|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Quantum mechanics methods | M1 | M2 | M3 | M4 | M5 | M6 | M7 | M8 | M9 | M10 |
| B3LYP/6-31+G(d) | -121213.48 | -120838.05 | -168424.52 | -168044.38 | -346413.07 | -346047.51 | -371086.12 | -370717.45 | -47955.79 | -47563.10 |
| B3LYP-D3/6-31+G(d) | -121213.88 | -120838.39 | -168422.97 | -168045.37 | -346413.40 | -346047.77 | -371087.73 | -370718.66 | -47955.79 | -47563.10 |
| B3LYP/6-311+G(d) | -121240.82 | -120865.66 | -168465.26 | -168085.42 | -346452.54 | -346087.54 | -371129.96 | -370762.00 | -47969.18 | -47576.55 |
| B3LYP-D3/6-311+G(d) | -121241.22 | -120866.00 | -168463.03 | -168086.41 | -346452.87 | -346087.79 | -371131.57 | -370763.21 | -47969.18 | -47576.55 |
| BLYP/6-311+G(d) | -121191.06 | -120819.62 | -168412.40 | -168036.11 | -346411.83 | -346050.56 | -371072.57 | -370708.28 | -47958.80 | -47570.38 |
| BLYP-D3/6-311+G(d) | -121191.53 | -120820.02 | -168411.94 | -168037.34 | -346412.22 | -346050.86 | -371074.62 | -370709.80 | -47958.80 | -47570.38 |
| BP86/6-311+G(d) | -121236.52 | -120864.47 | -168463.38 | -168086.33 | -346469.45 | -346107.11 | -371145.19 | -370780.33 | -47969.11 | -47578.57 |
| BP86-D3/6-311+G(d) | -121236.96 | -120864.84 | -168463.00 | -168087.45 | -346469.81 | -346107.39 | -371147.05 | -370781.71 | -47969.11 | -47578.57 |
| TPSS/6-311+G(d) | -121255.69 | -120879.47 | -168487.08 | -168105.74 | -346470.07 | -346103.82 | -371151.88 | -370782.88 | -47969.80 | -47576.39 |
| TPSSH-D3/6-311+G(d) | -121255.99 | -120879.71 | -168485.53 | -168106.49 | -346470.31 | -346104.01 | -371153.16 | -370783.83 | -47969.80 | -47576.39 |
| BH&HLYP/6-311+G(d) | -121163.21 | -120783.58 | -168364.99 | -167980.88 | -346378.31 | -346008.60 | -371038.40 | -370665.59 | -47941.01 | -47543.84 |
| HF/6-311+G(d) | -120485.89 | -120099.74 | -167483.34 | -167092.54 | -345443.44 | -345067.28 | -369944.14 | -369563.89 | -47713.67 | -47311.25 |
| HF/aug-cc-pVDZ | -120474.58 | -120089.13 | -167465.03 | -167075.11 | -345434.93 | -345059.62 | -369931.22 | -369551.75 | -47716.36 | -47311.37 |
| HF/aug-cc-pVTZ | -120504.40 | -120117.72 | -167507.34 | -167115.93 | -345467.16 | -345090.32 | -369970.69 | -369589.55 | -47728.39 | -47321.56 |
| MP2/6-311+G(d) | -120865.60 | -120489.93 | -167985.08 | -167604.24 | -345818.44 | -345451.17 | -370408.92 | -370039.35 | -47844.22 | -47452.84 |
| MP2/aug-cc-pVDZ | -120867.81 | -120494.98 | -167979.25 | -167601.28 | -345825.31 | -345461.76 | -370415.65 | -370049.67 | -47854.26 | -47462.91 |
| MP2/aug-cc-pVTZ | -120977.36 | -120603.57 | -168128.49 | -167749.35 | -345941.33 | -345576.90 | -370557.01 | -370189.99 | -47896.99 | -47503.85 |
| SCS-MP2/aug-cc-pVDZ | -120863.20 | -120486.71 | -167968.96 | -167587.70 | -345817.20 | -345450.09 | -370406.98 | -370037.16 | -47851.44 | -47457.91 |
