

Can popular DFT approximations and truncated coupled cluster theory describe the potential energy surface of the beryllium dimer?

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Supplementary Material

Table S1.

| | Hartree val HF | Hartree val CCSD | Hartree val CCSD(T) | Hartree val CCSDT | Hartree val CCSDT(Q) | Hartree val FCI | Hartree val pVDZ | Hartree val FCI | Hartree val pVTZ | Hartree val FCI | Hartree val FCI | Hartree val pVQZ | Hartree val FCI | Hartree val FCI | Hartree val FCI | Hartree val FCI | Hartree val FCI | Hartree val FCI | Hartree val FCI | Hartree val FCI | |
|-----------|----------------|------------------|---------------------|-------------------|----------------------|-----------------|------------------|-----------------|------------------|-----------------|-----------------|------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|--|
| | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | cc-pV[5,6]Z | |
| -1.600000 | 0.901319 | minus_1_60.out | -28.477736 | -28.588615 | -28.594179 | 39.278941 | 39.278911 | -28.521243 | -28.574260 | -28.591266 | -28.595713 | -28.603675 | -28.600379 | | | | | | | | |
| -1.400000 | 1.101319 | minus_1_40.out | -28.750630 | -28.857287 | -28.861750 | 39.645775 | 39.647220 | -28.817556 | -28.852506 | -28.862287 | -28.863854 | -28.869425 | -28.865497 | | | | | | | | |
| -1.200000 | 1.301319 | minus_1_20.out | -28.840347 | -28.983457 | -29.007065 | 39.808511 | 39.809211 | -28.952530 | -28.972901 | -28.979608 | -28.980460 | -28.984503 | -28.981353 | | | | | | | | |
| -1.000000 | 1.501319 | minus_1_00.out | -28.981479 | -29.111127 | -29.121215 | 40.001023 | 40.003555 | -29.103278 | -29.117441 | -29.122201 | -29.122994 | -29.125673 | -29.123826 | | | | | | | | |
| -0.900000 | 1.601319 | minus_0_90.out | -29.025719 | -29.151310 | -29.160348 | 40.054772 | 40.056463 | -29.144428 | -29.156518 | -29.160621 | -29.161342 | -29.163616 | -29.162099 | | | | | | | | |
| -0.800000 | 1.701319 | minus_0_80.out | -29.058007 | -29.180036 | -29.188363 | 40.093392 | 40.094717 | -29.174418 | -29.184894 | -29.188450 | -29.189125 | -29.191045 | -29.189834 | | | | | | | | |
| -0.700000 | 1.801319 | minus_0_70.out | -29.081414 | -29.200192 | -29.207931 | 40.120426 | 40.121531 | -29.195687 | -29.204874 | -29.207975 | -29.208613 | -29.210238 | -29.209282 | | | | | | | | |
| -0.600000 | 1.901319 | minus_0_60.out | -29.098280 | -29.214039 | -29.221239 | 40.138861 | 40.139808 | -29.210387 | -29.218565 | -29.221294 | -29.221900 | -29.223284 | -29.222536 | | | | | | | | |
| -0.500000 | 2.001319 | minus_0_50.out | -29.110373 | -29.223311 | -29.229989 | -29.230455 | -29.231063 | -29.220243 | -29.227649 | -29.230074 | -29.230655 | -29.232089 | -29.231264 | | | | | | | | |
| -0.400000 | 2.101319 | minus_0_40.out | -29.119015 | -29.229326 | -29.235486 | -29.236029 | -29.236558 | -29.226602 | -29.233419 | -29.235602 | -29.236162 | -29.236658 | -29.237494 | | | | | | | | |
| -0.300000 | 2.201319 | minus_0_30.out | -29.125191 | -29.233078 | -29.238722 | -29.239320 | -29.239778 | -29.230495 | -29.236864 | -29.238852 | -29.239396 | -29.240938 | -29.240193 | | | | | | | | |
