Gas phase enthalpies of formation, isomerization, and disproportionation of mono- through tetra-substituted tetrahedranes: A G4MP2/G4 theoretical study

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Abstract

Gas phase (298.15 K, 1 atm) enthalpies of formation ($\Delta_fH°_{(g)}$), enthalpies of disproportionation to two corresponding acetylene molecules ($\Delta_{rxn}H°_{(g),Td\rightarrow acet}$), and enthalpies of isomerization from a tetrahedrane geometry to a 1,3-cyclobutadiene structure ($\Delta_{isom}H°_{(g),Td\rightarrow CBD}$) were calculated for the mono- through tetra-substituted hydro, fluoro, chloro, bromo, methyl, ethynyl, and cyano carbon tetrahedrane derivatives at the G4MP2 and G4 levels of theory. All derivatives have endothermic $\Delta_fH°_{(g)}$ indicative of the cage strain in these systems. In all cases, $\Delta_{rxn}H°_{(g),Td\rightarrow acet}$ and $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ are predicted to be substantially exothermic. High quality linear regression fits within a homologous series were obtained between the number of substituents and the G4MP2/G4 estimated $\Delta_fH°_{(g)}$. Via calculations on lower homolog members, this strategy was employed to allow extrapolated G4 and/or G4MP2 $\Delta_fH°_{(g)}$ (as well as some $\Delta_{rxn}H°_{(g),Td\rightarrow acet}$ and $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$) to be obtained for the mono- through tetra-substituted t-butyl, trifluoromethyl, and trimethylsilyl carbon tetrahedrane derivatives.

Keywords: Tetrahedranes; 1,3-Cylobutadienes; Acetylenes; Enthalpy of formation; Isomerization; Disproportionation

Tetrahedrane (Figure 1) has long captured the imagination of theoreticians and experimentalists [1]. Although synthesis of the parent carbon tetrahedrane has not yet been achieved, a number of its substituted derivatives have been prepared [2-10]. While much theoretical work has focused on the parent system (see, e.g., ref. [11-24] and references therein), less computational effort has been undertaken on substituted tetrahedranes [25-27, 27-33]. Continued theoretical interest in the tetrahedranes is important because advances in computing power and model chemistries (particularly composite methods) are facilitating increasingly accurate thermodynamic studies on these compounds. In concert, synthetic chemists are illustrating that the successful isolation of many tetrahedrane derivatives are likely within practical reach.

Our initial theoretical efforts focused on the mono- through tetra-substituted hydro (i.e., parent system), fluoro, chloro, bromo, methyl, ethynyl, and cyano carbon tetrahedrane derivatives. These substituents encompass a range of electron-withdrawing and releasing abilities and impart minimal conformational complexity. The G4 [34] and G4MP2 [35] composite methods were employed using Gaussian 09 [36]. All calculations were conducted in the gas phase (1 atm) at 298.15 K. Geometries were visualized using Gabedit 2.2.12 [37] and Avogadro 1.01 (http://avogadro.openmolecules.net/). Except where noted otherwise, all compounds converged absent imaginary frequencies.

Gas phase (298.15 K, 1 atm) enthalpies of formation ($\Delta_fH°_{(g)}$) were calculated using the atomization approach [38-40] (Table 1). Prior work has established that G4MP2/G4 atomization $\Delta_fH°_{(g)}$ are expected to be at effective chemical accuracy [30, 34, 35, 41-48]. None of these compounds have been synthesized; thus, no experimental $\Delta_fH°_{(g)}$ are available for comparison. Excellent agreement between the G4MP2 and G4 $\Delta_fH°_{(g)}$ estimates was obtained, yielding a mean signed deviation (MSD) of 1.6 kJ/mol (G4-G4MP2), mean absolute deviation (MAD) of 3.3 kJ/mol, and a root mean squared deviation (RMSD) of 4.4 kJ/mol. Neither the G4MP2 (two imaginary frequencies) nor G4 (one imaginary frequency) methods converged on a tetrafluorotetrahedrane structure absent imaginary frequencies. A Gaussian-3 (G3) [49-51] calculation on this compound gave a structure with no imaginary frequencies, and a corresponding atomization $\Delta_fH°_{(g)}$ at this level of 70.2 kJ/mol.

Linearly regressing the number of fluorine substituents (n=1-3) against the G4MP2 and G4 $\Delta_fH°_{(g)}$ estimates provides high quality fits (G4MP2: r^2=0.9994, m=516.7, b=-114.6; G4: r^2=0.9994, m=520.5, b=-115.4; values in kJ/mol). Extrapolating these regressions to the n=4 (i.e., tetrafluoro-) member of the homologous series yields predicted G4MP2 and G4 $\Delta_fH°_{(g)}$ estimates of 58.3 and 58.9 kJ/mol, respectively. In light of the higher atomization $\Delta_fH°_{(g)}$ predictive ability of the G4MP2 and G4 methods versus the G3 level, and the high quality regression fits obtained over the mono- through trifluorinated range, we recommend the predicted G4MP2/G4 $\Delta_fH°_{(g)}$ estimates over the G3 estimate. To ensure there are likely no discontinuities in the linear relationship between the number of fluorine substituents and the predicted G4MP2/G4 $\Delta_fH°_{(g)}$ for the fluorinated tetrahedranes, we also conducted G3 calculations on the mono- through trifluorinated tetrahedranes, resulting in G3 atomization $\Delta_fH°_{(g)}$ estimates of 411.7 and 174.6 kJ/mol, respectively, for the mono- and tri-substituted derivatives (the difluorotetrahedrane would not converge at the G3 level despite several attempts). There is a high quality fit (r^2=0.9991, m=-114.5, b=524.2; values in kJ/mol) between the number of fluorine substituents and the G3 atomization $\Delta_fH°_{(g)}$ across the mono-, tri-, and tetrafluorinated range, further suggesting the linear regression extrapolation of the n=1-3 G4MP2/G4 $\Delta_fH°_{(g)}$ data to the n=4 homolog is valid.

With the exception of the chlorinated derivatives (for which there is negligible predicted variation in

$\Delta_fH°_{(g)}$ with increasing chlorination), similarly strong linear regressions were obtained between the number of substituents and the G4MP2/G4 $\Delta_fH°_{(g)}$ estimates within each homologous series for the other tetrahedrane derivatives (values in kJ/mol): methyl, G4MP2 (r^2=0.998, m=-32.6, b=530.2), G4 (r^2=0.99990, m=-34.0, b=534.5); ethynyl, G4MP2 (r^2=0.9999987, m=240.4, b=529.2), G4 (r^2=0.9999981, m=239.3, b=533.2); cyano, G4MP2 (r^2=0.9989, m=166.1, b=495.9), G4 (r^2=0.9988, m=162.8, b=499.4); and bromo, G4MP2 (r^2=0.99997, m=50.1, b=532.6), G4 (r^2=0.99993, m=48.8, b=537.4).

Increasing methyl and fluoro substitution is predicted to increase the thermodynamic stabilities of these substituted carbon tetrahedranes, versus increasing ethynyl, cyano, and bromo substitution decreasing the thermodynamic stability, and (as mentioned previously) no expected effect due to increasing chlorine substitution. All derivatives have endothermic $\Delta_fH°_{(g)}$ (ranging from about +60 to +1500 kJ/mol), indicative of the cage strain in these systems. Our G4MP2/G4 $\Delta_fH°_{(g)}$ of 400.2/399.1 kJ/mol for tetramethyltetrahedrane is in good agreement with the value of 429.7 kJ/mol reported by Balci et al. [26] at the B3LYP/6-311+G(d)//B3LYP/ 6-31G(d)+ZPC/6-31G(d) level using isodesmic reactions. A substantial number of prior theoretical works have estimated the $\Delta_fH°_{(g)}$ of the parent tetrahedrane at various levels of theory. This literature is summarized in our previous work [22], and our G4MP2/G4 $\Delta_fH°_{(g)}$ estimates for this compound are in excellent agreement with other high level calculations.

Tetrahedranes may disproportionate to two acetylenes, or may isomerize to a corresponding 1,3-cyclobutadiene. For each of the mono- through tetra-substituted carbon tetrahedrane derivatives discussed above, the enthalpies of these respective reactions were calculated at the G4MP2 and G4 levels. In all cases, the enthalpies of disproportionation to two corresponding acetylene molecules ($\Delta_{rxn}H°_{(g),Td\rightarrow acet}$) and enthalpies of isomerization to a 1,3-cyclobutadiene structure ($\Delta_{isom}H°_{(g),Td\rightarrow CBD}$) are predicted to be substantially exothermic. Increasing exothermicity with increasing substitution is predicted for all compounds and both $\Delta_{rxn}H°_{(g),Td\rightarrow acet}$ and $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$, with the exception of the acetylene disproportionations for the halogen derivatives. Negligible variation in $\Delta_{rxn}H°_{(g),Td\rightarrow acet}$ is expected with increasing fluorination or chlorination, whereas increasing bromination is estimated to modestly decrease the reaction exothermicity. For the disubstituted derivatives, disproportionation to two acetylenes can proceed via two pathways, leading either to (a) the parent unsubstituted acetylene (HC≡CH) and a disubstituted acetylene (RC≡CR) or (b) two monosubstituted acetylenes (HC≡CR). Similarly, isomerization to a 1,3-cyclobutadiene from a disubstituted tetrahedrane can result in (a) a cis-disubstituted 1,3-cyclobutadiene or (b) a trans-disubstituted 1,3-cyclobutadiene. For most derivatives, these competing pathways are expected to be effectively isoenergetic (i.e., $\Delta\Delta H°_{(g)}\leq$10-15 kJ/mol; or within the likely accuracy of the computational method).

The tetrafluoro-1,3-cyclobutadiene yields one imaginary frequency with both the G4MP2 and G4 methods, preventing us from using the linear regression derived G4MP2/G4 $\Delta_fH°_{(g)}$ estimates for the tetrafluorotetrahedrane, coupled with corresponding atomization $\Delta_fH°_{(g)}$ estimates at these levels for the tetrafluoro-1,3-cyclobutadiene, in order to obtain indirect $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ at these two levels of theory. Difluoroacetylene does converge absent imaginary frequencies at both the G4MP2 and G4 levels, giving atomization $\Delta_fH°_{(g)}$ estimates of 6.9 and 7.0 kJ/mol, respectively. Applying these difluoroacetylene $\Delta_fH°_{(g)}$ estimates to the corresponding G4MP2/G4 regression predicted $\Delta_fH°_{(g)}$ of 58.3 and 58.9 kJ/mol, respectively, results in G4MP2 and G4 estimated $\Delta_{rxn}H°_{g,Td\rightarrow acet}$ for tetrafluorotetrahedrane of -44.5 and -44.9 kJ/mol, respectively. These indirect G4MP2/G4 $\Delta_{rxn}H°_{g,Td\rightarrow acet}$ estimates are likely more accurate than the corresponding G3 estimate of -70.5 kJ/mol.

The high quality linear regression fits discussed above between the number of substituents and the G4MP2/G4 estimated $\Delta_fH°_{(g)}$ within a homologous series allows for reasonable confidence in using such regression approaches to estimate the $\Delta_fH°_{(g)}$ of higher substituted tetrahedrane homologs where only the $\Delta_fH°_{(g)}$ of less substituted members are known. As further validation of this approach, we used the n=1-3 G4MP2/G4 $\Delta_fH°_{(g)}$ regression trends for the methyl, ethynyl, cyano, and bromo substituted tetrahedranes to predict the $\Delta_fH°_{(g)}$ of the corresponding n=4 member, and then compared this extrapolated $\Delta_fH°_{(g)}$ to the calculated G4MP2/G4 $\Delta_fH°_{(g)}$ for the tetrasubstituted homolog. Estimated/actual $\Delta_fH°_{(g)}$ values were as follows (presented as G4MP2 [G4]; values in kJ/mol): methyl, 398.6/400.2 [397.7/399.1]; ethynyl, 1490.2/1490.9 [1489.7/1490.7]; cyano, 1146.2/1166.1 [1136.6/1156.7]; and bromo, 733.6/732.5 [733.6/732.0]. The $\Delta\Delta_fH°_{(g)}$ using this validation approach are on the order of 1 kJ/mol for the methyl, ethynyl, and bromo derivatives, and about 20 kJ/mol for the tetracyanotetrahedrane. We then applied this concept to the corresponding t-butyl, trifluoromethyl, and trimethylsilyl carbon tetrahedrane derivatives (Table 2). Namely, due to computational expense, G4MP2 and G4 calculations could only be completed and atomization $\Delta_fH°_{(g)}$ estimates obtained on the lower homolog members at each level of theory. Extrapolations of the linear relationship between the number of substituents and $\Delta_fH°_{(g)}$ within each homologous series allows reasonable quality $\Delta_fH°_{(g)}$ estimates to be obtained for all derivatives at one or both levels of theory.

The $\Delta_fH°_{(g)}$ of the t-butyl, trifluoromethyl, and trimethylsilyl substituted tetrahedranes all decline with increasing substitution. The tetra-t-butyltetrahedrane has only a modestly endothermic $\Delta_fH°_{(g)}$ (29.2 kJ/mol at the extrapolated G4MP2 level), consistent with the successful synthesis by Maier et al. [2] and our previous study showing a collective reference level DFT (B3LYP, mPW3LYP , and X3LYP) and MP2 tetrahedrane to 1,3-cyclobutadiene isomerization energy ($\Delta_{isom}E°_{(g),Td\rightarrow CBD}$) range of -1.2 to 2.0 kJ/mol (i.e., the tetra-t-butyltetrahedrane and tetra-t-butyl-1,3-cyclobutadiene are approximately isoenergetic) [31]. Our G4MP2 $\Delta_fH°_{(g)}$ of 29.2 kJ/mol for tetra-t-butyltetrahedrane differs substantially from the value of 133.5 kJ/mol reported by Balci et al. [26] at the B3LYP/6-311+G(d)//B3LYP/6-31G(d)+ZPC/6-31G(d) level using isodesmic reactions, but our value is in remarkable agreement with the experimental estimate of 25.9 kJ/mol [52]. In comparison, all trifluoromethyl derivatives and the tri- and tetrakis(trimethylsilyl)tetrahedranes are expected to have exothermic $\Delta_fH°_{(g)}$, again consistent with the successful synthesis of tetrakis(trimethylsilyl)tetrahedrane by Maier's group [4] and with the corresponding estimated reference level DFT/MP2 $\Delta_{isom}E°_{(g),Td\rightarrow CBD}$ for this compound of 19.6 to 32.3 kJ/mol [31] that suggests the tetrakis(trimethylsilyl)tetrahedrane is more thermodynamically stable than the tetrakis(trimethylsilyl)-1,3-cyclobutadiene.

Tri-t-butyl-mono(trimethylsilyl)tetrahedrane has also been synthesized [10]. In our prior work [31], we showed that - in the absence of access to the more computationally expensive composite methods - the B3LYP [53-55], mPW3LYP [56], and X3LYP [57] density functionals, as well as the MP2 [58-62] model chemistry, appear to best estimate $\Delta_{isom}E°_{(g),Td\rightarrow CBD}$. Calculations at the x/TZVP//B3LYP/6-31G(d) [53-55, 63-73, 73] level on tri-t-butyl-mono(trimethylsilyl)tetrahedrane and tri-t-butyl-mono(trimethylsilyl)-1,3-cyclobutadiene yield the following $\Delta_{isom}E°_{(g),Td\rightarrow CBD}$ estimates (values in kJ/mol): B3LYP, -2.5; mPW3LYP, -4.0; X3LYP, -2.9; and MP2, 0.3. The B2PLYPD [74, 75] and mPW2PLYPD [75, 76] functionals give systematically lower $\Delta_{isom}E°_{(g),Td\rightarrow CBD}$ estimates of -17.9 and -14.0 kJ/mol, respectively, as expected [31]. Consequently, consistent with the successful synthesis of tri-t-butyl-mono(trimethylsilyl)tetrahedrane, we find that this compound is approximately isoenergetic with its isomer tri-t-butyl-mono(trimethylsilyl)-1,3-cyclobutadiene.

Increasing substitution among the t-butyl and trimethylsilyl tetrahedranes has only a modest influence

on the expected $\Delta_{rxn}H°_{g,Td\rightarrow acet}$ (increasing by about 5 to 7 kJ/mol per substituent), and all mono- through tetra-substituted derivatives are expected to have substantially exothermic disproportionation enthalpies. In contrast, increasing trifluoromethylation significantly increases the $\Delta_{rxn}H°_{g,Td\rightarrow acet}$ such that the tri(trifluoromethyl)tetrahedrane disproportionation is predicted to be approximately isoenergetic, while the tetrakis(trifluoromethyl)tetrahedrane disproportionation is expected to be modestly endothermic. t-Butyl, trifluoromethyl, and trimethylsilyl substituted tetrahedrane $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ are expected to be strongly exothermic for the mono- and di-substituted homologs (and for the tri(trifluoromethyl) derivative). Projecting the mono- and di-(trimethylsilyl) $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ trend yields estimated $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ of -19.8 and 11.4 kJ/mol for the tri- and tetra-substituted members, respectively, in good agreement with our prior reference level DFT/MP2 $\Delta_{isom}E°_{(g),Td\rightarrow CBD}$ of 19.6 to 32.3 kJ/mol [31] for tetrakis(trimethylsilyl)tetrahedrane.

Both the t-butyl and trifluoromethyl derivatives show no significant $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ trends over their respective available G4MP2/G4 datasets. We expect the tetra-t-butyltetrahedrane $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ to be approximately isoenergetic [31] due to steric congestion on the 1,3-cyclobutadiene system, but do not expect a similarly isoenergetic $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ for tetrakis(trifluoromethyl)tetrahedrane due to the absence of steric bulk in the trifluoromethyl groups. Attempts to estimate $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ for tetrakis(trifluoromethyl)tetrahedrane obtained a converged tetrakis(trifluoromethyl)-1,3-cyclobutadiene structure with two imaginary frequencies at the B3LYP/6-31G(d) level, precluding any subsequent thermodynamic analysis. However, the minimum C-F···F-C distance between adjacent trifluoromethyl groups on this tetrakis(trifluoromethyl)-1,3-cyclobutadiene structure was 2.714 Å (B3LYP/6-31G(d)), which is longer than the C-H···H-C distance (2.671 Å) between adjacent methyl groups on tetramethyl-1,3-cyclobutadiene at the G4 level of theory. Thus, we do not expect the $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ for tetrakis(trifluoromethyl)tetrahedrane to be significantly different from that of the mono- through tri-substituted homologs (-113 to -120 kJ/mol).

Analogous calculations were performed for tri-t-butyltetrahedrane to investigate whether the steric influence that renders $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ isoenergetic for the tetra-t-butyl derivative also operates with three t-butyl substituents. As evidenced by the negligible change in $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ when moving from the mono- to di-t-butyl derivatives, the t-butyl effect is absent at these homologs. Calculations at the x/TZVP//B3LYP/6-31G(d) (x=B3LYP, mPW3LYP, X3LYP, and MP2) level of theory for tri-t-butyltetrahedrane and tri-t-butyl-1,3-cyclobutadiene yield the following $\Delta_{isom}E°_{(g),Td\rightarrow CBD}$ (values in kJ/mol): B3LYP, -83.4; mPW3LYP, -83.9; X3LYP, -83.2; and MP2, -78.0. When compared to the tetra-t-butyl $\Delta_{isom}E°_{(g),Td\rightarrow CBD}$ of -1.3, -2.0, -1.2, and -1.7 kJ/mol [31] at these four levels of theory, respectively, and the mono- and di-t-butyl G4MP2 $\Delta_{isom}H°_{(g),Td\rightarrow CBD}$ of -115.3 and -110.0/-120.8 kJ/mol, respectively, we see that the t-butyl effect is modestly in effect on the tri-t-butyl derivative, reducing the exothermicity of the tetrahedrane to 1,3-cyclobutadiene isomerization by about 35 kJ/mol compared to the lower homologs.

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Appendix A. Supplementary Material

Supplementary data is associated with this article.

Table 1. G4MP2 and G4 estimated gas phase (298.15 K, 1 atm) enthalpies of formation ($\Delta_fH°_g$), enthalpies of disproportionation to two corresponding acetylene molecules ($\Delta_{rxn}H°_{(g),Td\rightarrow acet}$), and enthalpies of isomerization from a tetrahedrane geometry (T_d) to a 1,3-cyclobutadiene structure ($\Delta_{isom}H°_{(g),Td\rightarrow CBD}$) at the G4MP2 and G4 levels of theory for various mono- through tetra-substituted carbon tetrahedrane derivatives.

	-H		-CH_3		-C≡CH		-C≡N		-F		-Cl		-Br	
	G4MP2	G4	G4MP2	G4	G4MP2	G4	G4MP2	G4	G4MP2	G4	G4MP2	G4	G4MP2	G4
$\Delta_fH°_{(g)}$ (kJ/mol)														
mono-	532.4 [22]	536.4 [22]	498.0	501.0	769.9	772.9	668.2	668.5	403.7	406.7	529.7	535.2	582.4	585.8
di-	532.4 [22]	536.4 [22]	464.5	466.2	1009.5	1011.3	821.5	818.4	284.2	286.4	529.0	535.9	632.9	635.2
tri-	532.4 [22]	536.4 [22]	431.8	432.2	1250.2	1250.9	988.4	982.1	174.5	175.9	529.7	538.1	683.2	684.3
tetra-	532.4 [22]	536.4 [22]	400.2	399.1	1490.9	1490.7	1166.1	1156.7	n/c[a]	n/c[b]	531.2	541.0	732.5	732.0
$\Delta_{rxn}H°_{(g),Td\rightarrow acet}$														
mono-	-78.4	-79.6	-86.6	-87.5	-84.6	-85.2	-67.8	-68.2	-70.6	-71.6	-78.9	-79.4	-74.6	-74.9
di-	-78.4	-79.6	-89.8[c]/-95.7	-89.9/-95.9	-100.3/-92.9	-98.2/-92.6	-61.4/-74.7	-61.3/-74.5	-50.3/-72.1	-51.0/-72.9	-76.6/-81.4	-77.0/-81.2	-70.9/-71.2	-70.6/-70.3
tri-	-78.4	-79.6	-99.7	-99.2	-109.7	-106.9	-81.9	-81.4	-61.6	-62.1	-80.6	-80.2	-67.4	-65.6
tetra-	-78.4	-79.6	-104.8	-103.3	-126.5	-121.3	-99.9	-99.4	n/c	n/c	-80.5	-79.9	-62.5	-59.4
$\Delta_{isom}H°_{(g),Td\rightarrow CBD}$														
mono-	-109.0	-107.3	-119.0	-117.2	-126.4	-124.1	-120.2	-118.0	-173.7	-172.2	-147.3	-145.6	-140.3	-138.8
di-	-109.0	-107.3	-127.4[d]/-130.2	-125.2/-127.9	-144.3/-143.5	-141.0/-140.0	-133.7/-136.7	-131.0/-133.9	-230.4/-241.7	-228.8/-240.4	-181.9/-183.7	-180.3/-182.0	-168.3/-169.1	-166.9/-167.5
tri-	-109.0	-107.3	-137.0	-134.1	-164.3	-159.8	-151.0	-147.7	-284.1	-282.4	-214.7	-213.2	-195.3	-193.8
tetra-	-109.0	-107.3	-145.6	-142.2	-184.3	-179.0	-169.4	-165.7	n/c	n/c	-244.4	-243.5	-219.2	-217.7

[a] Converged geometry at the G4MP2 level contained two imaginary frequencies. [b] Converged geometry at the G4 level contained one imaginary frequency. [c] For disubstituted tetrahedranes, disproportionation to two acetylene compounds can produce either (a) the parent unsubstituted acetylene (HC≡CH) and a disubstituted acetylene (RC≡CR) or (b) two monosubstituted acetylenes (HC≡CR). The value on the left of the "/" represents path (a); the value on the right of the "/" represents path (b). [d] For disubstituted tetrahedranes, isomerization to a 1,3-cyclobutadiene can result in (a) a cis-disubstituted 1,3-cyclobutadiene or (b) a trans-disubstituted 1,3-cyclobutadiene. The value on the left of the "/" represents path (a); the value on the right of the "/" represents path (b).

Table 2. G4MP2 and G4 estimated gas phase (298.15 K, 1 atm) enthalpies of formation ($\Delta_fH°_{(g)}$), enthalpies of disproportionation to two corresponding acetylene molecules ($\Delta_{rxn}H°_{(g),Td\rightarrow acet}$), and enthalpies of isomerization from a tetrahedrane geometry (T_d) to a 1,3-cyclobutadiene structure ($\Delta_{isom}H°_{(g),Td\rightarrow CBD}$) at the G4MP2 and G4 levels of theory for t-butyl, trifluoromethyl, and trimethylsilyl mono- through tetra-substituted carbon tetrahedrane derivatives.

	$-C(CH_3)_3$		$-CF_3$		$-Si(CH_3)_3$	
	G4MP2	G4	G4MP2	G4	G4MP2	G4
$\Delta_fH°_{(g)}$ (kJ/mol)						
mono-	408.4	411.1	-143.0	-142.6	333.8	336.2
di-	282.0	c/e[a]	-808.4	-811.6	130.9	c/e
tri-	155.6[b]	c/e	-1466.0	-1480.6[b]	-72.0[b]	c/e
tetra-	29.2[b]	c/e	-2128.8[b]	-2149.5[b]	-274.9[b]	c/e
$\Delta_{rxn}H°_{(g),Td\rightarrow acet}$						
mono-	-76.2	-76.6	-51.5	-51.3	-75.4	-76.6
di-	-70.5[c]/-71.6	n/a	-24.8/-34.7	-22.8/-33.0	n/c[d]/-68.0	n/a
tri-	-65.9[e]	n/a	-15.8	-4.5[f]	n/a[g]	n/a
tetra-	-60.2[h]	n/a	8.4[i]	23.9[j]	n/a[g]	n/a
$\Delta_{isom}H°_{(g),Td\rightarrow CBD}$						
mono-	-115.3	-113.4	-113.0	-111.5	-82.2	-80.9
di-	-110.0[k]/-120.8	n/a	-116.6/-120.0	-115.2/-118.2	-54.5/-51.0	n/a
tri-	n/a	n/a	-115.4	n/a	n/a	n/a
tetra-	n/a	n/a	n/a	n/a	n/a	n/a

[a] not completed due to computational expense. [b] estimated via extrapolation of the G4MP2 and G4 $\Delta_fH°_{(g)}$ trends from lower homologs. [c] For disubstituted tetrahedranes, disproportionation to two acetylene compounds can produce either (a) the parent unsubstituted acetylene (HC≡CH) and a disubstituted acetylene (RC≡CR) or (b) two monosubstituted acetylenes (HC≡CR). The value on the left of the "/" represents path (a); the value on the right of the "/" represents path (b). [d] calculation for the di(trimethylsilyl)acetylene failed to converge. [e] $\Delta_{rxn}H°_{(g),Td\rightarrow acet}$ obtained using G4MP2 atomization $\Delta_fH°_{(g)}$ of 105.2 and -15.5 kJ/mol, respectively, for the mono- and di-t-butylacetylenes and the regression estimated $\Delta_fH°_{(g)}$ of 155.6 kJ/mol for the tri-t-butyltetrahedrane. [f] $\Delta_{rxn}H°_{(g),Td\rightarrow acet}$ obtained using G4 atomization $\Delta_fH°_{(g)}$ of -422.3 and -1062.8 kJ/mol, respectively, for the mono- and di-(trifluoromethyl)acetylenes and the regression estimated $\Delta_fH°_{(g)}$ of -1480.6 kJ/mol for the tri(trifluoromethyl)tetrahedrane. [g] calculation for the di(trimethylsilyl)acetylene failed to converge. [h] $\Delta_{rxn}H°_{(g),Td\rightarrow acet}$ obtained using G4MP2 atomization $\Delta_fH°_{(g)}$ of -15.5 kJ/mol for the di-t-butylacetylene and the regression estimated $\Delta_fH°_{(g)}$ of 29.2 kJ/mol for the tetra-t-butyltetrahedrane. [i] $\Delta_{rxn}H°_{(g),Td\rightarrow acet}$ obtained using G4MP2 atomization $\Delta_fH°_{(g)}$ of -1060.2 kJ/mol for the di(trifluoromethyl)acetylene and the regression estimated $\Delta_fH°_{(g)}$ of -2128.8 kJ/mol for the tetra-t-butyltetrahedrane. [j] $\Delta_{rxn}H°_{(g),Td\rightarrow acet}$ obtained using G4 atomization $\Delta_fH°_{(g)}$ of -1062.8 kJ/mol for the di(trifluoromethyl)acetylene and the regression estimated $\Delta_fH°_{(g)}$ of -2149.5 kJ/mol for the

246 tetra(trifluoromethyl)tetrahedrane. [k] For disubstituted tetrahedranes, isomerization to a 1,3-cyclobutadiene can result in (a) a cis-disubstituted
247 1,3-cyclobutadiene or (b) a trans-disubstituted 1,3-cyclobutadiene. The value on the left of the "/" represents path (a); the value on the right
248 of the "/" represents path (b).
249

Figure Captions

Figure 1. Three- and two-dimensional representations of tetrahedrane.

Figure 2. General isomerization reaction for tetra-substituted tetrahedranes to the corresponding cyclobutadienes.

Figures

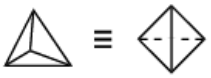

Figure 1.

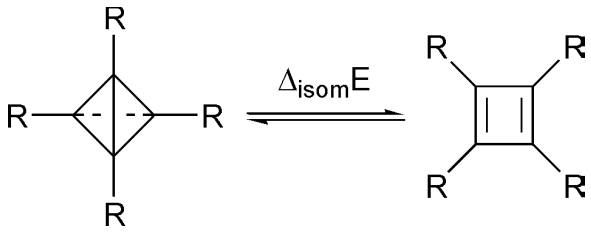

Figure 2.

