**SUPPORTING INFORMATION**

**TABLE 1 Cartesian coordinates of the optimized geometries**

**1,3-Butadiene**

6 -1.549183489 -0.492897259 0.077638860

6 -0.728115488 0.553030384 -0.104873515

6 0.728127071 0.553033406 0.104877238

6 1.549180213 -0.492906623 -0.077640900

1 1.160286392 1.505783795 0.413862811

1 -1.160281995 1.505775381 -0.413867354

1 1.185701601 -1.452197280 -0.439297815

1 2.615414737 -0.414374326 0.116296987

1 -1.185756365 -1.452201275 0.439315654

1 -2.615414219 -0.414345753 -0.116320379

**6Aa**

6 1.135408817 1.461803535 0.000000000

6 2.377218971 0.901224866 0.000000000

6 2.523395259 -0.520771783 0.000000000

6 1.406181714 -1.313579209 0.000000000

6 0.099907209 -0.743634664 0.000000000

7 0.000000000 0.668016140 0.000000000

6 -1.155359429 -1.339702113 0.000000000

15 -2.466398535 -0.168064527 0.000000000

6 -1.296961626 1.113899673 0.000000000

1 3.246988557 1.549530126 0.000000000

1 3.515293349 -0.962149905 0.000000000

1 1.482677709 -2.396756290 0.000000000

1 0.955433005 2.530693343 0.000000000

1 -1.280110865 -2.416253477 0.000000000

1 -1.463049218 2.184349305 0.000000000

**6Ab**

6 0.000000000 0.629868440 0.000000000

7 -1.166205425 1.421176507 0.000000000

6 -1.105857665 2.801698877 0.000000000

6 0.095514903 3.445969712 0.000000000

6 1.300266824 2.686565074 0.000000000

6 1.248412740 1.314877689 0.000000000

6 -2.330070146 0.682508331 0.000000000

15 -2.080236624 -1.021034918 0.000000000

6 -0.326235752 -0.738148662 0.000000000

6 0.590203673 -1.882877720 0.000000000

8 0.228561831 -3.048813000 0.000000000

1 0.115510139 4.530593177 0.000000000

1 2.259333155 3.195733173 0.000000000

1 2.147555495 0.714152284 0.000000000

1 -2.064035910 3.308078757 0.000000000

1 -3.266243517 1.227637009 0.000000000

8 1.910340685 -1.539225606 0.000000000

6 2.835553505 -2.640908603 0.000000000

1 3.826683971 -2.184776462 0.000000000

1 2.695117668 -3.258569855 0.891038950

1 2.695117668 -3.258569855 -0.891038950

**6Ac**

6 1.085017173 -1.547463964 0.000000000

7 0.000000000 -0.646005700 0.000000000

6 -1.296496114 -1.134074486 0.000000000

6 -1.542122529 -2.478777584 0.000000000

6 -0.471172698 -3.412700502 0.000000000

6 0.816776210 -2.941892837 0.000000000

6 0.424327996 0.684390037 0.000000000

6 -0.418401421 1.881739459 0.000000000

8 0.041926357 3.012416728 0.000000000

6 2.318106994 -0.891873833 0.000000000

15 2.174097295 0.839368490 0.000000000

1 -2.574020694 -2.813990225 0.000000000

1 -0.673751310 -4.479331322 0.000000000

1 1.668397947 -3.615215270 0.000000000

1 -2.074132379 -0.387904263 0.000000000

1 3.251170586 -1.443441703 0.000000000

8 -1.764047719 1.655472126 0.000000000

6 -2.588375045 2.837592308 0.000000000

1 -3.615472482 2.470340546 0.000000000

1 -2.391321783 3.438156161 0.891432139

1 -2.391321783 3.438156161 -0.891432139

**6Ad**

6 -1.042284052 0.066797303 0.000000000

7 0.000000000 1.014881894 0.000000000

6 -0.285818671 2.367806363 0.000000000

6 -1.577558132 2.814802502 0.000000000

6 -2.650196907 1.890152817 0.000000000

6 -2.379515314 0.543702910 0.000000000

6 1.268254405 0.416393395 0.000000000

6 2.571875028 1.094501675 0.000000000

8 3.625612936 0.480456694 0.000000000

6 -0.543353638 -1.254581778 0.000000000

6 -1.306337810 -2.512639509 0.000000000

8 -0.788539216 -3.617216513 0.000000000

15 1.209376711 -1.324847351 0.000000000

1 -1.756471018 3.884765328 0.000000000

1 -3.677352808 2.242407034 0.000000000

1 -3.169474673 -0.194055084 0.000000000

1 0.570319552 3.022006918 0.000000000

8 -2.658006441 -2.351373314 0.000000000

8 2.534117194 2.456102042 0.000000000