| -0.200000 | 2.301319 | minus_0_20.out | -29.129626 | -29.235306 | -29.240438 | -29.241067 | -29.241662 | -29.232706 | -29.238728 | -29.240562 | -29.241091 | -29.241283 | -29.241900 | | | | | | | | |
| -0.100000 | 2.401319 | minus_0_10.out | -29.132845 | -29.236548 | -29.241181 | -29.241817 | -29.242155 | -29.233706 | -29.239565 | -29.241275 | -29.241793 | -29.241979 | -29.242524 | | | | | | | | |
| -0.090000 | 2.411319 | minus_0_09.out | -29.133115 | -29.236634 | -29.241218 | -29.241853 | -29.242186 | -29.233885 | -29.239609 | -29.241308 | -29.241825 | -29.242011 | -29.242549 | | | | | | | | |
| -0.080000 | 2.421319 | minus_0_08.out | -29.133378 | -29.236715 | -29.241249 | -29.241884 | -29.242212 | -29.233946 | -29.239647 | -29.241336 | -29.241851 | -29.242036 | -29.242568 | | | | | | | | |
| -0.070000 | 2.431319 | minus_0_07.out | -29.133633 | -29.236790 | -29.241276 | -29.241909 | -29.242232 | -29.234002 | -29.239680 | -29.241358 | -29.241872 | -29.242057 | -29.242583 | | | | | | | | |
| -0.060000 | 2.441319 | minus_0_06.out | -29.133880 | -29.236860 | -29.241297 | -29.241930 | -29.242248 | -29.234052 | -29.239707 | -29.241375 | -29.241888 | -29.242072 | -29.242592 | | | | | | | | |
| -0.050000 | 2.451319 | minus_0_05.out | -29.134121 | -29.236925 | -29.241314 | -29.241946 | -29.242258 | -29.234097 | -29.239729 | -29.241388 | -29.241900 | -29.242083 | -29.242437 | | | | | | | | |
| -0.040000 | 2.461319 | minus_0_04.out | -29.134354 | -29.236985 | -29.241327 | -29.241957 | -29.242265 | -29.234137 | -29.239747 | -29.241396 | -29.241907 | -29.242090 | -29.242444 | | | | | | | | |
| -0.039000 | 2.462319 | minus_0_039.out | -29.134377 | -29.236991 | -29.241328 | -29.241958 | -29.242265 | -29.234140 | -29.239749 | -29.241396 | -29.241907 | -29.242090 | -29.242444 | | | | | | | | |
| -0.038000 | 2.463319 | minus_0_038.out | -29.134400 | -29.236997 | -29.241329 | -29.241959 | -29.242266 | -29.234141 | -29.239750 | -29.241397 | -29.241908 | -29.242091 | -29.242444 | | | | | | | | |
| -0.037000 | 2.464319 | minus_0_037.out | -29.134423 | -29.237003 | -29.241330 | -29.241959 | -29.242266 | -29.234148 | -29.239752 | -29.241397 | -29.241908 | -29.242091 | -29.242444 | | | | | | | | |
| -0.036000 | 2.465319 | minus_0_036.out | -29.134446 | -29.237008 | -29.241331 | -29.241960 | -29.242266 | -29.234151 | -29.239753 | -29.241398 | -29.241909 | -29.242091 | -29.242444 | | | | | | | | |
| -0.035000 | 2.466319 | minus_0_035.out | -29.134468 | -29.237014 | -29.241332 | -29.241961 | -29.242266 | -29.234155 | -29.239755 | -29.241398 | -29.241909 | -29.242091 | -29.242444 | | | | | | | | |
| -0.034000 | 2.467319 | minus_0_034.out | -29.134491 | -29.237020 | -29.241333 | -29.241962 | -29.242267 | -29.234158 | -29.239756 | -29.241399 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.033000 | 2.468319 | minus_0_033.out | -29.134514 | -29.237025 | -29.241334 | -29.241962 | -29.242267 | -29.234162 | -29.239757 | -29.241399 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.032000 | 2.469319 | minus_0_032.out | -29.134536 | -29.237031 | -29.241335 | -29.241963 | -29.242267 | -29.234165 | -29.239758 | -29.241399 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.031000 | 2.470319 | minus_0_031.out | -29.134559 | -29.237036 | -29.241335 | -29.241963 | -29.242267 | -29.234168 | -29.239760 | -29.241399 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.030000 | 2.471319 | minus_0_030.out | -29.134581 | -29.237042 | -29.241336 | -29.241964 | -29.242267 | -29.234171 | -29.239761 | -29.241400 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.029000 | 2.472319 | minus_0_029.out | -29.134603 | -29.237047 | -29.241337 | -29.241965 | -29.242267 | -29.234175 | -29.239762 | -29.241400 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.028000 | 2.473319 | minus_0_028.out | -29.134625 | -29.237052 | -29.241337 | -29.241965 | -29.242267 | -29.234178 | -29.239763 | -29.241400 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.027000 | 2.474319 | minus_0_027.out | -29.134648 | -29.237058 | -29.241338 | -29.241965 | -29.242267 | -29.234181 | -29.239764 | -29.241400 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.026000 | 2.475319 | minus_0_026.out | -29.134670 | -29.237063 | -29.241339 | -29.241966 | -29.242267 | -29.234184 | -29.239765 | -29.241400 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.025000 | 2.476319 | minus_0_025.out | -29.134692 | -29.237068 | -29.241339 | -29.241966 | -29.242267 | -29.234187 | -29.239766 | -29.241400 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.024000 | 2.477319 | minus_0_024.out | -29.134714 | -29.237074 | -29.241340 | -29.241966 | -29.242267 | -29.234190 | -29.239767 | -29.241400 | -29.241909 | -29.242092 | -29.242444 | | | | | | | | |
| -0.023000 | 2.478319 | minus_0_023.out | -29.134736 | -29.237079 | -29.241340 | -29.241967 | -29.242266 | -29.234193 | -29.239768 | -29.241400 | -29.241909 | -29.242091 | -29.242444 | | | | | | | | |
| -0.022000 | 2.479319 | minus_0_022.out | -29.134758 | -29.237084 | -29.241340 | -29.241967 | -29.242266 | -29.234196 | -29.239769 | -29.241400 | -29.241909 | -29.242091 | -29.242444 | | | | | | | | |
| -0.021000 | 2.480319 | minus_0_021.out | -29.134780 | -29.237089 | -29.241341 | -29.241967 | -29.242266 | -29.234199 | -29.239770 | -29.241400 | -29.241909 | -29.242091 | -29.242444 | | | | | | | | |
| -0.020000 | 2.481319 | minus_0_020.out | -29.134801 | -29.237094 | -29.241341 | -29.241967 | -29.242266 | -29.234202 | -29.239770 | -29.241400 | -29.241909 | -29.242090 | -29.242444 | | | | | | | | |
| -0.019000 | 2.482319 | minus_0_019.out | -29.134823 | -29.237100 | -29.241341 | -29.241967 | -29.242266 | -29.234205 | -29.239771 | -29.241399 | -29.241909 | -29.242087 | -29.242436 | | | | | | | | |
| -0.018000 | 2.483319 | plus_0_018.out | -29.135224 | -29.237188 | -29.241341 | -29.241963 | -29.242252 | -29.234251 | -29.239778 | -29.241389 | -29.241895 | -29.242077 | -29.242565 | | | | | | | | |
| -0.017000 | 2.511319 | plus_0_017.out | -29.135247 | -29.237229 | -29.241336 | -29.241956 | -29.242240 | -29.234269 | -29.239776 | -29.241379 | -29.241884 | -29.242066 | -29.242414 | | | | | | | | |