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Supplementary Material

Gas phase enthalpies of formation, isomerization, and disproportionation of mono- through tetra-substituted tetrahedranes: A G4MP2/G4 theoretical study

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G4MP2 archive entries

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,-0.0057832561,1.4294415835,2.4404600757,-0.0068990276,1.4301007137,0.
8264943832,2.2966081714,1.4358788738,5.7314331885,-1.1541876737,5.6777
76966,-1.6264764265,-1.1547043526,-2.814892281,-1.6342908364,-1.152980
6332,1.4314617382,0.8284568738,4.3189338879\PG=C01 [X(C4H1Br3)]\NImag=
0\\

tetrabromotetrahedrane
\\0,1\C,0,0.0129240851,0.0074551219,0.0051333671\C,0,
1.5018300061,0.0078303406,0.0051082902\C,0,0.7570179758,1.2970586849,0
.0050109904\C,0,0.7573387436,0.4375453263,1.220766438\Br,0,0.757260637
1,0.4379428224,3.062884521\Br,0,0.7567515242,3.0335638256,-0.609900488
1\Br,0,3.006998893,-0.8591937896,-0.6084023063\Br,0,-1.4909218648,-0.8
615023321,-0.6087008125\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1
=-10441.2232724\CCSD(T)/GTBas1=-10441.2622433\MP2/GTBas2=0.\MP2/GTBas3
=0.\HF/GTMP2LargeXP=-10440.8833218\MP2/GTMP2LargeXP=-10443.0685842\HF/
GFHFB3=-10441.1290552\HF/GFHFB4=-10441.1493402\G4MP2=-10443.5642293\Fr
eqCoord=0.0244229813,0.0140881387,0.009700658,2.8380474097,0.014797199
2,0.0096532696,1.4305566519,2.4510856928,0.0094693995,1.4311628152,0.8
268408374,2.3069142401,1.4310152153,0.8275919962,5.7880129214,1.430053
1314,5.732604837,-1.1525448908,5.6824043896,-1.6236409575,-1.149713737
5,-2.81743401,-1.6280034704,-1.1502778326\PG=C01 [X(C4Br4)]\NImag=0\\

monochlorotetrahedrane
\\0,1\C,0,0.0203858204,0.0123386448,0.0090031828\C,
0,1.4907647301,0.0063916713,0.0044575748\C,0,0.7449253185,1.2918994352
,0.0045039359\C,0,0.7451730387,0.4329708438,1.2173052808\Cl,0,-1.36579
67365,-0.7913192396,-0.5595253619\H,0,2.3673506782,-0.4937012814,-0.34
98288512\H,0,0.7456699321,2.3008905285,-0.3503991709\H,0,0.7461272186,
0.4334293974,2.2868834097\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBa
s1=-613.1289302\CCSD(T)/GTBas1=-613.1886607\MP2/GTBas2=0.\MP2/GTBas3=0
.\HF/GTMP2LargeXP=-612.5707165\MP2/GTMP2LargeXP=-613.4014638\HF/GFHFB3
=-612.5778233\HF/GFHFB4=-612.5919436\G4MP2=-613.5584944\FreqCoord=0.03
85236175,0.0233166596,0.0170135498,2.8171370685,0.0120785082,0.0084235
955,1.4077048415,2.4413361238,0.0085112054,1.4081729647,0.8181963183,2
.3003736009,-2.5809817851,-1.4953766465,-1.0573496983,4.4736444423,-0.
9329602134,-0.6610807222,1.4091119571,4.3480529605,-0.6621584703,1.409
9761034,0.8190628591,4.3215833421\PG=C01 [X(C4H3Cl1)]\NImag=0\\

dichlorotetrahedrane
\\0,1\C,0,0.0173232716,0.0086532133,0.0065949094\C,
0,1.4863372855,0.0091095339,0.0067568605\C,0,0.7514376861,1.2952922805
,0.0027145773\C,0,0.7515632864,0.4293700713,1.2224244302\Cl,0,2.879799
6964,-0.780680083,-0.5539083708\Cl,0,-1.3754242133,-0.7820597603,-0.55
45380699\H,0,0.7510866512,2.306336541,-0.3469724045\H,0,0.7513763362,0
.4327782033,2.2922280677\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas
1=-1072.1491505\CCSD(T)/GTBas1=-1072.2199994\MP2/GTBas2=0.\MP2/GTBas3=
0.\HF/GTMP2LargeXP=-1071.4894542\MP2/GTMP2LargeXP=-1072.5090082\HF/GFH
FB3=-1071.5037306\HF/GFHFB4=-1071.5204819\G4MP2=-1072.7245925\FreqCoor
d=0.032736239,0.0163522032,0.0124625727,2.8087704106,0.0172145243,0.01
27686159,1.4200114327,2.4477476722,0.0051298076,1.4202487828,0.8113918
444,2.3100473913,5.4420327437,-1.4752715542,-1.0467351235,-2.599175079
7,-1.4778787666,-1.0479250824,1.4193480729,4.3583444328,-0.6556828201,

1.4198954982,0.8178322804,4.3316832821\PG=C01 [X(C4H2Cl2)]\NImag=0\\

trichlorotetrahedrane

\\0,1\C,0,0.0136509451,0.0077404044,0.0052484744\C,
0,1.4938394542,0.0078147823,0.0056350557\C,0,0.7537280595,1.289746865,
0.0053862647\C,0,0.7533701131,0.4352371872,1.2271665878\Cl,0,0.7538515
625,2.8902308927,-0.547760937\Cl,0,2.8805414624,-0.7921425041,-0.54641
07841\Cl,0,-1.3724499474,-0.7924932249,-0.5479584042\H,0,0.7530683506,
0.4349655974,2.2975937428\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBa
s1=-1531.1687898\CCSD(T)/GTBas1=-1531.2505645\MP2/GTBas2=0.\MP2/GTBas3
=0.\HF/GTMP2LargeXP=-1530.4070351\MP2/GTMP2LargeXP=-1531.6163423\HF/GF
HFB3=-1530.4284041\HF/GFHFB4=-1530.4478238\G4MP2=-1531.8902383\FreqCoo
rd=0.0257965477,0.0146272445,0.0099181792,2.8229474549,0.0147677984,0.
010648712,1.4243396111,2.4372683556,0.0101785651,1.4236631905,0.822479
0867,2.3190087704,1.4245729979,5.461744848,-1.0351181572,5.4434344784,
-1.496932391,-1.032566738,-2.5935545316,-1.4975951572,-1.0354913161,1.
423092942,0.8219658562,4.3418229384\PG=C01 [X(C4H1Cl3)]\NImag=0\\

tetrachlorotetrahedrane

\\0,1\C,0,0.0101953896,0.0059343802,0.004190726\C,0,1
.5007994933,0.0062156189,0.0041604199\C,0,0.7553197984,1.2969632363,0.
0041060785\C,0,0.7554705983,0.4365640307,1.2212420995\Cl,0,0.755828477
5,0.4361241845,2.9119334544\Cl,0,0.755689959,2.8908288987,-0.559984642
1\Cl,0,2.8820301726,-0.7898867304,-0.5590147885\Cl,0,-1.3703338888,-0.
7911436189,-0.5591333477\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas
1=-1990.1881856\CCSD(T)/GTBas1=-1990.2807046\MP2/GTBas2=0.\MP2/GTBas3=
0.\HF/GTMP2LargeXP=-1989.3236405\MP2/GTMP2LargeXP=-1990.7237036\HF/GFH
FB3=-1989.3520429\HF/GFHFB4=-1989.3741589\G4MP2=-1991.0556906\FreqCoor
d=0.0192664942,0.0112143534,0.0079193244,2.8361000228,0.0117458175,0.0
078620541,1.4273475617,2.450905321,0.0077593639,1.4276325323,0.8249864
575,2.30781311,1.4283088259,0.8241552686,5.5027567461,1.4280470638,5.4
628749156,-1.0582176122,5.446247733,-1.4926695965,-1.0563848545,-2.589
5557605,-1.4950447714,-1.056608899\PG=C01 [X(C4Cl4)]\NImag=0\\

monocyanotetrahedrane

\\0,1\C,0,0.0124570935,0.0070180083,0.0049977505\C,0
,1.4975638901,0.0081781609,0.005773091\C,0,0.7670104885,1.2861790881,0
.0058442426\C,0,0.7671610266,0.4384057823,1.209198009\C,0,-1.126395770
9,-0.6439611984,-0.4536122154\N,0,-2.0769329955,-1.1870922886,-0.83641
49529\H,0,2.3490762617,-0.5220945014,-0.3678331575\H,0,0.7423221811,2.
2889848685,-0.3678216684\H,0,0.7425378248,0.4241820803,2.2792689011\\V
ersion=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-246.1223174\CCSD(T)/GTBa
s1=-246.1798175\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-245.41029
69\MP2/GTMP2LargeXP=-246.3806009\HF/GFHFB3=-245.4121379\HF/GFHFB4=-245
.4282363\G4MP2=-246.5339366\FreqCoord=0.0235404952,0.0132621138,0.0094
443797,2.8299856188,0.0154544844,0.010909561,1.4494397644,2.4305262344
,0.0110440179,1.4497242401,0.8284668636,2.2850530774,-2.1285795243,-1.
2169103051,-0.8572028577,-3.9248345578,-2.24327932,-1.5805951944,4.439
1107998,-0.9866156232,-0.6951039304,1.4027856247,4.3255545237,-0.69508
22189,1.4031931323,0.8015879622,4.3071940064\PG=C01 [X(C5H3N1)]\NImag=
0\\

dicyanotetrahedrane

\\0,1\C,0,0.0140770415,0.0015831338,0.0007797681\C,0
,1.5064061808,0.0005073149,0.0000787839\C,0,0.7611585872,1.2816074564,
0.0034958235\C,0,0.761113793,0.4384649962,1.2039734855\C,0,2.637394161
,-0.6643525428,-0.4667683151\C,0,-1.11804268,-0.6619511819,-0.46522568

88\N,0,-2.0612357551,-1.2123493812,-0.8517838851\N,0,3.5798319478,-1.2
156554885,-0.8538805382\H,0,0.7617472802,2.2789737182,-0.3872107281\H,
0,0.7616494436,0.409371975,2.2747412942\\Version=EM64L-G09RevA.02\Stat
e=1-A\MP2/GTBas1=-338.1293553\CCSD(T)/GTBas1=-338.1958595\MP2/GTBas2=0
.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-337.1618813\MP2/GTMP2LargeXP=-338.460
9472\HF/GFHFB3=-337.1656344\HF/GFHFB4=-337.1863537\G4MP2=-338.6695987\
FreqCoord=0.0266017532,0.0029916893,0.0014735482,2.8466951266,0.000958
6862,0.0001488799,1.4383812736,2.4218871025,0.006606149,1.4382966248,0
.8285787616,2.2751801589,4.9839526687,-1.2554443616,-0.882064283,-2.11
27944701,-1.2509064472,-0.8791491418,-3.8951710724,-2.2910083079,-1.60
96382673,6.7649019831,-2.2972559452,-1.6136003673,1.439493742,4.306636
1914,-0.7317222319,1.4393088576,0.7736009193,4.2986380693\PG=C01 [X(C6
H2N2)]\NImag=0\\

tricyanotetrahedrane
\\0,1\C,0,0.0149327783,0.0082211433,0.0032055517\C,0
,1.5064502337,0.0082430932,0.0029294469\C,0,0.7607147377,1.2997651664,
0.0026138229\C,0,0.7607412505,0.43899366,1.203421741\C,0,0.7611053732,
2.6095825877,-0.4737020889\C,0,2.6408329731,-0.647373891,-0.4722468029
\C,0,-1.1194063209,-0.6477039611,-0.4717591111\N,0,-2.0626459045,-1.19
15789468,-0.8656881335\N,0,3.583327032,-1.1922833907,-0.8665387506\N,0
,0.7620693501,3.6979115454,-0.86895853\H,0,0.7622784966,0.4401229935,2
.2757228545\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-430.130972
5\CCSD(T)/GTBas1=-430.2062654\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Larg
eXP=-428.9065788\MP2/GTMP2LargeXP=-430.5363008\HF/GFHFB3=-428.9121731\
HF/GFHFB4=-428.9375259\G4MP2=-430.800207\FreqCoord=0.0282188614,0.0155
357094,0.0060576148,2.8467783746,0.0155771887,0.0055358523,1.437542519
6,2.4562002016,0.0049394095,1.4375926214,0.8295777914,2.2741375128,1.4
382807137,4.9313964118,-0.8951672165,4.9904510819,-1.2233593595,-0.892
4171246,-2.1153713779,-1.2239831018,-0.8914955206,-3.8978358686,-2.251
7578751,-1.6359134888,6.7715067351,-2.2530890812,-1.6375209222,1.44010
2366,6.9880400845,-1.6420936426,1.4404975956,0.8317119225,4.3004929494
\PG=C01 [X(C7H1N3)]\NImag=0\\

tetracyanotetrahedrane
\\0,1\C,0,0.0157951032,0.0088163671,0.006156003\C,0,1.
5041332559,0.0080477965,0.0059464977\C,0,0.7606028639,1.2974192765,0.0
058803519\C,0,0.7602892196,0.4383177222,1.2212398616\C,0,0.7608632435,
0.4382979742,2.6162163928\C,0,0.7616177735,2.6124563341,-0.4595653505\
C,0,2.6427784313,-0.6502288715,-0.4588992406\C,0,-1.1235596852,-0.6483
58231,-0.458559965\N,0,-2.0687084559,-1.1937231305,-0.844177277\N,0,3.
5875016031,-1.1963312146,-0.8445287724\N,0,0.7623795988,3.7034231107,-
0.8458624983\N,0,0.7613070481,0.4380628663,3.7735539968\\Version=EM64L
-G09RevA.02\State=1-A\MP2/GTBas1=-522.1284505\CCSD(T)/GTBas1=-522.2123
479\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-520.6459617\MP2/GTMP2
LargeXP=-522.6077454\HF/GFHFB3=-520.6532979\HF/GFHFB4=-520.6832953\G4M
P2=-522.9268356\FreqCoord=0.0298484194,0.0166605193,0.0116331598,2.842
3999211,0.0152081313,0.011237252,1.4373311087,2.4517671121,0.011112254
6,1.4367384069,0.8283004542,2.307808881,1.4378231548,0.8282631358,4.94
39324867,1.4392490098,4.9368270056,-0.8684526526,4.9941274651,-1.22875
44908,-0.8671938874,-2.123220099,-1.2252194926,-0.8665527493,-3.909292
4304,-2.2558097951,-1.5952638611,6.7793955312,-2.2607383599,-1.5959280
912,1.4406886511,6.9984554334,-1.5984484678,1.4386618239,0.8278188463,
7.1309836016\PG=C01 [X(C8N4)]\NImag=0\\

monoethynyltetrahedrane
\\0,1\C,0,0.0143708035,0.008254859,0.0059134562\C,0,1.
5011055492,0.0093488207,0.0068496536\C,0,0.7697318584,1.2888372979,0.0
069946224\C,0,0.7695681855,0.4398572349,1.2116765908\C,0,-1.1248155416
,-0.6427971955,-0.4529505359\C,0,-2.1122412703,-1.2072084529,-0.850712
0269\H,0,2.3590551547,-0.5130962312,-0.3612293865\H,0,0.7548698895,2.2
932289851,-0.3610877081\H,0,0.7545155266,0.4310871317,2.2813445678\H,0
,-2.9819601554,-1.7041124495,-1.2008992333\\Version=EM64L-G09RevA.02\S
tate=1-A\MP2/GTBas1=-230.0303455\CCSD(T)/GTBas1=-230.0943493\MP2/GTBas
2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-229.3482102\MP2/GTMP2LargeXP=-230.
2835995\HF/GFHFB3=-229.3496701\HF/GFHFB4=-229.3653098\G4MP2=-230.43254
42\FreqCoord=0.0271568829,0.0155994228,0.0111748127,2.8366783846,0.017
6667107,0.0129439694,1.4545824082,2.4355495228,0.0132179208,1.45427311
12,0.8312097114,2.2897369183,-2.1255933236,-1.2147106586,-0.8559524646
,-3.9915575275,-2.2812933612,-1.6076127488,4.4579681747,-0.9696113568,
-0.6826246117,1.4264973571,4.3335747417,-0.6823568783,1.4258277082,0.8
146366184,4.3111164478,-5.6350880329,-3.2203058293,-2.2693706642\PG=C0
1 [X(C6H4)]\NImag=0\\

diethynyltetrahedrane
\\0,1\C,0,0.7504647987,0.3138416453,0.0001157804\C,0,-
0.7503299405,0.3135939876,-0.0000107512\C,0,-0.0001654342,1.3621135795
,0.7350281452\C,0,-0.0000391675,1.3620472844,-0.7350202572\C,0,-1.8791
584379,-0.4964024343,-0.0000864172\C,0,1.8793620666,-0.4960606762,0.00
02291205\C,0,2.8544729863,-1.2032943383,0.0003357826\C,0,-2.8542499976
,-1.2036498313,-0.0001513943\H,0,-0.0003206099,1.9657701795,1.61929167
24\H,0,-0.0000397986,1.9656090586,-1.6193516229\H,0,3.7133576782,-1.82
68783015,0.0008417483\H,0,-3.7133541435,-1.8269301532,-0.0003918068\\V
ersion=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-305.9525199\CCSD(T)/GTBa
s1=-306.0315724\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-305.04468
47\MP2/GTMP2LargeXP=-306.2735976\HF/GFHFB3=-305.0476152\HF/GFHFB4=-305
.0674257\G4MP2=-306.4726499\FreqCoord=1.418172942,0.5930747588,0.00021
87932,-1.4179180969,0.5926067536,-0.0000203168,-0.0003126254,2.5740216
272,1.3890018944,-0.0000740158,2.5738963476,-1.3889869881,-3.551094808
,-0.9380646525,-0.0001633048,3.5514796105,-0.9374188234,0.000432975,5.
3941721978,-2.2738967567,0.0006345372,-5.3937508103,-2.2745685411,-0.0
002860938,-0.0006058649,3.7147672794,3.0600177902,-0.0000752084,3.7144
62805,-3.0601310801,7.0172290452,-3.452299668,0.0015906738,-7.01722236
57,-3.4523976535,-0.0007404075\PG=C01 [X(C8H4)]\NImag=0\\

triethynyltetrahedrane
\\0,1\C,0,0.0129061994,0.0061039267,0.011987499\C,0,1
.5109527981,0.0058453509,0.0107775785\C,0,0.7621364165,1.3033814892,0.
0102859053\C,0,0.7630108538,0.4395286006,1.2124777558\C,0,0.761644845,
2.6089984455,-0.4630659128\C,0,2.6415218263,-0.6474854695,-0.462183136
9\C,0,-1.1184989217,-0.6470640006,-0.4591879366\C,0,-2.0977350099,-1.2
12457926,-0.8738992347\C,0,3.6199146024,-1.2130625305,-0.8786215805\C,
0,0.7615612256,3.7389482591,-0.8799141851\H,0,0.7638317134,0.440402232
9,2.2840644512\H,0,-2.9608855053,-1.7108039104,-1.2395130887\H,0,4.482
3338378,-1.7114001944,-1.2460045786\H,0,0.7616051186,4.7351657267,-1.2
468035361\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-381.8746048\
CCSD(T)/GTBas1=-381.9682596\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeX
P=-380.7401791\MP2/GTMP2LargeXP=-382.2637322\HF/GFHFB3=-380.7444732\HF
/GFHFB4=-380.768463\G4MP2=-382.5124604\FreqCoord=0.0243891823,0.011534
7497,0.0226530901,2.8552869882,0.0110461123,0.0203666717,1.4402291031,
2.4630340612,0.019437544,1.44188155,0.8305886828,2.2912509007,1.439300
1676,4.930292543,-0.8750677566,4.9917528258,-1.2235702124,-0.873399551

9,-2.113656642,-1.2227737516,-0.8677394436,-3.964144668,-2.2912134279,
-1.6514302213,6.8406472229,-2.2923559648,-1.6603541616,1.4391421498,7.
0655882348,-1.6627968302,1.4434327499,0.8322396085,4.3162562827,-5.595
2627158,-3.2329508578,-2.3423402758,8.4703833896,-3.2340776713,-2.3546
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tetraethynyltetrahedrane

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0.4395012267,2.6131533702\C,0,0.7602500667,2.6100009906,-0.4593185853\
C,0,2.6412836131,-0.6471989611,-0.4579603455\C,0,-1.1202349358,-0.6475
798582,-0.457186896\C,0,-2.1036600476,-1.2154001699,-0.8581077032\C,0,
3.6246224888,-1.2148917604,-0.859280054\C,0,0.7600679757,3.7451029148,
-0.8615972587\C,0,0.7614983263,0.4395300123,3.8174299911\H,0,-2.970618
8569,-1.7163153617,-1.2115143647\H,0,4.4918861717,-1.7152115523,-1.212
7702008\H,0,0.7598587638,4.7458717702,-1.216411249\H,0,0.7623670904,0.
43926225,4.8792341934\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-
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1.436986911,2.4592887358,0.0082133815,1.4376480321,0.8299649692,2.3145
932035,1.4386088653,0.8305369536,4.9381442128,1.4366644186,4.932187078
7,-0.8679863339,4.991302668,-1.2230287899,-0.8654196327,-2.1169372331,
-1.2237485812,-0.8639580251,-3.9753413666,-2.296773463,-1.6215885516,6
.8495438389,-2.2958127082,-1.6238039736,1.4363203165,7.0772188485,-1.6
281828558,1.4390232873,0.8305913504,7.2138972147,-5.6136560847,-3.2433
659912,-2.2894303553,8.4884346847,-3.2412800938,-2.2918035416,1.435924
9633,8.9683979074,-2.2986841257,1.4406650136,0.8300853531,9.2204163637
\PG=C01 [X(C12H4)]\NImag=0\\

monofluorotetrahedrane

\\0,1\C,0,0.0144506768,0.0087498649,0.0060851769\C,0
,1.4748779131,-0.0052816525,-0.0035469328\C,0,0.7169329455,1.289307781
2,-0.0040441075\C,0,0.7165731751,0.4205479417,1.2188091646\F,0,-1.0550
89492,-0.6174956316,-0.4390432151\H,0,2.3797189431,-0.4693813201,-0.33
29354569\H,0,0.7550571993,2.3052151519,-0.3343789744\H,0,0.7545786391,
0.4429378646,2.2868543452\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBa
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\HF/GTMP2LargeXP=-252.5139128\MP2/GTMP2LargeXP=-253.3986829\HF/GFHFB3=
-252.5169077\HF/GFHFB4=-252.535158\G4MP2=-253.5461573\FreqCoord=0.0273
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315,1.3548069226,2.4364386074,-0.0076422556,1.354127055,0.7947204355,2
.3032155293,-1.9938301855,-1.166897632,-0.8296714371,4.4970170758,-0.8
870021469,-0.6291568335,1.4268513214,4.3562253144,-0.6318846862,1.4259
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difluorotetrahedrane

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,0,1.4759668099,-0.006418574,-0.0042963858\C,0,0.7485520772,1.28561265
44,-0.0189894936\C,0,0.7483849096,0.3972954302,1.2230306075\F,0,2.5763
650811,-0.5918779352,-0.4228709047\F,0,-1.0797979919,-0.5913311605,-0.
4229789935\H,0,0.7487105966,2.3159262308,-0.3041917829\H,0,0.748369462
2,0.4602948546,2.2902312318\\Version=EM64L-G09RevA.02\State=1-A\MP2/GT
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=0.\HF/GTMP2LargeXP=-351.3735637\MP2/GTMP2LargeXP=-352.500496\HF/GFHFB
3=-351.3796575\HF/GFHFB4=-351.4046304\G4MP2=-352.6971819\FreqCoord=0.0
392100319,-0.011719137,-0.0081905999,2.7891730519,-0.0121293471,-0.008
1189925,1.4145584221,2.4294558298,-0.0358849423,1.4142425211,0.7507795
569,2.3111929002,4.8686244217,-1.1184872017,-0.7991101995,-2.040522483
5,-1.1174539472,-0.7993144577,1.4148579804,4.3764663202,-0.5748391615,
1.4142133298,0.8698312156,4.327909809\PG=C01 [X(C4H2F2)]\NImag=0\\

trifluorotetrahedrane

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0,1.4920432187,0.0082845524,-0.0109243438\C,0,0.7533960101,1.287645978
6,-0.0112479087\C,0,0.7531410125,0.4349635797,1.2313403878\F,0,0.75314
49295,2.5447549563,-0.3938655508\F,0,2.580765313,-0.6205994444,-0.3928
725429\F,0,-1.0739012871,-0.6204293158,-0.3938178689\H,0,0.7534313043,
0.4353928249,2.3005885418\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBa
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=-450.2383746\HF/GFHFB4=-450.2700716\G4MP2=-451.8446228\FreqCoord=0.02
7740233,0.015470939,-0.0207883379,2.8195530617,0.0156555352,-0.0206440
179,1.4237121288,2.4332982557,-0.0212554669,1.423230253,0.8219620434,2
.3268961093,1.4232376552,4.8088899428,-0.7442980242,4.8769396548,-1.17
27629881,-0.7424215111,-2.0293793264,-1.1724414917,-0.7442079184,1.423
778825,0.8227731992,4.3474822885\PG=C01 [X(C4H1F3)]\NImag=0\\

monomethyltetrahedrane

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0047157878\C,0,0.7537847911,0.4347948269,1.2130829743\C,0,-1.191758376
9,-0.6872975136,-0.486458671\H,0,2.3733721716,-0.4897743792,-0.3453846
105\H,0,0.7658704458,2.2990607588,-0.3461445945\H,0,0.7650518753,0.441
4611418,2.2826055153\H,0,-1.2221317544,-1.7247133391,-0.1347020315\H,0
,-1.2192819903,-0.7061667869,-1.5818151899\H,0,-2.1049701144,-0.191087
5707,-0.1389539653\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-193
.2814406\CCSD(T)/GTBas1=-193.3450401\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GT
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026726\HF/GFHFB4=-192.7175012\G4MP2=-193.636509\FreqCoord=0.0286153429
,0.0163382095,0.0110858794,2.8217189051,0.0127806682,0.0094266924,1.42
52900897,2.4353161751,0.0089115474,1.4244468183,0.8216431468,2.2923945
978,-2.2520969489,-1.2988040726,-0.9192736632,4.4850234158,-0.92553944
37,-0.6526823243,1.4472853959,4.344595197,-0.6541184861,1.4457385218,0
.8342406563,4.3134992933,-2.3094943141,-3.2592358686,-0.2545499491,-2.
3041090404,-1.3344618314,-2.9891975018,-3.977817034,-0.3611031759,-0.2
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dimethyltetrahedrane

