p   | 3   | f      | 6   | -120.1374  | -118.1289  | -120.2620  | -118.2533  |
| p   | 4   | e      | 1   | -1713.6219 | -1712.2389 | -1713.8172 | -1712.4000 |
| p   | 4   | e      | 2   | -1085.3338 | -1083.1320 | -1085.5230 | -1083.2935 |
| p   | 4   | e      | 3   | -990.1572  | -989.0906  | -989.8379  | -988.7540  |
| p   | 4   | e      | 4   | -584.6058  | -582.2643  | -584.7623  | -582.4036  |
| p   | 4   | e      | 5   | -517.4308  | -515.9667  | -517.3913  | -515.9132  |
| p   | 4   | e      | 6   | -486.6758  | -484.3335  | -486.7025  | -484.3382  |
| p   | 4   | e      | 7   | -466.6264  | -465.6147  | -466.3291  | -465.3303  |
| p   | 4   | e      | 8   | -246.4042  | -245.7078  | -246.3135  | -245.6232  |
| p   | 4   | e      | 9   | -169.3926  | -168.9900  | -169.2803  | -168.8895  |
| p   | 4   | e      | 10  | -164.1346  | -163.2778  | -164.1268  | -163.2709  |
| p   | 4   | e      | 11  | -138.6821  | -137.5338  | -138.7376  | -137.5967  |
| p   | 4   | e      | 12  | -91.7646   | -89.9697   | -91.9627   | -90.1686   |
| p   | 4   | e      | 13  | -69.1954   | -69.3391   | -69.0381   | -69.1905   |
| p   | 4   | e      | 14  | -24.1706   | -24.2514   | -24.2927   | -24.3849   |
| p   | 4   | e      | 15  | -0.5398    | -0.6185    | -0.5873    | -0.6800    |
| p   | 4   | f      | 1   | -1082.0685 | -1079.8421 | -1082.2434 | -1079.9890 |
| p   | 4   | f      | 2   | -509.7563  | -507.9354  | -509.7653  | -507.9274  |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| p   | 4   | f      | 3   | -481.3761  | -478.9785  | -481.4615  | -479.0518  |
| p   | 4   | f      | 4   | -161.9885  | -161.0487  | -161.9064  | -160.9677  |
| p   | 4   | f      | 5   | -138.7889  | -137.6201  | -138.8190  | -137.6568  |
| p   | 4   | f      | 6   | -91.3108   | -89.2809   | -91.4461   | -89.4149   |
| p   | 5   | e      | 1   | -1672.9672 | -1671.5887 | -1673.1707 | -1671.7579 |
| p   | 5   | e      | 2   | -1046.2995 | -1044.1221 | -1046.5037 | -1044.2985 |
| p   | 5   | e      | 3   | -953.4279  | -952.3610  | -953.1398  | -952.0554  |
| p   | 5   | e      | 4   | -546.2840  | -544.0005  | -546.4520  | -544.1499  |
| p   | 5   | e      | 5   | -488.5539  | -487.2051  | -488.5522  | -487.1929  |
| p   | 5   | e      | 6   | -449.1836  | -447.0443  | -449.1750  | -447.0100  |
| p   | 5   | e      | 7   | -429.6461  | -428.3497  | -429.4835  | -428.2014  |
| p   | 5   | e      | 8   | -219.4138  | -218.8010  | -219.3111  | -218.7041  |
| p   | 5   | e      | 9   | -145.3259  | -144.8495  | -145.3482  | -144.8810  |
| p   | 5   | e      | 10  | -137.8843  | -137.1764  | -137.9049  | -137.2015  |
| p   | 5   | e      | 11  | -109.9130  | -108.7645  | -110.0192  | -108.8773  |
| p   | 5   | e      | 12  | -58.3222   | -56.8480   | -58.4990   | -56.9939   |
| p   | 5   | e      | 13  | -50.7280   | -50.7354   | -50.6148   | -50.6655   |
