

A

cph006

b3lyp -419.7102154 uccsd(t) -418.6019879 ump2(3df,2p) -418.7551049 ump2(d,p) -418.4779541 rmp2(d,p) -418.514776589508 rccsd(t) -418.60483313 ----- ZPE 0.0882176 Thermal 0.0951963 S2: 0.757215 ----- G2M(UMP2,CC) Energy (0K): -418.7909211 T1 Diag: 0.03952695 G2M(UMP2,RCC) Energy (0K): -418.79376633 T1 Diag: 0.01703010	Geometry: C 0.000000000 2.276579527 0.939908204 C 0.000000000 -2.276579527 0.939908204 C 0.000000000 0.000000000 -0.403237321 C 0.000000000 -2.309028014 3.594126821 C 0.000000000 2.309028014 3.594126821 C 0.000000000 0.000000000 4.793097580 H 0.000000000 4.081882143 4.628247321 H 0.000000000 -4.081882143 4.628247321 H 0.000000000 -4.016013849 -0.145658200 H 0.000000000 4.016013849 -0.145658200 C 0.000000000 0.000000000 -3.343707873 O 0.000000000 2.142014019 -4.353156109 O 0.000000000 -2.142014019 -4.353156109	Frequencies: 59.2802 166.5088 212.3496 363.9897 410.6883 435.9200 500.4471 608.2261 633.9453 670.3256 743.4431 790.4001 805.9433 834.5261 956.8322 976.5940 991.6082 1039.7994 1072.2428 1109.7431 1150.0888 1279.8527 1303.0409 1329.4732 1371.1995 1455.4895 1553.7858 1598.2112 1670.7826 3140.2659 3140.7785 3173.0384 3174.2199
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B

cphG201

<p>b3lyp -570.1627048 uccsd(t) -568.7167903 ump2(3df,2p) -568.9464375 ump2(d,p) -568.5754363 rmp2(d,p) -568.604506191430 rccsd(t) -568.71740363 ----- ZPE 0.0964437 Thermal 0.1055352 S2: 0.759675 ----- G2M(UMP2,CC) Energy (OK): -568.9913478 T1 Diag: 0.03837182 G2M(UMP2,RCC) Energy (OK): -568.99196113 T1 Diag: 0.02679834</p>	<p>Geometry:</p> <p>C -2.086868031 0.016931946 0.000015118 C -0.552794026 -2.145209545 0.000026456 C 2.069660184 -1.977018251 0.000003779 C 3.156504044 0.422127023 -0.000005669 C 1.692642814 2.619613952 -0.000024566 C -0.923499712 2.394214978 0.000000000 H -2.143588160 4.038957014 0.000022677 H 2.626020124 4.444592397 -0.000013228 H 3.272344255 -3.629511943 0.000035905 H -1.501500795 -3.960514482 0.000103935 O 5.755552107 0.843860983 0.000034015 O 7.227318061 -1.193335596 0.000039684 C -5.014768125 -0.218161323 -0.000026456 O -6.181876212 1.839434850 -0.000081258 O -5.838310773 -2.436023279 -0.000001890</p>	<p>Frequencies:</p> <p>35.0489 75.1162 129.1457 168.0291 269.0115 292.6376 322.4467 418.1161 478.4439 490.4403 522.9133 633.6555 647.9454 651.5536 774.8062 776.0260 827.8765 835.1498 869.1315 971.4584 999.7419 1021.9130 1082.9191 1093.7639 1116.7817 1143.4438 1172.6143 1293.2542 1325.4938 1350.0548 1428.2713 1487.3010 1594.3354 1608.7174 1668.8493 3168.9865 3186.3418 3191.5680 3210.5845</p>
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B->T

cphG901

<p>b3lyp -570.0870295 uccsd(t) -568.6453982 ump2(3df,2p) -568.8631592 ump2(d,p) -568.4873047 rmp2(d,p) -568.539062144772 rccsd(t) -568.64687492 ----- ZPE 0.0940185 Thermal 0.1025255 S2: 0.781193 ----- G2M(UMP2,CC) Energy (OK): -568.9272342 T1 Diag: 0.03936328 G2M(UMP2,RCC) Energy (OK): -568.92871092 T1 Diag: 0.02091431</p>	<p>Geometry:</p> <p>C 1.837607485 3.084552721 0.097031768 C 3.369791763 1.035176857 0.480321139 C 2.492293654 -1.549722826 0.882143055 C -0.168317907 -1.979985121 0.341645477 C -1.747590380 0.073523575 0.094979525 C -0.778994244 2.590922241 0.094971966 H 2.597284948 4.931317819 -0.363005051 H 3.207609797 -2.540536473 2.552137501 H -1.001186353 -3.848650254 0.416138481 H -2.157477648 4.092971056 -0.083142281 C -4.665399337 -0.324842032 -0.135379980 O -5.928480945 1.674834035 -0.246099034 O -5.376915241 -2.574776421 -0.184425932 O 5.767170143 0.533303391 -0.308352282 O 4.952902271 -2.159968307 -0.968174727</p>	<p>Frequencies:</p> <p>-263.5302 47.8125 109.9684 173.2910 197.6458 294.9839 335.2912 418.5040 475.1149 496.7296 560.9298 585.3656 632.8031 648.6830 723.9798 754.4522 788.9184 805.5009 841.3955 878.9615 902.5576 968.3621 1011.1908 1070.6801 1097.7286 1186.5235 1212.1527 1276.4886 1314.4364 1322.4326 1351.9000 1426.6003 1521.0821 1584.4139 1680.5753 3014.2558 3168.7119 3190.7584 3198.1479</p>
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B->G