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0004293299\C,0,0.7553817574,0.4347405373,1.2124676749\C,0,2.7148408437
,-0.6770882232,-0.4784155581\C,0,-1.2033760097,-0.6781146846,-0.478531
6171\H,0,0.754910349,2.3012730023,-0.3458159671\H,0,0.7552630302,0.449
1202664,2.2822642587\H,0,2.7550745417,-1.7143488103,-0.1265988238\H,0,
3.6194427526,-0.1707649193,-0.122431278\H,0,2.7542966264,-0.6956081745
,-1.5735890097\H,0,-1.2429950528,-1.7154467543,-0.1268549545\H,0,-1.24
28736079,-0.6965097463,-1.5737059985\H,0,-2.1082566378,-0.1723650234,-
0.1224391974\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-232.45503
95\CCSD(T)/GTBas1=-232.5337018\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Lar
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F/GFHFB4=-231.772751\G4MP2=-232.8810498\FreqCoord=0.0299696755,0.01055
81366,0.0058136873,2.8255658697,0.0112806948,0.0059425649,1.4271345519
,2.4357736826,0.0008113159,1.4274646473,0.8215405543,2.2912318505,5.13
03056889,-1.2795113096,-0.9040743825,-2.2740510932,-1.2814510406,-0.90
42937022,1.4265738145,4.3487757314,-0.6534974702,1.4272402854,0.848714
3043,4.3128544117,5.2063363595,-3.2396497477,-0.2392371058,6.839755556
,-0.3226989306,-0.2313615854,5.2048663127,-1.3145089457,-2.973652274,-
2.3489202344,-3.2417245611,-0.2397211227,-2.3486907368,-1.3162126695,-
2.9738733508,-3.9840276632,-0.325722689,-0.231376551\PG=C01 [X(C6H8)]\
NImag=0\\

trimethyltetrahedrane
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0014367764\C,0,0.7573314049,0.4388062958,1.2121998364\C,0,0.7568472785
,2.6936774489,-0.4768754795\C,0,2.7117877972,-0.6921953938,-0.47238019
12\C,0,-1.1977154297,-0.6918123021,-0.4719909145\H,0,0.7575057106,0.44
02430811,2.2824748924\H,0,-0.1265004527,3.2355154127,-0.1191077624\H,0
,0.7548653695,2.7439977585,-1.57199321\H,0,1.6417718613,3.2350548737,-
0.1223536168\H,0,2.738267042,-1.7279124448,-0.1139494598\H,0,3.6224399
135,-0.1964962557,-0.1162169012\H,0,2.7567774977,-0.7197317813,-1.5674
026006\H,0,-1.2250498184,-1.7271045193,-0.1124042297\H,0,-1.2419691121
,-0.7206697543,-1.5670012486\H,0,-2.1084136269,-0.1952687899,-0.117044
4911\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-271.6284403\CCSD(
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34701816,-0.0027151139,1.4311489471,0.8292237245,2.2907257091,1.430234
0808,5.0903126687,-0.9011640558,5.1245362672,-1.3080597247,-0.89266919
2,-2.2633541473,-1.3073357864,-0.8919335656,1.4314783372,0.8319388552,
4.3132524517,-0.2390512113,6.1142380288,-0.2250810512,1.4264888156,5.1
854042729,-2.9706366496,3.1024991905,6.1133677361,-0.2312148271,5.1745
747881,-3.2652813023,-0.2153332721,6.8454193694,-0.3713241093,-0.21961
81152,5.20955448,-1.3600959558,-2.9619616552,-2.3150086559,-3.26375454
43,-0.2124132102,-2.3469814874,-1.3618684678,-2.9612032097,-3.98432432
97,-0.3690045352,-0.2211820336\PG=C01 [X(C7H10)]\NImag=0\\

tetramethyltetrahedrane
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058596358\C,0,0.7575503673,0.4371411497,1.2182150188\C,0,0.7585292078,
0.4365311508,2.6976978765\C,0,0.7573337231,2.6890939012,-0.4880768902\
C,0,2.7081036465,-0.6882456928,-0.4876756409\C,0,-1.1926613056,-0.6893
361129,-0.4876553786\H,0,1.6442578093,0.9436009439,3.0986454442\H,0,0.
7554624136,-0.5841241942,3.0985024431\H,0,-0.1231081586,0.9495198151,3
.1001278366\H,0,-0.1279821933,3.2369712772,-0.1438940238\H,0,0.7605307
075,2.7266205518,-1.583966543\H,0,1.6394656971,3.2387455787,-0.1386233
776\H,0,2.7432544113,-1.7269162115,-0.1379117619\H,0,3.6248662491,-0.1
950269368,-0.1431378681\H,0,2.7397510972,-0.7100497443,-1.5835430178\H
,0,-1.2262093026,-1.7286500033,-0.1396394967\H,0,-1.2252033612,-0.7094
15541,-1.5835412227\H,0,-2.1096995919,-0.1978652643,-0.1414361839\\Ver
sion=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-310.801574\CCSD(T)/GTBas1=
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MP2/GTMP2LargeXP=-311.1926876\HF/GFHFB3=-309.8565959\HF/GFHFB4=-309.88
14587\G4MP2=-311.3693095\FreqCoord=0.0284027802,0.0158059449,0.0109885
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0110731068,1.431562726,0.8260770543,2.3020927566,1.4334124665,0.824924
3235,5.0979101758,1.4311533278,5.0816510188,-0.9223316544,5.1175742313
,-1.3005958715,-0.9215734029,-2.2538032368,-1.302656467,-0.9215351129,
3.1071969515,1.7831473627,5.8555912724,1.4276170654,-1.1038347547,5.85
53210395,-0.2326407045,1.7943324082,5.8583925881,-0.2418512952,6.11698
9214,-0.2719202972,1.4371947528,5.1525661111,-2.9932629699,3.098141171
8,6.1203421578,-0.2619602193,5.1839995503,-3.2633986941,-0.2606154604,
6.8500044792,-0.3685474991,-0.2704913699,5.177379246,-1.3417995574,-2.
9924626232,-2.3171997635,-3.2666750859,-0.2638804061,-2.3152988097,-1.
3406010868,-2.9924592311,-3.9867544513,-0.3739111607,-0.2672756529\PG=
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mono-t-butyltetrahedrane
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.0040317494\C,0,0.7523206459,0.4348956703,1.2132021369\C,0,-1.20556115
88,-0.6954031937,-0.4918348192\C,0,-1.2025318632,-2.1474454833,0.02619
63542\C,0,-1.2000499009,-0.6943701471,-2.0336542743\C,0,-2.4607198153,
0.0366783775,0.0235105554\H,0,2.3754598517,-0.4877836035,-0.3411659973
\H,0,0.769863324,2.2983799841,-0.3454489227\H,0,0.7669589322,0.4449411
838,2.2825419871\H,0,-2.0905631786,-2.6836364694,-0.325480452\H,0,-1.2
014737087,-2.1721752635,1.1203781582\H,0,-0.3177555691,-2.6866094268,-
0.3264112801\H,0,-2.0873792475,-1.2056182089,-2.4223403259\H,0,-0.3145
881561,-1.2070876207,-2.4222093638\H,0,-1.1982642144,0.3280735192,-2.4
241874628\H,0,-3.3697001995,-0.4623467681,-0.3293752801\H,0,-2.4823262
292,1.0724010813,-0.3295569912\H,0,-2.483539044,0.0505340928,1.1177006
97\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-310.7883293\CCSD(T)
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-309.8674561\G4MP2=-311.3653407\FreqCoord=0.0240478508,0.0131392755,0.
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59013,0.0076189022,1.4216799849,0.8218337132,2.2926197825,-2.278180426
5,-1.3141215881,-0.929433111,-2.2724558875,-4.0580838487,0.0495039351,
-2.2677656585,-1.3121694128,-3.8430496273,-4.6500865406,0.0693120886,0
.0444285109,4.4889685594,-0.9217774228,-0.6447103008,1.4548308421,4.34
33087193,-0.6528038568,1.449342337,0.8408169827,4.3133792424,-3.950591
8711,-5.0713379674,-0.6150689158,-2.2704562653,-4.1048163606,2.1172078
843,-0.6004710027,-5.0769560427,-0.616827926,-3.9445751132,-2.27828823
56,-4.5775598166,-0.5944854596,-2.2810650215,-4.5773123342,-2.26439120
01,0.6199691028,-4.5810503996,-6.367810527,-0.87370877,-0.6224290743,-
4.6909167457,2.0265443482,-0.6227724586,-4.6932086335,0.0954955958,2.1
121482159\PG=C01 [X(C8H12)]\NImag=0\\

di-t-butyltetrahedrane
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,0,1.4967259737,-0.1350157531,-0.0954682821\C,0,0.7561318603,1.1519861
888,-0.0890511186\C,0,0.7559949205,0.2982658346,1.1163429582\C,0,2.769
4177047,-0.7728930907,-0.5471565511\C,0,-1.2581559755,-0.7719112786,-0
.5469209443\C,0,-1.3258720624,-2.2232410317,-0.0309307785\C,0,-1.32565
96639,-0.7665904182,-2.0872465466\C,0,-2.4469332586,0.0303492952,0.021
2599803\C,0,2.8365150879,-2.2242362163,-0.0311229696\C,0,3.9586357759,
0.0288331189,0.0208535027\C,0,2.8367332695,-0.7676553547,-2.0874909907
\H,0,0.7562829093,2.1622345249,-0.4415465658\H,0,0.756021873,0.3010238
617,2.1863186979\H,0,-2.2655996233,-2.6965206421,-0.3358460953\H,0,-1.
2683458199,-2.2533149621,1.061549116\H,0,-0.5012052028,-2.8215884314,-
0.4304696131\H,0,-2.2653744038,-1.2111708349,-2.4327019287\H,0,-0.5009
796954,-1.3420625336,-2.5190574369\H,0,-1.2679997933,0.2540434788,-2.4

780231881\H,0,-3.3969812591,-0.4145915173,-0.2940570329\H,0,-2.4234366
13,1.0666102267,-0.3300500185\H,0,-2.423614648,0.042652663,1.115386229
7\H,0,3.7759745478,-2.6979742317,-0.3361522305\H,0,2.0115077315,-2.822
2056168,-0.4305241766\H,0,2.7791268471,-2.2542433505,1.0613663489\H,0,
4.9084374275,-0.4165701043,-0.2945531328\H,0,3.935447334,0.0411939926,
1.1149816582\H,0,3.9355865103,1.0650894891,-0.3304991052\H,0,3.7762007
233,-1.2126796746,-2.4330478636\H,0,2.7794938836,0.2529920425,-2.47829
49165\H,0,2.0117356443,-1.3427636486,-2.5191800077\\Version=EM64L-G09R
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P=-468.0817246\HF/GFHFB3=-466.0325923\HF/GFHFB4=-466.0709498\G4MP2=-46
8.3400476\FreqCoord=0.0281342329,-0.2544441127,-0.1802175086,2.8284021
862,-0.2551427971,-0.1804089076,1.4288821363,2.1769384056,-0.168282226
,1.4286233577,0.5636407421,2.1095824614,5.2334410094,-1.4605562713,-1.
0339760333,-2.3775702261,-1.4587009153,-1.0335308011,-2.5055350852,-4.
2013166774,-0.0584507005,-2.5051337101,-1.4486459465,-3.9443243448,-4.
6240337242,0.0573518562,0.0401755404,5.3602366879,-4.2031973036,-0.058
813889,7.4807374764,0.0544866982,0.0394074091,5.3606489913,-1.45065838
49,-3.9447862773,1.4291675775,4.0860310872,-0.8344020843,1.4286742904,
0.568852658,4.1315435783,-4.2813628147,-5.0956855253,-0.634657143,-2.3
968262414,-4.2581481695,2.0060371058,-0.9471405697,-5.332029395,-0.813
4696774,-4.2809372117,-2.2887811782,-4.5971404082,-0.9467144224,-2.536
1306418,-4.7603286687,-2.3961723459,0.4800726008,-4.6827851765,-6.4193
642583,-0.7834644247,-0.5556872596,-4.5796314989,2.015601219,-0.623704
1451,-4.5799679364,0.0806018519,2.1077745065,7.1355577801,-5.098432411
5,-0.6352356547,3.8011987268,-5.3331957064,-0.8135727873,5.2517886296,
-4.2599025694,2.0056917262,9.2756024784,-0.7872034123,-0.5566247526,7.
4369176716,0.0778453643,2.1070099772,7.4371806767,2.0127274414,-0.6245
527961,7.1359851898,-2.2916324719,-4.5977941305,5.252482228,0.47808567
42,-4.6832986686,3.8016294194,-2.537455557,-4.760560294\PG=C01 [X(C12H
20)]\NImag=0\\

mono(trimethylsilyl)tetrahedrane
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,0,1.4261596456,-0.1585482012,0.5017057375\C,0,1.0954836905,1.01290974
23,-0.315020023\C,0,0.5960235955,0.9131738201,1.0595794406\Si,0,-1.481
9566361,-0.8334988945,-0.6029975886\C,0,-2.1102770075,-2.0131532261,0.
7261841712\C,0,-1.0628854283,-1.8036989695,-2.1637120784\C,0,-2.807287
2027,0.4493061537,-0.9907062304\H,0,2.1665168749,-0.9004095655,0.71669
75014\H,0,1.4390350423,1.6771434064,-1.0801963928\H,0,0.3399300363,1.4
577194644,1.9442210982\H,0,-3.0115741929,-2.53896058,0.3917565661\H,0,
-2.3615278893,-1.4785229952,1.6480707278\H,0,-1.3590865429,-2.76964379
71,0.9757350764\H,0,-1.9457543967,-2.3222553663,-2.5540784143\H,0,-0.2
942917559,-2.5589091824,-1.9694820925\H,0,-0.6887461637,-1.1454728496,
-2.9546493614\H,0,-3.7234512868,-0.0288807068,-1.3547279879\H,0,-2.470
5911213,1.1499591437,-1.7617709795\H,0,-3.0689584664,1.0338178268,-0.1
02603372\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-561.8246016\C
CSD(T)/GTBas1=-561.9365703\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP
=-560.9605669\MP2/GTMP2LargeXP=-562.2532294\HF/GFHFB3=-560.9619826\HF/
GFHFB4=-560.9879983\G4MP2=-562.4477874\FreqCoord=0.0459944322,0.031605
2478,0.0096266456,2.695051152,-0.2996126792,0.9480864432,2.0701641581,
1.9141220104,-0.5953015698,1.1263213643,1.7256484317,2.0023149588,-2.8
00492183,-1.5750846426,-1.1395003013,-3.9878456086,-3.8043082608,1.372
2892057,-2.00856237,-3.4084970786,-4.0888232585,-5.3050039895,0.849065
5803,-1.8721634535,4.0941235558,-1.7015274862,1.3543619978,2.719382125
6,3.1693417236,-2.0412753521,0.6423746729,2.7546905663,3.6740454174,-5
.6910504534,-4.7979401585,0.7403126207,-4.4626409659,-2.7940035422,3.1

144023232,-2.568301357,-5.2338682621,1.8438720727,-3.6769429316,-4.388
4266529,-4.826508725,-0.5561308217,-4.8356375536,-3.7217817785,-1.3015
416245,-2.1646299784,-5.5834781118,-7.0363032013,-0.0545766264,-2.5600
648818,-4.6687406056,2.1731078456,-3.3292646601,-5.7994910146,1.953632
5639,-0.1938922733\PG=C01 [X(C7H12Si1)]\NImag=0\\

di(trimethylsilyl)tetrahedrane
\\0,1\C,0,0.0200074034,0.167352123,-0.3101643865\
C,0,1.5325552047,0.1037760271,-0.1943131286\C,0,0.8547767565,1.3626578
993,-0.6041715899\C,0,0.7304303724,0.9043937046,0.7688436912\Si,0,3.02
09816005,-0.9491983189,-0.4108644263\Si,0,-1.5008882422,-0.7592937255,
-0.7565477928\C,0,-1.6629266057,-2.272644703,0.3552079466\C,0,-1.39967
93912,-1.3009695742,-2.5590115247\C,0,-2.9958075157,0.3641696433,-0.51
70383618\C,0,2.8853245924,-2.4644294874,0.7018709382\C,0,4.5505054182,
0.0468568435,0.0611144459\C,0,3.1501975305,-1.4907958374,-2.2115463446
\H,0,0.9400946791,2.2111019616,-1.2517308708\H,0,0.6637323414,1.193354
7902,1.7976876383\H,0,-2.5711557865,-2.8385460183,0.1194522852\H,0,-1.
7149428245,-1.9877415052,1.4110851519\H,0,-0.8110189411,-2.9501590972,
0.2362647166\H,0,-2.3018549202,-1.846818133,-2.8570643928\H,0,-0.54240
91954,-1.95990127,-2.7317104106\H,0,-1.296701753,-0.4407496231,-3.2284
652419\H,0,-3.924696158,-0.1565238696,-0.7754033113\H,0,-2.9296613055,
1.2565126028,-1.1480236083\H,0,-3.0814331788,0.6985744169,0.5220195513
\H,0,3.7682584232,-3.1057411732,0.6026056764\H,0,2.0076872381,-3.06890
36117,0.4503046853\H,0,2.8001751111,-2.1788343085,1.755406295\H,0,5.46
11472707,-0.551196644,-0.0562519702\H,0,4.504444585,0.3792337953,1.103
3234573\H,0,4.6560269625,0.9377572792,-0.5665446739\H,0,4.0384722842,-
2.1118074099,-2.3728411677\H,0,3.2223630434,-0.6288236834,-2.882774675
1\H,0,2.2771950004,-2.0767630935,-2.5172186015\\Version=EM64L-G09RevA.
02\State=1-A\MP2/GTBas1=-969.5427118\CCSD(T)/GTBas1=-969.7182454\MP2/G
TBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-968.2697087\MP2/GTMP2LargeXP=-
970.214515\HF/GFHFB3=-968.2726722\HF/GFHFB4=-968.3131485\G4MP2=-970.50
5795\FreqCoord=0.0378085131,0.3162496802,-0.5861257467,2.8961096205,0.
1961082705,-0.3671985971,1.6152939745,2.5750502424,-1.1417188421,1.380
3133629,1.7090564181,1.4529040153,5.7088278775,-1.7937248685,-0.776421
2435,-2.8362677338,-1.4348571956,-1.4296681348,-3.1424758638,-4.294676
086,0.6712457393,-2.6450107232,-2.4584762025,-4.8358309526,-5.66125575
15,0.6881808918,-0.977060904,5.4524732841,-4.657096805,1.3263438538,8.
5992090066,0.0885466016,0.1154895656,5.9530105971,-2.8171958526,-4.179
2169215,1.7765214825,4.1783771594,-2.365428538,1.2542723508,2.25511373
28,3.3971373089,-4.8587802814,-5.3640745902,0.225732105,-3.2407722718,
-3.7562870678,2.6665644873,-1.5326036872,-5.5749927422,0.4464756093,-4
.3498753967,-3.4899804886,-5.3990692465,-1.0250048313,-3.7036766479,-5
.1621845503,-2.4504111892,-0.8328960808,-6.1009151368,-7.4166008934,-0
.2957872468,-1.465299901,-5.5362575295,2.3744647018,-2.1694502137,-5.8
230648048,1.3201143315,0.986473988,7.1209764178,-5.8690002569,1.138759
6946,3.7939790404,-5.7993873544,0.8509525316,5.2915640841,-4.117400132
1,3.3172371495,10.320072713,-1.0416107025,-0.106300818,8.5121666464,0.
7166480135,2.0849791703,8.7986158264,1.7721044369,-1.0706142757,7.6316
066124,-3.99073765,-4.4840199638,6.0893836527,-1.1883045474,-5.4476546
388,4.303274902,-3.9245134897,-4.7568537734\PG=C01 [X(C10H20Si2)]\NIma
g=0\\

mono(trifluoromethyl)tetrahedrane
\\0,1\C,0,-0.58989,0.00003,-0.00026\C,0,-1.79241,-0.
85276,0.00182\C,0,-1.79256,0.42783,0.73754\C,0,-1.79267,0.4248,-0.7393
4\C,0,0.87426,0.0001,-0.00004\F,0,1.36833,-0.62071,1.08415\F,0,1.36851
,1.24942,-0.00454\F,0,1.36872,-0.6287,-1.07943\H,0,-2.12979,-1.86769,0

.00402\H,0,-2.13004,0.93734,1.61529\H,0,-2.13059,0.93026,-1.61926\\Ver
sion=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-490.3659261\CCSD(T)/GTBas1
=-490.4304307\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-489.3952415
\MP2/GTMP2LargeXP=-490.9361325\HF/GFHFB3=-489.4036525\HF/GFHFB4=-489.4
390338\G4MP2=-491.1964901\FreqCoord=-1.1147305485,0.0000566918,-0.0004
913288,-3.3871640178,-1.6114828571,0.0034393016,-3.3874474768,0.808481
5314,1.393748612,-3.3876553466,0.8027556612,-1.3971501191,1.6521119689
,0.0001889726,-0.000075589,2.5857689594,-1.1729719079,2.048746587,2.58
61091101,2.3610616249,-0.0085793566,2.5865059526,-1.1880708197,-2.0398
270796,-4.0247198206,-3.5294226011,0.0075966991,-4.0251922521,1.771315
8934,3.0524557252,-4.0262316015,1.7579366324,-3.0599579379\PG=C01 [X(C
5H3F3)]\NImag=0\\

di(trifluoromethyl)tetrahedrane

\\0,1\C,0,0.0202170531,-0.0235599148,-0.0080008245\C
,0,1.4908634898,-0.0143609863,-0.0207617293\C,0,0.7477820637,1.2603196
82,-0.0158926692\C,0,0.7630527149,0.4105561915,1.1906405133\C,0,2.6917
37747,-0.702129067,-0.5187935407\C,0,-1.1804681046,-0.7244285736,-0.48
7893086\F,0,-1.2284376355,-0.7477004442,-1.8266490299\F,0,-2.296100482
9,-0.1215225169,-0.0511384805\F,0,-1.2088827233,-1.99293355,-0.0575495
079\F,0,2.7399297827,-1.9703983001,-0.0895150104\F,0,3.8072051773,-0.0
875042669,-0.0982448703\F,0,2.7202871902,-0.7244637435,-1.8581165448\H
,0,0.737855758,2.2615438992,-0.3931006631\H,0,0.7728579698,0.392681590
5,2.2604154434\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-826.619
4931\CCSD(T)/GTBas1=-826.7002364\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2L
argeXP=-825.1358383\MP2/GTMP2LargeXP=-827.5750234\HF/GFHFB3=-825.15244
92\HF/GFHFB4=-825.2117779\G4MP2=-827.9977457\FreqCoord=0.0382046935,-0
.0445217866,-0.0151193672,2.8173236972,-0.0271383312,-0.0392339824,1.4
131033075,2.3816590388,-0.0300327922,1.441960656,0.7758387641,2.249984
4928,5.0866471634,-1.3268316466,-0.9803777115,-2.2307614262,-1.3689716
069,-0.9219843148,-2.3214107025,-1.412949069,-3.4518664075,-4.33900108
63,-0.2296442759,-0.096637723,-2.2844572739,-3.7660986105,-0.108752809
,5.1777169126,-3.7235131599,-0.1691588545,7.1945751168,-0.1653590999,-
0.1856558988,5.1405977924,-1.3690380685,-3.5113313926,1.3943453082,4.2
736986071,-0.7428525959,1.4604899025,0.7420606634,4.2715661346\PG=C01
[X(C6H2F6)]\NImag=0\\

tri(trifluoromethyl)tetrahedrane

\\0,1\C,0,0.0198524875,0.0057165451,-0.0339843702\C,
0,1.4931364186,0.0138134851,-0.0307659036\C,0,0.7493971578,1.285701913
5,-0.0285400445\C,0,0.7515835632,0.431365607,1.1747785971\C,0,0.742923
5745,2.6792910501,-0.5157721794\C,0,2.7026857691,-0.6745612942,-0.5232
377728\C,0,-1.1795507894,-0.6967526007,-0.5312931647\F,0,-1.2078158877
,-0.7142977472,-1.867715677\F,0,-2.2950045983,-0.0953746956,-0.1019092
367\F,0,-1.2012897511,-1.963378662,-0.1004657447\F,0,2.736546469,-1.94
14822952,-0.0943632121\F,0,3.8091793901,-0.0614111223,-0.0873638108\F,
0,2.7375889031,-0.6896142589,-1.8595964335\F,0,0.7497459211,2.72282427
64,-1.8519754292\F,0,1.8187305242,3.341632045,-0.075020704\F,0,-0.3457
568497,3.3278500513,-0.0864388449\H,0,0.749547698,0.4285777027,2.24516
39309\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-1162.8696799\CCS
D(T)/GTBas1=-1162.9667867\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=
-1160.8728933\MP2/GTMP2LargeXP=-1164.2110709\HF/GFHFB3=-1160.8973389\H
F/GFHFB4=-1160.9806558\G4MP2=-1164.796176\FreqCoord=0.0375157645,0.010
8027048,-0.0642211524,2.8216189101,0.0261037038,-0.058139132,1.4161553
931,2.429624505,-0.0539328678,1.4202871004,0.8151628604,2.2200098153,1
.4039220935,5.0631263149,-0.9746681661,5.1073359269,-1.2747361059,-0.9
887760929,-2.2290279518,-1.3166715978,-1.0039985775,-2.2824412468,-1.3

498271195,-3.5294711236,-4.3369301645,-0.1802320546,-0.1925805478,-2.2
701086359,-3.7102479664,-0.1898527433,5.1713233762,-3.6688698298,-0.17
8320628,7.1983058383,-0.1160502027,-0.1650936764,5.1732932913,-1.30318
20867,-3.5141279769,1.4168144602,5.1453921904,-3.499726366,3.436902600
3,6.3147694019,-0.1417685849,-0.6533857545,6.2887252082,-0.1633457442,
1.4164398727,0.8098944847,4.2427449528\PG=C01 [X(C7H1F9)]\NImag=0\\

1,3-cyclobutadiene
\\0,1\C,0,-4.7643548182,2.7839695499,0.\C,0,-4.7107481
777,1.4532659396,0.\C,0,-3.1867271613,2.8475341974,0.\C,0,-3.133123008
,1.5168261778,0.\H,0,-5.5525843738,3.5240738214,0.\H,0,-5.4368846974,0
.6521541999,0.\H,0,-2.4605921243,3.6486466137,0.\H,0,-2.3448956393,0.7
767195003,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-154.1452
147\CCSD(T)/GTBas1=-154.2051961\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2La
rgeXP=-153.6934742\MP2/GTMP2LargeXP=-154.3233988\HF/GFHFB3=-153.694688
1\HF/GFHFB4=-153.7059809\G4MP2=-154.4332877\FreqCoord=-9.0033258062,5.
2609400117,0.,-8.9020239369,2.746274624,0.,-6.0220415952,5.381059787,0
.,-5.9207444257,2.8663860673,0.,-10.4928637963,6.6595343945,0.,-10.274
2230942,1.2323928343,0.,-4.6498452397,6.8949428555,0.,-4.4312105684,1.
4677871376,0.\PG=CS [SG(C4H4)]\NImag=0\\

monobromo-1,3-cyclobutadiene
\\0,1\C,0,-3.6237056585,2.4627523366,0.\C,0,-3.5554
820769,1.13536368,0.\C,0,-2.0465133925,2.4948844278,0.\C,0,-1.97595997
72,1.166510431,0.\Br,0,-0.8061067856,3.8895447475,0.\H,0,-1.1926158571
,0.425022807,0.\H,0,-4.3911510711,3.2207366087,0.\H,0,-4.274905181,0.3
283149613,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-2725.937
0982\CCSD(T)/GTBas1=-2725.9935122\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2
LargeXP=-2725.5132049\MP2/GTMP2LargeXP=-2726.5298289\HF/GFHFB3=-2725.5
76093\HF/GFHFB4=-2725.5895939\G4MP2=-2726.7381835\FreqCoord=-6.8478112
807,4.6539274494,0.,-6.7188873958,2.1455264165,0.,-3.8673498392,4.7146
483017,0.,-3.7340232065,2.2043852458,0.,-1.5233210587,7.3501743544,0.,
-2.2537173517,0.8031767055,0.,-8.2980729326,6.0863101366,0.,-8.0784000
361,0.6204253621,0.\PG=CS [SG(C4H3Br1)]\NImag=0\\

cis-dibromo-1,3-cyclobutadiene
\\0,1\C,0,-3.4460169932,2.318072477,0.\C,0,-3.40080
53136,0.9899704589,0.\C,0,-1.8637600782,2.36907779,0.\C,0,-1.823333528
9,1.0408180018,0.\Br,0,-0.6448618462,3.7667236427,0.\H,0,-1.0519616294
,0.2864775368,0.\Br,0,-4.7526328577,3.63402356,0.\H,0,-4.1220377527,0.
1875465328,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-5297.72
67236\CCSD(T)/GTBas1=-5297.7795552\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP
2LargeXP=-5297.3299756\MP2/GTMP2LargeXP=-5298.7349474\HF/GFHFB3=-5297.
4544407\HF/GFHFB4=-5297.4701994\G4MP2=-5299.0417588\FreqCoord=-6.51202
83665,4.3805221377,0.,-6.426590674,1.8707730469,0.,-3.5219961252,4.476
9082105,0.,-3.4456010186,1.9668609776,0.,-1.218612283,7.118076103,0.,-
1.9879193818,0.5413640878,0.,-8.9811745112,6.8673092889,0.,-7.78952246
19,0.3544115842,0.\PG=CS [SG(C4H2Br2)]\NImag=0\\

trans-dibromo-1,3-cyclobutadiene
\\0,1\C,0,-3.434563629,2.5449983657,0.\C,0,-3.33410
38901,1.2199924901,0.\C,0,-1.85785474,2.5708559414,0.\C,0,-1.757391704
4,1.2458478027,0.\Br,0,-0.6499281552,3.9887506021,0.\H,0,-0.9830109874
,0.4977486189,0.\H,0,-4.2089451451,3.2930972398,0.\Br,0,-4.5420317488,
-0.1979010607,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-5297
.7273132\CCSD(T)/GTBas1=-5297.7798947\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/G
TMP2LargeXP=-5297.3314021\MP2/GTMP2LargeXP=-5298.7353879\HF/GFHFB3=-52

