

N->R

pyG_2x3

b3lyp -382.0976024 uccsd(t) -381.104824 ump2(3df,2p) -381.2207126 ump2(d,p) -380.9849578 rmp2(d,p) -381.028052230893 rccsd(t) -381.10820220 ----- ZPE 0.0912803 Thermal 0.0983205 S2: 0.755568 ----- G2M(UMP2,CC) Energy (OK): -381.2492985 T1 Diag: 0.04554452 G2M(UMP2,RCC) Energy (OK): -381.25267670 T1 Diag: 0.01852322	Geometry: C 2.930167765 1.050266320 -0.950454765 C 0.997233046 2.268353549 0.307581274 C -2.542469663 -0.939651201 -0.902028643 C -0.883297678 -1.643351197 1.217868020 C 1.479443912 -2.832593646 0.822871795 C 3.291143251 -1.559430350 -0.571861363 H 4.201809833 2.231003112 -2.040834302 H -1.669455874 -1.074802524 -2.801033330 H -1.907559477 -1.970515703 2.968735186 H 5.027671175 -2.447792494 -1.193647401 O -0.163918624 4.053328381 0.871515236 O -4.741141450 -0.329985867 -0.653393597 H 1.954679798 -4.586199025 1.777960169	Frequencies: -373.4753 106.0546 136.1390 242.0314 283.6985 328.4790 416.7462 467.1951 532.4349 626.2922 683.6159 782.5181 798.7200 899.7018 931.4487 949.0227 1006.3663 1033.8613 1078.8250 1124.8552 1175.3070 1334.0485 1376.1738 1425.2687 1482.4458 1512.1487 1718.8911 2034.3150 2906.3365 3144.6829 3156.6156 3175.8383 3197.3585
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R

pyG_2x4

b3lyp -382.1357666 uccsd(t) -381.155967 ump2(3df,2p) -381.2800447 ump2(d,p) -381.0470849 rmp2(d,p) -381.067997498489 rccsd(t) -381.15626718 ----- ZPE 0.0932138 Thermal 0.1002012 S2: 0.775577 ----- G2M(UMP2,CC) Energy (OK): -381.2957130 T1 Diag: 0.02790907 G2M(UMP2,RCC) Energy (OK): -381.29601318 T1 Diag: 0.01719956	Geometry: C -3.368956504 -0.457302385 -0.746046869 C -1.609706513 1.480810184 0.099915490 C 3.172474119 0.929293612 -0.053297836 C 0.724889495 0.044094870 1.171705791 C 0.042396006 -2.672896670 0.786898969 C -2.325154937 -2.850468566 -0.309556038 H -5.187700742 -0.038304749 -1.576532371 H 0.875632949 0.550917528 3.182771237 H -3.243735692 -4.616908964 -0.780472010 O -1.832422076 3.770151031 0.022455616 O 4.712094470 -0.457752140 -0.992678806 H 3.436973417 3.003880313 -0.014004760 H 1.265782027 -4.239948285 1.252300720	Frequencies: 70.9830 128.1139 194.3868 253.2232 397.4604 489.6895 595.8922 614.3457 650.9878 730.5501 763.0833 802.6025 815.9195 928.1055 970.5424 999.4116 1051.2934 1067.0007 1100.9184 1166.5039 1180.2333 1258.0070 1313.6006 1396.8780 1416.2158 1465.3063 1703.3713 1795.8591 2937.5626 3000.6072 3199.3616 3225.9905 3232.1201
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R->M

pyG_2x5

b3lyp -382.0723462 uccsd(t) -381.0914114 ump2(3df,2p) -381.2032436 ump2(d,p) -380.9712085 rmp2(d,p) -381.001063709193 rccsd(t) -381.09340622 ----- ZPE 0.0880134 Thermal 0.096063 S2: 0.782802 ----- G2M(UMP2,CC) Energy (OK): -381.2354331 T1 Diag: 0.04518032 G2M(UMP2,RCC) Energy (OK): -381.23742792 T1 Diag: 0.01953784	Geometry: C -2.520785055 0.243923959 -1.876662455 C -1.204182624 1.671462763 0.192417584 C 3.692252740 0.299013256 -0.254489418 C -0.598943028 -0.280172686 2.188287742 C -1.623794422 -2.494241962 1.428090604 C -2.777530806 -2.166102358 -1.103779585 H -3.160007596 1.104414533 -3.612710388 H 0.265204165 0.171611699 3.981826814 H -3.677015878 -3.682715292 -2.139383520 O -0.781388527 3.926667598 0.288840860 O 5.062022616 -1.341452330 -0.808749872 H 4.125107739 2.347007730 0.039174023 H -1.600454414 -4.265340535 2.447170774	Frequencies: -171.3771 26.6909 74.0562 103.3969 222.0308 237.2198 296.1587 454.4578 484.7856 646.8441 666.9063 734.4409 747.6129 810.0158 853.9776 925.5278 960.4058 976.3603 1033.2511 1085.7547 1094.3163 1131.9947 1301.3096 1358.7019 1476.3429 1610.1223 1750.3171 1930.7959 2748.5371 3201.4523 3213.0724 3234.7511 3241.8103
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M

pyG_2x6b

<p>b3lyp -268.181045 uccsd(t) -267.4796362 ump2(3df,2p) -267.5703898 ump2(d,p) -267.4069979 rmp2(d,p) -267.406997682929 rccsd(t) -267.47963798 ----- ZPE 0.073744 Thermal 0.0784656 S2: 0.0 ----- G2M(UMP2,CC) Energy (0K): -267.5692841 T1 Diag: 0.01506520 G2M(UMP2,RCC) Energy (0K): -267.56928588 T1 Diag: 0.01506285</p>	<p>Geometry:</p> <p>C 0.000000000 2.276643777 -0.167388161 C 0.000000000 -2.276643777 -0.167388161 C 0.000000000 0.000000000 1.555900341 C 0.000000000 -1.420692326 -2.546062032 C 0.000000000 1.420692326 -2.546062032 H 0.000000000 4.201494248 0.508827658 H 0.000000000 -4.201494248 0.508827658 H 0.000000000 2.543658300 -4.254969718 H 0.000000000 -2.543658300 -4.254969718 O 0.000000000 0.000000000 3.839785549</p>	<p>Frequencies:</p> <table><tr><td>209.2796</td><td>452.9560</td><td>461.3809</td></tr><tr><td>644.1118</td><td>658.9938</td><td>730.8401</td></tr><tr><td>738.7064</td><td>841.7125</td><td>850.4287</td></tr><tr><td>953.7481</td><td>966.1207</td><td>966.4876</td></tr><tr><td>1094.0397</td><td>1096.2094</td><td>1131.4352</td></tr><tr><td>1303.0989</td><td>1349.1482</td><td>1580.8993</td></tr><tr><td>1650.9425</td><td>1791.6672</td><td>3200.0461</td></tr><tr><td>3210.4918</td><td>3242.4200</td><td>3244.6954</td></tr></table>	209.2796	452.9560	461.3809	644.1118	658.9938	730.8401	738.7064	841.7125	850.4287	953.7481	966.1207	966.4876	1094.0397	1096.2094	1131.4352	1303.0989	1349.1482	1580.8993	1650.9425	1791.6672	3200.0461	3210.4918	3242.4200	3244.6954
209.2796	452.9560	461.3809																								
644.1118	658.9938	730.8401																								
738.7064	841.7125	850.4287																								
953.7481	966.1207	966.4876																								
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1303.0989	1349.1482	1580.8993																								
1650.9425	1791.6672	3200.0461																								
3210.4918	3242.4200	3244.6954																								