cphG1501

<p>b3lyp -570.1240004 uccsd(t) -568.676382 ump2(3df,2p) -568.913258 ump2(d,p) -568.5351846 rmp2(d,p) -568.570278922940 rccsd(t) -568.67651502 ----- ZPE 0.0941204 Thermal 0.1030146 S2: 0.77335 ----- G2M(UMP2,CC) Energy (OK): -568.9603350 T1 Diag: 0.03495732 G2M(UMP2,RCC) Energy (OK): -568.96046802 T1 Diag: 0.02527105</p>	<p>Geometry:</p> <p>C 1.999445520 -2.215507358 -0.776584843 C 3.368741075 0.078695755 -0.365599645 C 1.992540461 2.350900566 0.136502477 C -0.588789530 -2.231339483 -0.577396371 C -1.953893672 0.006820022 -0.047662672 C -0.597642897 2.288061503 0.287438683 H 3.078919448 -3.900447648 -1.210142820 H 3.066345210 4.077337352 0.378842846 H -1.678621046 3.997271545 0.609733364 H -1.656048267 -3.962980575 -0.814857467 C -4.825544178 -0.031849444 0.116514844 O -5.764263744 -1.955823082 1.125037114 O -5.916794878 1.866707377 -0.784737122 O 5.910870587 -0.333801224 1.726569067 O 5.872720796 0.212184119 -1.017224459</p>	<p>Frequencies:</p> <p>-365.9074 52.0053 79.7837 167.5435 191.0193 218.7255 314.6296 357.1887 395.9737 431.8875 497.1091 584.7151 621.3325 676.9200 742.2273 769.6074 796.5397 798.4391 845.5992 863.5924 966.2523 978.7409 1005.2901 1107.1877 1124.4547 1173.1295 1255.9873 1292.7709 1315.0073 1344.1848 1451.8665 1470.3106 1509.3533 1568.8179 1596.8010 3178.9405 3180.1233 3194.0624 3195.9745</p>
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C

cphG301

b3lyp -495.0174528	Geometry:	Frequencies:
uccsd(t) -493.7356077		
ump2(3df,2p) -493.9298269	C 1.285159278 -0.000045353 -0.000168186	54.6263 90.5675 177.3789
ump2(d,p) -493.6030539	C -0.084491545 -2.271772063 0.376176443	226.4738 329.6766 370.5577
rmp2(d,p) -493.643672053599	C -2.675995821 -2.294044376 0.399444640	384.8725 452.5884 533.7070
rccsd(t) -493.73651027	C -4.131370291 -0.000024566 0.000011338	609.8527 615.1083 702.7859
-----	C -2.676020388 2.293982015 -0.399546686	752.3946 789.3866 792.7591
ZPE 0.0923546	C -0.084531229 2.271713482 -0.376380533	814.0116 864.1134 965.9774
Thermal 0.1004506	H 0.994925690 3.997328237 -0.614623976	981.0304 991.4702 1100.8367
S2: 0.772056	H -3.738774018 4.022873555 -0.697361855	1123.5857 1176.7412 1267.9891
-----	H -3.738741893 -4.022945365 0.697231464	1298.4803 1347.1860 1414.0017
G2M(UMP2,CC) Energy (0K): -493.9700261	H 0.994954036 -3.997441621 0.614123198	1453.5188 1485.4888 1525.8865
T1 Diag: 0.03652378	O -6.506485807 -0.000041574 0.000120942	1565.9746 1597.9386 3159.6289
	C 4.156348691 -0.000090707 -0.000026456	3160.0173 3180.1490 3182.2383
G2M(UMP2,RCC) Energy (0K): -493.97092867	O 5.174914855 1.847692953 1.075135116	
T1 Diag: 0.02073918	O 5.175700981 -1.847417053 -1.074811973	

G

cphG706

b3lyp -570.1299955 uccsd(t) -568.6918336 ump2(3df,2p) -568.9389265 ump2(d,p) -568.5621097 rmp2(d,p) -568.585668217339 rccsd(t) -568.69185945 ----- ZPE 0.0948609 Thermal 0.1039164 S2: 0.770887 ----- G2M(UMP2,CC) Energy (OK): -568.9737895 T1 Diag: 0.03052181 G2M(UMP2,RCC) Energy (OK): -568.97381535 T1 Diag: 0.02032933	Geometry: C -2.356322190 -0.000051023 -2.015785982 C 2.356322190 0.000051023 -2.015785982 C 0.000000000 0.000000000 -3.471186908 C 2.308478104 -0.017767205 0.562070692 C -2.308478104 0.017767205 0.562070692 C 0.000000000 0.000000000 1.940816767 H -4.100694367 0.003161512 -3.090125524 H 4.100694367 -0.003161512 -3.090125524 H 4.044314388 -0.075239446 1.648502591 H -4.044314388 0.075239446 1.648502591 O 0.000000000 -1.409089408 -5.794206455 O 0.000000000 1.409089408 -5.794206455 C 0.000000000 0.000000000 4.815160133 O -1.809979689 1.142749517 5.832898597 O 1.809979689 -1.142749517 5.832898597	Frequencies: 54.4771 69.0716 166.5435 196.1191 287.1981 303.1153 355.8220 401.1608 450.4924 474.8012 543.8461 573.7062 607.7353 696.7709 719.5128 760.6894 774.6436 783.6246 824.5947 868.6489 969.3494 976.5479 986.0615 1099.3570 1108.3859 1171.1040 1219.3829 1278.2579 1298.4915 1333.4580 1422.8830 1446.8461 1506.1794 1580.4749 1606.8432 3172.1448 3172.6497 3188.0307 3190.1048
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G->U