97.4559354\HF/GFHFB4=-5297.4716634\G4MP2=-5299.0421864\FreqCoord=-6.49
03846447,4.8093499198,0.,-6.3005432509,2.3054516905,0.,-3.5108366533,4
.8582136564,0.,-3.3209890295,2.3543111504,0.,-1.2281862194,7.537646250
3,0.,-1.8576215518,0.9406085727,0.,-7.9537536326,6.2230519121,0.,-8.58
31960921,-0.373978806,0.\PG=CS [SG(C4H2Br2)]\NImag=0\\

tribromo-1,3-cyclobutadiene

\\0,1\C,0,-3.5803268031,2.6475525929,0.\C,0,-3.5029
563554,1.322531084,0.\C,0,-2.0044657794,2.7014792523,0.\C,0,-1.9204501
378,1.3721365312,0.\Br,0,-0.8043692531,4.1132729818,0.\Br,0,-0.6005502
524,0.0830360181,0.\H,0,-4.3481132624,3.4032068105,0.\Br,0,-4.68763815
64,-0.1022452709,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-7
869.5160921\CCSD(T)/GTBas1=-7869.5647086\MP2/GTBas2=0.\MP2/GTBas3=0.\H
F/GTMP2LargeXP=-7869.1462895\MP2/GTMP2LargeXP=-7870.9403556\HF/GFHFB3=
-7869.3323032\HF/GFHFB4=-7869.3503178\G4MP2=-7871.3452282\FreqCoord=-6
.765837124,5.0031493231,0.,-6.6196281671,2.499221551,0.,-3.7878913658,
5.1050559405,0.,-3.6291248124,2.5929622609,0.,-1.520037598,7.772959445
4,0.,-1.1348755061,0.1569153333,0.,-8.2167432607,6.4311288454,0.,-8.85
83523256,-0.1932155603,0.\PG=CS [SG(C4H1Br3)]\NImag=0\\

tetrabromo-1,3-cyclobutadiene

\\0,1\C,0,-3.4218541328,2.5248577371,0.\C,0,-3.357353
0132,1.1958283035,0.\C,0,-1.8414830126,2.6015627343,0.\C,0,-1.77696652
68,1.2725321823,0.\Br,0,-0.6632668114,4.0211881233,0.\Br,0,-0.46587052
25,-0.025292956,0.\Br,0,-4.7329465114,3.8226906514,0.\Br,0,-4.53557946
92,-0.2237867759,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-1
0441.3045812\CCSD(T)/GTBas1=-10441.3488263\MP2/GTBas2=0.\MP2/GTBas3=0.
\HF/GTMP2LargeXP=-10440.9606182\MP2/GTMP2LargeXP=-10443.1453386\HF/GFH
FB3=-10441.2080953\HF/GFHFB4=-10441.2283932\G4MP2=-10443.6480049\FreqC
oord=-6.4663671778,4.7712896476,0.,-6.3444777263,2.2597879956,0.,-3.47
98985722,4.9162410853,0.,-3.3579800829,2.4047373199,0.,-1.2533926267,7
.5989442818,0.,-0.8803677009,-0.0477967599,0.,-8.9439727082,7.22383842
19,0.,-8.5710030507,-0.4228957186,0.\PG=CS [SG(C4Br4)]\NImag=0\\

monochloro-1,3-cyclobutadiene

\\0,1\C,0,-3.3595680989,2.4448085529,0.\C,0,-3.3089
183181,1.1150544701,0.\C,0,-1.787216066,2.5591844762,0.\C,0,-1.7333879
724,1.2307769705,0.\H,0,-1.0908750341,3.383051244,0.\H,0,-0.9421217625
,0.4945313415,0.\Cl,0,-4.6032096262,3.6198781729,0.\H,0,-4.0218231217,
0.3059047719,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-613.1
812047\CCSD(T)/GTBas1=-613.2507824\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP
2LargeXP=-612.6267767\MP2/GTMP2LargeXP=-613.4474781\HF/GFHFB3=-612.635
216\HF/GFHFB4=-612.6492104\G4MP2=-613.6146529\FreqCoord=-6.3486636317,
4.6200186123,0.,-6.2529494174,2.1071475717,0.,-3.377348905,4.836157783
6,0.,-3.27562855,2.325831405,0.,-2.0614550596,6.3930403446,0.,-1.78035
21149,0.9345287996,0.,-8.6988055258,6.8405783811,0.,-7.600144255,0.578
0762417,0.\PG=CS [SG(C4H3Cl1)]\NImag=0\\

cis-dichloro-1,3-cyclobutadiene

\\0,1\C,0,-3.4917416549,2.3320290261,0.\C,0,-3.4186
712075,1.0048815269,0.\C,0,-1.9135544128,2.4187490466,0.\C,0,-1.840714
0199,1.0915945909,0.\Cl,0,-0.8327615051,3.7313871951,0.\H,0,-1.0515562
03,0.3565111053,0.\Cl,0,-4.709892201,3.5182415224,0.\H,0,-4.1224987957
,0.1877159866,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-1072
.2147314\CCSD(T)/GTBas1=-1072.2940051\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/G
TMP2LargeXP=-1071.5568108\MP2/GTMP2LargeXP=-1072.5693844\HF/GFHFB3=-10
71.5724296\HF/GFHFB4=-1071.5891623\G4MP2=-1072.7939246\FreqCoord=-6.59

84354546,4.4068961934,0.,-6.4603523205,1.8989508819,0.,-3.6160937806,4
.5707732822,0.,-3.4784453867,2.0628148249,0.,-1.5736911787,7.051299894
5,0.,-1.9871532369,0.6737083524,0.,-8.9004063754,6.6485129468,0.,-7.79
03937071,0.3547318054,0.\PG=CS [SG(C4H2Cl2)]\NImag=0\\

trans-dichloro-1,3-cyclobutadiene
\\0,1\C,0,-3.4835291214,2.4996886313,0.\C,0,-3.4624
188049,1.1699997738,0.\C,0,-1.912861401,2.6223352309,0.\C,0,-1.8917503
389,1.2926456804,0.\H,0,-1.2097247497,3.4374681184,0.\Cl,0,-0.67677497
77,0.0956153921,0.\Cl,0,-4.6985045798,3.6967195572,0.\H,0,-4.165556026
6,0.3548676158,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-107
2.2153813\CCSD(T)/GTBas1=-1072.2943281\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/
GTMP2LargeXP=-1071.5586372\MP2/GTMP2LargeXP=-1072.5702911\HF/GFHFB3=-1
071.5742612\HF/GFHFB4=-1071.5909811\G4MP2=-1072.7947208\FreqCoord=-6.5
829160153,4.7237269306,0.,-6.5430232985,2.2109791481,0.,-3.6147841781,
4.9554954149,0.,-3.5748900523,2.4427463229,0.,-2.2860484732,6.49587333
43,0.,-1.2789193614,0.1806869052,0.,-8.87888689,6.9857875532,0.,-7.871
7600815,0.6706026074,0.\PG=CS [SG(C4H2Cl2)]\NImag=0\\

trichloro-1,3-cyclobutadiene
\\0,1\C,0,-3.3909754772,2.6603047781,0.\C,0,-3.3495
67556,1.328582684,0.\C,0,-1.8156627991,2.7547314909,0.\C,0,-1.77125782
72,1.4275929171,0.\H,0,-1.119326877,3.5761849977,0.\Cl,0,-0.5768406877
,0.2222602604,0.\Cl,0,-4.6024521334,3.8491722918,0.\Cl,0,-4.4389366423
,0.03356058,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-1531.2
470459\CCSD(T)/GTBas1=-1531.3356237\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTM
P2LargeXP=-1530.4860224\MP2/GTMP2LargeXP=-1531.6904831\HF/GFHFB3=-1530
.5088091\HF/GFHFB4=-1530.5282748\G4MP2=-1531.9721341\FreqCoord=-6.4080
149752,5.0272474606,0.,-6.3297653444,2.5106574176,0.,-3.43110544,5.205
6880874,0.,-3.3471922042,2.6977596426,0.,-2.1152212507,6.7580102462,0.
,-1.0900709221,0.4200110224,0.,-8.6973740719,7.2738814697,0.,-8.388374
5752,0.0634203051,0.\PG=CS [SG(C4H1Cl3)]\NImag=0\\

tetrachloro-1,3-cyclobutadiene
\\0,1\C,0,-3.5101437233,2.5416148199,0.\C,0,-3.453579
6292,1.21190543,0.\C,0,-1.9288182934,2.6089060861,0.\C,0,-1.8722414516
,1.2791959454,0.\Cl,0,-0.8477477913,3.9084253453,0.\Cl,0,-0.6848335509
,0.0760996605,0.\Cl,0,-4.6975478446,3.7447179698,0.\Cl,0,-4.5346577158
,-0.087605257,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-1990
.2780925\CCSD(T)/GTBas1=-1990.3759777\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/G
TMP2LargeXP=-1989.4127906\MP2/GTMP2LargeXP=-1990.8102367\HF/GFHFB3=-19
89.4427272\HF/GFHFB4=-1989.4649486\G4MP2=-1991.1489677\FreqCoord=-6.63
32103241,4.802955945,0.,-6.5263196773,2.2901693616,0.,-3.6449383346,4.
9301180091,0.,-3.5380235981,2.4173300072,0.,-1.6020111553,7.3858535134
,0.,-1.2941478577,0.1438075171,0.,-8.8770789223,7.0764914079,0.,-8.569
2611893,-0.1655499435,0.\PG=CS [SG(C4Cl4)]\NImag=0\\

monocyano-1,3-cyclobutadiene
\\0,1\C,0,-4.1391762194,1.7895086412,-1.5940434281\C
,0,-3.1763568962,2.6846673946,-1.8626473025\C,0,-3.0291707049,0.823761
4704,-0.9913363634\C,0,-2.0973282312,1.733736447,-1.2712226514\C,0,-5.
5262932908,1.7187808385,-1.7637458313\H,0,-3.1670460141,3.6686292583,-
2.3106663965\H,0,-3.0624920542,-0.1600823694,-0.5468660931\H,0,-1.0272
460421,1.8037633856,-1.1473715172\N,0,-6.6773006221,1.6204551693,-1.88
64599011\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-246.1622505\C
CSD(T)/GTBas1=-246.2317231\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP
=-245.4564059\MP2/GTMP2LargeXP=-246.4144908\HF/GFHFB3=-245.459346\HF/G

FHFB4=-245.4753363\G4MP2=-246.5797641\FreqCoord=-7.8219094705,3.381681
2443,-3.012305523,-6.0024446341,5.0732861338,-3.5198932839,-5.72430304
2,1.5566835779,-1.8733542324,-3.9633759677,3.2762870713,-2.4022626651,
-10.4431808496,3.2480250672,-3.3329965892,-5.9848496169,6.9327045812,-
4.3665266738,-5.7872712666,-0.3025118369,-1.0334271472,-1.9412136907,3
.4086188074,-2.1682179401,-12.6182694828,3.0622164805,-3.5648925737\PG
=C01 [X(C5H3N1)]\NImag=0\\

cis-dicyano-1,3-cyclobutadiene
\\0,1\C,0,-4.1601256089,1.8579612858,-1.6304973452\C
,0,-3.1771704441,2.7376103881,-1.878102222\C,0,-3.0606598017,0.8597491
191,-1.0291268177\C,0,-2.1236818348,1.7809985298,-1.3023707955\C,0,-5.
5454790358,1.7971165103,-1.8036826864\H,0,-3.143727915,3.726130138,-2.
3112112735\C,0,-3.1040104658,-0.4195297078,-0.4683564301\H,0,-1.053255
6423,1.8279072215,-1.1687241495\N,0,-6.6963929715,1.7126329107,-1.9325
067958\N,0,-3.1767962802,-1.4828763957,-0.0075614843\\Version=EM64L-G0
9RevA.02\State=1-A\MP2/GTBas1=-338.1745837\CCSD(T)/GTBas1=-338.2521705
\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-337.2111638\MP2/GTMP2Lar
geXP=-338.5009089\HF/GFHFB3=-337.2159336\HF/GFHFB4=-337.2366416\G4MP2=
-338.7205496\FreqCoord=-7.8614980793,3.5110379958,-3.0811934428,-6.003
9820168,5.1733338921,-3.5490988492,-5.7838088111,1.624690378,-1.944767
8415,-4.0131770611,3.3655994645,-2.461124127,-10.4794366533,3.39605803
34,-3.4084663079,-5.9407847956,7.0413654962,-4.3675563421,-5.865729694
,-0.7927962523,-0.8850653855,-1.990364712,3.454244045,-2.2085685675,-1
2.6543487942,3.2364071675,-3.651908594,-6.0032749496,-2.8022302767,-0.
0142891344\PG=C01 [X(C6H2N2)]\NImag=0\\

trans-dicyano-1,3-cyclobutadiene
\\0,1\C,0,-4.1622995887,1.8373091482,-1.6212053639\C
,0,-3.2214823782,2.7570944306,-1.8824167255\C,0,-3.0641804308,0.887136
3066,-1.0308178027\C,0,-2.1235308909,1.807391745,-1.2909785379\C,0,-5.
5495321868,1.7363558069,-1.7918803559\H,0,-3.2092744034,3.745572679,-2
.3179668186\C,0,-0.7363895829,1.908606863,-1.1197119261\N,0,-6.6969194
885,1.6173262221,-1.9173686711\H,0,-3.0763326758,-0.1014965089,-0.5956
171858\N,0,0.410931626,2.0278233077,-0.9937966125\\Version=EM64L-G09Re
vA.02\State=1-A\MP2/GTBas1=-338.1733055\CCSD(T)/GTBas1=-338.2530905\MP
2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-337.2139085\MP2/GTMP2LargeX
P=-338.4997091\HF/GFHFB3=-337.2186774\HF/GFHFB4=-337.2393899\G4MP2=-33
8.7217825\FreqCoord=-7.8656063057,3.4720111116,-3.063634143,-6.0877194
367,5.2101533963,-3.5572520792,-5.7904618359,1.6764446619,-1.94796334,
-4.0128918186,3.4154754129,-2.4395958801,-10.4870959987,3.2812369442,-
3.3861631355,-6.0646497077,7.0781065741,-4.3803224723,-1.3915746388,3.
6067442663,-2.115948888,-12.6553437673,3.0563036273,-3.6233016842,-5.8
134262509,-0.1918006053,-1.1255533612,0.7765482325,3.8320306973,-1.878
0034294\PG=C01 [X(C6H2N2)]\NImag=0\\

tricyano-1,3-cyclobutadiene
\\0,1\C,0,-4.1791302789,1.8923143512,-1.6500785988\C
,0,-3.216696074,2.7944997639,-1.8904056622\C,0,-3.091513943,0.90844866
68,-1.056718232\C,0,-2.1438867494,1.8386805341,-1.3116883792\C,0,-5.56
44451427,1.8047979558,-1.8269232226\H,0,-3.1812542689,3.7867691159,-2.
3132788598\C,0,-0.7575522992,1.924572531,-1.1341064294\N,0,-6.71220010
21,1.6998720753,-1.9594398544\C,0,-3.127926462,-0.3751458721,-0.508117
5732\N,0,0.3901982619,2.0319696774,-1.0027469351\N,0,-3.1977929417,-1.
4430287994,-0.0578462535\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas
1=-430.1819441\CCSD(T)/GTBas1=-430.2680651\MP2/GTBas2=0.\MP2/GTBas3=0.
\HF/GTMP2LargeXP=-428.9607394\MP2/GTMP2LargeXP=-430.5828089\HF/GFHFB3=

-428.9673638\HF/GFHFB4=-428.9927807\G4MP2=-430.8577784\FreqCoord=-7.89
74117007,3.575955881,-3.1181966494,-6.0786746325,5.2808392323,-3.57234
89815,-5.8421146882,1.7167191861,-1.996908058,-4.0513588163,3.47460265
54,-2.4787318084,-10.5152774011,3.4105738616,-3.4523845564,-6.01169932
74,7.1559565576,-4.3714635139,-1.4315663769,3.6369150065,-2.1431505571
,-12.684219942,3.2122926833,-3.7028046986,-5.9109243771,-0.7089229581,
-0.9602030566,0.7373678526,3.8398662006,-1.8949170879,-6.0429528895,-2
.7269292328,-0.109313577\PG=C01 [X(C7H1N3)]\NImag=0\\

tetracyano-1,3-cyclobutadiene
\\0,1\C,0,-4.1717328702,1.8731026103,-1.6356175734\C,0
,-3.2117556633,2.7926861545,-1.8795082615\C,0,-3.0933197939,0.90144205
43,-1.054474361\C,0,-2.1333382054,1.8210246498,-1.2983532024\C,0,-5.55
55860633,1.7862752357,-1.8124640237\C,0,-3.1607048021,4.0803788748,-2.
420897521\C,0,-0.7494863997,1.9078540172,-1.1215039646\N,0,-6.70338180
99,1.6808048595,-1.9448750308\C,0,-3.1443705684,-0.3862525138,-0.51308
75476\N,0,0.3983092751,2.0133277314,-0.9890934231\N,0,-3.2227057104,-1
.4553163462,-0.0691754005\N,0,-3.0823673886,5.1494426725,-2.8648096903
\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-522.1869098\CCSD(T)/G
TBas1=-522.2802193\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-520.70
50162\MP2/GTMP2LargeXP=-522.6624658\HF/GFHFB3=-520.7135618\HF/GFHFB4=-
520.7436322\G4MP2=-522.9913314\FreqCoord=-7.8834326243,3.5396509522,-3
.0908692719,-6.0693386095,5.277412007,-3.5517558787,-5.8455272519,1.70
34786074,-1.9926677564,-4.031424957,3.4412378694,-2.4535319763,-10.498
5361673,3.3755709934,-3.4250606305,-5.9728664628,7.7107985919,-4.57483
33104,-1.4163240357,3.6053215941,-2.1193353501,-12.6675557849,3.176260
8672,-3.675281171,-5.9419992345,-0.7299114691,-0.9695949472,0.75269544
6,3.804638028,-1.8691156896,-6.0900311995,-2.750149331,-0.1307225622,-
5.8248302053,9.731036388,-5.4137057375\PG=C01 [X(C8N4)]\NImag=0\\

monoethynyl-1,3-cyclobutadiene
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,-3.2556410566,2.7460632127,-1.8730251419\C,0,-3.0527452438,0.87540056
15,-1.0297171815\C,0,-2.1504014724,1.8178761743,-1.2983717232\C,0,-5.5
738734634,1.6908768012,-1.7760281151\C,0,-6.7655843859,1.5227971714,-1
.8885586369\H,0,-7.8139842419,1.3940813785,-1.9953802304\H,0,-3.271346
5751,3.7367328005,-2.3053316176\H,0,-1.0815856185,1.9141837174,-1.1739
070057\H,0,-3.0499217522,-0.1156393817,-0.5992126922\\Version=EM64L-G0
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9984,5.1893074157,-3.5395045582,-5.7688524643,1.6542673179,-1.94588346
73,-4.0636698586,3.435288113,-2.4535669755,-10.5330943452,3.1952940788
,-3.3562067419,-12.7851016183,2.8776696098,-3.5688586097,-14.766290223
8,2.6344320123,-3.7707221665,-6.1819491127,7.0614016246,-4.3564454027,
-2.0439006083,3.617282994,-2.2183627462,-5.7635168384,-0.2185267616,-1
.1323478836\PG=C01 [X(C6H4)]\NImag=0\\

cis-diethynyl-1,3-cyclobutadiene
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,-3.2579562538,2.7147060036,-1.8547830109\C,0,-3.1337968977,0.82219939
45,-1.026394499\C,0,-2.2078330169,1.7642415317,-1.285830226\C,0,-5.621
1712114,1.742218291,-1.8050189818\C,0,-6.8161650776,1.6105805318,-1.93
38068199\C,0,-3.1927180705,-0.4557232684,-0.4891125087\C,0,-3.30322682
95,-1.5688955941,-0.0302591399\H,0,-3.3877189139,-2.5467376898,0.37475
95468\H,0,-7.8662058933,1.5066375659,-2.0519991401\H,0,-3.226215326,3.

7094086901,-2.2751434959\H,0,-1.1382842563,1.8196282474,-1.1439057159\
\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-306.0008242\CCSD(T)/GT
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00925212,-6.1566450726,5.1300508782,-3.5050319266,-5.9220178927,1.5537
316822,-1.9396045074,-4.1721997491,3.3339333271,-2.4298669805,-10.6224
741355,3.2923154337,-3.4109915402,-12.8806852731,3.0435561201,-3.65436
52835,-6.0333627728,-0.8611921697,-0.9242886896,-6.2421940626,-2.96478
30038,-0.0571814874,-6.4018609624,-4.812636766,0.7081929092,-14.864974
8432,2.8471323811,-3.8777163997,-6.0966634119,7.0097665392,-4.29939812
03,-2.1510455058,3.4385990513,-2.1616685248\PG=C01 [X(C8H4)]\NImag=0\\

trans-diethynyl-1,3-cyclobutadiene
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,-3.3126736082,2.7399447309,-1.8538301404\C,0,-3.1451330264,0.86497328
12,-1.0154117277\C,0,-2.2066551991,1.7967353801,-1.2571652276\C,0,-5.6
278463996,1.6795360202,-1.7925043223\C,0,-6.8174894874,1.5214828319,-1
.9279932414\H,0,-7.8644111751,1.3965681684,-2.053736106\H,0,-3.3083578
264,3.7321197014,-2.2815610417\C,0,-0.8299522668,1.9253324872,-1.07696
44987\H,0,-3.1494364301,-0.1271900399,-0.5876562374\C,0,0.3596863608,2
.0834194575,-0.9414902733\H,0,1.4066486143,2.2080583567,-0.8158126287\
\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-305.9991178\CCSD(T)/GT
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9562\MP2/GTMP2LargeXP=-306.3157974\HF/GFHFB3=-305.1017923\HF/GFHFB4=-3
05.1216472\G4MP2=-306.5274986\FreqCoord=-8.0335273078,3.4169075972,-3.
0466817703,-6.2600458871,5.1777451607,-3.5032312623,-5.9434400714,1.63
45626137,-1.9188500776,-4.1699739961,3.3953378016,-2.375697984,-10.635
0884132,3.1738631085,-3.3873422612,-12.8831880449,2.8751858682,-3.6433
792123,-14.8615833174,2.6391313642,-3.8809987895,-6.2518902416,7.05268
41308,-4.3115255243,-1.5683824876,3.6383511156,-2.0351679574,-5.951572
3258,-0.2403543422,-1.1105093489,0.6797087156,3.9370921946,-1.77915877
34,2.6581806462,4.1726255797,-1.541662444\PG=C01 [X(C8H4)]\NImag=0\\

triethynyl-1,3-cyclobutadiene
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0,-3.2783480873,2.7671810972,-1.8808458653\C,0,-3.1207621875,0.8801223
113,-1.0489455418\C,0,-2.1867715433,1.834452317,-1.3128147589\C,0,-5.6
105568485,1.7334579015,-1.7999760056\C,0,-0.8096133301,1.9518975227,-1
.149836651\C,0,-6.80286591,1.5803797561,-1.9191960437\C,0,-3.148867267
8,-0.3944667893,-0.5078103369\C,0,0.3838183929,2.0946339963,-1.0261215
591\C,0,-3.2258670959,-1.5085420359,-0.0429591396\H,0,-3.2797340779,-2
.4865546915,0.3671089259\H,0,-7.8517740625,1.4561006981,-2.028443154\H
,0,1.4337179908,2.2044412642,-0.9107840386\H,0,-3.2652604676,3.7606356
481,-2.303850941\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-381.9
285077\CCSD(T)/GTBas1=-382.0329464\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP
2LargeXP=-380.7985187\MP2/GTMP2LargeXP=-382.3150689\HF/GFHFB3=-380.803
6654\HF/GFHFB4=-380.8277453\G4MP2=-382.5752108\FreqCoord=-8.0023013776
,3.5025525933,-3.0956452089,-6.1951800532,5.2292144338,-3.5542835836,-
5.8973858602,1.6631901319,-1.9822198023,-4.132399332,3.4666124829,-2.4
808603574,-10.6024158967,3.2757606968,-3.4014616963,-1.5299474675,3.68
85517573,-2.1728763679,-12.8555534887,2.9864849249,-3.626754918,-5.950
4967649,-0.7454342002,-0.9596224643,0.7253116473,3.9582846016,-1.93908
87257,-6.0960053524,-2.8507313077,-0.0811810087,-6.197799196,-4.698907
3814,0.6937353309,-14.8377026353,2.7516315413,-3.8332020372,2.70933435
45,4.1657902654,-1.7211323992,-6.1704480363,7.1065714604,-4.3536473294
\PG=C01 [X(C10H4)]\NImag=0\\

tetraethynyl-1,3-cyclobutadiene
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0,-3.2092553156,2.7961713886,-1.8808432377\C,0,-3.0958472807,0.8980117
033,-1.0530563899\C,0,-2.1296143375,1.823430195,-1.2986759833\C,0,-5.5
498652212,1.7770392303,-1.8079052935\C,0,-3.1504659864,4.0751823889,-2
.417674379\C,0,-0.755220586,1.9170973961,-1.1261053218\C,0,-6.74472260
51,1.6523664438,-1.9395080997\C,0,-3.1546431569,-0.3809834685,-0.51618
81578\C,0,0.4396409731,2.0417546008,-0.9945270948\C,0,-3.2522202669,-1
.4942310607,-0.0560732118\C,0,-3.0528932317,5.1884413932,-2.8777624559
\H,0,-3.3249411349,-2.4726475221,0.3503601999\H,0,-7.7952760591,1.5549
11633,-2.0603977552\H,0,1.4901983008,2.1391318434,-0.8736089578\H,0,-2
.9801773548,6.1668620536,-3.2841866442\\Version=EM64L-G09RevA.02\State
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372\HF/GFHFB3=-456.5056121\HF/GFHFB4=-456.5338342\G4MP2=-458.622819\Fr
eqCoord=-7.8905075074,3.5351518372,-3.0902638867,-6.064613637,5.283998
145,-3.5542786181,-5.8503035098,1.6969961834,-1.9899881794,-4.02438786
65,3.4457836911,-2.4541419439,-10.4877253424,3.3581174727,-3.416445879
,-5.9535179053,7.7009786567,-4.5687424549,-1.4271600775,3.6227890486,-
2.128030655,-12.7456785659,3.12252005,-3.6651391409,-5.9614116134,-0.7
199544166,-0.9754542513,0.830801036,3.8583570261,-1.879383841,-6.14580
56282,-2.8236874839,-0.1059630136,-5.7691321209,9.8047332897,-5.438182
9171,-6.2832281529,-4.6726266399,0.6620848257,-14.730936882,2.93835714
72,-3.8935874821,2.8160666722,4.0423733462,-1.6508816775,-5.6317190281
,11.6536803805,-6.2062133269\PG=C01 [X(C12H4)]\NImag=0\\

monofluoro-1,3-cyclobutadiene
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18424,1.1663940089,0.\C,0,-1.9025685207,2.6097211779,0.\C,0,-1.8693642
835,1.2799280556,0.\H,0,-1.1903788978,3.4190183929,0.\H,0,-1.087374354
7,0.5344287506,0.\F,0,-4.3956645325,3.4181118776,0.\H,0,-4.1663853155,
0.3617876216,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-253.1
648008\CCSD(T)/GTBas1=-253.2242143\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP
2LargeXP=-252.5824943\MP2/GTMP2LargeXP=-253.455864\HF/GFHFB3=-252.5867
006\HF/GFHFB4=-252.6048965\G4MP2=-253.6123542\FreqCoord=-6.5507776915,
4.7126937336,0.,-6.5220530787,2.2041652399,0.,-3.5953334532,4.93165830
95,0.,-3.5325865384,2.4187134949,0.,-2.2494901112,6.4610084059,0.,-2.0
548397344,1.0099239761,0.,-8.3066021384,6.4592953403,0.,-7.8733272104,
0.683679523,0.\PG=CS [SG(C4H3F1)]\NImag=0\\

cis-difluoro-1,3-cyclobutadiene
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20491,1.1677709037,0.\C,0,-1.9357887598,2.5569796016,0.\C,0,-1.8585674
555,1.2363339811,0.\F,0,-1.1021220394,3.5660096571,0.\H,0,-1.086636224
6,0.4867282124,0.\F,0,-4.4159309521,3.4242743426,0.\H,0,-4.1683151024,
0.3549687058,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-352.1
782223\CCSD(T)/GTBas1=-352.2372394\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP
2LargeXP=-351.4638183\MP2/GTMP2LargeXP=-352.5817768\HF/GFHFB3=-351.470
9382\HF/GFHFB4=-351.4960494\G4MP2=-352.7848864\FreqCoord=-6.6121657554
,4.7057669063,0.,-6.5445034156,2.2067671939,0.,-3.6581106071,4.8319911
744,0.,-3.5121834903,2.336332633,0.,-2.0827088194,6.7387816391,0.,-2.0
534448706,0.9197830225,0.,-8.3449001211,6.4709407115,0.,-7.8769739792,
0.6707936396,0.\PG=CS [SG(C4H2F2)]\NImag=0\\

trans-difluoro-1,3-cyclobutadiene
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555,1.2363339811,0.\F,0,-1.1021220394,3.5660096571,0.\H,0,-1.086636224
6,0.4867282124,0.\F,0,-4.4159309521,3.4242743426,0.\H,0,-4.1683151024,
0.3549687058,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-352.1
782223\CCSD(T)/GTBas1=-352.2372394\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP
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9382\HF/GFHFB4=-351.4960494\G4MP2=-352.7848864\FreqCoord=-6.6121657554
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744,0.,-3.5121834903,2.336332633,0.,-2.0827088194,6.7387816391,0.,-2.0
534448706,0.9197830225,0.,-8.3449001211,6.4709407115,0.,-7.8769739792,
0.6707936396,0.\PG=CS [SG(C4H2F2)]\NImag=0\\

trifluoro-1,3-cyclobutadiene
\\0,1\C,0,-3.4836019846,2.5412065085,0.\C,0,-3.44407
57727,1.2167433347,0.\C,0,-1.8936966245,2.652166002,0.\C,0,-1.87417158
9,1.3299843824,0.\H,0,-1.1999483934,3.4722280656,0.\F,0,-0.9690914946,
0.3918428604,0.\F,0,-4.39281464,3.4800254099,0.\F,0,-4.2721695014,0.19
90534366,0.\\Version=EM64L-G09RevA.02\State=1-A'\MP2/GTBas1=-451.18469
07\CCSD(T)/GTBas1=-451.2441264\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2Lar
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\HF/GFHFB4=-450.3834017\G4MP2=-451.9528352\FreqCoord=-6.5830537068,4.8
021843482,0.,-6.5083599912,2.2993116765,0.,-3.578567999,5.0118674027,0
.,-3.5416710292,2.5133062437,0.,-2.2675738371,6.5615601149,0.,-1.83131
75225,0.7404756932,0.,-8.3012166221,6.5762949603,0.,-8.0732303509,0.37
6156481,0.\PG=CS [SG(C4H1F3)]\NImag=0\\

monomethyl-1,3-cyclobutadiene
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5,0.0029726487\C,0,-1.7986886663,1.2078680476,-0.001900238\H,0,-1.1173
650814,3.3386328322,0.0059195999\H,0,-1.0115808806,0.4659910706,-0.004
5060433\C,0,-4.4847816826,3.5098394911,0.0056498477\H,0,-4.0950368895,
0.3371496048,-0.0048239196\H,0,-5.4836443622,3.0632181222,0.0040095931
\H,0,-4.3991692073,4.1666721896,-0.870994475\H,0,-4.3994088939,4.16064
63236,0.886806557\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-193.
3212282\CCSD(T)/GTBas1=-193.3958759\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTM
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03762\HF/GFHFB4=-192.7650576\G4MP2=-193.681902\FreqCoord=-6.4861051685
,4.6702467266,0.0043146432,-6.3653313699,2.1506745269,-0.003848959,-3.
4868036498,4.7974595433,0.0056174919,-3.3990289777,2.2825398146,-0.003
5909294,-2.1115139942,6.3091017111,0.0111864227,-1.9116108257,0.880595
5037,-0.0085151878,-8.475009146,6.6326354085,0.0106766648,-7.738498225
2,0.6371204189,-0.0091158869,-10.3625860547,5.7886433362,0.0075770328,
-8.3132250141,7.8738693239,-1.645941021,-8.313677956,7.8624820874,1.67
58215256\PG=C01 [X(C5H6)]\NImag=0\\

cis-dimethyl-1,3-cyclobutadiene
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-3.4862199896,1.0647002356,-0.0804996159\C,0,-1.9382023587,2.438324678
2,-0.0574188522\C,0,-1.9233060245,1.1084343786,-0.1618643434\C,0,-0.94
51785775,3.5360990575,-0.0260383147\H,0,-1.147539803,0.3609859559,-0.2
61976556\C,0,-4.5789996562,3.434131411,0.1627376355\H,0,-4.2252937062,
0.274872513,-0.102120001\H,0,-5.5782757859,2.9879723244,0.1819113505\H
,0,-4.543584492,4.1543025219,-0.6662640984\H,0,-4.4492195315,4.0181336
534,1.0843013162\H,0,-1.1063160125,4.2506433419,-0.8449023269\H,0,0.07