| p   | 5   | e      | 14  | -7.7992    | -8.0052    | -7.8771    | -8.0924    |
| p   | 5   | f      | 1   | -1041.3209 | -1039.1042 | -1041.5006 | -1039.2556 |
| p   | 5   | f      | 2   | -476.9944  | -475.2406  | -477.0092  | -475.2396  |
| p   | 5   | f      | 3   | -440.6849  | -438.2696  | -440.7871  | -438.3578  |
| p   | 5   | f      | 4   | -134.2851  | -133.4836  | -134.1997  | -133.4006  |
| p   | 5   | f      | 5   | -109.9574  | -108.7858  | -110.0083  | -108.8427  |
| p   | 5   | f      | 6   | -55.7294   | -53.6967   | -55.8738   | -53.8386   |
| p   | 6   | e      | 1   | -1624.2811 | -1622.9082 | -1624.4946 | -1623.0871 |
| p   | 6   | e      | 2   | -999.6731  | -997.5272  | -999.9008  | -997.7271  |
| p   | 6   | e      | 3   | -909.4166  | -908.3473  | -909.1668  | -908.0795  |
| p   | 6   | e      | 4   | -500.7168  | -498.5152  | -500.9133  | -498.6910  |
| p   | 6   | e      | 5   | -453.5133  | -452.2657  | -453.5990  | -452.3453  |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| p   | 6   | e      | 6   | -405.5917  | -403.7023  | -405.5564  | -403.6445  |
| p   | 6   | e      | 7   | -384.6923  | -383.0749  | -384.6701  | -383.0616  |
| p   | 6   | e      | 8   | -187.8794  | -187.3813  | -187.7756  | -187.2839  |
| p   | 6   | e      | 9   | -115.4064  | -114.8647  | -115.5910  | -115.0538  |
| p   | 6   | e      | 10  | -107.4654  | -106.8872  | -107.5565  | -106.9875  |
| p   | 6   | e      | 11  | -75.1659   | -74.0324   | -75.3417   | -74.2140   |
| p   | 6   | e      | 12  | -31.8870   | -32.2321   | -31.7203   | -32.0773   |
| p   | 6   | e      | 13  | -18.6187   | -17.0825   | -18.8939   | -17.3598   |
| p   | 6   | f      | 1   | -992.5603  | -990.3554  | -992.7456  | -990.5119  |
| p   | 6   | f      | 2   | -437.3322  | -435.6497  | -437.3585  | -435.6610  |
| p   | 6   | f      | 3   | -392.6572  | -390.2308  | -392.7794  | -390.3377  |
| p   | 6   | f      | 4   | -101.9670  | -101.2987  | -101.8858  | -101.2209  |
| p   | 6   | f      | 5   | -75.0565   | -73.9038   | -75.1349   | -73.9873   |
| p   | 6   | f      | 6   | -13.7462   | -11.7420   | -13.8971   | -11.8896   |
| p   | 7   | e      | 1   | -1567.6184 | -1566.2521 | -1567.8438 | -1566.4424 |
| p   | 7   | e      | 2   | -945.5812  | -943.4744  | -945.8489  | -943.7157  |
| p   | 7   | e      | 3   | -858.1476  | -857.0726  | -857.9439  | -856.8501  |
| p   | 7   | e      | 4   | -448.2081  | -446.1309  | -448.4584  | -446.3553  |
| p   | 7   | e      | 5   | -412.3867  | -411.2085  | -412.6467  | -411.4721  |
| p   | 7   | e      | 6   | -356.0199  | -354.3418  | -355.9894  | -354.2954  |
| p   | 7   | e      | 7   | -331.7381  | -329.8469  | -331.8450  | -329.9544  |
| p   | 7   | e      | 8   | -152.5037  | -152.1410  | -152.4271  | -152.0730  |
| p   | 7   | e      | 9   | -79.5164   | -78.9618   | -79.8244   | -79.2624   |