cphG4401

<p>b3lyp -570.1183852 uccsd(t) -568.6803298 ump2(3df,2p) -568.9229845 ump2(d,p) -568.5464222 rmp2(d,p) -568.569625612715 rccsd(t) -568.68014660 ----- ZPE 0.0935082 Thermal 0.1024851 S2: 0.767996 ----- G2M(UMP2,CC) Energy (OK): -568.9633839 T1 Diag: 0.03323458 ----- G2M(UMP2,RCC) Energy (OK): -568.96320070 T1 Diag: 0.02301438</p>	<p>Geometry:</p> <p>H 3.109138058 -3.999807558 -0.927001374 C 2.035017725 -2.298215001 -0.537993691 C 3.554746818 0.000000000 0.000000000 C 2.035017725 2.298216891 0.537991802 C -0.537135756 2.261645021 0.508551758 C -0.537135756 -2.261643131 -0.508553648 C -1.904106947 0.000001890 -0.000001890 H 3.109139948 3.999809448 0.926997595 H -1.622760741 3.967054825 0.840147672 H -1.622762631 -3.967051045 -0.840149561 O 5.635390091 -0.371678894 1.579474675 O 5.635390091 0.371678894 -1.579474675 C -4.768886409 0.000001890 0.000000000 O -5.775267619 1.801545841 -1.156211926 O -5.775243053 -1.801553400 1.156215705</p>	<p>Frequencies:</p> <p>-959.0335 49.3154 70.5782 161.5322 193.9025 255.1329 307.7017 329.0458 401.9760 442.2598 474.7087 563.9335 598.1926 659.3288 739.0974 753.4639 770.0596 781.9816 826.2670 871.2414 968.9364 972.3116 980.4105 1096.3809 1123.1703 1174.6786 1235.2184 1267.5305 1306.0480 1356.5793 1417.9846 1447.6612 1511.3173 1598.5592 1622.6177 3170.3771 3170.5529 3186.5305 3188.7787</p>
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U

cphG4501

b3lyp -570.1428797 uccsd(t) -568.6856392 ump2(3df,2p) -568.9479684 ump2(d,p) -568.5647097 rmp2(d,p) -568.533579279641 rccsd(t) -568.65129786 ----- ZPE 0.0943042 Thermal 0.1040115 S2: 0.758575 ----- G2M(UMP2,CC) Energy (OK): -568.9745937 T1 Diag: 0.03148532 G2M(UMP2,RCC) Energy (OK): -568.94025236 T1 Diag: 0.05337313	Geometry: H 3.151672014 -4.101497500 -0.004956752 C 2.065283579 -2.362399549 -0.002910178 C 3.657175644 0.000000000 -0.000015118 C 2.065283579 2.362399549 0.002883722 C -0.496068227 2.348602659 0.002834589 C -0.496068227 -2.348602659 -0.002887502 C -1.835449417 0.000000000 -0.000100155 H 3.151673904 4.101497500 0.004941634 H -1.589968324 4.081723406 0.004847148 H -1.589968324 -4.081723406 -0.004884942 O 5.338164516 -0.002424519 1.981203994 O 5.338162627 0.002424519 -1.981232340 C -4.673224693 0.000000000 -0.000034015 O -5.641231235 0.004843368 -2.144372397 O -5.640717229 -0.004845258 2.144578377	Frequencies: 40.4280 59.7057 98.1248 183.1684 188.2208 195.6262 282.8251 373.2207 427.0981 450.2263 456.4393 570.8276 618.2310 719.8670 737.6614 789.4534 789.8935 790.3279 846.0547 924.4512 966.1192 983.6727 1003.8317 1079.7058 1124.2940 1157.0061 1214.0184 1226.7116 1334.0329 1412.3090 1413.7536 1442.4611 1516.4697 1635.2848 1646.6034 3162.2170 3162.8048 3184.3224 3187.3080
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U->H

cphG1405

b3lyp -570.1405838 uccsd(t) -568.6820251 ump2(3df,2p) -568.9277681 ump2(d,p) -568.5480685 rmp2(d,p) -568.581563960732 rccsd(t) -568.68300047 ----- ZPE 0.0931649 Thermal 0.1022354 S2: 0.797461 ----- G2M(UMP2,CC) Energy (OK): -568.9685598 T1 Diag: 0.04620050 G2M(UMP2,RCC) Energy (OK): -568.96953517 T1 Diag: 0.03110352	Geometry: H -3.086285600 4.134718886 1.116087371 C -2.097384357 2.400700518 0.645358481 C -3.814867620 0.183889250 0.000192752 C -2.234223205 -2.168572230 -0.677994052 C 0.354900016 -2.181734172 -0.650411609 C 0.448363981 2.290450116 0.609049284 C 1.747956987 -0.009692405 -0.023530870 H -3.368346122 -3.779692258 -1.211295553 H 1.360582028 -3.896745674 -1.151323204 H 1.581959664 3.944036071 1.033513898 O -4.636989194 -1.005079189 2.131594069 O -5.326920646 0.683924012 -1.917954860 C 4.601373526 -0.043291736 -0.034472384 O 5.591353803 -0.830209602 1.949923357 O 5.556975905 0.747263853 -2.038080971	Frequencies: -166.2868 22.4980 75.9877 171.7846 184.6603 236.2958 272.7053 357.0260 394.3654 411.9653 477.7839 579.0300 627.5780 654.9153 756.8979 769.6820 780.4120 788.5710 820.6358 883.5475 934.7091 972.8878 979.9373 1066.8702 1135.6462 1142.6312 1190.9356 1201.7547 1296.6873 1397.5488 1402.0502 1431.1769 1464.0005 1625.1430 1651.6347 3159.9702 3160.9103 3180.2110 3233.6196
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T

cphG801

<p>b3lyp -570.1962684 uccsd(t) -568.7514503 ump2(3df,2p) -568.9772212 ump2(d,p) -568.6053906 rmp2(d,p) -568.635909977192 rccsd(t) -568.75303223 ----- ZPE 0.0954597 Thermal 0.1048513 S2: 0.770378 ----- G2M(UMP2,CC) Energy (OK): -569.0278212 T1 Diag: 0.04025838 G2M(UMP2,RCC) Energy (OK): -569.02940313 T1 Diag: 0.02337474</p>	<p>Geometry:</p> <p>C -2.192694584 2.842580849 0.149545367 C -3.841527877 0.705831607 -0.454212683 C -2.682226248 -1.961756822 -0.221067722 C 0.190410695 -2.008340461 -0.411310231 C 1.584790474 0.115199595 -0.123128886 C 0.341630359 2.533737238 0.287168452 H -3.076555400 4.685458780 0.316292911 H 1.091405658 -3.833077021 -0.609824071 H 1.591699313 4.111021720 0.675845433 H -3.578803032 -3.209144255 -1.628033077 O -6.056799018 0.950212880 -1.067030081 O -2.877914948 -2.824677584 2.214946109 C 4.508497266 0.004363378 -0.174142042 O 5.486615732 -1.793945362 -1.325852641 O 5.512969853 1.775416598 1.044009437</p>	<p>Frequencies:</p> <p>43.4948 78.4179 114.1069 179.6083 223.4705 245.5301 329.9949 356.3200 413.1664 449.5717 530.9494 574.2657 607.6172 696.7534 748.3461 758.2017 786.5831 848.1203 886.0785 948.8235 969.1309 1024.3741 1067.6811 1070.7155 1150.3368 1225.2576 1247.5549 1290.6245 1306.8574 1312.8836 1407.8745 1530.6060 1619.6721 1646.7068 1711.4699 2944.3912 3161.1000 3184.7508 3210.5541</p>
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T->H