41415616,3.1466465986,-0.1116789656\H,0,-1.0113926222,4.1146219219,0.9
056614761\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-232.4969315\
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P=-231.8037909\MP2/GTMP2LargeXP=-232.7806996\HF/GFHFB3=-231.8045352\HF
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456189,0.0481904653,-6.5880010194,2.011991859,-0.1521222279,-3.6626716
481,4.6077658649,-0.1085059056,-3.634521656,2.0946374118,-0.3058792796
,-1.7861286582,6.6822587975,-0.0492052837,-2.1685359543,0.6821645944,-
0.4950639441,-8.6530553128,6.4895678712,0.3075295626,-7.9846479357,0.5
19433771,-0.1929788347,-10.541413529,5.6464493857,0.3437626329,-8.5861
303514,7.8504940396,-1.2590566782,-8.4078064196,7.5931721702,2.0490325
331,-2.0906342801,8.0325518047,-1.596634007,0.1401072465,5.9463003083,
-0.2110426599,-1.9112550688,7.7755085727,1.711452159\PG=C01 [X(C6H8)]\
NImag=0\\

trans-dimethyl-1,3-cyclobutadiene
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-3.576098077,1.1446460099,0.0010595741\C,0,-2.0403091626,2.5345991155,
0.0037965838\C,0,-1.997665742,1.2002796636,0.0017590175\C,0,-0.9570930
61,0.1493526553,0.0007026253\C,0,-4.659315829,3.5298912468,0.004063183
4\H,0,-4.313765139,0.353469207,-0.0004445892\H,0,-5.664319069,3.097463
7617,0.0029532612\H,0,-4.5632901035,4.1839332493,-0.8735607718\H,0,-4.
56409134,4.1812335523,0.8837855142\H,0,0.0479105478,0.5817792445,0.001
7435736\H,0,-1.0523504381,-0.5021174542,-0.8789141841\H,0,-1.053087790
2,-0.5045614185,0.878432587\H,0,-1.3026425373,3.3257763371,0.005259687
2\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-232.497368\CCSD(T)/G
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56901\MP2/GTMP2LargeXP=-232.7814913\HF/GFHFB3=-231.8064595\HF/GFHFB4=-
231.8245263\G4MP2=-232.9307692\FreqCoord=-6.8384318154,4.6845646214,0.
0055632363,-6.7578459898,2.1630674778,0.0020023048,-3.8556255437,4.789
6981849,0.0071745036,-3.7750411574,2.268199847,0.0033240614,-1.8086437
69,0.2822356157,0.0013277694,-8.8048308834,6.6705277353,0.0076783039,-
8.1518347143,0.6679599976,-0.0008401518,-10.7040117697,5.8533582162,0.
0055808549,-8.6233685605,7.9064879994,-1.6507906192,-8.624882678,7.901
3863115,1.670112582,0.0905378143,1.0994034419,0.0032948765,-1.98865412
38,-0.948864475,-1.6609071022,-1.9900475175,-0.9534828982,1.6599970157
,-2.4616376446,6.2848064564,0.0099393684\PG=C01 [X(C6H8)]\NImag=0\\

trimethyl-1,3-cyclobutadiene
\\0,1\C,0,-3.5417414079,2.5518819387,0.0030115341\C,0
,-3.5027791146,1.2148022311,-0.0019442291\C,0,-1.967982379,2.607197644
,0.0058696082\C,0,-1.9143270626,1.2739754292,0.00115953\C,0,-0.8599316
891,0.2342009264,-0.0004820555\C,0,-4.5849999296,3.6029693552,0.005164
9432\C,0,-4.4849815808,0.1040695274,-0.008150079\H,0,-5.5906118806,3.1
712034418,0.0020680243\H,0,-4.4937909859,4.2595551009,-0.8714454395\H,
0,-4.4964929042,4.2532228023,0.8867608216\H,0,0.1383271942,0.682728031
7,0.0026497128\H,0,-0.9387811267,-0.4174775154,-0.8815230538\H,0,-0.94
16998807,-0.4231281608,0.8761032717\H,0,-1.2326131994,3.4012509271,0.0
10021112\H,0,-5.5113672056,0.4845690703,-0.008610198\H,0,-4.3692749619
,-0.5479276307,0.8689982565\H,0,-4.3659418857,-0.5409531194,-0.8900117
596\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-271.6723632\CCSD(T
)/GTBas1=-271.7764736\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-270
.8580923\MP2/GTMP2LargeXP=-272.0087823\HF/GFHFB3=-270.8586725\HF/GFHFB
4=-270.8801476\G4MP2=-272.1776426\FreqCoord=-6.6929212944,4.8223579877
,0.0056909747,-6.6192932306,2.2956435224,-0.0036740606,-3.7189477307,4
.9268895215,0.0110919519,-3.6175538771,2.4074646613,0.0021911942,-1.62
50353854,0.4425756109,-0.0009109528,-8.6643941862,6.8086253465,0.00976

03281,-8.4753868988,0.1966629056,-0.0154014173,-10.5647253695,5.992706
0167,0.0039079996,-8.4920342617,8.0493925887,-1.6467932204,-8.49714014
73,8.0374262785,1.6757350982,0.2614005138,1.2901690031,0.0050072316,-1
.7740392281,-0.7889181708,-1.6658371515,-1.7795548739,-0.799596343,1.6
555952476,-2.3293013747,6.4274327614,0.0189371573,-10.4149746363,0.915
7028353,-0.0162709161,-8.2567330774,-1.0354331626,1.6421687148,-8.2504
34476,-1.0222532463,-1.6818784807\PG=C01 [X(C7H10)]\NImag=0\\

tetramethyl-1,3-cyclobutadiene
\\0,1\C,0,-3.610579164,2.4895390511,0.048530157\C,0,-
3.564325735,1.1537452265,0.001479539\C,0,-2.0290820525,2.5458399623,0.
0042899146\C,0,-1.9828211264,1.2100551407,-0.0427248812\C,0,-0.9284765
153,0.1694514702,-0.1085629867\C,0,-4.6649298282,3.53015559,0.11405638
51\C,0,-4.5441034941,0.0407519796,-0.008303484\H,0,-5.6644125834,3.083
7619226,0.1280406173\H,0,-4.6146513598,4.2142015958,-0.7446568102\H,0,
-4.5637637592,4.1553714678,1.0122067043\H,0,0.0710042881,0.6158529263,
-0.1222793916\H,0,-1.0295867451,-0.4553807613,-1.0069888905\H,0,-0.978
8375859,-0.5149646996,0.749850234\C,0,-1.0493853209,3.6589048224,0.014
2227565\H,0,-5.5719918494,0.4149779145,0.0345844735\H,0,-4.3976971138,
-0.6371447325,0.8442431211\H,0,-4.4489428025,-0.5765768269,-0.91255629
07\H,0,-1.1956759254,4.3366516605,-0.8384399631\H,0,-0.0214578418,3.28
47507864,-0.0282941259\H,0,-1.1449334855,4.2762755037,0.9184029216\\Ve
rsion=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-310.8474974\CCSD(T)/GTBas
1=-310.9663652\MP2/GTBas2=0.\MP2/GTBas3=0.\HF/GTMP2LargeXP=-309.910836
4\MP2/GTMP2LargeXP=-311.2361875\HF/GFHFB3=-309.911241\HF/GFHFB4=-309.9
361174\G4MP2=-311.4249666\FreqCoord=-6.8230058011,4.7045470038,0.09170
87059,-6.7355994875,2.1802625052,0.0027959235,-3.8344093804,4.81094030
68,0.0081067638,-3.7469888994,2.2866728216,-0.0807383245,-1.7545663347
,0.3202168716,-0.2051543131,-8.8154398044,6.6710272717,0.2155353316,-8
.5871111234,0.0770100808,-0.0156913107,-10.7041884862,5.8274654927,0.2
419617005,-8.7204272688,7.9636868848,-1.4071974342,-8.6242636401,7.852
5140545,1.9127934611,0.1341786589,1.1637933689,-0.2310745619,-1.945636
9783,-0.8605449251,-1.902933222,-1.8497349659,-0.9731422503,1.41701158
29,-1.9830508643,6.9143280605,0.0268771145,-10.5295386101,0.7841946095
,0.0653551834,-8.3104431605,-1.2040290515,1.5953882884,-8.4072834777,-
1.0895722974,-1.7244814703,-2.2595000426,8.1950839722,-1.5844219091,-0
.0405494445,6.207279401,-0.0534681491,-2.1636107279,8.0809895708,1.735
5300014\PG=C01 [X(C8H12)]\NImag=0\\

mono-t-butyl-1,3-cyclobutadiene
\\0,1\C,0,-1.1802831278,1.5374635001,-0.2379489093\C,
0,-0.0736282157,0.6897260396,0.5326469209\C,0,-0.2908425905,1.80701430
24,-1.1972623304\C,0,0.7965072894,0.9710119039,-0.4351412347\C,0,-2.60
73964086,1.8510783915,0.0621826451\H,0,-0.3064978653,2.3685938101,-2.1
207332805\H,0,-0.0447692924,0.1246123367,1.4540519109\H,0,1.8329248843
,0.7289427595,-0.6290655003\C,0,-3.4001096047,0.5276171543,0.169143661
7\C,0,-3.1995250394,2.7282826445,-1.053467016\C,0,-2.6836295024,2.5960
114746,1.4151694943\H,0,-2.2438542437,1.999754858,2.221155147\H,0,-3.7
266434816,2.8017819243,1.6798491763\H,0,-2.147144797,3.5485209143,1.36
88577006\H,0,-3.1555125551,2.2164982882,-2.0200160768\H,0,-2.651363253
3,3.6714015743,-1.143669795\H,0,-4.2476485708,2.9642625352,-0.84219974
81\H,0,-3.3824034652,-0.0174964835,-0.7794158553\H,0,-4.4449473945,0.7
281020623,0.430653397\H,0,-2.9797327657,-0.1247499903,0.9412996927\\Ve
rsion=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-310.8274186\CCSD(T)/GTBas
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9\MP2/GTMP2LargeXP=-311.2202559\HF/GFHFB3=-309.8888511\HF/GFHFB4=-309.
9137001\G4MP2=-311.4093528\FreqCoord=-2.2304118708,2.9053849544,-0.449

6582722,-0.1391371633,1.3033933215,1.006556806,-0.5496128438,3.4147621
498,-2.2624979137,1.5051806398,1.8349465702,-0.8222977626,-4.927265132
1,3.4980312104,0.1175081695,-0.5791970257,4.4759936212,-4.0076051011,-
0.0846017017,0.2354831892,2.7477598946,3.4637260535,1.377502182,-1.188
7615152,-6.4252759747,0.9970519246,0.3196351977,-6.0462260798,5.155707
0113,-1.9907641503,-5.0713248016,4.9057507248,2.6742827758,-4.24027000
26,3.7789890146,4.1973749265,-7.0423355752,5.2946005209,3.1744548877,-
4.057515634,6.7057327048,2.5867661691,-5.9630545381,4.1885747388,-3.81
72771692,-5.0103504275,6.9379434992,-2.1612226989,-8.0268925076,5.6016
443774,-1.5915268732,-6.3918162202,-0.033063562,-1.4728825102,-8.39973
32507,1.3759134946,0.8138169786,-5.6308788764,-0.2357433168,1.77879862
82\PG=C01 [X(C8H12)]\NImag=0\\

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,0,-0.2535447994,0.4267548234,-0.3628265129\C,0,-0.0749946361,2.493559
7679,-0.4778518354\C,0,0.7445762506,1.2145741141,-0.7699321221\C,0,-2.
5118209478,2.1446004373,0.3845501513\H,0,0.1247841163,3.550722071,-0.5
868915525\C,0,-0.4005778967,-1.0586880802,-0.2000840674\H,0,1.74454617
98,1.0357838779,-1.1407317986\C,0,-2.8917753769,1.4012982133,1.6824512
313\C,0,-3.5338588665,1.7927785984,-0.7238982833\C,0,-2.5650851979,3.6
635840693,0.6415583033\H,0,-1.8688038994,3.9542014551,1.4339605572\H,0
,-3.5737957333,3.962686069,0.9449867052\H,0,-2.3070149348,4.2253477155
,-0.2614845125\H,0,-3.5084679478,0.7297153525,-0.9760392304\H,0,-3.323
9148686,2.3593752885,-1.6359621074\H,0,-4.5505134067,2.03614007,-0.394
2824606\H,0,-2.9428605199,0.3202998365,1.5270928601\H,0,-3.8765071066,
1.7307180859,2.0320303468\H,0,-2.1663227439,1.5973604664,2.4782008163\
C,0,-1.7225667149,-1.5610557614,-0.8178058414\C,0,-0.3652964659,-1.429
1374945,1.3027178696\C,0,0.780180753,-1.7523191242,-0.9077957958\H,0,0
.7823169469,-1.5317370014,-1.9794828783\H,0,0.7144406016,-2.8380260376
,-0.7815184091\H,0,1.73732466,-1.4243384973,-0.4906963716\H,0,-2.59178
07462,-1.1535044837,-0.2946732631\H,0,-1.7798698753,-2.6531266724,-0.7
50695524\H,0,-1.7980383806,-1.2816272033,-1.8733332978\H,0,-1.15983963
4,-0.9291523992,1.8622056889\H,0,0.5915156801,-1.1414860546,1.74853366
84\H,0,-0.4929225104,-2.5102631958,1.4305371795\\Version=EM64L-G09RevA
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-468.1137374\HF/GFHFB3=-466.073258\HF/GFHFB4=-466.1117099\G4MP2=-468.3
81802\FreqCoord=-2.128137721,3.3657188267,-0.1237005538,-0.4791302334,
0.8064497421,-0.6856427432,-0.1417193236,4.7121450572,-0.903009101,1.4
070451987,2.2952124437,-1.4549608516,-4.7466536862,4.0527074909,0.7266
944704,0.2358078055,6.7098922882,-1.109064304,-0.7569825197,-2.0006305
318,-0.378104091,3.2967145059,1.9573478621,-2.1556706905,-5.4646635001
,2.6480698537,3.1793720591,-6.6780254499,3.3878605679,-1.3679695035,-4
.8473085316,6.9231705558,1.2123694914,-3.5315275659,7.4723578243,2.709
7927385,-6.7534951908,7.488391421,1.785766072,-4.3596264113,7.98474999
86,-0.4941341165,-6.6300435673,1.3789621711,-1.8444468403,-6.281288790
6,4.4585731399,-3.0915203468,-8.5992241027,3.8477471005,-0.7450858695,
-5.5612004299,0.6052789714,2.8857872852,-7.3255367836,3.2705831957,3.8
399808492,-4.0937567014,3.018573817,4.6831208451,-3.2551793368,-2.9499
678672,-1.5454290701,-0.6903102778,-2.7006784708,2.461780002,1.4743279
573,-3.3114032421,-1.7154854387,1.4783647787,-2.8945634403,-3.74068052
47,1.3500970752,-5.363091969,-1.476855761,3.2830678112,-2.6916096805,-
0.9272817567,-4.8977558068,-2.1798075672,-0.5568517659,-3.3634666166,-
5.0136828066,-1.4186089496,-3.3978001157,-2.4219244187,-3.5400868884,-
2.1917792663,-1.7558435703,3.5190587551,1.1178026386,-2.1570960278,3.3
042497674,-0.9314885494,-4.7437099616,2.7033234922\PG=C01 [X(C12H20)]\

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,0,-0.2584926563,1.1751549335,0.5545173111\C,0,-0.5951459418,2.0668758
201,-1.2873661521\C,0,0.5645785158,1.3539528066,-0.4821097727\C,0,-2.8
387305107,2.1964307301,0.0881520446\H,0,-0.6856606044,2.5120666073,-2.
2683628306\C,0,1.9851870632,1.0453828217,-0.8209885029\C,0,-3.57755373
53,0.8738446061,0.3980800306\C,0,-3.5198916831,2.9142637314,-1.0886732
277\C,0,-2.8688043654,3.0976679722,1.3443060758\H,0,-2.3654755833,2.61
66778843,2.1890738648\H,0,-3.9027884905,3.3045472798,1.6416496432\H,0,
-2.3695690353,4.0525158572,1.1534837488\H,0,-3.5083117063,2.2903577296
,-1.9879771461\H,0,-3.0102750879,3.8543974989,-1.322207335\H,0,-4.5631
881485,3.1441981637,-0.8486119724\H,0,-3.5920884805,0.218544145,-0.478
1298601\H,0,-4.613249141,1.0747228282,0.6935646562\H,0,-3.0930999759,0
.3319616622,1.2166183306\H,0,-0.1683376722,0.7290618648,1.5351457251\C
,0,2.7242236157,2.3679221003,-1.1303411634\C,0,2.0152676013,0.14459700
47,-2.0775236329\C,0,2.6662097141,0.3269516601,0.3555652109\H,0,2.6547
473236,0.9505115209,1.2550890251\H,0,3.7094268457,0.0967844274,0.11536
11584\H,0,2.1564419605,-0.6132043424,0.5887396255\H,0,2.2400760514,2.9
10118187,-1.9488389085\H,0,3.7599856856,2.1669632035,-1.4255579227\H,0
,2.7386600131,3.0229648898,-0.253930368\H,0,1.5122362562,0.6260661072,
-2.9222044389\H,0,1.5156980614,-0.8101572396,-1.8871613785\H,0,3.04926
0981,-0.0623883799,-2.3747713544\\Version=EM64L-G09RevA.02\State=1-A\M
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/GFHFB3=-466.083152\HF/GFHFB4=-466.1215595\G4MP2=-468.3862673\FreqCoor
d=-2.6798714061,3.5674928695,-0.4737741528,-0.4884803279,2.2207209881,
1.0478858539,-1.1246628391,3.9058292507,-2.4327694602,1.0668987753,2.5
586000014,-0.9110554364,-5.3644232303,4.1506525497,0.1665832223,-1.295
7107624,4.7471179154,-4.2865845199,3.7514598719,1.9754872371,-1.551443
4288,-6.7605967855,1.6513269881,0.7522622368,-6.6516312984,5.507160331
4,-2.0572942486,-5.4212545794,5.853744118,2.540370322,-4.4701010266,4.
9448045793,4.1367500891,-7.3752014016,6.244689352,3.1022682318,-4.4778
365297,7.6581451194,2.179768384,-6.6297483137,4.3281488552,-3.75673236
45,-5.6885955008,7.2837556801,-2.4986097541,-8.6231758934,5.9416734368
,-1.603644221,-6.7880634733,0.412988582,-0.9035344916,-8.7177774592,2.
030931814,1.3106472557,-5.8451118561,0.6273166282,2.2990754531,-0.3181
120982,1.3777272583,2.9010049945,5.1480365584,4.4747242736,-2.13603523
56,3.8083038509,0.2732487385,-3.9259507009,5.0384061724,0.6178490963,0
.671920871,5.0167453936,1.7962064607,2.3717745299,7.0098008483,0.18289
60616,0.2180009958,4.0750847267,-1.1587882707,1.1125566558,4.233130254
,5.4993263878,-3.6827718142,7.1053432094,4.0949669947,-2.6939140604,5.
1753173959,5.712575751,-0.4798588523,2.8577123725,1.1830934837,-5.5221
660938,2.8642542361,-1.5309753074,-3.566218174,5.7622681618,-0.1178969
519,-4.487667488\PG=C01 [X(C12H20)]\NImag=0\\

mono(trimethylsilyl)-1,3-cyclobutadiene
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0,-3.5644706265,-0.7883564927,-0.0514946062\C,0,-2.7489486723,1.144230
7092,-0.0484433082\C,0,-2.292063394,-0.395234989,-0.0423330415\H,0,-4.
9819802011,1.196339016,-0.0657202029\Si,0,-1.9207742167,2.8050579126,-
0.0446655565\H,0,-1.332496703,-0.89617712,-0.0341076264\H,0,-4.0760804
632,-1.7419794246,-0.0538588163\C,0,-3.2492432382,4.1423274661,-0.0564
250401\C,0,-0.8235837217,2.9684284714,-1.5718092124\C,0,-0.8464633741,
2.9726448774,1.4982106528\H,0,-3.8847507575,4.0692424653,-0.9448478779
\H,0,-2.7963794418,5.1398182106,-0.0559260798\H,0,-3.8961011371,4.0734

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3141326337,3.9304773951,1.5053053001\H,0,-0.0943068968,2.1781990704,1.
5507051303\H,0,-1.4122332764,2.9116210636,-2.4930364681\H,0,-0.0707026
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FB4=-561.0219617\G4MP2=-562.4791675\FreqCoord=-7.5922808266,1.32686264
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39,2.1622826732,-0.0915445856,-4.3313720939,-0.7468858874,-0.079997854
7,-9.4145781796,2.2607531023,-0.1241931849,-3.6297372327,5.3007912417,
-0.0844056694,-2.5180538417,-1.6935293233,-0.064454073,-7.702675771,-3
.2918640416,-0.1017784126,-6.1401798592,7.8278644636,-0.1066278727,-1.
5563476815,5.609516856,-2.9702889445,-1.5995839586,5.6174847086,2.8312
078231,-7.3411150261,7.6897538277,-1.7855037265,-5.2843913087,9.712848
7909,-0.1056849744,-7.3625641351,7.6977645705,1.5573368616,-2.73782794
9,5.5148700437,4.5555696805,-0.5936246472,7.4275258482,2.8446147636,-0
.1782142075,4.116199706,2.9304080092,-2.6687341282,5.502166413,-4.7111
561641,-0.1336087142,4.1080750628,-3.0441953437,-0.5503646573,7.419596
0009,-2.9735689589\PG=C01 [X(C7H12Si1)]\NImag=0\\

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,0,-3.4733233113,0.0031536841,-0.9187439612\C,0,-2.7292002294,1.852544
9317,-0.3259720061\C,0,-2.2404454086,0.2915610627,-0.4686888747\H,0,-4
.8614662322,1.9849412161,-0.9743367928\Si,0,-2.0209426113,3.4935525633
,0.1851086466\Si,0,-0.7175446502,-0.7263530488,-0.1519740337\C,0,-3.41
92029007,4.7593688451,0.1793657439\C,0,-0.6771672178,4.0313945658,-1.0
267627288\C,0,-1.2737811027,3.369398826,1.9134108347\H,0,-3.8853475568
,4.8375118094,-0.8082612635\H,0,-3.0448613769,5.7540744671,0.445208266
7\H,0,-4.201973619,4.4975094267,0.8983260035\H,0,-2.0146107211,3.03651
40482,2.6472255822\H,0,-0.8897820437,4.3411823276,2.2437514468\H,0,-0.
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.0329526505\H,0,0.126732627,3.2915545768,-1.0970849341\H,0,-0.22613832
09,4.9801127075,-0.7141919324\H,0,-3.9507327263,-0.9135978353,-1.24760
02814\C,0,0.7624687899,0.0200184615,-1.0537235363\C,0,-1.0415448131,-2
.4730467522,-0.785722501\C,0,-0.3430141963,-0.7845948705,1.6973365767\
H,0,-1.2257453334,-2.4817787067,-1.8647016542\H,0,-1.9105659452,-2.923
1055537,-0.2947733461\H,0,-0.1815262089,-3.12333965,-0.5914546864\H,0,
0.5790373087,0.09648363,-2.1301252079\H,0,1.6580973585,-0.5949844803,-
0.9103971752\H,0,0.9937222005,1.0242796281,-0.6833021929\H,0,-0.207934
3173,0.2177018627,2.1165284281\H,0,0.5751906361,-1.3503450846,1.892320
4564\H,0,-1.1557446703,-1.2662747662,2.2503981474\\Version=EM64L-G09Re
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5,-4.233828238,0.5509705595,-0.8856936148,-9.1868397832,3.7509952883,-
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26083381,-0.287189303,-6.4613570752,8.9939036826,0.3389521335,-1.27966
05878,7.6182316629,-1.9403003609,-2.4070974373,6.3672410136,3.61582245
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1,0.8413216962,-7.9405793575,8.4990610965,1.6975901246,-3.8070625273,5
.7381799499,5.0025313624,-1.6814443805,8.2036456921,4.2400757446,-0.82
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23775446,-3.6104463952,-5.523868954,-0.5570408954,-0.3430348208,-5.902
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091,-1.1243577211,-1.7204013333,1.8778628111,1.9356079806,-1.291254010
6,-0.3929389134,0.4113968992,3.9996590815,1.0869527765,-2.5517823949,3
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168,-0.0492578934\C,0,-2.1384075874,0.0482198109,0.4270500939\H,0,-4.5
52003855,1.4310736194,-0.9514068407\Si,0,-1.7238681276,3.1945274075,-0
.0498183104\H,0,-1.2670573847,-0.3816569904,0.9100052591\Si,0,-4.09561
23198,-2.1449320886,0.0086167855\C,0,-2.9178620617,4.4178644993,-0.844
7183002\C,0,-0.1096096954,3.1397667797,-1.0267572837\C,0,-1.3469843316
,3.7193025878,1.7238202847\H,0,-3.1505639446,4.1384753474,-1.877389380
8\H,0,-2.4873542504,5.4249857399,-0.8646245405\H,0,-3.8618395927,4.473
8094443,-0.2930036731\H,0,-2.262853267,3.7970424928,2.3185057187\H,0,-
0.848156696,4.6947050011,1.7490886089\H,0,-0.688593424,3.00050698,2.22
33661108\H,0,-0.2873278902,2.8726377861,-2.0734533104\H,0,0.5858667,2.
402731056,-0.6110863241\H,0,0.3943164704,4.1127451342,-1.0109512842\C,
0,-5.7101037382,-2.0893272416,0.985123948\C,0,-2.9022491707,-3.3684661
753,0.8041488824\C,0,-4.4719318746,-2.6702232168,-1.7649841949\H,0,-5.
5325005866,-1.8216218067,2.0316945147\H,0,-6.2142361022,-3.0622073755,
0.9698174162\H,0,-6.4053573399,-1.3523870122,0.5689187678\H,0,-5.12907
76997,-1.9509732938,-2.2655069344\H,0,-4.9718658553,-3.6450621056,-1.7
900497386\H,0,-3.55566901,-2.7493694975,-2.3588856069\H,0,-2.670928997
7,-3.0898136925,1.8373248806\H,0,-1.9575649675,-3.4236525839,0.2535646
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978983699,-3.2576386503,6.0367819241,-0.0941429631,-2.3943914517,-0.72
12271886,1.7196607192,-7.7395856308,-4.0533342211,0.0162833648,-5.5139
601901,8.3485539959,-1.5962862469,-0.2071323057,5.9332993348,-1.940290
071,-2.5454314921,7.0284632963,3.2575482404,-5.9537030195,7.8205850142
,-3.5477517745,-4.7004183287,10.2517373232,-1.6339035894,-7.2978191992
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.6027838732,8.8717067267,3.305298453,-1.3012529883,5.6701364521,4.2015
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55,-3.9482562886,1.8616144687,-5.484456102,-6.3654785592,1.5196211578,
-8.4507265278,-5.0459905934,-3.3353367572,-10.4549109387,-3.4423663324
,3.8393462184,-11.7432043583,-5.7867333017,1.8326893154,-12.1043711558
,-2.5556410788,1.075100663,-9.6925521667,-3.6868052178,-4.2811876582,-
9.395464836,-6.8881691169,-3.3827037702,-6.7192406482,-5.1955553885,-4
.4576477759,-5.0473243261,-5.8389016804,3.4720408414,-3.699261676,-6.4
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7085,-0.9953556019\C,0,-2.075852273,1.7468067101,-1.1990775652\H,0,-3.
1022519843,3.7369578973,-2.2216011514\H,0,-3.0854050586,-0.1582130703,
-0.5873087639\C,0,-5.5444664622,1.7914965519,-1.8603149197\H,0,-1.0112
95366,1.8003888287,-1.0248015035\F,0,-5.9762502296,2.9303148162,-2.417
4315676\F,0,-6.2381668351,1.6000923391,-0.7225897004\F,0,-5.8743818116
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91234846,-5.7256378552,1.5877227796,-1.8809494924,-3.9227922884,3.3009
862892,-2.2659282103,-5.8624066455,7.061826996,-4.1982177526,-5.830570
5698,-0.2989793736,-1.1098527192,-10.4775231666,3.3854378511,-3.515485
7192,-1.9110712812,3.4022418189,-1.9365941822,-11.2934762355,5.5374924
858,-4.5682836078,-11.7884268895,3.0237363082,-1.3654966402,-11.100972
8238,1.471468181,-5.0710277385\PG=C01 [X(C5H3F3)]\NImag=0\\