6 3.819746150 3.109754639 0.000000000

1 3.597227345 4.177395574 0.000000000

1 4.386394065 2.830931856 0.891616002

1 4.386394065 2.830931856 -0.891616002

6 -3.426306840 -3.569414873 0.000000000

1 -4.469597540 -3.250934631 0.000000000

1 -3.202295363 -4.161157854 -0.891269385

1 -3.202295363 -4.161157854 0.891269385

**6Ba**

7 0.000000000 0.691286879 0.000000000

6 1.155512695 1.447786127 0.000000000

6 2.375636821 0.836144959 0.000000000

6 2.462840575 -0.587955601 0.000000000

6 1.321059601 -1.347264114 0.000000000

6 0.037925359 -0.727924772 0.000000000

7 -1.140226341 -1.322729568 0.000000000

15 -2.395963181 -0.191371566 0.000000000

6 -1.299613481 1.146186581 0.000000000

1 3.271633717 1.446626319 0.000000000

1 3.438484732 -1.064928081 0.000000000

1 1.344438858 -2.431511811 0.000000000

1 1.017971188 2.522988083 0.000000000

1 -1.471665769 2.215658733 0.000000000

**6Bb**

6 -1.497640561 -1.129655105 0.000000000

7 -0.132539212 -0.765602865 0.000000000

6 0.863680221 -1.722256851 0.000000000

6 0.533601335 -3.050536530 0.000000000

6 -0.826800933 -3.457753727 0.000000000

6 -1.821740390 -2.511113706 0.000000000

6 0.000000000 0.622458402 0.000000000

15 -1.585403936 1.356905184 0.000000000

7 -2.362711286 -0.120733612 0.000000000

1 1.333594990 -3.783268613 0.000000000

1 -1.075380887 -4.514980088 0.000000000

1 -2.874901675 -2.768878251 0.000000000

1 1.874172235 -1.338858917 0.000000000

6 1.304389676 1.281080847 0.000000000

8 1.156754399 2.626992680 0.000000000

8 2.400154185 0.733974565 0.000000000

6 2.371183964 3.397285770 0.000000000

1 2.047921018 4.438445976 0.000000000

1 2.963549157 3.176762497 0.892148179

1 2.963549157 3.176762497 -0.892148179

**6Ca**

7 0.000000000 -0.636390025 0.000000000

6 1.138916368 -1.408876761 0.000000000

6 2.369691001 -0.814436780 0.000000000

6 2.476972560 0.606258297 0.000000000

6 1.341259164 1.377201740 0.000000000

6 0.055984072 0.766476806 0.000000000

6 -1.235995893 1.294766847 0.000000000

15 -2.398118281 -0.004986169 0.000000000

7 -1.219615311 -1.196731623 0.000000000

1 3.256289095 -1.439122331 0.000000000

1 3.457451768 1.072917599 0.000000000

1 1.392975080 2.461451479 0.000000000

1 0.957780790 -2.476234998 0.000000000

1 -1.436378949 2.359291457 0.000000000

**6Cb**

6 -0.015280176 -0.783462523 0.000000000

7 -1.335439252 -1.239140227 0.000000000

6 -1.647939066 -2.576792641 0.000000000

6 -0.647787858 -3.509888407 0.000000000

6 0.710411810 -3.091140205 0.000000000

6 1.022740583 -1.751698103 0.000000000

7 -2.310312266 -0.304820754 0.000000000

15 -1.652699248 1.223933398 0.000000000

6 0.000000000 0.625405846 0.000000000

1 -0.908176836 -4.562843339 0.000000000

1 1.502593422 -3.833922555 0.000000000

1 2.043944992 -1.390859646 0.000000000

1 -2.709181723 -2.790263330 0.000000000

6 1.232203031 1.417755535 0.000000000

8 0.965079848 2.748228389 0.000000000

8 2.370974462 0.973241804 0.000000000

6 2.106563790 3.622266795 0.000000000

1 1.694553369 4.631885995 0.000000000

1 2.716554485 3.454144728 0.891802494

1 2.716554485 3.454144728 -0.891802494

**6D**

7 0.000000000 0.661506117 0.000000000

6 1.156920455 1.398832231 0.000000000

6 2.364722683 0.754050248 0.000000000

6 2.416004737 -0.667555306 0.000000000

6 1.256496531 -1.406184551 0.000000000

6 -0.002099445 -0.748734990 0.000000000

7 -1.221362549 -1.275662252 0.000000000

15 -2.330449497 -0.026297918 0.000000000

7 -1.225330092 1.222037059 0.000000000

1 3.275681552 1.342433917 0.000000000

1 3.380007254 -1.167729487 0.000000000

1 1.257335759 -2.490477079 0.000000000

1 1.018296648 2.472629163 0.000000000