| -0.016000 | 2.521319 | plus_0_016.out | -29.135624 | -29.237268 | -29.241329 | -29.241946 | -29.242225 | -29.234284 | -29.239772 | -29.241366 | -29.241870 | -29.242050 | -29.242399 | | | | | | | | |
| -0.015000 | 2.531319 | plus_0_015.out | -29.135816 | -29.237303 | -29.241318 | -29.241933 | -29.242208 | -29.234296 | -29.239764 | -29.241350 | -29.241853 | -29.242033 | -29.242380 | | | | | | | | |
| -0.014000 | 2.541319 | plus_0_014.out | -29.136003 | -29.237336 | -29.241306 | -29.241917 | -29.242188 | -29.234305 | -29.239754 | -29.241331 | -29.241833 | -29.242013 | -29.242360 | | | | | | | | |
| -0.013000 | 2.551319 | plus_0_013.out | -29.136185 | -29.237366 | -29.241290 | -29.241899 | -29.242166 | -29.234310 | -29.239741 | -29.241311 | -29.241811 | -29.241990 | -29.242336 | | | | | | | | |
| -0.012000 | 2.561319 | plus_0_012.out | -29.136362 | -29.237394 | -29.241273 | -29.241879 | -29.242141 | -29.234314 | -29.239726 | -29.241288 | -29.241787 | -29.241965 | -29.242217 | | | | | | | | |
| -0.011000 | 2.571319 | plus_0_011.out | -29.136535 | -29.237420 | -29.241254 | -29.241857 | -29.242115 | -29.234314 | -29.239709 | -29.241263 | -29.241767 | -29.241939 | -29.242284 | | | | | | | | |
| -0.010000 | 2.581319 | plus_0_010.out | -29.136703 | -29.237443 | -29.241233 | -29.241833 | -29.242086 | -29.234313 | -29.239690 | -29.241236 | -29.241733 | -29.241911 | -29.242255 | | | | | | | | |
| -0.009000 | 2.591319 | plus_0_009.out | -29.136867 | -29.237465 | -29.241211 | -29.241807 | -29.242057 | -29.234309 | -29.239669 | -29.241207 | -29.241703 | -29.241880 | -29.242224 | | | | | | | | |
| -0.010000 | 2.601319 | plus_0_010.out | -29.137027 | -29.237484 | -29.241187 | -29.241779 | -29.242025 | -29.234304 | -29.239646 | -29.241177 | -29.241672 | -29.241849 | -29.242191 | | | | | | | | |
| -0.020000 | 2.701319 | plus_0_20.out | | | | | | | | | | | | | | | | | | | |

| hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree | Hartree |
|-------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|------------|------------|------------|----------------|------------|------------|------------|------------|---------|
| val | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA | GGA |
| FCI | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z | V5Z |
| cc-pV[5,6]Z | BLYP | BLYP-D3BJ | PBE | PBE-D3BJ | N12 | B3LYP | B3LYP-D3BJ | B3PW91 | B3PW91-D3BJ | PBE0 | PBE0-D3BJ | BHandHLYP | BHandHLYP-LM06 | M062X | M062X | M06HF | M06HF | |
| -28.700688 | -28.704247 | -28.634523 | -28.636001 | -28.791210 | -28.722859 | -28.725837 | -28.686819 | -28.689704 | -28.642381 | -28.643711 | -28.697633 | -28.700295 | -28.702913 | -28.699204 | -28.699204 | -28.710792 | -28.710792 | |
| -28.966192 | -28.969750 | -28.903202 | -28.904679 | -29.05980 | -28.988871 | -28.991849 | -28.956067 | -28.958951 | -28.912082 | -28.913411 | -28.964624 | -28.967286 | -28.973458 | -28.969186 | -28.969186 | -28.978102 | -28.978102 | |
| -29.123888 | -29.127445 | -29.063487 | -29.064963 | -29.219431 | -29.146864 | -29.149840 | -29.116589 | -29.119472 | -29.072977 | -29.074306 | -29.123106 | -29.125765 | -29.132586 | -29.128691 | -29.128691 | -29.139364 | -29.139364 | |