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7193,-1.015287856\C,0,-2.1202094865,1.9606548265,-1.0893122622\H,0,-3.
1543565569,3.9166155391,-2.1516859668\C,0,-3.065496115,-0.4012518391,-
0.5264737187\C,0,-5.511724676,1.7998625617,-2.0749247277\H,0,-1.083884
6814,2.0568146186,-0.8014714924\F,0,-5.9506145429,2.8856800414,-2.7216
467734\F,0,-6.2824130935,1.6225324634,-0.9894757343\F,0,-5.7000883985,
0.7321737663,-2.8668175075\F,0,-4.056546918,-0.5779556135,0.3618334098
\F,0,-1.9101909882,-0.732679646,0.0611575318\F,0,-3.2831775036,-1.2643
422448,-1.5320994644\\Version=EM64L-G09RevA.02\State=1-A\MP2/GTBas1=-8
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2.0585018488,-5.960870018,7.4013307367,-4.0660972012,-5.7929481187,-0.
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0482452074,3.8868163352,-1.5145616239,-11.2450318084,5.4531449854,-5.1
431670321,-11.8720402004,3.0661419976,-1.869838153,-10.7716060064,1.38
36079,-5.417499962,-7.6657627203,-1.0921778264,0.6837660503,-3.6097378
292,-1.384563874,0.115570986,-6.2043063275,-2.3892605809,-2.895248396\
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76,-1.0985077596\C,0,-2.1479172992,1.9161237557,-1.3074936621\H,0,-3.2
412293345,3.8829716925,-2.2943671172\C,0,-5.6180962928,1.8354656245,-1
.9108747376\C,0,-0.6880932931,2.0193804661,-1.0815614181\F,0,-6.101147
363,2.9605006969,-2.4492978554\F,0,-6.2760975931,1.6069455921,-0.76155
74696\F,0,-5.9144387648,0.8171694144,-2.7363433601\F,0,-0.2050558231,0
.8943701117,-0.543070872\F,0,-0.3916572798,3.0377405999,-0.2562148109\
F,0,-0.030149549,2.2477580101,-2.2309451838\H,0,-3.0650588471,-0.02792
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G4 archive entries

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2.2103420896,-2.8651465665,-10.8103189976,-0.9471692191,-0.0139754171,
-6.6061940221,3.3738346683,0.8202583807,-10.0107003278,3.3755266673,-4
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monobromotetrahedrane
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C,0,0.7509388377,0.4328420625,1.2147844961\Br,0,-1.4933573522,-0.86025
08329,-0.6038782841\H,0,2.3629200124,-0.5027090295,-0.3562602169\H,0,0
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\HF/GFHFB1=-2725.5352693\HF/GFHFB2=-2725.5377305\G4=-2727.5760941\Freq
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974,-0.9499823902,-0.6732342419,1.4170305491,4.340400514,-0.6726635637
,1.4191376049,0.8171794695,4.3163905596\PG=C01 [X(C4H3Br1)]\NImag=0\\

dibromotetrahedrane
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96\C,0,0.7564505213,0.4277754549,1.2151513593\Br,0,3.0072438121,-0.859
6593895,-0.6084210156\Br,0,-1.4942850462,-0.8597450433,-0.6084398115\H
,0,0.7564557384,2.2973873906,-0.3595892084\H,0,0.7564793757,0.42726874
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37895017,-1.6246826759,-1.1497846121,1.4294941773,4.3414329893,-0.6795
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tribromotetrahedrane
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95\C,0,0.7567763198,0.4373618013,1.2153124869\Br,0,0.7598365957,3.0329
437728,-0.6107698979\Br,0,3.0045508221,-0.8606925714,-0.6110430497\Br,
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GTBas3=-7869.7382024\HF/GTLargeXP=-7869.0770887\MP2/GTLargeXP=-7873.26
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82,0.8264940255,2.2966077661,1.4358830716,5.7314331071,-1.1541878373,5
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,0,0.757142532,0.4384183476,1.2208076687\Br,0,0.7584327662,0.437203429
5,3.0628529813\Br,0,0.7566146818,3.0340989613,-0.6098689191\Br,0,3.005
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0.6095830146\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-10441.223
2734\MP4/GTBas1=-10441.2741016\CCSD(T)/G3Bas1=-10441.2622386\MP2/GTBas
2=-10441.2411302\MP4/GTBas2=-10441.2927622\MP2/GTBas3=-10441.4746735\M
P4/GTBas3=-10441.5561609\HF/GTLargeXP=-10440.884307\MP2/GTLargeXP=-104
46.1944401\HF/GFHFB1=-10441.1493442\HF/GFHFB2=-10441.152314\G4=-10446.
6637223\FreqCoord=0.0241551469,0.0145516965,0.0103393602,2.8376602703,
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7920291,0.8284906085,2.3069921547,1.4332302184,0.8261947461,5.78795331
99,1.4297945367,5.733616097,-1.152485234,5.6799966509,-1.6260069298,-1
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monochlorotetrahedrane
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73,0.0063916581,0.0044575931\C,0,0.7449253141,1.2918994638,0.004503932
9\C,0,0.7451730653,0.4329708586,1.2173052534\Cl,0,-1.3657967418,-0.791
3192663,-0.5595253777\H,0,2.367350675,-0.4937012955,-0.3498287801\H,0,
0.7456699184,2.3008905501,-0.3503991733\H,0,0.7461272761,0.4334293598,
2.2868833828\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-613.12893
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FB1=-612.591112\HF/GFHFB2=-612.5945467\G4=-614.0256097\FreqCoord=0.038
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,1.4077048331,2.4413361777,0.0085111998,1.408173015,0.8181963462,2.300
3735491,-2.5809817952,-1.4953766971,-1.0573497282,4.4736444362,-0.9329
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121,0.8190627879,4.3215832913\PG=C01 [X(C4H3Cl1)]\NImag=0\\

dichlorotetrahedrane
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6,0.0091095404,0.0067568661\C,0,0.7514376865,1.2952922865,0.0027145804
\C,0,0.7515632866,0.429370075,1.2224244362\Cl,0,2.879799669,-0.7806801

039,-0.5539083874\Cl,0,-1.3754241858,-0.7820597808,-0.5545380861\H,0,0
.7510866506,2.3063365488,-0.346972398\H,0,0.7513763356,0.4327782141,2.
2922280739\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-1072.149150
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2.1611767\MP4/GTBas2=-1072.2339375\MP2/GTBas3=-1072.3605983\MP4/GTBas3
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127686265,1.4200114334,2.4477476835,0.0051298136,1.4202487833,0.811391
8514,2.3100474025,5.442032692,-1.4752715938,-1.046735155,-2.5991750278
,-1.4778788052,-1.047925113,1.4193480716,4.3583444475,-0.655682808,1.4
19895497,0.817832301,4.3316832938\PG=C01 [X(C4H2Cl2)]\NImag=0\\

trichlorotetrahedrane
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78,0.0078147097,0.0056349929\C,0,0.7537279378,1.2897466366,0.005386083
5\C,0,0.7533698052,0.4352370905,1.2271664757\Cl,0,0.7538530487,2.89023
08561,-0.5477607533\Cl,0,2.8805418471,-0.7921413734,-0.5464110681\Cl,0
,-1.372450436,-0.7924939342,-0.5479577747\H,0,0.7530680061,0.434965710
8,2.2975936439\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-1531.16
87898\MP4/GTBas1=-1531.2532668\CCSD(T)/G3Bas1=-1531.2505645\MP2/GTBas2
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TBas3=-1531.5350345\HF/GTLargeXP=-1530.4077442\MP2/GTLargeXP=-1532.727
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22478904,2.3190085586,1.4245758065,5.4617447789,-1.0351178101,5.443435
2053,-1.4969302543,-1.0325672747,-2.5935554551,-1.4975964976,-1.035490
1266,1.423092291,0.8219660706,4.3418227516\PG=C01 [X(C4H1Cl3)]\NImag=0
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tetrachlorotetrahedrane
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,0.0061312207,0.0041533465\C,0,0.7554711236,1.2971264098,0.004091438\C
,0,0.7555982503,0.4366069162,1.2213786746\Cl,0,0.7555163992,0.43618438
72,2.9122227986\Cl,0,0.7553987241,2.8910914262,-0.5600175346\Cl,0,2.88
20606079,-0.7902601603,-0.5593199106\Cl,0,-1.3703748879,-0.7912079626,
-0.5591506008\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-1990.188
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-1990.2046519\MP4/GTBas2=-1990.3025887\MP2/GTBas3=-1990.4858734\MP4/GT
Bas3=-1990.6172988\HF/GTLargeXP=-1989.3244166\MP2/GTLargeXP=-1992.1460
029\HF/GFHFB1=-1989.3706515\HF/GFHFB2=-1989.3776291\G4=-1992.4572756\F
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967097,5.4633710207,-1.0582797701,5.4463052472,-1.4933752767,-1.056961
4518,-2.5896332376,-1.4951663635,-1.0566415025\PG=C01 [X(C4Cl4)]\NImag
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monocyanotetrahedrane
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,0.767161034,0.4384057791,1.2091979804\C,0,-1.1263957403,-0.6439611832
,-0.4536121996\N,0,-2.0769329819,-1.187092283,-0.836414947\H,0,2.34907
62248,-0.5220945015,-0.3678331602\H,0,0.7423221683,2.2889848488,-0.367
8216678\H,0,0.7425378014,0.4241820751,2.2792688783\\Version=EM64L-G09R
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T)/G3Bas1=-246.1798175\MP2/GTBas2=-246.1359391\MP4/GTBas2=-246.1983\MP
2/GTBas3=-246.2883054\MP4/GTBas3=-246.3575748\HF/GTLargeXP=-245.410861
5\MP2/GTLargeXP=-246.6474823\HF/GFHFB1=-245.4282363\HF/GFHFB2=-245.431
5307\G4=-246.7724663\FreqCoord=0.0235405546,0.0132621366,0.0094443985,
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440423,1.4497242541,0.8284668576,2.2850530233,-2.1285794664,-1.2169102
765,-0.8572028278,-3.9248345322,-2.2432793093,-1.5805951833,4.43911073
01,-0.9866156233,-0.6951039354,1.4027856004,4.3255544865,-0.6950822179
,1.403193088,0.8015879524,4.3071939633\PG=C01 [X(C5H3N1)]\NImag=0\\

dicyanotetrahedrane
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\C,0,0.7611137933,0.438464994,1.20397348\C,0,2.6373942051,-0.664352507
,-0.46676829\C,0,-1.1180426966,-0.6619511665,-0.4652256779\N,0,-2.0612
357674,-1.2123493731,-0.8517838792\N,0,3.5798319452,-1.2156555087,-0.8
538805523\H,0,0.7617472678,2.2789737104,-0.3872107351\H,0,0.761649431,
0.4093719656,2.2747412891\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBa
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MP4/GTBas3=-338.4225018\HF/GTLargeXP=-337.1626025\MP2/GTLargeXP=-338.8
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8285787575,2.2751801485,4.9839527521,-1.255444294,-0.8820642356,-2.112
7945014,-1.250906418,-0.8791491212,-3.8951710957,-2.2910082925,-1.6096
382561,6.7649019781,-2.2972559834,-1.613600394,1.4394937186,4.30663617
66,-0.731722245,1.4393088338,0.7736009015,4.2986380596\PG=C01 [X(C6H2N
2)]\NImag=0\\

tricyanotetrahedrane
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C,0,0.7607412423,0.4389936605,1.2034215497\C,0,0.7611054976,2.60958270
62,-0.4737020867\C,0,2.6408329403,-0.6473740063,-0.4722468423\C,0,-1.1
194064823,-0.6477038985,-0.4717591457\N,0,-2.0626460084,-1.1915792643,
-0.865687833\N,0,3.5833272487,-1.1922833517,-0.8665385166\N,0,0.762069
4135,3.6979117648,-0.8689583136\H,0,0.7622784644,0.440122954,2.2757227
53\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-430.1309725\MP4/GTB
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,1.4382809486,4.9313966359,-0.8951672125,4.9904510199,-1.2233595775,-0
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tetracyanotetrahedrane
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0,0.7602425066,0.4382792201,1.2216901475\C,0,0.7608118933,0.4383292866
,2.6165296433\C,0,0.7617964902,2.6125831782,-0.4597182778\C,0,2.642930
1782,-0.6506586776,-0.4588307715\C,0,-1.1239042561,-0.6484456958,-0.45

86154354\N,0,-2.0692011144,-1.193811112,-0.8443049265\N,0,3.5881167418
,-1.1958494896,-0.8450418631\N,0,0.7624779235,3.7036925687,-0.84604132
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monoethynyltetrahedrane

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,0,0.7695680803,0.4398571231,1.2116767058\C,0,-1.1248154007,-0.6427973
578,-0.4529505459\C,0,-2.1122412128,-1.2072085065,-0.8507119904\H,0,2.
3590553311,-0.5130959255,-0.3612295658\H,0,0.754869827,2.2932288144,-0
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diethynyltetrahedrane

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7\C,0,-0.0000390073,1.3620474351,-0.7350202763\C,0,-1.8791586988,-0.49
64021983,-0.000086393\C,0,1.879361705,-0.4960608594,0.0002290674\C,0,2
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6053,1.9656091579,-1.6193516051\H,0,3.7133575379,-1.8268783524,0.00084
18719\H,0,-3.7133538743,-1.8269305542,-0.0003918532\\Version=EM64L-G09
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29926,-3.0601310466,7.0172287801,-3.4522997641,0.0015909074,-7.0172218
569,-3.4523984112,-0.0007404953\PG=C01 [X(C8H4)]\NImag=0\\

triethynyltetrahedrane
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,0,0.7630110111,0.4395291439,1.2124779861\C,0,0.7616446879,2.608998502
6,-0.4630659612\C,0,2.6415217114,-0.6474855769,-0.4621828711\C,0,-1.11
84987727,-0.6470641915,-0.4591873772\C,0,-2.0977346514,-1.2124581391,-
0.8738991287\C,0,3.6199142403,-1.2130626169,-0.8786219395\C,0,0.761560
9832,3.738948199,-0.8799145527\H,0,0.7638320164,0.4404032089,2.2840647
203\H,0,-2.9608845355,-1.710804127,-1.2395145849\H,0,4.4823329425,-1.7
114011105,-1.2460051828\H,0,0.761604874,4.7351660262,-1.2468030505\\Ve
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,-2.1136563604,-1.2227741124,-0.8677383865,-3.9641439906,-2.2912138305
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tetraethynyltetrahedrane
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C,0,0.7608687923,0.4390015264,1.2248501264\C,0,0.7612471184,0.43945317
04,2.6131784279\C,0,0.7603836618,2.6098858048,-0.4591956059\C,0,2.6414
023216,-0.6474293495,-0.4579785839\C,0,-1.1202188799,-0.6476018733,-0.
4572198498\C,0,-2.1036549637,-1.2153953171,-0.858142753\C,0,3.62468614
43,-1.2151677684,-0.8593556937\C,0,0.7602846574,3.7450459644,-0.861297
5131\C,0,0.7614050083,0.4397769324,3.8174509375\H,0,-2.9705851911,-1.7
165082523,-1.2113336434\H,0,4.4919059385,-1.7148477486,-1.2138592678\H
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33,4.8792533172\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-457.79
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18,-1.2237901838,-0.8640202987,-3.9753317594,-2.2967642925,-1.62165478
61,6.8496641304,-2.2963342878,-1.6239469118,1.4367297855,7.0771112278,
-1.6276164187,1.4388469418,0.8310579618,7.2139367977,-5.6135924657,-3.
2437305017,-2.2890888416,8.4884720385,-3.2405926045,-2.29386158,1.4359
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8\C,0,0.7165733059,0.4205482243,1.2188090856\F,0,-1.0550895273,-0.6174

948382,-0.4390429046\H,0,2.3797191631,-0.4693823652,-0.3329357351\H,0,
0.7550561882,2.305215049,-0.3343788639\H,0,0.7545780348,0.442937899,2.
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03427\MP4/GTBas2=-253.1730196\MP2/GTBas3=-253.2801253\MP4/GTBas3=-253.
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=-252.535158\HF/GFHFB2=-252.5394183\G4=-253.7481221\FreqCoord=0.027309
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30321538,-1.9938302523,-1.1668961327,-0.8296708503,4.4970174914,-0.887
0041218,-0.6291573592,1.4268494107,4.35622512,-0.6318844774,1.42594583
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difluorotetrahedrane
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01,-0.0064185764,-0.0042963874\C,0,0.7485520773,1.285612653,-0.0189894
947\C,0,0.7483849097,0.3972954289,1.2230306064\F,0,2.5763650848,-0.591
8779303,-0.4228709012\F,0,-1.0797979955,-0.5913311556,-0.42297899\H,0,
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2.3111928983,4.8686244285,-1.1184871924,-0.7991101928,-2.0405224903,-1
.117453938,-0.799314451,1.4148579802,4.3764663187,-0.5748391643,1.4142
133297,0.8698312122,4.3279098084\PG=C01 [X(C4H2F2)]\NImag=0\\

trifluorotetrahedrane
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4\C,0,0.7531410119,0.4349635798,1.231340394\F,0,0.7531449293,2.5447549
545,-0.3938655557\F,0,2.5807653093,-0.6205994448,-0.3928725506\F,0,-1.
0739012834,-0.6204293158,-0.3938178772\H,0,0.7534313051,0.4353928268,2
.3005885469\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-451.079036
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1=-450.2700716\HF/GFHFB2=-450.278238\G4=-452.1391738\FreqCoord=0.02774
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07,1.4237121285,2.4332982562,-0.0212554626,1.4232302519,0.8219620437,2
.3268961211,1.4232376547,4.8088899393,-0.7442980334,4.8769396478,-1.17
27629889,-0.7424215257,-2.0293793193,-1.1724414917,-0.7442079341,1.423
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monomethyltetrahedrane
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57,-0.4864586719\H,0,2.373372174,-0.4897743799,-0.3453846155\H,0,0.765
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055134\H,0,-1.2221317651,-1.7247133383,-0.1347020235\H,0,-1.2192819802
,-0.7061667885,-1.5818151906\H,0,-2.1049701145,-0.1910875669,-0.138953
9757\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-193.2814406\MP4/G
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36,-2.2520969486,-1.2988040764,-0.9192736648,4.4850234203,-0.925539444
9,-0.6526823338,1.447285383,4.3445951995,-0.6541184563,1.4457385346,0.
8342406772,4.3134992897,-2.3094943343,-3.2592358671,-0.254549934,-2.30
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dimethyltetrahedrane
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0,0.7553817574,0.4347405446,1.2124676821\C,0,2.7148408262,-0.677088227
4,-0.4784155615\C,0,-1.2033759922,-0.6781146888,-0.4785316205\H,0,0.75
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2264266\H,0,2.7550745126,-1.7143488138,-0.1265988249\H,0,3.6194427443,
-0.1707649339,-0.1224312923\H,0,2.7542965939,-0.6956081807,-1.57358901
31\H,0,-1.2429950233,-1.715446758,-0.1268549565\H,0,-1.2428735759,-0.6
965097516,-1.573706002\H,0,-2.1082566294,-0.1723650384,-0.122439211\\V
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trimethyltetrahedrane
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C,0,0.7573312964,0.4388064737,1.2122002837\C,0,0.7568476026,2.69367726
99,-0.4768756102\C,0,2.7117875945,-0.6921951641,-0.472380321\C,0,-1.19
77154569,-0.6918123576,-0.4719908342\H,0,0.7575058032,0.4402433099,2.2
824753152\H,0,-0.1265002844,3.2355148268,-0.1191077571\H,0,0.754865170
1,2.7439971398,-1.5719933677\H,0,1.6417730211,3.2350539081,-0.12235466
3\H,0,2.7382670932,-1.7279124179,-0.1139504166\H,0,3.6224394917,-0.196
4964352,-0.1162161187\H,0,2.7567777815,-0.719730052,-1.5674027398\H,0,
-1.2250497607,-1.727104649,-0.1124044116\H,0,-1.2419689598,-0.72066948
29,-1.5670011577\H,0,-2.1084140613,-0.1952692522,-0.1170447752\\Versio
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eXP=-270.8070185\MP2/GTLargeXP=-272.2771228\HF/GFHFB1=-270.8274021\HF/
GFHFB2=-270.8315163\G4=-272.3981966\FreqCoord=0.0301240211,0.017716591
,0.0006838863,2.8313712322,0.0173716304,0.0002285086,1.4311190767,2.44
34706836,-0.0027141091,1.4311487421,0.8292240606,2.2907265543,1.430234
6933,5.0903123305,-0.9011643027,5.1245358842,-1.3080592907,-0.89266943
72,-2.2633541987,-1.3073358912,-0.8919334138,1.4314785122,0.8319392876

,4.3132532508,-0.2390508933,6.1142369215,-0.2250810411,1.4264884388,5.
1854031037,-2.9706369477,3.1025013822,6.1133659114,-0.2312168042,5.174
5748849,-3.2652812515,-0.2153350801,6.8454185722,-0.3713244485,-0.2196
166366,5.2095550162,-1.360092688,-2.9619619182,-2.3150085469,-3.263754
7894,-0.2124135541,-2.3469811995,-1.361867955,-2.9612030379,-3.9843251
505,-0.3690054088,-0.2211825703\PG=C01 [X(C7H10)]\NImag=0\\

tetramethyltetrahedrane

\\0,1\C,0,0.0152321667,0.0081058821,0.0055719438\C,0,1.5004273502
,0.008326722,0.0052141469\C,0,0.7577905302,1.2945151851,0.0052546965\C
,0,0.7579224188,0.4372282828,1.2180593541\C,0,0.7580157584,0.437241201
9,2.6978321146\C,0,0.7574524427,2.6896938523,-0.4879254482\C,0,2.70876
20898,-0.689110638,-0.4881075038\C,0,-1.1929214004,-0.6897922724,-0.48
75357539\H,0,1.6427529784,0.9463683239,3.0984310992\H,0,0.7565793074,-
0.5836124929,3.0981316881\H,0,-0.1253904347,0.9487955593,3.0982270331\
H,0,-0.1269330529,3.236863904,-0.1402754951\H,0,0.7576706324,2.7273685
446,-1.5838389274\H,0,1.6411931949,3.2376217114,-0.1398000998\H,0,2.74
19284926,-1.7282265283,-0.1394337632\H,0,3.6249948012,-0.1964517578,-0
.1414082063\H,0,2.7403577269,-0.708751626,-1.5840144613\H,0,-1.2252567
638,-1.7289636031,-0.138981994\H,0,-1.2247670816,-0.7093457324,-1.5834
377186\H,0,-2.1094111576,-0.1977745185,-0.140562705\\Version=EM64L-G09
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2\MP2/GTBas3=-311.0736778\MP4/GTBas3=-311.196678\HF/GTLargeXP=-309.857
9933\MP2/GTLargeXP=-311.5455796\HF/GFHFB1=-309.8814407\HF/GFHFB2=-309.
8861627\G4=-311.6813445\FreqCoord=0.0287846235,0.0153178972,0.01052944
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0099299373,1.4322658015,0.826241712,2.3017985929,1.4324421878,0.826266
1257,5.0981638492,1.4313776753,5.0827847621,-0.9220454704,5.118818509,
-1.3022303811,-0.9223895056,-2.2542947448,-1.3035184834,-0.9213090548,
3.1043532332,1.788376953,5.8551862191,1.4297276887,-1.1028677793,5.854
6204142,-0.2369535812,1.7929637631,5.8548005901,-0.2398687072,6.116786
308,-0.2650822689,1.4317899942,5.1539796128,-2.9930218114,3.1014056696
,6.1182183565,-0.264183902,5.181493927,-3.265874834,-0.2634916261,6.85
02474073,-0.3712400206,-0.2672227829,5.1785256101,-1.3393464694,-2.993
3535223,-2.3153997261,-3.2672677037,-0.262637906,-2.3144743609,-1.3404
691678,-2.9922636366,-3.9862093895,-0.3737396759,-0.2656250169\PG=C01
[X(C8H12)]\NImag=0\\

mono-t-butyltetrahedrane

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,0.0059106856,0.0060906168\C,0,0.7537692825,1.2877901628,0.0039976665\
C,0,0.7523530776,0.4349462045,1.2132189132\C,0,-1.2052904514,-0.695455
4698,-0.4918326242\C,0,-1.2026331008,-2.1476784473,0.0259142452\C,0,-1
.2003019356,-0.6943209739,-2.0334614596\C,0,-2.4604185379,0.0366932474
,0.0234700849\H,0,2.3762590852,-0.4872861009,-0.3407308776\H,0,0.76999
07621,2.2985960991,-0.3453953853\H,0,0.7669313455,0.4450473096,2.28267
99883\H,0,-2.0903716697,-2.6835802156,-0.3268789393\H,0,-1.2028493678,
-2.1728561784,1.1201301069\H,0,-0.3176714539,-2.687070406,-0.325989559
8\H,0,-2.0878973034,-1.2054012702,-2.4216211989\H,0,-0.3151642913,-1.2
074171933,-2.4223198595\H,0,-1.1988605987,0.3282976212,-2.4235525864\H
,0,-3.3692065624,-0.4633882533,-0.3286100587\H,0,-2.4827913905,1.07202
24263,-0.3308810468\H,0,-2.4827740428,0.0520689303,1.1176553244\\Versi
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8974904\CCSD(T)/G3Bas1=-310.8981916\MP2/GTBas2=-310.805792\MP4/GTBas2=
-310.9158128\MP2/GTBas3=-311.0632137\MP4/GTBas3=-311.1859634\HF/GTLarg
eXP=-309.8443441\MP2/GTLargeXP=-311.5395422\HF/GFHFB1=-309.8674488\HF/

GFHFB2=-309.8722023\G4=-311.6759757\FreqCoord=0.0246713398,0.013004759
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35707243,0.0075544948,1.4217412719,0.8219292091,2.2926514852,-2.277668
8636,-1.3142203755,-0.929428963,-2.2726471988,-4.058524087,0.048970826
4,-2.2682419351,-1.3120764889,-3.8426852604,-4.6495172089,0.0693401884
,0.0443520327,4.4904788918,-0.9208372791,-0.6438880436,1.4550716653,4.
3437171174,-0.6527026858,1.4492902057,0.8410175312,4.3136400269,-3.950
2299716,-5.0712316631,-0.6177116739,-2.2730558843,-4.1061031034,2.1167
391353,-0.600312048,-5.0778271672,-0.6160309902,-3.945554097,-2.277878
281,-4.5762008634,-0.5955741975,-2.2816878235,-4.5775211407,-2.2655182
031,0.6203925941,-4.579850657,-6.3668776881,-0.8756768919,-0.620983015
4,-4.6917957731,2.0258287941,-0.625274561,-4.6917629908,0.0983960182,2
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mono(trimethylsilyl)tetrahedrane
\\0,1\C,0,0.0241746975,0.0168170202,0.0055006885\C,0,1.4258618
112,-0.1590060514,0.5023409917\C,0,1.0960217005,1.0119553502,-0.315621
8873\C,0,0.5965526241,0.9139292183,1.0590517769\Si,0,-1.4820790859,-0.
8334606487,-0.6027422894\C,0,-2.1107169088,-2.0131732058,0.7262015291\
C,0,-1.0623699541,-1.8031185975,-2.1635883552\C,0,-2.8077419395,0.4489
921041,-0.9905839439\H,0,2.1657278528,-0.9011030056,0.718232479\H,0,1.
4401233759,1.6751960121,-1.0814179455\H,0,0.3408927758,1.4596670692,1.
9431020463\H,0,-3.0121127643,-2.5388883292,0.3917430932\H,0,-2.3621002
049,-1.4785644759,1.6480602659\H,0,-1.3595369987,-2.7696354482,0.97575
12228\H,0,-1.9445393771,-2.323411986,-2.5531259654\H,0,-0.2920986278,-
2.5568341859,-1.9701657564\H,0,-0.6902925773,-1.1441349141,-2.95486716
99\H,0,-3.7232443234,-0.0295155533,-1.3558629487\H,0,-2.470671594,1.15
05630254,-1.7606679129\H,0,-3.070750482,1.0325266023,-0.1022399188\\Ve
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61.9349078\CCSD(T)/G3Bas1=-561.9365713\MP2/GTBas2=-561.8437041\MP4/GTB
as2=-561.9546427\MP2/GTBas3=-562.1113043\MP4/GTBas3=-562.2372545\HF/GT
LargeXP=-560.9614176\MP2/GTLargeXP=-562.8536387\HF/GFHFB1=-560.9858339
\HF/GFHFB2=-560.9924333\G4=-563.007789\FreqCoord=0.0456835577,0.031779
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,1.9123184706,-0.5964389286,1.1273210833,1.7270759274,2.0013178189,-2.
8007235796,-1.5750123686,-1.1390178558,-3.9886769016,-3.8043460171,1.3
723220073,-2.0075882651,-3.4074003343,-4.0885894556,-5.3058633174,0.84
84721125,-1.8719323656,4.0926325201,-1.7028378981,1.3572626851,2.72143
8778,3.1656616817,-2.0435837521,0.6441939869,2.7583710061,3.6719307157
,-5.6920682059,-4.7978036242,0.7402871606,-4.4637224857,-2.7940819293,
3.1143825531,-2.569152595,-5.2338524851,1.8439025849,-3.6746468774,-4.
3906123473,-4.8247088573,-0.5519864104,-4.8317163786,-3.723073716,-1.3
044639226,-2.1621016468,-5.5838897101,-7.0359120971,-0.0557763123,-2.5
622096468,-4.6688926769,2.1742490166,-3.3271801664,-5.8028774334,1.951
1925032,-0.1932054464\PG=C01 [X(C7H12Si1)]\NImag=0\\

mono(trifluoromethyl)tetrahedrane
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2\C,0,-1.79256,0.42783,0.73754\C,0,-1.79267,0.4248,-0.73934\C,0,0.8742
6,0.0001,-0.00004\F,0,1.36833,-0.62071,1.08415\F,0,1.36851,1.24942,-0.
00454\F,0,1.36872,-0.6287,-1.07943\H,0,-2.12979,-1.86769,0.00402\H,0,-
2.13004,0.93734,1.61529\H,0,-2.13059,0.93026,-1.61926\\Version=EM64L-G
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573\MP2/GTBas3=-490.6827462\MP4/GTBas3=-490.7710062\HF/GTLargeXP=-489.
3961117\MP2/GTLargeXP=-491.303756\HF/GFHFB1=-489.4390338\HF/GFHFB2=-48
9.4478868\G4=-491.5300431\FreqCoord=-1.1147305485,0.0000566918,-0.0004