cphG4301

<p>b3lyp -570.1938813 uccsd(t) -568.752314 ump2(3df,2p) -569.0044607 ump2(d,p) -568.6337245 rmp2(d,p) -568.633043987619 rccsd(t) -568.75106874 ----- ZPE 0.0938762 Thermal 0.1027922 S2: 0.756976 ----- G2M(UMP2,CC) Energy (OK): -569.0291740 T1 Diag: 0.02361055 G2M(UMP2,RCC) Energy (OK): -569.02792874 T1 Diag: 0.02405945</p>	<p>Geometry:</p> <p>C -2.653940828 -1.960001267 -0.362430575 C -3.814998011 0.876060027 -0.367727477 C 0.462168430 2.494517862 0.381804047 C -2.066638512 2.886562335 0.286482482 C 1.661107064 0.068840833 -0.076804139 C 0.213930226 -1.981024470 -0.438061194 H -2.889965732 4.753855527 0.487611703 H -3.472025947 -2.820540973 -2.083324794 H 1.760349811 4.033977586 0.778107963 H 1.116833813 -3.807320054 -0.680499829 C 4.597550610 -0.067918647 -0.094903936 O 5.523582555 -2.154922738 -0.672105665 O 5.663601812 1.969156990 0.486264328 O -3.535012408 -2.979769297 1.797915677 O -6.015954478 1.157761501 -0.921080862</p>	<p>Frequencies:</p> <p>-125.9783 52.7572 88.8357 167.5276 206.3370 240.8827 318.6974 327.3637 429.5670 442.4948 452.2415 522.9465 593.6786 641.2936 722.3882 747.9381 762.7656 832.7146 851.6908 901.5768 945.3055 1001.1278 1036.6129 1068.5045 1139.3511 1175.9742 1213.6501 1279.3899 1295.3351 1312.0005 1404.2574 1571.4390 1646.6193 1681.8427 1734.4649 2897.4374 3157.5524 3167.8195 3174.5186</p>
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H

cphG1001

<p>b3lyp -570.2444999 uccsd(t) -568.7992707 ump2(3df,2p) -569.0462414 ump2(d,p) -568.6704656 rmp2(d,p) -568.696461997950 rccsd(t) -568.79996723 ----- ZPE 0.0964717 Thermal 0.1057033 S2: 0.772518 ----- G2M(UMP2,CC) Energy (OK): -569.0785748 T1 Diag: 0.03114130 ----- G2M(UMP2,RCC) Energy (OK): -569.07927133 T1 Diag: 0.02016173</p>	<p>Geometry:</p> <p>C 3.233884549 -1.723931009 0.000000000 C -0.713553028 -4.348182350 0.000000000 C 2.472555465 0.718553244 0.000000000 C -2.522338410 -2.290983019 0.000000000 C 0.000000000 1.762925508 0.000000000 C -2.209261813 0.297095183 0.000000000 H 5.228460245 -2.187187922 0.000000000 H -4.436175557 -3.022804030 0.000000000 H 3.970040592 2.121886546 0.000000000 H -3.915720414 1.440789564 0.000000000 C -0.254638706 4.688514467 0.000000000 O 1.794174019 5.873508812 0.000000000 O -2.477260883 5.505091585 0.000000000 O 1.900856618 -3.945234157 0.000000000 O -1.328581405 -6.555442942 0.000000000</p>	<p>Frequencies:</p> <p>30.7811 65.1366 97.3765 201.3237 208.2587 296.4503 368.5091 372.9365 475.0322 521.3535 523.3536 563.5735 664.7279 708.0009 761.2999 786.8723 789.6111 812.2551 822.4767 883.9878 966.5560 1016.0971 1041.2273 1061.9741 1079.0104 1245.0152 1296.0958 1309.7858 1335.7184 1432.7211 1451.3779 1510.8303 1592.9699 1656.8087 1731.8514 3148.0477 3158.9613 3173.0668 3184.7377</p>
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H->I

cphG1102

<p>b3lyp -570.1759658 uccsd(t) -568.7404837 ump2(3df,2p) -568.9812301 ump2(d,p) -568.6082082 rmp2(d,p) -568.637268042466 rccsd(t) -568.74058306 ----- ZPE 0.0943045 Thermal 0.103001 S2: 0.79077 ----- G2M(UMP2,CC) Energy (OK): -569.0192011 T1 Diag: 0.03430459 G2M(UMP2,RCC) Energy (OK): -569.01930046 T1 Diag: 0.02215067</p>	<p>Geometry:</p> <p>C -1.980338499 2.400451075 1.189229221 C -2.433243492 -1.578631857 1.418502134 C 0.189384573 -1.942589330 1.003624100 H -2.806052443 3.584672521 2.649789099 C 0.689850193 2.416906810 0.542512026 H -3.344053693 -2.988157791 2.617410532 H 1.790757394 4.136047363 0.334256648 H 1.101649863 -3.695438818 1.550943589 C 4.608195437 -0.298824283 -0.399176299 O -3.692848004 1.946293193 -0.844666007 O 5.316793604 -2.559201298 -0.316217322 O 5.822338807 1.665334381 -0.890132817 O -6.002875683 -1.591209874 -1.482730145 C -4.243455617 -0.549547477 -0.487617372 C 1.788009733 0.097757423 0.252524103</p>	<p>Frequencies:</p> <p>-695.8085 43.0508 75.5664 138.7038 183.4592 273.3597 362.0182 383.2939 471.2580 492.8817 518.1966 555.5189 644.1258 730.2435 743.7297 765.3270 796.9015 815.5793 851.7748 860.8310 920.8011 963.7839 990.2422 1087.6462 1110.9096 1129.2937 1193.5180 1257.0355 1327.2513 1350.3030 1363.8515 1411.3200 1545.3400 1670.7037 1805.3927 3085.7972 3137.8910 3162.5826 3175.3933</p>
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I