| SCS-MP2/aug-cc-pVTZ | -120976.21 | -120598.49 | -168122.04 | -167739.36 | -345936.69 | -345568.43 | -370552.67 | -370181.54 | -47895.25 | -47499.78 |
| CCSD(T)/aug-cc-pVDZ | -120906.99 | -120530.69 | -168021.95 | -167641.00 | -345863.19 | -345495.87 | -370464.60 | -370094.89 | -47862.42 | -47467.23 |
| CCSD(T)/aug-cc-pVTZ | -121020.01 | -120642.48 | -168175.03 | -167792.66 | -345982.67 | -345614.22 | -370610.29 | -370239.27 | -47906.23 | -47509.09 |
| SCCDFTB | -6738.56 | -6495.41 | -8822.64 | -8579.00 | -6709.76 | -6482.16 | -8271.32 | -8043.37 | -2558.93 | -2275.42 |
| AM1 | -46.53 | -42.62 | -92.71 | -92.20 | -34.55 | -45.02 | -38.47 | -47.64 | -59.00 | -13.71 |
| PM3 | -52.87 | -48.11 | -92.77 | -91.94 | -37.03 | -48.75 | -41.48 | -52.61 | -53.24 | -16.94 |

**Table S2** Molecular energies of molecular No.1 (M1) to molecular No.29 (M29) (in kcal∙mol-1) calculated by 24 quantum mechanics methods

using the structure optimized at the B3LYP/6-311+G(d) level as starting structures (continue)

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Quantum mechanics methods | M11 | M12 | M13 | M14 | M15 | M16 | M17 | M18 | M19 | M20 |
| B3LYP/6-31+G(d) | -143759.80 | -143410.40 | -143382.99 | -106615.38 | -155163.59 | -154810.43 | -129119.75 | -128875.65 | -251563.66 | -251230.11 |
| B3LYP-D3/6-31+G(d) | -143759.96 | -143410.45 | -143383.15 | -106615.41 | -155164.78 | -154811.26 | -129120.16 | -128875.89 | -251568.27 | -251233.85 |
| B3LYP/6-311+G(d) | -143796.33 | -143447.27 | -143419.49 | -106643.44 | -155199.23 | -154846.12 | -129152.27 | -128907.54 | -251615.78 | -251282.49 |
| B3LYP-D3/6-311+G(d) | -143796.49 | -143447.32 | -143419.65 | -106643.48 | -155200.42 | -154846.95 | -129152.68 | -128907.77 | -251620.39 | -251286.23 |
| BLYP/6-311+G(d) | -143759.98 | -143414.00 | -143386.65 | -106618.18 | -155151.71 | -154803.13 | -129107.07 | -128864.73 | -251529.92 | -251199.02 |
| BLYP-D3/6-311+G(d) | -143760.16 | -143414.06 | -143386.85 | -106618.23 | -155153.24 | -154804.19 | -129107.55 | -128865.01 | -251535.68 | -251203.68 |
| BP86/6-311+G(d) | -143796.89 | -143449.61 | -143422.37 | -106645.22 | -155198.07 | -154849.78 | -129152.53 | -128909.24 | -251614.35 | -251284.58 |
| BP86-D3/6-311+G(d) | -143797.06 | -143449.66 | -143422.55 | -106645.26 | -155199.45 | -154850.75 | -129152.97 | -128909.50 | -251619.62 | -251288.84 |
| TPSS/6-311+G(d) | -143812.25 | -143462.37 | -143433.76 | -106655.28 | -155221.44 | -154867.75 | -129166.04 | -128920.77 | -251656.91 | -251322.43 |
| TPSSH-D3/6-311+G(d) | -143812.36 | -143462.40 | -143433.88 | -106655.31 | -155222.38 | -154868.42 | -129166.33 | -128920.94 | -251660.54 | -251325.35 |