913288,-3.3871640178,-1.6114828571,0.0034393016,-3.3874474768,0.808481
5314,1.393748612,-3.3876553466,0.8027556612,-1.3971501191,1.6521119689
,0.0001889726,-0.000075589,2.5857689594,-1.1729719079,2.048746587,2.58
61091101,2.3610616249,-0.0085793566,2.5865059526,-1.1880708197,-2.0398
270796,-4.0247198206,-3.5294226011,0.0075966991,-4.0251922521,1.771315
8934,3.0524557252,-4.0262316015,1.7579366324,-3.0599579379\PG=C01 [X(C
5H3F3)]\NImag=0\\

di(trifluoromethyl)tetrahedrane
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789,-0.0143608929,-0.0207616538\C,0,0.7477820679,1.2603197828,-0.01589
2601\C,0,0.7630527104,0.4105562895,1.1906405872\C,0,2.6917376046,-0.70
21291099,-0.5187935586\C,0,-1.1804679626,-0.7244286045,-0.48789312\F,0
,-1.2284373959,-0.7477004056,-1.8266490638\F,0,-2.2961004231,-0.121522
7143,-0.0511385486\F,0,-1.2088824228,-1.9929335988,-0.0575496004\F,0,2
.7399295478,-1.9703983188,-0.0895149631\F,0,3.8072051166,-0.0875043934
,-0.0982450375\F,0,2.7202868861,-0.7244638477,-1.8581165596\H,0,0.7378
557699,2.2615439817,-0.3931006357\H,0,0.7728579589,0.3926816455,2.2604
155139\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-826.6194931\MP4
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37\MP4/GTBas2=-826.7794298\MP2/GTBas3=-827.1291128\MP4/GTBas3=-827.253
2331\HF/GTLargeXP=-825.1371646\MP2/GTLargeXP=-828.1335296\HF/GFHFB1=-8
25.211778\HF/GFHFB2=-825.2271854\G4=-828.5091672\FreqCoord=0.038204713
,-0.0445215957,-0.0151192436,2.8173236767,-0.0271381546,-0.0392338397,
1.4131033153,2.3816592293,-0.0300326634,1.4419606476,0.7758389493,2.24
99846325,5.0866468943,-1.3268317276,-0.9803777453,-2.2307611579,-1.368
9716654,-0.9219843789,-2.3214102497,-1.412948996,-3.4518664714,-4.3390
009733,-0.229644649,-0.0966378516,-2.284456706,-3.7660987028,-0.108752
9838,5.1777164687,-3.7235131952,-0.169158765,7.1945750022,-0.165359338
9,-0.1856562148,5.1405972175,-1.3690382652,-3.5113314206,1.3943453307,
4.2736987629,-0.7428525441,1.460489882,0.7420607675,4.2715662678\PG=C0
1 [X(C6H2F6)]\NImag=0\\

1,3-cyclobutadiene
\\0,1\C,0,-4.7643604946,2.7838248168,0.\C,0,-4.7107641651,1.453413
5332,0.\C,0,-3.1867125954,2.8473843128,0.\C,0,-3.1331177733,1.51697266
35,0.\H,0,-5.5531579249,3.5230605246,0.\H,0,-5.4375416354,0.6531142392
,0.\H,0,-2.4599347958,3.6476832345,0.\H,0,-2.3443206154,0.7777366754,0
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as1=-154.2016361\CCSD(T)/G3Bas1=-154.2051628\MP2/GTBas2=-154.1555298\M
P4/GTBas2=-154.2115427\MP2/GTBas3=-154.2620526\MP4/GTBas3=-154.324149\
HF/GTLargeXP=-153.6939018\MP2/GTLargeXP=-154.4987227\HF/GFHFB1=-153.70
6021\HF/GFHFB2=-153.7083201\G4=-154.5882875\FreqCoord=-9.003336533,5.2
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0.,-5.9207345336,2.8666628851,0.,-10.4939476508,6.6576195411,0.,-10.27
54645271,1.2342070455,0.,-4.6486030688,6.8931223326,0.,-4.4301239308,1
.46970932,0.\PG=CS [SG(C4H4)]\NImag=0\\

monobromo-1,3-cyclobutadiene
\\0,1\C,0,-3.6237056592,2.4627523372,0.\C,0,-3.5554820801,1.135
363678,0.\C,0,-2.0465133914,2.4948844287,0.\C,0,-1.9759599756,1.166510
4301,0.\Br,0,-0.8061067774,3.8895447483,0.\H,0,-1.19261585,0.425022810
2,0.\H,0,-4.3911510764,3.2207366057,0.\H,0,-4.2749051898,0.3283149618,
0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-2725.9370982\MP4/G
TBas1=-2725.9932813\CCSD(T)/G3Bas1=-2725.9935122\MP2/GTBas2=-2725.9483
867\MP4/GTBas2=-2726.0044901\MP2/GTBas3=-2726.0854596\MP4/GTBas3=-2726
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4.7146483035,0.,-3.7340232035,2.2043852441,0.,-1.5233210432,7.35017435
58,0.,-2.2537173383,0.8031767116,0.,-8.2980729426,6.0863101309,0.,-8.0
784000528,0.6204253631,0.\PG=CS [SG(C4H3Br1)]\NImag=0\\0

cis-dibromo-1,3-cyclobutadiene
\\0,1\C,0,-3.4460169983,2.3180724807,0.\C,0,-3.400805309,0.9899
704594,0.\C,0,-1.8637600789,2.3690777829,0.\C,0,-1.8233335135,1.040817
9958,0.\Br,0,-0.6448618692,3.7667236085,0.\H,0,-1.0519616028,0.2864775
293,0.\Br,0,-4.7526328942,3.634023602,0.\H,0,-4.1220377342,0.187546541
4,0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-5297.7267236\MP4
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93287\MP4/GTBas2=-5297.7956956\MP2/GTBas3=-5297.9072857\MP4/GTBas3=-52
97.9818252\HF/GTLargeXP=-5297.3306305\MP2/GTLargeXP=-5300.3847577\HF/G
FHFB1=-5297.4701994\HF/GFHFB2=-5297.4728064\G4=-5300.6685553\FreqCoord
=-6.512028376,4.3805221446,0.,-6.4265906652,1.870773048,0.,-3.52199612
64,4.4769081973,0.,-3.4456009894,1.9668609662,0.,-1.2186123263,7.11807
60384,0.,-1.9879193316,0.5413640736,0.,-8.9811745802,6.8673093682,0.,-
7.7895224271,0.3544116004,0.\PG=CS [SG(C4H2Br2)]\NImag=0\\

trans-dibromo-1,3-cyclobutadiene
\\0,1\C,0,-3.4345636163,2.5449983757,0.\C,0,-3.3341038946,1.219
992513,0.\C,0,-1.8578547356,2.5708559193,0.\C,0,-1.7573917166,1.245847
7924,0.\Br,0,-0.6499281053,3.9887505648,0.\H,0,-0.9830109396,0.4977487
106,0.\H,0,-4.2089451929,3.2930971459,0.\Br,0,-4.542031799,-0.19790102
17,0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-5297.7273132\MP
4/GTBas1=-5297.7832114\CCSD(T)/G3Bas1=-5297.7798947\MP2/GTBas2=-5297.7
399133\MP4/GTBas2=-5297.7959986\MP2/GTBas3=-5297.9074363\MP4/GTBas3=-5
297.9818421\HF/GTLargeXP=-5297.3320477\MP2/GTLargeXP=-5300.3850766\HF/
GFHFB1=-5297.4716634\HF/GFHFB2=-5297.4742576\G4=-5300.6689178\FreqCoor
d=-6.4903846209,4.8093499388,0.,-6.3005432594,2.3054517337,0.,-3.51083
6645,4.8582136145,0.,-3.3209890526,2.3543111309,0.,-1.2281861251,7.537
6461798,0.,-1.8576214615,0.9406087461,0.,-7.9537537229,6.2230517348,0.
,-8.5831961869,-0.3739787324,0.\PG=CS [SG(C4H2Br2)]\NImag=0\\

tribromo-1,3-cyclobutadiene
\\0,1\C,0,-3.5803268057,2.6475525913,0.\C,0,-3.5029563657,1.322
5310785,0.\C,0,-2.0044657786,2.7014792536,0.\C,0,-1.9204501367,1.37213
65313,0.\Br,0,-0.8043692289,4.1132729684,0.\Br,0,-0.6005502269,0.08303
60405,0.\H,0,-4.3481132731,3.4032068017,0.\Br,0,-4.6876381844,-0.10224
52653,0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-7869.5160921
\MP4/GTBas1=-7869.5719661\CCSD(T)/G3Bas1=-7869.5647086\MP2/GTBas2=-786
9.5304971\MP4/GTBas2=-7869.586847\MP2/GTBas3=-7869.7288143\MP4/GTBas3=
-7869.8095117\HF/GTLargeXP=-7869.1470849\MP2/GTLargeXP=-7873.327563\HF
/GFHFB1=-7869.3503178\HF/GFHFB2=-7869.3530984\G4=-7873.7080328\FreqCoo
rd=-6.7658371291,5.0031493199,0.,-6.6196281866,2.4992215407,0.,-3.7878
913643,5.105055943,0.,-3.6291248102,2.5929622611,0.,-1.5200375523,7.77
295942,0.,-1.1348754579,0.1569153756,0.,-8.216743281,6.4311288288,0.,-
8.8583523786,-0.1932155497,0.\PG=CS [SG(C4H1Br3)]\NImag=0\\

tetrabromo-1,3-cyclobutadiene
\\0,1\C,0,-3.4220274844,2.5247103357,0.\C,0,-3.3574193299,1.19574
61377,0.\C,0,-1.841410927,2.6016487859,0.\C,0,-1.7768026453,1.27268485
64,0.\Br,0,-0.6632169622,4.0213453192,0.\Br,0,-0.4661146582,-0.0252966
117,0.\Br,0,-4.7327153986,3.8226918582,0.\Br,0,-4.5356125944,-0.223950
6815,0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-10441.3045738

\MP4/GTBas1=-10441.3603806\CCSD(T)/G3Bas1=-10441.3488168\MP2/GTBas2=-10441.3207613\MP4/GTBas2=-10441.3772917\MP2/GTBas3=-10441.5500013\MP4/GTBas3=-10441.6370133\HF/GTLargeXP=-10440.9615621\MP2/GTLargeXP=-10446.2701068\HF/GFHFB1=-10441.2283926\HF/GFHFB2=-10441.2313613\G4=-10446.746968\FreqCoord=-6.4666947647,4.7710110994,0.,-6.3446030467,2.2596327248,0.,-3.4797623502,4.9164036994,0.,-3.3576703918,2.405025832,0.,-1.2532984252,7.599241339,0.,-0.8808290505,-0.0478036682,0.,-8.9435359683,7.2238407024,0.,-8.5710656483,-0.4232054553,0.\PG=CS [SG(C4Br4)]\NImag=0\\

monochloro-1,3-cyclobutadiene
\\0,1\C,0,-3.3595680945,2.4448085556,0.\C,0,-3.3089183187,1.115054473,0.\C,0,-1.7872160634,2.5591844761,0.\C,0,-1.7333879696,1.2307769729,0.\H,0,-1.090875035,3.3830512492,0.\H,0,-0.9421217666,0.494531333,0.\Cl,0,-4.6032096299,3.6198781687,0.\H,0,-4.0218231223,0.3059047716,0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-613.1812047\MP4/GTBas1=-613.2487744\CCSD(T)/G3Bas1=-613.2507824\MP2/GTBas2=-613.1925032\MP4/GTBas2=-613.2600697\MP2/GTBas3=-613.3421225\MP4/GTBas3=-613.4226444\HF/GTLargeXP=-612.6272639\MP2/GTLargeXP=-613.9342735\HF/GFHFB1=-612.6484462\HF/GFHFB2=-612.6518224\G4=-614.0811095\FreqCoord=-6.3486636234,4.6200186174,0.,-6.2529494184,2.1071475773,0.,-3.3773489001,4.8361577833,0.,-3.2756285446,2.3258314094,0.,-2.0614550613,6.3930403544,0.,-1.7803521227,0.9345287834,0.,-8.6988055328,6.8405783732,0.,-7.6001442561,0.5780762411,0.\PG=CS [SG(C4H3Cl1)]\NImag=0\\

cis-dichloro-1,3-cyclobutadiene
\\0,1\C,0,-3.4917416523,2.3320290262,0.\C,0,-3.41867121,1.00488
15255,0.\C,0,-1.9135544166,2.4187490455,0.\C,0,-1.8407140167,1.0915945899,0.\Cl,0,-0.8327615154,3.7313871948,0.\H,0,-1.0515561973,0.3565111049,0.\Cl,0,-4.7098921925,3.5182415271,0.\H,0,-4.1224987991,0.187715986,0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-1072.2147314\MP4/GTBas1=-1072.2936402\CCSD(T)/G3Bas1=-1072.2940051\MP2/GTBas2=-1072.2270723\MP4/GTBas2=-1072.3063796\MP2/GTBas3=-1072.4197717\MP4/GTBas3=-1072.5188829\HF/GTLargeXP=-1071.5574065\MP2/GTLargeXP=-1073.3678007\HF/GFHFB1=-1071.5875548\HF/GFHFB2=-1071.5920907\G4=-1073.5719026\FreqCoord=-6.5984354497,4.4068961935,0.,-6.4603523254,1.8989508791,0.,-3.6160937877,4.5707732802,0.,-3.4784453805,2.0628148231,0.,-1.5736911981,7.0512998939,0.,-1.9871532263,0.6737083516,0.,-8.9004063593,6.6485129556,0.,-7.7903937135,0.3547318044,0.\PG=CS [SG(C4H2Cl2)]\NImag=0\\

trans-dichloro-1,3-cyclobutadiene
\\0,1\C,0,-3.483529128,2.4996886369,0.\C,0,-3.4624188082,1.1699997784,0.\C,0,-1.9128614001,2.6223352279,0.\C,0,-1.8917503313,1.2926456769,0.\H,0,-1.2097247403,3.4374681117,0.\Cl,0,-0.6767749558,0.0956153865,0.\Cl,0,-4.6985045986,3.6967195597,0.\H,0,-4.1655560377,0.3548676262,0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-1072.2153813\MP4/GTBas1=-1072.2940076\CCSD(T)/G3Bas1=-1072.2943281\MP2/GTBas2=-1072.227907\MP4/GTBas2=-1072.3068985\MP2/GTBas3=-1072.4203945\MP4/GTBas3=-1072.5193235\HF/GTLargeXP=-1071.559226\MP2/GTLargeXP=-1073.368607\HF/GFHFB1=-1071.5894283\HF/GFHFB2=-1071.593908\G4=-1073.5726602\FreqCoord=-6.5829160278,4.7237269413,0.,-6.5430233049,2.2109791567,0.,-3.6147841764,4.9554954094,0.,-3.5748900379,2.4427463161,0.,-2.2860484554,6.4958733217,0.,-1.27891932,0.1806868945,0.,-8.8788869255,6.9857875579,0.,-7.8717601024,0.670602619,0.\PG=CS [SG(C4H2Cl2)]\NImag=0\\

trichloro-1,3-cyclobutadiene
\\0,1\C,0,-3.3909754815,2.6603047819,0.\C,0,-3.3495675598,1.328

5826852,0.\C,0,-1.815662798,2.7547314905,0.\C,0,-1.7712578256,1.427592
9151,0.\H,0,-1.1193268709,3.5761849951,0.\Cl,0,-0.5768406795,0.2222602
57,0.\Cl,0,-4.6024521427,3.8491723008,0.\Cl,0,-4.4389366421,0.03356057
45,0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-1531.2470459\MP
4/GTBas1=-1531.3371302\CCSD(T)/G3Bas1=-1531.3356237\MP2/GTBas2=-1531.2
609831\MP4/GTBas2=-1531.3518122\MP2/GTBas3=-1531.4960488\MP4/GTBas3=-1
531.613664\HF/GTLargeXP=-1530.4867266\MP2/GTLargeXP=-1532.8005227\HF/G
FHFB1=-1530.5258091\HF/GFHFB2=-1530.5315255\G4=-1533.0616704\FreqCoord
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4378,5.2056880866,0.,-3.3471922011,2.6977596388,0.,-2.1152212391,6.758
0102413,0.,-1.0900709066,0.4200110159,0.,-8.6973740895,7.2738814868,0.
,-8.3883745748,0.0634202947,0.\PG=CS [SG(C4H1Cl3)]\NImag=0\\

tetrachloro-1,3-cyclobutadiene
\\0,1\C,0,-3.5101337601,2.5415700135,0.\C,0,-3.4535547283,1.21196
48189,0.\C,0,-1.9288393193,2.6088490958,0.\C,0,-1.8722570625,1.2792441
153,0.\Cl,0,-0.8483744175,3.9078816482,0.\Cl,0,-0.6854896017,0.0765624
693,0.\Cl,0,-4.6969001874,3.7442536093,0.\Cl,0,-4.5340209378,-0.087065
789,0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-1990.2780995\M
P4/GTBas1=-1990.3795134\CCSD(T)/G3Bas1=-1990.3759477\MP2/GTBas2=-1990.
2934997\MP4/GTBas2=-1990.3960193\MP2/GTBas3=-1990.5710748\MP4/GTBas3=-
1990.7073137\HF/GTLargeXP=-1989.4136623\MP2/GTLargeXP=-1992.2321094\HF
/GFHFB1=-1989.4616185\HF/GFHFB2=-1989.468575\G4=-1992.55022\FreqCoord=
-6.6331914964,4.802871273,0.,-6.5262726214,2.2902815903,0.,-3.64497806
77,4.9300103131,0.,-3.5380530984,2.417421035,0.,-1.6031953072,7.384826
0749,0.,-1.2953876141,0.1446820991,0.,-8.8758550277,7.0756138937,0.,-8
.5680578533,-0.1645304967,0.\PG=CS [SG(C4Cl4)]\NImag=0\\

monocyano-1,3-cyclobutadiene
\\0,1\C,0,-4.1391762264,1.7895086855,-1.5940434533\C,0,-3.176356
8823,2.6846674198,-1.8626473047\C,0,-3.0291707148,0.8237614832,-0.9913
363639\C,0,-2.0973282292,1.7337364488,-1.2712226588\C,0,-5.5262933052,
1.7187808334,-1.7637458399\H,0,-3.1670459581,3.6686292883,-2.310666390
9\H,0,-3.0624920944,-0.1600823504,-0.5468660961\H,0,-1.0272460336,1.80
37633516,-1.1473715146\N,0,-6.6773006311,1.6204550751,-1.8864598625\\V
ersion=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-246.1622505\MP4/GTBas1=-
246.2329456\CCSD(T)/G3Bas1=-246.2317231\MP2/GTBas2=-246.1762127\MP4/GT
Bas2=-246.246986\MP2/GTBas3=-246.3205522\MP4/GTBas3=-246.3990986\HF/GT
LargeXP=-245.4569631\MP2/GTLargeXP=-246.6799863\HF/GFHFB1=-245.4753363
\HF/GFHFB2=-245.4786269\G4=-246.8174781\FreqCoord=-7.8219094837,3.3816
81328,-3.0123055706,-6.0024446078,5.0732861814,-3.519893288,-5.7243030
607,1.5566836021,-1.8733542334,-3.963375964,3.2762870749,-2.402262679,
-10.4431808768,3.2480250576,-3.3329966054,-5.984849511,6.9327046381,-4
.3665266632,-5.7872713425,-0.3025118009,-1.0334271531,-1.9412136746,3.
408618743,-2.1682179352,-12.6182694998,3.0622163025,-3.5648925008\PG=C
01 [X(C5H3N1)]\NImag=0\\

cis-dicyano-1,3-cyclobutadiene
\\0,1\C,0,-4.1601256037,1.8579612659,-1.6304973389\C,0,-3.177170
46,2.7376103832,-1.8781022142\C,0,-3.0606598193,0.8597491239,-1.029126
819\C,0,-2.1236818405,1.7809985142,-1.3023707974\C,0,-5.5454790204,1.7
971165022,-1.8036826859\H,0,-3.1437279486,3.7261301322,-2.3112112612\C
,0,-3.1040104715,-0.4195296924,-0.4683564324\H,0,-1.0532556505,1.82790
71907,-1.1687241516\N,0,-6.6963929543,1.7126329562,-1.9325068197\N,0,-
3.1767962313,-1.4828763761,-0.0075614796\\Version=EM64L-G09RevB.01\Sta
te=1-A\MP2/GTBas1=-338.1745837\MP4/GTBas1=-338.2593935\CCSD(T)/G3Bas1=
-338.2521705\MP2/GTBas2=-338.1921014\MP4/GTBas2=-338.2774074\MP2/GTBas

3=-338.3744925\MP4/GTBas3=-338.4693177\HF/GTLargeXP=-337.2118877\MP2/G
TLargeXP=-338.8565582\HF/GFHFB1=-337.2366416\HF/GFHFB2=-337.2409435\G4
=-339.0408408\FreqCoord=-7.8614980693,3.511037958,-3.081193431,-6.0039
820469,5.1733338828,-3.5490988344,-5.7838088445,1.6246903873,-1.944767
844,-4.0131770719,3.365599435,-2.4611241305,-10.4794366242,3.396058018
,-3.408466307,-5.9407848591,7.0413654854,-4.3675563189,-5.8657297047,-
0.7927962233,-0.8850653898,-1.9903647274,3.4542439867,-2.2085685715,-1
2.6543487619,3.2364072534,-3.6519086392,-6.0032748571,-2.8022302397,-0
.0142891257\PG=C01 [X(C6H2N2)]\NImag=0\\

trans-dicyano-1,3-cyclobutadiene

\\0,1\C,0,-4.1622995891,1.8373091462,-1.6212053643\C,0,-3.221482
3905,2.7570944346,-1.882416723\C,0,-3.0641804186,0.8871363055,-1.03081
77941\C,0,-2.1235308909,1.807391747,-1.29097854\C,0,-5.5495321871,1.73
63557983,-1.7918803575\H,0,-3.209274419,3.7455726822,-2.3179668137\C,0
,-0.7363895834,1.9086068677,-1.1197119336\N,0,-6.6969194906,1.61732624
31,-1.9173686891\H,0,-3.0763326579,-0.1014965081,-0.5956171747\N,0,0.4
10931627,2.0278232834,-0.99379661\\Version=EM64L-G09RevB.01\State=1-A\
MP2/GTBas1=-338.1733055\MP4/GTBas1=-338.2586281\CCSD(T)/G3Bas1=-338.25
30905\MP2/GTBas2=-338.1908195\MP4/GTBas2=-338.2766514\MP2/GTBas3=-338.
3731223\MP4/GTBas3=-338.4684374\HF/GTLargeXP=-337.2146328\MP2/GTLargeX
P=-338.8553248\HF/GFHFB1=-337.2393899\HF/GFHFB2=-337.2436821\G4=-339.0
420168\FreqCoord=-7.8656063064,3.4720111078,-3.0636341437,-6.08771946,
5.210153404,-3.5572520744,-5.7904618128,1.67644466,-1.9479633237,-4.01
28918185,3.4154754168,-2.439595884,-10.4870959993,3.281236928,-3.38616
31386,-6.0646497372,7.0781065802,-4.3803224631,-1.3915746397,3.6067442
753,-2.1159489023,-12.6553437712,3.056303667,-3.6233017183,-5.81342621
71,-0.1918006038,-1.1255533402,0.7765482344,3.8320306515,-1.8780034246
\PG=C01 [X(C6H2N2)]\NImag=0\\

tricyano-1,3-cyclobutadiene

\\0,1\C,0,-4.1791302892,1.8923143583,-1.6500785758\C,0,-3.216696
0842,2.7944997519,-1.8904057684\C,0,-3.0915139737,0.9084486058,-1.0567
18267\C,0,-2.1438867474,1.8386805113,-1.3116883374\C,0,-5.5644451828,1
.8047979714,-1.826923149\H,0,-3.1812542749,3.7867690919,-2.3132790323\
C,0,-0.7575522225,1.9245725704,-1.134106347\N,0,-6.7122001202,1.699872
0362,-1.9594397098\C,0,-3.1279264979,-0.3751458839,-0.5081176426\N,0,0
.3901984031,2.0319697372,-1.0027468119\N,0,-3.1977930103,-1.4430287505
,-0.0578463589\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-430.181
9441\MP4/GTBas1=-430.2811383\CCSD(T)/G3Bas1=-430.2680651\MP2/GTBas2=-4
30.2033003\MP4/GTBas2=-430.3033387\MP2/GTBas3=-430.4236121\MP4/GTBas3=
-430.5350044\HF/GTLargeXP=-428.9616294\MP2/GTLargeXP=-431.0285563\HF/G
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.8974117203,3.5759558946,-3.1181966059,-6.0786746519,5.2808392096,-3.5
723491823,-5.8421147463,1.7167190707,-1.9969081242,-4.0513588124,3.474
6026122,-2.4787317294,-10.5152774769,3.4105738911,-3.4523844174,-6.011
6993386,7.1559565121,-4.37146384,-1.431566232,3.6369150808,-2.14315040
14,-12.6842199763,3.2122926094,-3.7028044254,-5.9109244448,-0.70892298
04,-0.9602031878,0.7373681193,3.8398663137,-1.8949168551,-6.0429530191
,-2.7269291403,-0.1093137761\PG=C01 [X(C7H1N3)]\NImag=0\\

tetracyano-1,3-cyclobutadiene

\\0,1\C,0,-4.1715250914,1.8729761753,-1.6355365626\C,0,-3.21161451
1,2.7924985164,-1.8794011612\C,0,-3.0934609792,0.9016327026,-1.0545722
578\C,0,-2.1335460478,1.8211488231,-1.2984433322\C,0,-5.5550481598,1.7
882639346,-1.813238913\C,0,-3.162831506,4.0798220289,-2.4209791776\C,0
,-0.7500230178,1.9058594627,-1.1207458381\N,0,-6.7030740386,1.68364321