| -29.202552 | -29.206106 | -29.143900 | -29.145375 | -29.299581 | -29.225265 | -29.228238 | -29.196659 | -29.199540 | -29.153355 | -29.154683 | -29.201410 | -29.204065 | -29.210611 | -29.207227 | -29.207227 | -29.219176 | -29.219176 | |
| -29.221815 | -29.225365 | -29.163784 | -29.165257 | -29.319501 | -29.265963 | -29.268933 | -29.216168 | -29.219047 | -29.172966 | -29.174293 | -29.220018 | -29.222669 | -29.229013 | -29.226171 | -29.226171 | -29.238187 | -29.238187 | |
| -29.277058 | -29.280604 | -29.217448 | -29.218919 | -29.374995 | -29.295459 | -29.298426 | -29.226352 | -29.229228 | -29.183210 | -29.184536 | -29.229256 | -29.231902 | -29.272312 | -29.230544 | -29.230544 | -29.248088 | -29.248088 | |
| -29.297496 | -29.301037 | -29.238394 | -29.239863 | -29.396223 | -29.316195 | -29.319156 | -29.287088 | -29.289962 | -29.243736 | -29.245060 | -29.288274 | -29.290913 | -29.292160 | -29.297330 | -29.297330 | -29.324226 | -29.324226 | |
| -29.311497 | -29.315033 | -29.252857 | -29.254323 | -29.411104 | -29.330486 | -29.333442 | -29.301867 | -29.304738 | -29.258640 | -29.259962 | -29.303086 | -29.305717 | -29.305923 | -29.311834 | -29.311834 | -29.339290 | -29.339290 | |
| -29.231163 | -29.320796 | -29.324330 | -29.262560 | -29.264024 | -29.421328 | -29.340074 | -29.311895 | -29.314766 | -29.268780 | -29.270103 | -29.313203 | -29.315827 | -29.315516 | -29.321676 | -29.321676 | -29.349426 | -29.349426 | |
| -29.236651 | -29.326693 | -29.330234 | -29.268793 | -29.270259 | -29.428144 | -29.346266 | -29.349224 | -29.318470 | -29.275455 | -29.276782 | -29.319942 | -29.322565 | -29.322103 | -29.328131 | -29.328131 | -29.356026 | -29.356026 | |
| -29.239867 | -29.330162 | -29.333731 | -29.272520 | -29.273998 | -29.432455 | -29.350041 | -29.353022 | -29.322560 | -29.279634 | -29.280973 | -29.324285 | -29.326921 | -29.326439 | -29.332224 | -29.332224 | -29.360095 | -29.360095 | |
| -29.241546 | -29.331932 | -29.335593 | -29.274464 | -29.275979 | -29.434933 | -29.352129 | -29.355184 | -29.324889 | -29.327873 | -29.282040 | -29.283415 | -29.326962 | -29.329655 | -29.329072 | -29.329072 | -29.346488 | -29.346488 | |
| -29.242235 | -29.332548 | -29.336508 | -29.275164 | -29.276802 | -29.436096 | -29.353072 | -29.356037 | -29.325995 | -29.328203 | -29.283209 | -29.284702 | -29.328507 | -29.331407 | -29.330444 | -29.330444 | -29.336668 | -29.336668 | |
| -29.242266 | -29.332562 | -29.336574 | -29.275182 | -29.276820 | -29.436156 | -29.353119 | -29.356465 | -29.326055 | -29.329333 | -29.283275 | -29.284778 | -29.328616 | -29.331552 | -29.330529 | -29.330529 | -29.336744 | -29.336744 | |
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| -29.288548 | -29.205987 | -29.213598 | -29.221208 | -29.225463 | -29.229717 | -29.231944 | -29.234170 |
| -29.288520 | -29.205952 | -29.213559 | -29.221166 | -29.225422 | -29.229678 | -29.231906 | -29.234134 |
| -29.288498 | -29.205923 | -29.213528 | -29.221133 | -29.225390 | -29.229646 | -29.231876 | -29.234106 |
| -29.288482 | -29.205900 | -29.213503 | -29.221106 | -29.225364 | -29.229621 | -29.231852 | -29.234083 |
| -29.288470 | -29.205882 | -29.213483 | -29.221084 | -29.225343 | -29.229601 | -29.231832 | -29.234064 |