| p   | 7   | e      | 10  | -73.0241   | -72.5164   | -73.3096   | -72.8228   |
| p   | 7   | e      | 11  | -34.5495   | -33.4575   | -34.8290   | -33.7423   |
| p   | 7   | e      | 12  | -10.6654   | -11.1332   | -10.5609   | -11.0431   |
| p   | 7   | f      | 1   | -935.8628  | -933.6706  | -936.0548  | -933.8345  |
| p   | 7   | f      | 2   | -390.9532  | -389.3438  | -391.0000  | -389.3782  |
| p   | 7   | f      | 3   | -337.3684  | -334.9385  | -337.5178  | -335.0722  |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| p   | 7   | f      | 4   | -65.3695   | -64.8141   | -65.3031   | -64.7545   |
| p   | 7   | f      | 5   | -34.2391   | -33.1393   | -34.3546   | -33.2596   |
| p   | 8   | e      | 1   | -1503.0436 | -1501.6846 | -1503.2832 | -1501.8888 |
| p   | 8   | e      | 2   | -884.1788  | -882.1242  | -884.5188  | -882.4371  |
| p   | 8   | e      | 3   | -799.6406  | -798.5538  | -799.4915  | -798.3855  |
| p   | 8   | e      | 4   | -389.3092  | -387.4551  | -389.6161  | -387.7220  |
| p   | 8   | e      | 5   | -365.0837  | -363.8971  | -365.6923  | -364.5247  |
| p   | 8   | e      | 6   | -300.3470  | -298.8004  | -300.3543  | -298.7974  |
| p   | 8   | e      | 7   | -271.0221  | -268.9440  | -271.2514  | -269.1667  |
| p   | 8   | e      | 8   | -114.0220  | -113.8003  | -114.0257  | -113.8135  |
| p   | 8   | e      | 9   | -39.1590   | -38.7776   | -39.2819   | -38.8927   |
| p   | 8   | e      | 10  | -33.4480   | -32.8572   | -34.3120   | -33.7369   |
| p   | 8   | f      | 1   | -871.3179  | -869.1425  | -871.5191  | -869.3142  |
| p   | 8   | f      | 2   | -338.0542  | -336.5256  | -338.1362  | -336.5939  |
| p   | 8   | f      | 3   | -274.9388  | -272.5155  | -275.1274  | -272.6879  |
| p   | 8   | f      | 4   | -24.7657   | -24.3112   | -24.7300   | -24.2795   |
| p   | 9   | e      | 1   | -1430.6303 | -1429.2795 | -1430.8881 | -1429.5015 |
| p   | 9   | e      | 2   | -815.6569  | -813.6665  | -816.1238  | -814.1074  |
| p   | 9   | e      | 3   | -733.9028  | -732.7961  | -733.8208  | -732.6947  |
| p   | 9   | e      | 4   | -325.5931  | -324.2662  | -325.7977  | -324.4125  |
| p   | 9   | e      | 5   | -310.5955  | -309.1171  | -311.9827  | -310.5460  |
| p   | 9   | e      | 6   | -238.3578  | -236.8709  | -238.4261  | -236.9316  |
| p   | 9   | e      | 7   | -202.8896  | -200.7004  | -203.2571  | -201.0579  |
| p   | 9   | e      | 8   | -73.0521   | -72.9597   | -73.2084   | -73.1275   |
| p   | 9   | f      | 1   | -799.0327  | -796.8756  | -799.2448  | -797.0577  |
| p   | 9   | f      | 2   | -278.8611  | -277.4165  | -278.9973  | -277.5388  |
| p   | 9   | f      | 3   | -205.5318  | -203.1258  | -205.7799  | -203.3573  |
| p   | 10  | e      | 1   | -1350.4602 | -1349.1183 | -1350.7442 | -1349.3662 |
| p   | 10  | e      | 2   | -740.2244  | -738.3134  | -740.9264  | -738.9917  |

| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D  | MRCI/CCVM  | FCI/CCVM   |
|-----|-----|--------|-----|------------|------------|------------|------------|
| p   | 10  | e      | 3   | -660.9047  | -659.7676  | -660.9306  | -659.7739  |
| p   | 10  | e      | 4   | -261.4765  | -260.8329  | -261.7910  | -261.1584  |
| p   | 10  | e      | 5   | -245.0862  | -243.1896  | -247.5509  | -245.6305  |
| p   | 10  | e      | 6   | -169.8163  | -168.3318  | -169.9986  | -168.5119  |
| p   | 10  | e      | 7   | -127.6305  | -125.3873  | -128.2454  | -125.9909  |
| p   | 10  | e      | 8   | -30.0705   | -30.0973   | -30.5068   | -30.5446   |
| p   | 10  | f      | 1   | -719.1266  | -716.9898  | -719.3554  | -717.1884  |
| p   | 10  | f      | 2   | -213.6282  | -212.2721  | -213.8525  | -212.4833  |
| p   | 10  | f      | 3   | -129.3500  | -126.9722  | -129.7011  | -127.3085  |
| p   | 11  | e      | 1   | -1262.6702 | -1261.3384 | -1262.9486 | -1261.5800 |
| p   | 11  | e      | 2   | -658.8099  | -657.0035  | -659.2418  | -657.4080  |
| p   | 11  | e      | 3   | -580.7735  | -579.5947  | -580.8077  | -579.6082  |
| p   | 11  | e      | 4   | -198.0492  | -197.6262  | -198.1619  | -197.7348  |
| p   | 11  | e      | 5   | -171.4865  | -169.6774  | -172.8307  | -171.0057  |
| p   | 11  | e      | 6   | -94.7340   | -93.2254   | -94.9419   | -93.4286   |
| p   | 11  | e      | 7   | -46.1455   | -43.8979   | -46.6227   | -44.3591   |
| p   | 11  | f      | 1   | -631.7675  | -629.6541  | -631.9932  | -629.8488  |
| p   | 11  | f      | 2   | -142.8919  | -141.6323  | -143.0247  | -141.7520  |
| p   | 11  | f      | 3   | -46.9259   | -44.5974   | -47.1915   | -44.8447   |
| p   | 12  | e      | 1   | -1167.3070 | -1165.9859 | -1167.6105 | -1166.2522 |
| p   | 12  | e      | 2   | -570.8072  | -569.1205  | -571.4352  | -569.7222  |
| p   | 12  | e      | 3   | -493.3064  | -492.0719  | -493.4369  | -492.1821  |
| p   | 12  | e      | 4   | -130.8967  | -130.5866  | -131.3208  | -131.0026  |
| p   | 12  | e      | 5   | -90.8206   | -89.2291   | -92.5842   | -90.9799   |
| p   | 12  | e      | 6   | -12.9718   | -11.4241   | -13.3094   | -11.7600   |
| p   | 12  | f      | 1   | -537.0794  | -534.9920  | -537.3217  | -535.2029  |
| p   | 12  | f      | 2   | -66.7091   | -65.5547   | -66.9125   | -65.7453   |
| p   | 13  | e      | 1   | -1064.5107 | -1063.2009 | -1064.8522 | -1063.5051 |
| p   | 13  | e      | 2   | -476.9356  | -475.3866  | -477.9066  | -476.3328  |



| o/p | $J$ | parity | $n$ | MRCI/DVR3D | FCI/DVR3D | MRCI/CCVM | FCI/CCVM  |
|-----|-----|--------|-----|------------|-----------|-----------|-----------|
| p   | 13  | e      | 3   | -398.5522  | -397.2506 | -398.8232 | -397.5033 |
| p   | 13  | e      | 4   | -60.0428   | -59.8436  | -60.8527  | -60.6428  |