cphG2302

<p>b3lyp -570.2219224 uccsd(t) -568.792399 ump2(3df,2p) -569.0504055 ump2(d,p) -568.6769643 rmp2(d,p) -568.691976962411 rccsd(t) -568.79223124 ----- ZPE 0.0965811 Thermal 0.1052827 S2: 0.77477 ----- G2M(UMP2,CC) Energy (OK): -569.0692591 T1 Diag: 0.02390370 G2M(UMP2,RCC) Energy (OK): -569.06909134 T1 Diag: 0.01851403</p>	<p>Geometry:</p> <p>C -2.044182897 2.162440068 1.071157243 C -2.373199334 -0.673485165 1.710300415 C 0.182162040 -1.779231955 1.144291534 H -2.841756928 3.589625493 2.324391488 C 0.621648088 2.445135539 0.281860211 H -3.199019102 -1.211635704 3.526603127 H 1.516461757 4.190225811 -0.284991488 H 0.673611777 -3.753786003 1.304827548 C 4.649028639 -0.343847008 -0.349916808 O -3.941653126 1.814847623 -1.086673784 O 5.844758518 1.606218079 -0.947690096 O 5.361774755 -2.593598093 -0.198232271 O -5.722283478 -2.123271715 -1.424316821 C -4.292134962 -0.655547885 -0.465696549 C 1.841668506 0.103203613 0.338748527</p>	<p>Frequencies:</p> <p>43.3826 87.0221 145.6435 178.8282 251.9938 330.8029 393.2992 478.5034 493.9230 517.6424 667.4349 679.7799 693.1404 735.1142 760.1618 770.7231 826.4981 844.1184 863.9544 919.9286 939.7630 1003.2939 1033.3851 1103.5356 1122.6811 1187.6702 1209.4117 1255.6362 1264.7839 1308.3160 1327.3023 1339.5361 1477.7827 1677.8344 1854.7406 3052.5154 3090.9267 3229.5547 3233.6520</p>
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I->F

cphG1804

b3lyp -570.2150536 uccsd(t) -568.7752063 ump2(3df,2p) -569.0322882 ump2(d,p) -568.6548752 rmp2(d,p) -568.674985778939 rccsd(t) -568.77535620 ----- ZPE 0.0953883 Thermal 0.1039864 S2: 0.770889 ----- G2M(UMP2,CC) Energy (OK): -569.0572310 T1 Diag: 0.02847072 G2M(UMP2,RCC) Energy (OK): -569.05738090 T1 Diag: 0.02285025	Geometry: C 4.344865880 -0.594513510 -0.435014955 C 2.356276837 -0.365038397 1.693085010 C -0.110955270 -1.635788513 1.129574346 C -1.879353425 0.119041408 0.332555894 C -0.746077105 2.548488440 0.276582206 C 1.795729264 2.384669972 1.062895360 H 3.139625010 -0.783380299 3.558858862 H -0.460450669 -3.643756699 1.255072949 H -1.733695224 4.233940846 -0.317162185 H 2.870038570 3.951672454 1.816765695 O 4.152614592 1.610090128 -1.551402793 O 5.753033102 -2.326564673 -0.936128752 C -4.662281289 -0.445234594 -0.334353024 O -5.960547708 1.472279960 -0.808481531 O -5.245696437 -2.734333557 -0.287172232	Frequencies: -326.3694 34.2429 85.4765 128.3935 181.3210 256.1918 338.8544 385.8170 467.3233 491.5636 524.9426 670.6754 703.1547 748.9674 769.4289 807.6592 844.5517 855.2368 901.5020 907.2035 934.5911 977.2760 1010.9003 1083.1294 1125.4835 1160.7357 1222.3561 1241.2036 1267.3216 1324.7950 1368.8209 1383.2337 1493.1376 1675.8569 1773.2573 3060.6215 3199.4109 3232.4166 3233.5806
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F

cphG2401

b3lyp -381.6084364 uccsd(t) -380.6001039 ump2(3df,2p) -380.759844 ump2(d,p) -380.5012353 rmp2(d,p) -380.516908829583 rccsd(t) -380.59939956 ----- ZPE 0.0804454 Thermal 0.0873364 S2: 0.759012 ----- G2M(UMP2,CC) Energy (0K): -380.7782672 T1 Diag: 0.03385737 G2M(UMP2,RCC) Energy (0K): -380.77756286 T1 Diag: 0.02295649	Geometry: C -4.030600645 -1.327742367 -0.389514130 H -5.705986480 -2.461451434 -0.708753124 C -4.030583638 1.327748036 0.389635072 H -5.705954355 2.461464662 0.708928868 C -1.563999707 2.107180697 0.618095403 H -0.886370373 3.966083505 1.122138274 C -1.564028053 -2.107184476 -0.618065167 H -0.886428954 -3.966089174 -1.122138274 C 0.050121206 -0.000009449 -0.000001890 C 2.877943294 0.000000000 -0.000032125 O 3.921950841 1.740046594 -1.229531410 O 3.922001864 -1.740042814 1.229423696	Frequencies: 55.1231 108.2829 187.6722 304.7884 394.6769 548.5371 635.2052 686.4071 703.6211 720.4386 725.2154 794.4851 850.9573 854.4966 907.8208 987.8677 1051.1345 1071.3255 1140.9582 1228.4963 1274.6197 1376.8124 1391.0778 1493.4225 1504.3240 1519.9253 3166.4085 3183.1015 3220.5076 3223.7593
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H->N