| -29.288450 | -29.205850 | -29.213448 | -29.221047 | -29.225306 | -29.229565 | -29.231799 | -29.234032 |
| -29.288438 | -29.205830 | -29.213427 | -29.221024 | -29.225284 | -29.229544 | -29.231778 | -29.234012 |
| -29.288430 | -29.205818 | -29.213414 | -29.221010 | -29.225271 | -29.229531 | -29.231766 | -29.234000 |
| -29.288425 | -29.205810 | -29.213406 | -29.221001 | -29.225262 | -29.229523 | -29.231758 | -29.233993 |
| -29.288422 | -29.205806 | -29.213401 | -29.220996 | -29.225256 | -29.229517 | -29.231753 | -29.233988 |
| -29.288419 | -29.205802 | -29.213397 | -29.220992 | -29.225253 | -29.229514 | -29.231749 | -29.233985 |
| -29.288417 | -29.205800 | -29.213395 | -29.220989 | -29.225250 | -29.229511 | -29.231747 | -29.233982 |
| -29.288416 | -29.205798 | -29.213393 | -29.220988 | -29.225248 | -29.229509 | -29.231745 | -29.233981 |
| -29.288415 | -29.205797 | -29.213392 | -29.220986 | -29.225247 | -29.229508 | -29.231744 | -29.233980 |
| -29.288414 | -29.205797 | -29.213391 | -29.220985 | -29.225246 | -29.229507 | -29.231743 | -29.233979 |
| -29.288413 | -29.205795 | -29.213390 | -29.220984 | -29.225245 | -29.229506 | -29.231742 | -29.233978 |
| -29.288413 | -29.205795 | -29.213389 | -29.220984 | -29.225245 | -29.229506 | -29.231741 | -29.233977 |
| -29.288412 | -29.205795 | -29.213389 | -29.220983 | -29.225244 | -29.229505 | -29.231741 | -29.233977 |
| -29.288412 | -29.205794 | -29.213389 | -29.220983 | -29.225244 | -29.229505 | -29.231741 | -29.233977 |
| -29.288412 | -29.205794 | -29.213389 | -29.220983 | -29.225244 | -29.229505 | -29.231741 | -29.233977 |
| -29.288412 | -29.205794 | -29.213388 | -29.220982 | -29.225243 | -29.229504 | -29.231740 | -29.233976 |
| -14.644206 | -14.602897 | -14.606694 | -14.610491 | -14.612622 | -14.614752 | -14.615870 | -14.616988 |

Table S2. Relative errors in the vibrational transition frequencies (see Table 1 of the main text for the absolute errors).

| Basis set | $\Delta\nu_1$ | $\Delta\nu_2$ | $\Delta\nu_3$ | $\Delta\nu_4$ | $\Delta\nu_5$ |
|-------------|---------------|---------------|---------------|---------------|---------------|
| cc-pVDZ | 75.9 | 80.9 | 82.6 | 83.5 | 84.0 |
| cc-pVTZ | 9.2 | 10.2 | 11.8 | 13.6 | 15.7 |
| cc-pVQZ | 2.4 | 2.7 | 3.4 | 4.1 | 4.9 |
| cc-pV5Z | 1.1 | 1.1 | 1.4 | 1.7 | 2.0 |
| cc-pV6Z | 0.6 | 0.7 | 0.8 | 1.0 | 1.2 |
| cc-pV{T,Q}Z | 2.3 | 2.5 | 2.5 | 2.6 | 2.5 |
| cc-pV{Q,5}Z | 0.2 | 0.5 | 0.5 | 0.7 | 0.8 |

Table S3. Relative errors in the vibrational transition frequencies (see Table 2 of the main text for the absolute errors).

| Basis set | $\Delta\nu_1$ | $\Delta\nu_2$ | $\Delta\nu_3$ | $\Delta\nu_4$ | $\Delta\nu_5$ |
|----------------------|---------------|---------------|---------------|---------------|---------------|
| HF/cc-pV{Q,5}Z | 98.6 | 98.2 | 97.8 | 97.3 | 96.7 |
| CCSD/cc-pV{Q,5}Z | 88.2 | 88.5 | 88.9 | 89.3 | 89.7 |
| CCSD(T)/cc-pV{Q,5}Z | 10.3 | 11.7 | 13.7 | 16.4 | 19.4 |
| CCSDT/cc-pV{Q,5}Z | 4.8 | 5.2 | 5.9 | 6.6 | 7.5 |
| CCSDT(Q)/cc-pV{Q,5}Z | 0.9 | 0.9 | 1.1 | 1.2 | 1.4 |