| p   | 13  | e      | 5   | -6.1851    | -4.8368   | -8.5661   | -7.2042   |
| p   | 13  | f      | 1   | -435.2569  | -433.1982 | -435.5294 | -433.4396 |
| p   | 14  | e      | 1   | -954.4838  | -953.1870 | -954.8103 | -953.4754 |
| p   | 14  | e      | 2   | -378.3631  | -376.9692 | -379.0683 | -377.6471 |
| p   | 14  | e      | 3   | -296.7130  | -295.3439 | -297.0282 | -295.6395 |
| p   | 14  | f      | 1   | -326.5725  | -324.5477 | -326.8346 | -324.7777 |
| p   | 15  | e      | 1   | -837.2689  | -835.9837 | -837.6374 | -836.3158 |
| p   | 15  | e      | 2   | -274.3015  | -273.0648 | -275.3233 | -274.0618 |
| p   | 15  | e      | 3   | -187.6862  | -186.2493 | -188.2086 | -186.7562 |
| p   | 15  | f      | 1   | -211.1955  | -209.2084 | -211.4927 | -209.4736 |
| p   | 16  | e      | 1   | -713.0577  | -711.7883 | -713.5047 | -712.1975 |
| p   | 16  | e      | 2   | -165.5621  | -164.4891 | -167.0648 | -165.9642 |
| p   | 16  | e      | 3   | -71.7484   | -70.2558  | -72.6480  | -71.1456  |
| p   | 16  | f      | 1   | -89.4432   | -87.4997  | -89.8072  | -87.8322  |
| p   | 17  | e      | 1   | -582.0194  | -580.7651 | -582.6044 | -581.3130 |
| p   | 17  | e      | 2   | -52.5453   | -51.6334  | -54.7052  | -53.7642  |
| p   | 18  | e      | 1   | -444.3289  | -443.0900 | -445.1540 | -443.8803 |
| p   | 19  | e      | 1   | -300.0312  | -298.8077 | -301.4026 | -300.1488 |
| p   | 20  | e      | 1   | -149.5301  | -148.3249 | -151.6385 | -150.4075 |

TABLE S6. Bound states calculated for  $J = 0$  for *para*-H<sub>2</sub><sup>+</sup>-He using DVR3D, CCVM and TDWP methods on the FCI PES of this work. Zero corresponds to the energy of H<sub>2</sub><sup>+</sup>( $v = 0, j = 0$ ). DVR3D\* are the bound states when using the masses for H and He as in other previous work (Ref.1).

| $J$ | DVR3D    | DVR3D*   | CCVM     | TDWP     | CCVM on PES Ref. <sup>?</sup> |
|-----|----------|----------|----------|----------|-------------------------------|
| 1   | -1793.76 | -1793.26 | -1793.91 | -1793.58 | -1775.7165                    |
| 2   | -1062.71 | -1062.12 | -1062.31 | -1062.09 | -1041.9418                    |
| 3   | -659.67  | -659.00  | -659.82  | -659.52  | -625.8204                     |
| 4   | -538.84  | -538.24  | -538.27  | -538.09  | -512.0368                     |
| 5   | -300.65  | -300.16  | -300.62  | -300.46  | -272.8832                     |
| 6   | -214.31  | -213.80  | -214.01  | -213.84  | -185.6895                     |
| 7   | -109.87  | -109.38  | -109.83  | -109.68  | -93.5363                      |
| 8   | -60.72   | -60.27   | -60.79   | -60.63   | -43.9115                      |
| 9   | -16.07   | -15.70   | -16.01   | -15.83   | -3.6274                       |
| 10  | -1.15    | -0.82    | -1.53    | -0.58    | —                             |

## REFERENCES

- <sup>1</sup>T. Szidarovszky and K. Yamanouchi, Mol. Phys. **115**, 1916 (2017).