cphG1308

b3lyp -570.191497 uccsd(t) -568.7490793 ump2(3df,2p) -568.9970139 ump2(d,p) -568.6267758 rmp2(d,p) -568.644176854445 rccsd(t) -568.74882197 ----- ZPE 0.0908772 Thermal 0.1012346 S2: 0.778681 ----- G2M(UMP2,CC) Energy (OK): -569.0284402 T1 Diag: 0.02729380 G2M(UMP2,RCC) Energy (OK): -569.02818287 T1 Diag: 0.02077948	Geometry: C -0.799446 -0.048594 0.006411 C -0.246953 1.189032 -0.219530 C 1.142042 1.666137 -0.071253 C -0.172876 -1.257038 0.365295 C 1.206691 -1.664672 0.343871 C 2.277659 -1.123842 -0.219841 H -0.972632 1.950167 -0.517755 H 1.771935 1.633114 -0.991535 H 1.454015 -2.620021 0.805876 O 3.253071 -0.715830 -0.719179 O 1.620830 2.147776 0.937391 H -0.871778 -2.025192 0.676336 C -2.379949 -0.117590 -0.106713 O -2.919938 0.895471 -0.598222 O -2.897033 -1.177251 0.309714	Frequencies: -269.3439 23.1333 61.9272 110.8669 119.9440 136.8076 212.2914 216.7884 308.9828 376.6326 405.5508 442.7906 485.6516 548.2139 596.6038 652.2693 726.3261 776.0457 782.7547 819.0284 836.8209 921.7165 974.7287 1053.0804 1108.3767 1178.6105 1272.2575 1313.9019 1368.6856 1404.0258 1424.0203 1485.4387 1686.9148 1732.7354 2146.4179 2817.7634 3074.5327 3113.7870 3174.0715
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N

cphG2602

b3lyp -570.2129141 uccsd(t) -568.7641157 ump2(3df,2p) -569.0039974 ump2(d,p) -568.6321915 rmp2(d,p) -568.664312675235 rccsd(t) -568.76455979 ----- ZPE 0.0928195 Thermal 0.1035071 S2: 0.773592 ----- G2M(UMP2,CC) Energy (OK): -569.0431021 T1 Diag: 0.03335314 G2M(UMP2,RCC) Energy (OK): -569.04354619 T1 Diag: 0.02148144	Geometry: C -2.066789690 -3.434316462 -0.497636700 C -4.103065973 -2.394615600 0.536255143 C -2.135819496 2.883652157 -0.975850795 C 0.466274805 -2.467765009 -0.759437469 C 1.462536532 -0.117951036 -0.131549505 C 0.200212704 2.175293985 0.201592204 H -2.413257749 -5.382816855 -1.056360687 H 1.218986738 3.648086061 1.201699524 H 1.852041213 -3.847329336 -1.370346243 O -5.983557013 -1.629185810 1.384744066 O -3.189651730 4.952367478 -0.736413045 C 4.425213256 -0.103441719 0.278407682 O 5.593094241 -1.582159975 -1.144051538 O 5.184646945 1.367757318 1.943452935 H -2.985398791 1.466701488 -2.267529628	Frequencies: 41.4584 64.0570 85.1385 132.4686 148.6847 197.4325 227.4274 249.7834 325.2887 364.8011 387.6002 448.6084 507.6119 576.1027 603.7948 689.8085 771.0415 778.7668 855.4751 877.5501 887.7193 942.3401 1003.4619 1057.0091 1169.5069 1182.9269 1293.2668 1299.1039 1381.1076 1400.4241 1456.5873 1491.8865 1632.1709 1695.5380 2156.8751 2880.2857 3131.2803 3171.1346 3177.5261
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N->R

cphG2801

b3lyp -570.2053716 uccsd(t) -568.7544729 ump2(3df,2p) -568.993091 ump2(d,p) -568.6194171 rmp2(d,p) -568.661845045606 rccsd(t) -568.75704972 ----- ZPE 0.0925064 Thermal 0.1023639 S2: 0.758232 ----- G2M(UMP2,CC) Energy (OK): -569.0356404 T1 Diag: 0.04067068 G2M(UMP2,RCC) Energy (OK): -569.03821722 T1 Diag: 0.02212112	Geometry: C -1.810979354 -3.351578582 -0.707029694 C -3.435958634 -1.971173328 0.749346331 C -2.267729939 2.476839474 -1.277851707 C 0.700496910 -2.537514801 -1.155660126 C 1.463129906 -0.226657532 -0.186727618 C -0.400911068 1.555569639 0.509345443 H -2.497135133 -5.191414054 -1.309546194 H -0.020108576 2.788778456 2.105844660 H 2.059217558 -3.793458913 -2.029856883 O -5.386337415 -1.540268527 1.718361986 O -3.691706609 4.272217249 -0.918452253 C 4.311304344 0.226784143 0.368188570 O 5.684891467 -0.412623591 -1.446417168 O 4.818843209 1.142254409 2.465593714 H -2.303600721 1.469849772 -3.116802787	Frequencies: -287.1852 57.1833 80.3819 103.9552 153.1407 172.0508 236.7609 278.5286 312.7987 349.7228 393.9596 472.7603 506.5778 595.6348 646.2871 691.3488 757.8661 783.2226 877.2199 895.5540 919.6986 960.9710 1004.9887 1062.3268 1098.7796 1148.1946 1271.3288 1298.7075 1372.7700 1412.0694 1453.7571 1483.2954 1670.1966 1684.1393 2015.1646 2884.4068 3140.0650 3160.8736 3198.9241
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R