Table S4. Evaluation of DFT and MPn methods for the shape of the potential energy surface of Be₂, equilibrium bond distances (re), bond dissociation energies (De), and vibrational frequencies. The reference values are calculated at the FCI/cc-pV{5,6}Z levels of theory (bond distances are in a.u. and bond energies and frequencies are in cm⁻¹).^a

| Type | Functional | R ² ^b | Δr_e | ΔD_e | $\Delta \nu_1$ | $\Delta \nu_2$ | $\Delta \nu_3$ | $\Delta \nu_4$ | $\Delta \nu_5$ |
|--------|------------|-----------------------------|--------------|--------------|----------------|----------------|----------------|----------------|----------------|
| GGA | BLYP | 0.8064 | -0.085 | -1290.174 | 46.78 | 101.125 | 163.454 | 235.977 | 318.978 |
| GGA | BLYP-D3BJ | 0.7625 | 0.2 | -2323.988 | 36.364 | 72.667 | 120.458 | 181.839 | 256.335 |
| GGA | PBE | 0.7382 | -0.079 | -2576.361 | 58.383 | 125.636 | 202.287 | 290.857 | 392.034 |
| GGA | PBE-D3BJ | 0.7289 | 0.02 | -2964.997 | 38.968 | 94.896 | 163.484 | 245.619 | 341.377 |
| GGA | N12 | 0.8204 | 0.026 | -1752.263 | 45.261 | 99.689 | 163.907 | 239.873 | 327.995 |
| HGGA | B3LYP | 0.9356 | 0.026 | -619.270 | 22.422 | 51.104 | 86.024 | 128.973 | 180.074 |
| HGGA | B3PW91 | 0.8822 | 0.047 | -1212.996 | 30.505 | 68.757 | 114.823 | 170.561 | 236.219 |
| HGGA | BHandHLYP | 0.5539 | 0.386 | 498.028 | -42.004 | -81.466 | -118.521 | -151.357 | -179.521 |
| HGGA | D3BJ | 0.8468 | 0.455 | -415.307 | -9.524 | -15.846 | -17.321 | -10.859 | 4.713 |
| HGGA | PBE0 | 0.8749 | 0.062 | -1434.832 | 29.742 | 67.396 | 113.034 | 168.502 | 234.041 |
| HMGGGA | M06 | 0.9501 | 0.098 | -949.926 | 27.188 | 50.012 | 70.837 | 99.474 | 137.54 |
| HMGGGA | M06-2X | 0.8783 | 0.509 | -55.882 | -38.831 | -70.061 | -91.022 | -98.893 | -93.739 |
| HMGGGA | M06-HF | 0.1825 | 1.136 | 112.225 | -43.462 | -75.849 | -97.899 | -108.312 | -107.583 |
| HMGGGA | PW6B95 | 0.9651 | 0.104 | -654.804 | 11.739 | 30.001 | 54.709 | 87.652 | 128.853 |
| HMGGGA | MN15 | 0.643 | 0.698 | -107.060 | -69.353 | -129.857 | -178.219 | -212.425 | -232.480 |
| RS | CAM-B3LYP | 0.6137 | 0.362 | 454.028 | -40.881 | -79.105 | -114.731 | -145.819 | -171.727 |
| RS | LC-BLYP | 0.0294 | 2.408 | 777.054 | -102.861 | -194.360 | -274.694 | -342.427 | -397.987 |
| RS | LC-PBE | 0.4897 | 0.695 | 195.407 | -49.771 | -90.779 | -122.800 | -143.875 | -153.763 |
| RS | LC-wPBE | 0.44 | 0.695 | 269.578 | -50.663 | -93.126 | -127.180 | -150.827 | -163.802 |
| RS | wB97X-D | 0.546 | 0.638 | 136.953 | -41.691 | -77.611 | -109.141 | -134.581 | -151.489 |
| MPn | MP2 | 0.5299 | 0.464 | 432.593 | -65.352 | -128.958 | -186.928 | -234.305 | -269.411 |
| MPn | MP2.5 | 0.6569 | 0.377 | 348.472 | -55.871 | -110.758 | -161.835 | -204.054 | -235.035 |
| MPn | MP3 | 0.7787 | 0.299 | 258.517 | -46.792 | -92.848 | -136.290 | -172.529 | -198.838 |
| MPn | MP3.5 | 0.8877 | 0.2 | 179.377 | -33.937 | -67.728 | -100.639 | -129.046 | -150.127 |
| MPn | MP4 | 0.962 | 0.119 | 89.587 | -21.478 | -42.752 | -63.791 | -82.048 | -95.555 |
| MPn | MP4.5 | 0.9752 | 0.089 | 86.65 | -17.725 | -35.489 | -53.519 | -69.628 | -82.116 |
| MPn | MP5 | 0.9859 | 0.062 | 82.163 | -13.865 | -27.929 | -42.650 | -56.220 | -67.335 |