| BH&HLYP/6-311+G(d) | -143713.28 | -143360.97 | -143332.33 | -106579.44 | -155101.84 | -154742.52 | -129072.17 | -128825.04 | -251458.13 | -251121.02 |
| HF/6-311+G(d) | -142990.04 | -142633.47 | -142602.71 | -106036.48 | -154266.32 | -153896.93 | -128369.60 | -128119.35 | -250055.91 | -249710.63 |
| HF/aug-cc-pVDZ | -142977.52 | -142591.00 | -142616.88 | -106026.17 | -154251.28 | -153882.76 | -128365.67 | -128115.20 | -250034.07 | -249689.07 |
| HF/aug-cc-pVTZ | -143012.72 | -142624.68 | -142650.73 | -106051.96 | -154287.29 | -153917.46 | -128397.08 | -128144.56 | -250089.77 | -249743.57 |
| MP2/6-311+G(d) | -143406.59 | -143058.94 | -143028.65 | -106350.57 | -154746.72 | -154390.33 | -128769.20 | -128528.59 | -250866.34 | -250538.07 |
| MP2/aug-cc-pVDZ | -143400.66 | -143049.49 | -143025.68 | -106346.30 | -154739.20 | -154385.33 | -128775.93 | -128535.27 | -250851.83 | -250524.77 |
| MP2/aug-cc-pVTZ | -143525.36 | -143172.85 | -143149.29 | -106438.48 | -154872.94 | -154518.32 | -128891.24 | -128649.38 | -251066.39 | -250738.67 |
| SCS-MP2/aug-cc-pVDZ | -143389.73 | -143036.21 | -143011.52 | -106337.95 | -154729.86 | -154370.79 | -128767.23 | -128524.88 | -250830.11 | -250495.68 |
| SCS-MP2/aug-cc-pVTZ | -143517.33 | -143162.31 | -143137.82 | -106432.35 | -154867.33 | -154507.19 | -128885.78 | -128642.08 | -251050.64 | -250715.15 |
| CCSD(T)/aug-cc-pVDZ | -143430.76 | -143076.89 | -143052.72 | -106368.53 | -154782.31 | -154423.67 | -128810.94 | -128568.88 | -250922.90 | -250586.96 |
| CCSD(T)/aug-cc-pVTZ | -143558.37 | -143202.99 | -143179.02 | -106462.94 | -154919.78 | -154560.07 | -128929.49 | -128686.09 | -251143.42 | -250806.44 |
| SCCDFTB | -7280.96 | -7056.11 | -7036.31 | -5354.64 | -7958.71 | -7736.32 | -6819.80 | -6718.13 | -12744.11 | -12546.35 |
| AM1 | -100.04 | -113.74 | -99.90 | -44.80 | -7.43 | -30.88 | 157.42 | 25.44 | 27.52 | -16.28 |
| PM3 | -100.31 | -118.44 | -99.65 | -40.54 | -15.94 | -33.63 | 167.37 | 20.83 | 15.20 | -23.17 |

**Table S2** Molecular energies of molecular No.1 (M1) to molecular No.29 (M29) (in kcal∙mol-1) calculated by 24 quantum mechanics methods

using the structure optimized at the B3LYP/6-311+G(d) level as starting structures (continue)

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Quantum mechanics methods | M21 | M22 | M23 | M24 | M25 | M26 | M27 | M28 | M29 |
| B3LYP/6-31+G(d) | -72233.49 | -178867.24 | -240677.62 | -491931.72 | -467260.73 | -289266.70 | -264603.59 | -431423.92 | -383451.96 |
| B3LYP-D3/6-31+G(d) | -72233.50 | -178868.03 | -240681.52 | -491938.72 | -467264.76 | -289273.53 | -264607.34 | -431437.26 | -383461.27 |
| B3LYP/6-311+G(d) | -72252.69 | -178913.08 | -240736.49 | -492002.98 | -467327.59 | -289334.52 | -264667.05 | -431531.72 | -383544.85 |