cphG2901

<p>b3lyp -570.2448417 uccsd(t) -568.8081462 ump2(3df,2p) -569.0575084 ump2(d,p) -568.6858936 rmp2(d,p) -568.706038431408 rccsd(t) -568.80797073 ----- ZPE 0.0951536 Thermal 0.1048374 S2: 0.767384 ----- G2M(UMP2,CC) Energy (OK): -569.0846074 T1 Diag: 0.02806984 G2M(UMP2,RCC) Energy (OK): -569.08443193 T1 Diag: 0.02101592</p>	<p>Geometry:</p> <p>C 2.097148141 -3.636828963 0.637731547 C 3.271971979 -1.321302180 -0.231054924 C 1.312732272 2.970092009 0.743401253 C 1.059045988 0.558901621 -0.797577811 C -1.258610516 -0.967628596 -0.160862937 C -0.527343195 -3.361645154 0.642771446 H 3.166462900 -5.303484262 1.151364778 H 1.140888137 1.090893542 -2.794848257 H -1.882344861 -4.796151378 1.186067709 O 5.525013077 -0.873964321 -0.520494827 O 2.178582109 4.918010367 -0.074065926 C -3.901186531 0.093471524 -0.143859181 O -5.634806166 -1.366923949 -0.807755876 O -4.004102905 2.348668799 0.598759725 H 0.734956066 2.792057131 2.742593550</p>	<p>Frequencies:</p> <p>47.4338 60.6602 94.9834 148.5156 176.0589 237.3236 295.9323 344.7600 362.7418 453.3097 497.2948 598.3392 642.4831 699.3303 753.0214 760.6301 777.1801 800.0368 910.8847 949.6474 994.5016 1037.7823 1056.3344 1115.8602 1163.3425 1194.2172 1243.4723 1278.7140 1343.3385 1410.2532 1418.4501 1452.1079 1606.6987 1673.9941 1772.9020 2941.1879 3056.9646 3189.9691 3206.9335</p>
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R->ID_M

cphG3001

<p>b3lyp -570.1799079 uccsd(t) -568.7437381 ump2(3df,2p) -569.0013657 ump2(d,p) -568.6281192 rmp2(d,p) -568.639082723549 rccsd(t) -568.74353752 ----- ZPE 0.0905322 Thermal 0.1008521 S2: 0.771648 ----- G2M(UMP2,CC) Energy (OK): -569.0264524 T1 Diag: 0.03004433 G2M(UMP2,RCC) Energy (OK): -569.02625182 T1 Diag: 0.02194093</p>	<p>Geometry:</p> <p>C 2.344435813 -2.413607348 2.032086760 C 3.122447399 -1.537947943 -0.565434404 C 1.650883646 3.372263525 0.723472201 C 0.751929587 -0.596261507 -1.764448627 C -1.218795876 -1.103594392 -0.181254972 C -0.182226291 -2.189695588 2.196693244 H 3.658868838 -3.157184345 3.408385640 H 0.656419048 0.143420765 -3.664392508 H -1.373059889 -2.656966279 3.791977368 O 5.225737150 -1.722362537 -1.497730791 O 2.253821555 5.324951551 -0.166012441 C -3.940893456 -0.242803352 -0.335528434 O -4.347619211 1.391256062 1.362902611 O -5.386031279 -1.120069024 -1.955059633 H -0.076188088 2.950393504 1.877713142</p>	<p>Frequencies:</p> <p>-202.8622 41.6923 60.4734 90.2729 95.7988 170.8901 185.2302 222.8084 261.8212 360.3414 372.7839 478.7611 564.3911 629.1684 670.6229 709.8881 734.3900 755.6378 786.1411 840.9262 880.1649 883.7987 944.9568 1064.7294 1081.4267 1095.2804 1146.1762 1233.9091 1329.0932 1353.1493 1503.8421 1601.8362 1651.5108 1725.4231 1857.0325 2706.1261 3197.8727 3221.8596 3228.8290</p>
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M

cphG2501

<p>b3lyp -456.2806091 uccsd(t) -455.1202063 ump2(3df,2p) -455.3375346 ump2(d,p) -455.0341946 rmp2(d,p) -455.034193773948 rccsd(t) -455.12020827 ----- ZPE 0.0751756 Thermal 0.0826204 S2: 0.0 ----- G2M(UMP2,CC) Energy (OK): -455.3483707 T1 Diag: 0.01947431 G2M(UMP2,RCC) Energy (OK): -455.34837267 T1 Diag: 0.01947392</p>	<p>Geometry:</p> <p>C -3.577939427 -0.518482269 0.129442461 C -3.027484882 2.233514558 -0.429419476 H -4.483409262 3.650709001 -0.646634047 C -0.514665022 2.479071241 -0.565201968 H 0.585204719 4.169990624 -0.890739420 C -1.079352985 -1.787093215 0.290828852 H -0.823270528 -3.778050086 0.655413714 C 0.736445171 -0.050092860 -0.145807489 O -5.675737634 -1.455412264 0.355200483 C 3.594527443 -0.280168907 0.025541538 O 4.623653397 -2.185496617 -0.893970851 O 4.543619716 1.578015806 1.169978581</p>	<p>Frequencies:</p> <p>45.7404 112.3297 170.6534 245.4218 356.6388 385.4886 476.3147 597.0076 663.8766 686.3860 733.8895 740.0496 803.2480 851.6696 861.8268 877.5053 948.3666 1051.5714 1084.0097 1143.1797 1236.6498 1314.6099 1354.0309 1573.2723 1631.9526 1653.8984 1733.9729 3202.3437 3228.4136 3233.9718</p>
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S

cphG7001

<p>b3lyp -570.253237 uccsd(t) -568.8095898 ump2(3df,2p) -569.0501043 ump2(d,p) -568.677084 rmp2(d,p) -568.708860904401 rccsd(t) -568.80994575 ----- ZPE 0.0956333 Thermal 0.1052237 S2: 0.767636 ----- G2M(UMP2,CC) Energy (OK): -569.0869768 T1 Diag: 0.03263271 G2M(UMP2,RCC) Energy (OK): -569.0555558 T1 Diag: 0.02019927</p>	<p>Geometry:</p> <p>C -2.729140589 1.679520555 -0.251004763 C -3.781619779 -1.003837639 0.191982947 C -1.945299197 -2.996897775 0.255498532 C 0.662466172 -2.598218473 0.095782659 C 1.746464104 -0.222564385 -0.004658175 C 0.096177611 2.073439637 0.059443225 O -6.084734840 -1.341603508 0.391762904 O -4.128575386 3.408300602 -0.809288444 H -2.691467009 -4.902272728 0.416866026 H 1.930625474 -4.209659755 0.058902764 H 0.729515545 3.496146411 -1.303181596 H 0.383546375 2.984370780 1.906949095 C 4.598943338 0.119549744 0.003968425 O 5.784922230 -1.311898903 -1.459760524 O 5.398365522 1.785885680 1.479084864</p>	<p>Frequencies:</p> <p>36.2780 48.7694 72.0302 166.7066 206.5960 307.4840 336.2120 349.9535 377.7232 458.6231 516.1975 573.0495 594.9442 632.2420 681.3524 766.8907 773.5642 836.9106 911.9455 922.6345 964.3767 1053.2605 1115.1306 1119.7131 1165.9702 1262.8965 1309.4598 1343.3649 1355.4274 1396.6075 1461.8849 1521.3420 1599.9848 1609.5225 1755.3381 2998.5074 3055.2421 3150.1682 3169.8568</p>
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X

cphG7202

<p>b3lyp -569.6598047 uccsd(t) 0.0 ump2(3df,2p) -568.5014994 ump2(d,p) 0.0 rmp2(d,p) -568.129917526239 rccsd(t) -568.22965603 ----- ZPE 0.0856813 Thermal 0.0947747 S2: 0.0 ----- G2M(UMP2,CC) Energy (OK): -568.4158181 T1 Diag: 0.0 G2M(UMP2,RCC) Energy (OK): -568.515556603761 T1 Diag: 0.01941167</p>	<p>Geometry:</p> <p>C 3.730428988 -0.969641155 -0.075589045 C 2.614256579 1.765994423 0.176375699 C -0.123801628 2.012616911 0.110902357 C -1.657127301 -0.024008970 -0.149399858 C -0.590938148 -2.574836892 -0.368065738 C 1.915498216 -3.038048451 -0.370537500 O 4.069413730 3.547737824 0.376875641 O 6.010122783 -1.295998747 -0.018814113 H -0.918758389 3.897754788 0.223996797 H -1.956735820 -4.094000957 -0.514494947 H 2.685682557 -4.929040699 -0.566581468 C -4.548977089 0.170963523 0.008794785 O -5.468863645 -1.624841330 1.266443431 O -5.591452069 2.006482860 -1.016729350</p>	<p>Frequencies:</p> <p>42.5088 62.6341 115.1196 177.6450 248.8784 311.5551 353.7338 356.6740 467.6781 478.2853 551.3722 596.8519 618.3123 688.9632 755.8636 776.5646 791.3292 847.7095 896.1905 934.9384 994.2782 1064.5737 1140.1894 1170.2150 1263.2280 1299.0257 1342.4130 1407.8510 1594.5751 1643.7140 1664.2988 1693.9051 1727.4011 3158.1707 3181.5925 3191.5035</p>
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T->S

cphG6901

<p>b3lyp -570.1845533 ccsd(t) -568.7335453 mp2(3df,2p) -568.9680522 mp2(d,p) -568.5935986 ----- ZPE 0.0912173 Thermal 0.1002482 S2: 0.775413 ----- G2M(MP2,cc) Energy (0K): -569.0167816 G2M(MP2,cc) Enthalpy (298K): -569.0077507 T1 Diag: 0.03892981</p>	<p>Geometry:</p> <p>C -1.416504 0.882606 0.167316 C -1.984742 -0.538920 -0.038810 C -1.004262 -1.619336 -0.101837 C 0.338835 -1.396054 -0.095083 C 0.913788 -0.083181 -0.020760 C 0.086690 1.010579 0.073825 O -3.191735 -0.727449 -0.122900 O -2.175385 1.908522 0.057201 H -1.408443 -2.620587 -0.216702 H 1.041691 -2.220346 -0.147182 H 0.489554 2.014578 0.140453 H -0.938760 0.806210 1.273673 C 2.442342 0.103355 -0.035156 O 3.061605 -0.898395 0.402620 O 2.875400 1.200553 -0.430322</p>	<p>Frequencies:</p> <p>-975.6550 44.7602 78.8512 152.3863 177.3019 274.1431 315.4813 333.4228 380.9070 465.0080 474.7338 537.2115 595.4887 609.2575 678.7737 750.9794 761.5359 798.6048 857.3150 903.6176 937.6394 1006.9154 1020.8720 1037.7057 1077.8514 1133.1414 1211.7099 1266.1408 1306.9339 1386.6103 1418.4900 1494.6470 1591.8800 1623.7873 1683.0019 2118.3930 3154.3842 3182.9068 3196.9964</p>
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S->X

cphG7101

b3lyp -570.1620989 uccsd(t) -568.7278635 ump2(3df,2p) -568.9919723 ump2(d,p) -568.617894 rmp2(d,p) -568.628033006196 rccsd(t) -568.72820915 ----- ZPE 0.0863241 Thermal 0.0966848 S2: 0.762037 ----- G2M(UMP2,CC) Energy (OK): -569.0156177 T1 Diag: 0.02659346 G2M(UMP2,RCC) Energy (OK): -569.005824343804 T1 Diag: 0.01951257	Geometry: C -2.612578502 1.718180573 -0.303565606 C -3.727601957 -1.001210919 0.077533573 C -1.909598491 -3.063006064 0.396209429 C 0.598716261 -2.601926116 0.384332501 C 1.665281469 -0.060603517 0.129393328 C 0.125602537 1.983101279 -0.119413684 O -6.008450375 -1.321956026 0.090262769 O -4.054545365 3.468100985 -0.724853591 H -2.679285834 -4.949052898 0.636129059 H 1.961155889 -4.121898984 0.551777354 H 0.922450914 3.860617890 -0.312260236 H -0.328271885 3.038662612 4.397838683 C 4.550980199 0.131094081 -0.067019137 O 5.446256851 -1.664408416 -1.343655751 O 5.614132562 1.960496375 0.945959107	Frequencies: -198.0681 43.3296 64.5617 107.2716 134.3819 171.9030 186.4815 254.5281 312.4722 353.4795 353.8471 467.6198 475.9272 557.9852 596.6783 614.5143 687.5461 755.4581 775.7479 794.2844 847.7636 891.4898 935.9114 995.2723 1065.1194 1139.1241 1168.8365 1261.3253 1296.6134 1342.0167 1409.5434 1573.3298 1637.6079 1659.9592 1697.4061 1728.5403 3159.0366 3183.3537 3191.6220
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