| B3LYP-D3/6-311+G(d) | -72252.69 | -178913.86 | -240740.39 | -492009.99 | -467331.62 | -289341.35 | -264670.81 | -431545.06 | -383554.16 |
| BLYP/6-311+G(d) | -72230.28 | -178862.66 | -240658.08 | -491898.56 | -467239.98 | -289233.69 | -264582.95 | -431411.19 | -383437.87 |
| BLYP-D3/6-311+G(d) | -72230.28 | -178863.60 | -240662.87 | -491907.23 | -467244.83 | -289242.18 | -264587.55 | -431427.75 | -383449.51 |
| BP86/6-311+G(d) | -72253.72 | -178916.87 | -240736.94 | -492021.79 | -467347.79 | -289334.97 | -264669.85 | -431535.68 | -383547.03 |
| BP86-D3/6-311+G(d) | -72253.72 | -178917.74 | -240741.31 | -492029.77 | -467352.25 | -289342.75 | -264674.06 | -431550.88 | -383557.70 |
| TPSS/6-311+G(d) | -72258.58 | -178933.34 | -240766.69 | -492043.01 | -467363.18 | -289373.37 | -264700.05 | -431582.86 | -383593.34 |
| TPSSH-D3/6-311+G(d) | -72258.58 | -178933.91 | -240769.64 | -492048.56 | -467366.20 | -289378.73 | -264702.89 | -431593.34 | -383600.69 |
| BH&HLYP/6-311+G(d) | -72202.20 | -178800.33 | -240588.54 | -491829.57 | -467171.32 | -289153.89 | -264503.43 | -431293.37 | -383332.73 |
| HF/6-311+G(d) | -71811.34 | -177860.11 | -239309.29 | -490043.27 | -465544.68 | -287581.92 | -263089.82 | -429110.37 | -381385.98 |
| HF/aug-cc-pVDZ | -71804.21 | -177843.02 | -239283.44 | -490019.32 | -465525.09 | -287552.83 | -263066.46 | -429084.54 | -381361.52 |
| HF/aug-cc-pVTZ | -71821.62 | -177885.30 | -239342.08 | -490084.50 | -465583.22 | -287620.92 | -263127.51 | -429183.50 | -381449.20 |
| MP2/6-311+G(d) | -72034.50 | -178407.80 | -240046.04 | -490915.92 | -466326.91 | -288488.21 | -263911.14 | -430373.46 | -382506.65 |
| MP2/aug-cc-pVDZ | -72041.66 | -178410.94 | -240048.18 | -490929.65 | -466340.56 | -288489.95 | -263911.97 | -430375.78 | -382502.79 |
| MP2/aug-cc-pVTZ | -72106.99 | -178568.74 | -240262.17 | -491176.81 | -466562.61 | -288745.11 | -264142.78 | -430745.34 | -382829.52 |
| SCS-MP2/aug-cc-pVDZ | -72037.63 | -178396.50 | -240031.23 | -490908.91 | -466320.56 | -288468.34 | -263889.79 | -430339.76 | -382472.04 |
| SCS-MP2/aug-cc-pVTZ | -72104.72 | -178558.08 | -240250.61 | -491163.47 | -466549.15 | -288730.65 | -264126.57 | -430717.83 | -382806.44 |
| CCSD(T)/aug-cc-pVDZ | -72060.15 | -178452.08 | -240109.44 | -491012.91 | -466412.61 | -288567.52 | -263976.90 | -430469.08 | -382589.17 |
| CCSD(T)/aug-cc-pVTZ | -72127.24 | -178613.66 | -240328.82 | -491267.47 | -466641.19 | -288829.83 | -264213.69 | -430847.15 | -382923.58 |
| SCCDFTB | -3841.67 | -9210.97 | -12687.58 | -14783.65 | -13222.92 | -15326.67 | -13785.35 | -21873.58 | -19300.17 |
| AM1 | -37.82 | -96.75 | -155.86 | -88.62 | -85.14 | -143.14 | -150.68 | -107.65 | -39.70 |
| PM3 | -37.06 | -94.33 | -149.36 | -94.50 | -91.23 | -145.12 | -152.81 | -72.61 | -15.43 |