79,-1.946051984\C,0,-3.142244627,-0.3856895696,-0.5129895775\N,0,0.398
0038523,2.0104792526,-0.9879393769\N,0,-3.2196571341,-1.454940405,-0.0
68851986\N,0,-3.0854184309,5.1490750086,-2.8651118297\\Version=EM64L-G
09RevB.01\State=1-A\MP2/GTBas1=-522.186977\MP4/GTBas1=-522.3004199\CCS
D(T)/G3Bas1=-522.280232\MP2/GTBas2=-522.2121545\MP4/GTBas2=-522.326798
4\MP2/GTBas3=-522.4707118\MP4/GTBas3=-522.5985403\HF/GTLargeXP=-520.70
59471\MP2/GTLargeXP=-523.1983871\HF/GFHFB1=-520.7435078\HF/GFHFB2=-520
.7498319\G4=-523.4765957\FreqCoord=-7.8830399793,3.5394120247,-3.09071
61837,-6.0690718702,5.2770574226,-3.5515534885,-5.8457940534,1.7038388
804,-1.9928527547,-4.0318177223,3.4414725228,-2.453702297,-10.49751967
71,3.3793290897,-3.4265249591,-5.9768853508,7.7097463056,-4.574987619,
-1.417338097,3.6015524323,-2.1179026986,-12.6669741815,3.1816245874,-3
.6775052901,-5.9379817876,-0.7288476588,-0.9694098105,0.7521182807,3.7
992551833,-1.8669348583,-6.0842702252,-2.7494389051,-0.1301113973,-5.8
305958398,9.730341604,-5.4142766982\PG=C01 [X(C8N4)]\NImag=0\\

monoethynyl-1,3-cyclobutadiene
\\0,1\C,0,-4.1970062333,1.8200877053,-1.6177773634\C,0,-3.25564103
22,2.746063203,-1.8730252345\C,0,-3.0527452875,0.8754006141,-1.0297171
144\C,0,-2.1504014646,1.8178761586,-1.2983716941\C,0,-5.5738734654,1.6
908768125,-1.7760281486\C,0,-6.765584377,1.5227971202,-1.8885586461\H,
0,-7.8139842338,1.394081346,-1.9953801756\H,0,-3.2713465345,3.73673275
92,-2.3053317999\H,0,-1.0815855917,1.9141836886,-1.1739069569\H,0,-3.0
499218284,-0.1156392745,-0.5992125548\\Version=EM64L-G09RevB.01\State=
1-A\MP2/GTBas1=-230.0726987\MP4/GTBas1=-230.1474072\CCSD(T)/G3Bas1=-23
0.1481671\MP2/GTBas2=-230.0874697\MP4/GTBas2=-230.161945\MP2/GTBas3=-2
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-4.0636698438,3.4352880833,-2.4535669206,-10.5330943489,3.1952941001,-
3.3562068052,-12.7851016014,2.877669513,-3.5688586271,-14.7662902085,2
.6344319509,-3.7707220629,-6.1819490359,7.0614015466,-4.3564457472,-2.
0439005575,3.6172829395,-2.2183626541,-5.7635169823,-0.218526559,-1.13
2347624\PG=C01 [X(C6H4)]\NImag=0\\

cis-diethynyl-1,3-cyclobutadiene
\\0,1\C,0,-4.2475594824,1.8302361999,-1.6299147461\C,0,-3.25795509
05,2.7147019119,-1.8547867342\C,0,-3.1338015311,0.8221993756,-1.026394
7938\C,0,-2.2078349273,1.7642383615,-1.2858293981\C,0,-5.6211724705,1.
7422215026,-1.8050200032\C,0,-6.8161664707,1.6105831108,-1.933807181\C
,0,-3.1927246575,-0.4557232298,-0.4891101663\C,0,-3.3032265966,-1.5688
932422,-0.0302544955\H,0,-3.38770373,-2.546734965,0.3747658223\H,0,-7.
8662074962,1.5066450511,-2.0520023814\H,0,-3.2262113175,3.7094029224,-
2.2751508875\H,0,-1.1382864224,1.8196235329,-1.143903789\\Version=EM64
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24505\MP2/GTBas3=-306.2063229\MP4/GTBas3=-306.3077291\HF/GTLargeXP=-30
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-305.1244396\G4=-306.8428367\FreqCoord=-8.0267241548,3.4586451764,-3.0
800924901,-6.1566428744,5.1300431458,-3.5050389626,-5.9220266486,1.553
7316465,-1.9396050644,-4.1722033592,3.3339273363,-2.4298654161,-10.622
476515,3.2923215028,-3.4109934705,-12.8806879058,3.0435609937,-3.65436
59658,-6.0333752204,-0.8611920967,-0.9242842631,-6.2421936225,-2.96477
85596,-0.0571727108,-6.401832269,-4.8126316168,0.7082047681,-14.864977
8722,2.847146526,-3.8777225249,-6.0966558369,7.0097556399,-4.299412088
3,-2.151049599,3.4385901422,-2.1616648835\PG=C01 [X(C8H4)]\NImag=0\\

trans-diethynyl-1,3-cyclobutadiene
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92,2.7399445511,-1.8538307017\C,0,-3.1451331501,0.8649738571,-1.015411
0493\C,0,-2.2066549606,1.7967355472,-1.2571653061\C,0,-5.627846848,1.6
795360158,-1.7925041129\C,0,-6.8174900845,1.521482828,-1.9279928758\H,
0,-7.864411599,1.3965675097,-2.0537368937\H,0,-3.3083578029,3.73211930
84,-2.2815622918\C,0,-0.8299518305,1.9253326628,-1.0769647753\H,0,-3.1
494365322,-0.1271892295,-0.5876547095\C,0,0.3596869157,2.0834192929,-0
.9414906238\H,0,1.4066490861,2.2080579521,-0.8158121213\\Version=EM64L
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CCSD(T)/G3Bas1=-306.0903575\MP2/GTBas2=-306.0179435\MP4/GTBas2=-306.11
10118\MP2/GTBas3=-306.2042795\MP4/GTBas3=-306.3062163\HF/GTLargeXP=-30
5.0987326\MP2/GTLargeXP=-306.6682467\HF/GFHFB1=-305.1216471\HF/GFHFB2=
-305.1256479\G4=-306.8425051\FreqCoord=-8.0335276082,3.4169077485,-3.0
466817402,-6.2600456433,5.1777448209,-3.503232323,-5.9434403052,1.6345
637021,-1.9188487954,-4.1699735453,3.3953381175,-2.3756981323,-10.6350
892606,3.1738631001,-3.3873418654,-12.8831891733,2.8751858609,-3.64337
85215,-14.8615841184,2.6391301194,-3.8810002782,-6.2518901971,7.052683
3881,-4.3115278866,-1.5683816631,3.6383514475,-2.03516848,-5.951572518
7,-0.2403528108,-1.1105064617,0.6797097643,3.9370918835,-1.7791594358,
2.6581815378,4.1726248149,-1.5416614851\PG=C01 [X(C8H4)]\NImag=0\\

triethynyl-1,3-cyclobutadiene
\\0,1\C,0,-4.2346354224,1.8534709632,-1.6381448702\C,0,-3.2783479
978,2.7671810586,-1.8808457321\C,0,-3.1207620674,0.880122235,-1.048945
4123\C,0,-2.1867714818,1.8344522544,-1.3128146749\C,0,-5.6105567833,1.
7334578421,-1.7999760688\C,0,-0.8096132411,1.9518976011,-1.1498366224\
C,0,-6.8028658609,1.5803797333,-1.9191961945\C,0,-3.1488672494,-0.3944
668782,-0.5078102096\C,0,0.383818466,2.0946342527,-1.026121608\C,0,-3.
2258674333,-1.5085421371,-0.0429590687\H,0,-3.2797346049,-2.4865548511
,0.367108819\H,0,-7.8517740267,1.4561006525,-2.0284431811\H,0,1.433718
0735,2.2044416594,-0.9107844089\H,0,-3.2652603707,3.760635614,-2.30385
07674\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-381.9285077\MP4/
GTBas1=-382.0393417\CCSD(T)/G3Bas1=-382.0329464\MP2/GTBas2=-381.952585
4\MP4/GTBas2=-382.0633347\MP2/GTBas3=-382.1783002\MP4/GTBas3=-382.2995
037\HF/GTLargeXP=-380.7994755\MP2/GTLargeXP=-382.756081\HF/GFHFB1=-380
.8277453\HF/GFHFB2=-380.8326131\G4=-382.9701873\FreqCoord=-8.002301221
,3.5025525156,-3.0956451707,-6.1951798841,5.2292143609,-3.5542833319,-
5.8973856333,1.6631899877,-1.9822195576,-4.1323992159,3.4666123647,-2.
4808601989,-10.6024157734,3.2757605844,-3.4014618158,-1.5299472992,3.6
885519056,-2.1728763139,-12.8555533959,2.9864848818,-3.6267552029,-5.9
504967302,-0.7454343682,-0.9596222237,0.7253117856,3.9582850862,-1.939
0888181,-6.0960059899,-2.850731499,-0.0811808748,-6.1978001918,-4.6989
076829,0.6937351288,-14.8377025677,2.7516314551,-3.8332020883,2.709334
5108,4.1657910123,-1.7211330989,-6.1704478532,7.106571396,-4.353647001
4\PG=C01 [X(C10H4)]\NImag=0\\

tetraethynyl-1,3-cyclobutadiene
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697,2.7962101357,-1.8807748776\C,0,-3.0957919912,0.8980010764,-1.05311
65847\C,0,-2.129628532,1.8234530458,-1.2987092337\C,0,-5.5498697317,1.
776864418,-1.8078873004\C,0,-3.1505463813,4.0752586674,-2.417491108\C,
0,-0.7552443859,1.9172603486,-1.1262087275\C,0,-6.7447091002,1.6520911
134,-1.9394805988\C,0,-3.1546114181,-0.3810160783,-0.5163272937\C,0,0.
4396045148,2.0419966439,-0.9946665218\C,0,-3.2522046782,-1.4942814736,
-0.0562819189\C,0,-3.0529482021,5.18854826,-2.8774772444\H,0,-3.324883

6319,-2.472726996,0.350083727\H,0,-7.7952496311,1.5544167642,-2.060291
6387\H,0,1.4901582913,2.1394535573,-0.8737950001\H,0,-2.980004254,6.16
70278616,-3.2837133356\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=
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TBas2=-457.8857965\MP4/GTBas2=-458.0145975\MP2/GTBas3=-458.1511544\MP4
/GTBas3=-458.2919913\HF/GTLargeXP=-456.5002382\MP2/GTLargeXP=-458.8428
898\HF/GFHFB1=-456.53384\HF/GFHFB2=-456.5395833\G4=-459.0977951\FreqCo
ord=-7.8905458476,3.5351153155,-3.0902933596,-6.0647996882,5.284071366
4,-3.5541494364,-5.8501990277,1.6969761015,-1.9901019311,-4.0244146903
,3.4458268727,-2.4542047779,-10.4877338661,3.3577871252,-3.4164118769,
-5.9536698296,7.7011228021,-4.5683961229,-1.4272050528,3.6230969843,-2
.1282260634,-12.7456530453,3.121999751,-3.6650871718,-5.9613516359,-0.
7200160402,-0.9757171801,0.8307321397,3.8588144212,-1.8796473198,-6.14
57761699,-2.8237827506,-0.1063574129,-5.7692359999,9.8049352387,-5.437
6439455,-6.283119488,-4.6727768239,0.6615623677,-14.7308869402,2.93742
19808,-3.893386951,2.8159910652,4.0429812973,-1.6512332464,-5.63139191
5,11.6539937123,-6.2053189032\PG=C01 [X(C12H4)]\NImag=0\\

monofluoro-1,3-cyclobutadiene
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940071,0.\C,0,-1.9025685209,2.6097211793,0.\C,0,-1.8693642833,1.279928
0561,0.\H,0,-1.1903788965,3.4190183949,0.\H,0,-1.0873743537,0.53442875
15,0.\F,0,-4.39566453,3.4181118774,0.\H,0,-4.1663853193,0.3617876198,0
.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-253.1648008\MP4/GTB
as1=-253.2238779\CCSD(T)/G3Bas1=-253.2242143\MP2/GTBas2=-253.1841334\M
P4/GTBas2=-253.2436482\MP2/GTBas3=-253.3355524\MP4/GTBas3=-253.4036048
\HF/GTLargeXP=-252.5830084\MP2/GTLargeXP=-253.6803317\HF/GFHFB1=-252.6
048965\HF/GFHFB2=-252.6091514\G4=-253.8137536\FreqCoord=-6.5507776905,
4.7126937316,0.,-6.5220530814,2.2041652364,0.,-3.5953334536,4.93165831
21,0.,-3.532586538,2.4187134958,0.,-2.2494901088,6.4610084097,0.,-2.05
48397325,1.0099239779,0.,-8.3066021338,6.4592953399,0.,-7.8733272175,0
.6836795198,0.\PG=CS [SG(C4H3F1)]\NImag=0\\

cis-difluoro-1,3-cyclobutadiene
\\0,1\C,0,-3.4990074178,2.4901845842,0.\C,0,-3.4632020587,1.1677
708881,0.\C,0,-1.9357887574,2.5569795914,0.\C,0,-1.8585674516,1.236333
969,0.\F,0,-1.1021220428,3.5660096588,0.\H,0,-1.0866361803,0.486728244
1,0.\F,0,-4.4159309401,3.4242743439,0.\H,0,-4.1683151512,0.3549687205,
0.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-352.1782223\MP4/GT
Bas1=-352.2404607\CCSD(T)/G3Bas1=-352.2372394\MP2/GTBas2=-352.2057262\
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2\HF/GTLargeXP=-351.4644512\MP2/GTLargeXP=-352.8553611\HF/GFHFB1=-351.
4960494\HF/GFHFB2=-351.5022643\G4=-353.0325371\FreqCoord=-6.6121657565
,4.7057668844,0.,-6.5445034338,2.2067671644,0.,-3.6581106026,4.8319911
551,0.,-3.5121834831,2.3363326102,0.,-2.0827088259,6.7387816424,0.,-2.
0534447869,0.9197830825,0.,-8.3449000986,6.4709407138,0.,-7.8769740714
,0.6707936675,0.\PG=CS [SG(C4H2F2)]\NImag=0\\

trans-difluoro-1,3-cyclobutadiene
\\0,1\C,0,-3.4705684056,2.4969318668,0.\C,0,-3.472394748,1.16741
77832,0.\C,0,-1.9099918978,2.6533957803,0.\C,0,-1.9118241964,1.3238825
592,0.\H,0,-1.2062196171,3.464950531,0.\F,0,-0.9947848019,0.3964256941
,0.\F,0,-4.3876104033,3.4243838716,0.\H,0,-4.1761659299,0.3558619138,0
.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-352.1819328\MP4/GTB
as1=-352.2433597\CCSD(T)/G3Bas1=-352.2405478\MP2/GTBas2=-352.2097783\M
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\HF/GTLargeXP=-351.4719939\MP2/GTLargeXP=-352.8598862\HF/GFHFB1=-351.5
03617\HF/GFHFB2=-351.5098313\G4=-353.0371609\FreqCoord=-6.5584238121,4
.7185174008,0.,-6.5618750989,2.206099893,0.,-3.6093616029,5.0141913469
,0.,-3.6128241455,2.501775469,0.,-2.2794247325,6.5478075676,0.,-1.8798
708367,0.7491359938,0.,-8.29138204,6.4711476912,0.,-7.891809893,0.6724
815582,0.\PG=CS [SG(C4H2F2)]\NImag=0\\

trifluoro-1,3-cyclobutadiene
\\0,1\C,0,-3.483601982,2.5412065053,0.\C,0,-3.4440757694,1.21674
33329,0.\C,0,-1.8936966235,2.6521660086,0.\C,0,-1.8741715966,1.3299843
894,0.\H,0,-1.1999483883,3.4722280692,0.\F,0,-0.9690915181,0.391842862
,0.\F,0,-4.3928146309,3.4800254031,0.\F,0,-4.2721694911,0.1990534296,0
.\\Version=EM64L-G09RevB.01\State=1-A'\MP2/GTBas1=-451.1846907\MP4/GTB
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P4/GTBas2=-451.2886898\MP2/GTBas3=-451.4636963\MP4/GTBas3=-451.5447973
\HF/GTLargeXP=-450.3420944\MP2/GTLargeXP=-452.0245001\HF/GFHFB1=-450.3
834017\HF/GFHFB2=-450.3915848\G4=-452.2467381\FreqCoord=-6.5830537019,
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52,0.,-3.5416710436,2.5133062569,0.,-2.2675738276,6.5615601216,0.,-1.8
313175669,0.7404756962,0.,-8.301216605,6.5762949473,0.,-8.0732303314,0
.3761564678,0.\PG=CS [SG(C4H1F3)]\NImag=0\\

monomethyl-1,3-cyclobutadiene
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1\C,0,-1.7986899589,1.2078683171,-0.0018938638\H,0,-1.1173588615,3.338
6334506,0.0059135662\H,0,-1.0115855787,0.4659873163,-0.0044929469\C,0,
-4.4847788966,3.5098423351,0.0056534922\H,0,-4.095026235,0.3371498531,
-0.0048391071\H,0,-5.4836511972,3.0632250172,0.0040227004\H,0,-4.39918
86736,4.1666610774,-0.8710005276\H,0,-4.3994130301,4.1606461603,0.8868
09228\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-193.3212283\MP4/
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5\MP4/GTBas2=-193.4043121\MP2/GTBas3=-193.4753155\MP4/GTBas3=-193.5546
026\HF/GTLargeXP=-192.749912\MP2/GTLargeXP=-193.7719623\HF/GFHFB1=-192
.7650576\HF/GFHFB2=-192.7679728\G4=-193.8758743\FreqCoord=-6.486103503
2,4.6702495137,0.0043168875,-6.3653108059,2.1506771409,-0.0038657917,-
3.4867941925,4.7974619929,0.0056101227,-3.3990314203,2.282540324,-0.00
35788839,-2.1115022405,6.3091028797,0.0111750206,-1.9116197037,0.88058
84092,-0.0084904392,-8.4750038812,6.632640783,0.0106835519,-7.73847809
12,0.6371208882,-0.0091445872,-10.3625989711,5.7886563659,0.007601802,
-8.3132618001,7.8738483249,-1.6459524588,-8.3136857723,7.8624817788,1.
6758265731\PG=C01 [X(C5H6)]\NImag=0\\

cis-dimethyl-1,3-cyclobutadiene
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4,1.0645907481,-0.0811861749\C,0,-1.938242117,2.4385683137,-0.05816553
46\C,0,-1.9230415861,1.1088390484,-0.1640297719\C,0,-0.9454838502,3.53
64124164,-0.0257705802\H,0,-1.1473265848,0.3614050329,-0.2648290071\C,
0,-4.578979452,3.4337055366,0.1640249705\H,0,-4.2246418033,0.274403163

,-0.1033735681\H,0,-5.5781734007,2.9873739149,0.1847660201\H,0,-4.5448
290185,4.1530710971,-0.6657964785\H,0,-4.4485323725,4.018786307,1.0848
248328\H,0,-1.1070486473,4.2521251317,-0.8436128562\H,0,0.0738989663,3
.1473045415,-0.1126952297\H,0,-1.0110516102,4.1135571261,0.906806278\\
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TLargeXP=-231.8043601\MP2/GTLargeXP=-233.0442618\HF/GFHFB1=-231.822619
8\HF/GFHFB2=-231.8261514\G4=-233.1626046\FreqCoord=-6.6796139891,4.522
828239,0.0498643918,-6.587507893,2.0117849575,-0.1534196364,-3.6627467
803,4.6082262693,-0.1099169308,-3.6340219399,2.095402127,-0.3099713466
,-1.78670554,6.68285096,-0.0486993389,-2.1681330302,0.6829565353,-0.50
04542954,-8.6530171324,6.4887630852,0.3099622732,-7.9834160179,0.51854
6828,-0.1953477331,-10.541220049,5.6453185558,0.3491571767,-8.58848216
59,7.8481669838,-1.2581730045,-8.4065078772,7.5944055069,2.0500218362,
-2.0920187592,8.0353519816,-1.5941972604,0.1396488078,5.9475436403,-0.
2129631206,-1.9106106495,7.7734964003,1.713615521\PG=C01 [X(C6H8)]\NIm
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trans-dimethyl-1,3-cyclobutadiene
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1,1.1447137623,0.0003735695\C,0,-2.0403004183,2.5345339073,0.003118694
1\C,0,-1.997650081,1.2002513408,0.0016515076\C,0,-0.9571142202,0.14938
14114,0.0010358038\C,0,-4.6592950323,3.5298611117,0.004399517\H,0,-4.3
138100332,0.3535000522,-0.0013707926\H,0,-5.6642482486,3.0973364871,0.
0033132285\H,0,-4.5633808651,4.1841407259,-0.8730284196\H,0,-4.5639313
869,4.1809560425,0.8842640071\H,0,0.0478394351,0.5819047332,0.00209630
3\H,0,-1.0522634455,-0.5023362334,-0.8783773254\H,0,-1.0532464035,-0.5
042755143,0.8789169986\H,0,-1.3025966296,3.3257493391,0.0043444912\\Ve
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LargeXP=-231.806265\MP2/GTLargeXP=-233.0450833\HF/GFHFB1=-231.8245288\
HF/GFHFB2=-231.8280563\G4=-233.1636553\FreqCoord=-6.8384601092,4.68461
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94,4.7895749593,0.0058934777,-3.7750115625,2.2681463248,0.0031208971,-
1.8086837541,0.2822899569,0.0019573856,-8.8047915834,6.6704707882,0.00
83138823,-8.1519195521,0.6680182867,-0.0025904227,-10.7038779386,5.853
1177021,0.0062610944,-8.623540075,7.9068800735,-1.6497846193,-8.624580
4105,7.900861894,1.6710168026,0.0904034307,1.0996405811,0.0039614386,-
1.9884897317,-0.9492779077,-1.6598925864,-1.9903472531,-0.9529426175,1
.6609124209,-2.4615508916,6.2847554375,0.0082098985\PG=C01 [X(C6H8)]\N
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trimethyl-1,3-cyclobutadiene
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3,1.2147848679,-0.0019474529\C,0,-1.9680447131,2.6072042548,0.00585805
23\C,0,-1.9143083671,1.2739844022,0.0011594986\C,0,-0.85992567,0.23420
44991,-0.0004939697\C,0,-4.5849651916,3.6029842292,0.0051740446\C,0,-4
.4849827008,0.1040418534,-0.0081382438\H,0,-5.5906078778,3.1712610241,
0.0021221021\H,0,-4.4937829473,4.2595292847,-0.8714646425\H,0,-4.49642
58327,4.2532485024,0.8867521464\H,0,0.1383609596,0.6826996351,0.002755
667\H,0,-0.9386964329,-0.4173766253,-0.8816102683\H,0,-0.9417619505,-0
.4231941761,0.8760255544\H,0,-1.2327159675,3.401299173,0.0100004521\H,
0,-5.5113905593,0.4845156643,-0.0087007786\H,0,-4.3693424036,-0.547877
7304,0.8690724255\H,0,-4.3658756203,-0.5410357812,-0.8899435278\\Versi
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geXP=-270.8587558\MP2/GTLargeXP=-272.3164339\HF/GFHFB1=-270.8801477\HF
/GFHFB2=-270.8842978\G4=-272.4494212\FreqCoord=-6.692900572,4.82232961
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,4.9269020142,0.0110701145,-3.6175185478,2.4074816177,0.0021911349,-1.
6250240109,0.4425823624,-0.0009334675,-8.664328541,6.8086534544,0.0097
775273,-8.4753890153,0.1966106092,-0.015379052,-10.5647178054,5.992814
8314,0.0040101919,-8.492019071,8.0493438031,-1.6468295088,-8.497013400
6,8.0374748447,1.6757187044,0.261464321,1.2901153414,0.005207456,-1.77
387918,-0.7887275162,-1.666001963,-1.7796721689,-0.7997210939,1.655448
3833,-2.3294955782,6.427523933,0.0188981157,-10.4150187685,0.915601912
6,-0.0164420886,-8.2568605236,-1.0353388647,1.6423088738,-8.2503092525
,-1.0224094546,-1.6817495412\PG=C01 [X(C7H10)]\NImag=0\\

tetramethyl-1,3-cyclobutadiene
\\0,1\C,0,-3.6108013218,2.4893644369,0.0484004265\C,0,-3.56414911
81,1.1534670076,0.0038952587\C,0,-2.0293174292,2.5461355977,0.00222889
77\C,0,-1.9826841205,1.2102646494,-0.0431063625\C,0,-0.9278680845,0.17
0160534,-0.1095709841\C,0,-4.6656247245,3.5295088802,0.1141240857\C,0,
-4.5437859545,0.0402961653,-0.0020539543\H,0,-5.6648304298,3.082566086
5,0.1300749292\H,0,-4.6169779084,4.2126551169,-0.7453937836\H,0,-4.563
5332756,4.1558637665,1.0113858178\H,0,0.0713150023,0.6171384696,-0.125
9572025\H,0,-1.0304124767,-0.456039147,-1.0068889951\H,0,-0.97603765,-
0.5131399502,0.7498515926\C,0,-1.049651865,3.6592786053,0.0089202538\H
,0,-5.5716373021,0.4144699182,0.0419918202\H,0,-4.3957363304,-0.636056
0837,0.8514385851\H,0,-4.4501740139,-0.5787537427,-0.9052935101\H,0,-1
.1973696602,4.3359235468,-0.844397105\H,0,-0.0217960972,3.285089653,-0
.0348847846\H,0,-1.14357724,4.2780264895,0.9123350143\\Version=EM64L-G
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738\MP2/GTBas3=-311.1132028\MP4/GTBas3=-311.2442415\HF/GTLargeXP=-309.
9115822\MP2/GTLargeXP=-311.5879136\HF/GFHFB1=-309.9361092\HF/GFHFB2=-3
09.9408793\G4=-311.7356893\FreqCoord=-6.8234256185,4.7042170306,0.0914
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68,0.0042120063,-3.7467299957,2.2870687357,-0.0814592197,-1.7534165671
,0.321556808,-0.2070591522,-8.8167529682,6.6698051672,0.2156632672,-8.
5865110604,0.0761487165,-0.0038814111,-10.7049781016,5.82520569,0.2458
05993,-8.7248238084,7.9607644633,-1.4085901121,-8.6238280891,7.8534443
643,1.9112422104,0.1347658235,1.1662226935,-0.2380246172,-1.9471973848
,-0.8617890936,-1.9027444469,-1.844443854,-0.9696939738,1.4170141503,-
1.9835545596,6.915034408,0.0168568368,-10.5288686128,0.7832346357,0.07
93530401,-8.3067378169,-1.2019718033,1.6089857449,-8.40961013,-1.09368
6072,-1.710756804,-2.2627007377,8.1937080367,-1.5956792758,-0.04118865
45,6.2079197662,-0.0659226892,-2.1610477955,8.0842984544,1.7240633185\
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mono-t-butyl-1,3-cyclobutadiene
\\0,1\C,0,-1.1790531601,1.5425550132,-0.2362268689\C,0,-0.0690504
49,0.7006148863,0.5361559596\C,0,-0.2888241416,1.8187187808,-1.1929039
021\C,0,0.8016538752,0.9887348792,-0.4290964872\C,0,-2.6085982654,1.84
74202979,0.060925558\H,0,-0.3058586446,2.3808372907,-2.1160002537\H,0,
-0.038976794,0.1341436392,1.4566627842\H,0,1.840090061,0.7534855769,-0
.6206413467\C,0,-3.3934768376,0.5191321854,0.1653009317\C,0,-3.2034522
139,2.7216645121,-1.0556284699\C,0,-2.6922010713,2.5909166771,1.414228
0755\H,0,-2.2507555544,1.9966850286,2.2208028142\H,0,-3.7369958743,2.7
904065807,1.6767396397\H,0,-2.1612066901,3.5465689058,1.3697232678\H,0

,-3.153507903,2.2109210908,-2.0224518458\H,0,-2.6612050562,3.668398308
7,-1.143578106\H,0,-4.2536735987,2.9505994142,-0.8470284656\H,0,-3.371
0338236,-0.0249462396,-0.7837460903\H,0,-4.4399093185,0.7130899389,0.4
253752881\H,0,-2.97046454,-0.131516767,0.9374775174\\Version=EM64L-G09
RevB.01\State=1-A\MP2/GTBas1=-310.8274195\MP4/GTBas1=-310.9446166\CCSD
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6862\MP2/GTLargeXP=-311.5715037\HF/GFHFB1=-309.9137021\HF/GFHFB2=-309.
9184638\G4=-311.7192546\FreqCoord=-2.2280875688,2.9150065198,-0.446404
0875,-0.130486438,1.3239702598,1.0131879281,-0.5457985282,3.4368804085
,-2.2542616779,1.5149062775,1.8684381397,-0.8108748453,-4.9295363123,3
.4911184155,0.1151326191,-0.5779890737,4.4991304464,-3.9986609766,-0.0
736554662,0.2534947406,2.75269373,3.4772662751,1.4238813854,-1.1728421
719,-6.4127418613,0.9810176572,0.3123734905,-6.0536473641,5.1432005535
,-1.9948487062,-5.0875227194,4.8961229528,2.672503752,-4.2533115899,3.
7731878777,4.1967091141,-7.0618987622,5.2731042369,3.1685787153,-4.084
0887608,6.7020439434,2.588401854,-5.9592662945,4.178035363,-3.82188010
55,-5.0289487396,6.9322681497,-2.1610494319,-8.0382781602,5.5758248206
,-1.6006518267,-6.3703307113,-0.0471415608,-1.4810654685,-8.3902126668
,1.3475446927,0.8038427982,-5.6133644681,-0.2485306715,1.7715757636\PG
=C01 [X(C8H12)]\NImag=0\\

mono(trimethylsilyl)-1,3-cyclobutadiene

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706265,-0.7883564927,-0.0514946062\C,0,-2.7489486723,1.1442307092,-0.0
484433082\C,0,-2.292063394,-0.395234989,-0.0423330415\H,0,-4.981980201
1,1.196339016,-0.0657202029\Si,0,-1.9207742167,2.8050579126,-0.0446655
565\H,0,-1.332496703,-0.89617712,-0.0341076264\H,0,-4.0760804632,-1.74
19794246,-0.0538588163\C,0,-3.2492432382,4.1423274661,-0.0564250401\C,
0,-0.8235837217,2.9684284714,-1.5718092124\C,0,-0.8464633741,2.9726448
774,1.4982106528\H,0,-3.8847507575,4.0692424653,-0.9448478779\H,0,-2.7
963794418,5.1398182106,-0.0559260798\H,0,-3.8961011371,4.0734815678,0.
8241071733\H,0,-1.4487961517,2.9183435354,2.410703647\H,0,-0.314132633
7,3.9304773951,1.5053053001\H,0,-0.0943068968,2.1781990704,1.550705130
3\H,0,-1.4122332764,2.9116210636,-2.4930364681\H,0,-0.0707026864,2.173
8996944,-1.6109187944\H,0,-0.2912404331,3.9262811006,-1.5735449212\\Ve
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61.9702949\CCSD(T)/G3Bas1=-561.9749678\MP2/GTBas2=-561.8708173\MP4/GTB
as2=-561.9905165\MP2/GTBas3=-562.1292548\MP4/GTBas3=-562.2649989\HF/GT
LargeXP=-560.9944078\MP2/GTLargeXP=-562.8715365\HF/GFHFB1=-561.0198512
\HF/GFHFB2=-561.0264059\G4=-563.0386796\FreqCoord=-7.5922808266,1.3268
626443,-0.1086221227,-6.7358732928,-1.4897778662,-0.0973107031,-5.1947
601439,2.1622826732,-0.0915445856,-4.3313720939,-0.7468858874,-0.07999
78547,-9.4145781796,2.2607531023,-0.1241931849,-3.6297372327,5.3007912
417,-0.0844056694,-2.5180538417,-1.6935293233,-0.064454073,-7.70267577
1,-3.2918640416,-0.1017784126,-6.1401798592,7.8278644636,-0.1066278727
,-1.5563476815,5.609516856,-2.9702889445,-1.5995839586,5.6174847086,2.
8312078231,-7.3411150261,7.6897538277,-1.7855037265,-5.2843913087,9.71
28487909,-0.1056849744,-7.3625641351,7.6977645705,1.5573368616,-2.7378
27949,5.5148700437,4.5555696805,-0.5936246472,7.4275258482,2.844614763
6,-0.1782142075,4.116199706,2.9304080092,-2.6687341282,5.502166413,-4.
7111561641,-0.1336087142,4.1080750628,-3.0441953437,-0.5503646573,7.41
95960009,-2.9735689589\PG=C01 [X(C7H12Si1)]\NImag=0\\

mono(trifluoromethyl)-1,3-cyclobutadiene

\\0,1\C,0,-4.0888832915,1.8356046886,-1.6087857339\C,0,-3.132798
4155,2.7384584419,-1.8093235959\C,0,-3.0298789964,0.840186946,-0.99536

04723\C,0,-2.0758531516,1.7468087134,-1.199074553\H,0,-3.1022539581,3.
7369573147,-2.2216030074\H,0,-3.0854018571,-0.1582137623,-0.5873159184
\C,0,-5.5444658308,1.7914984774,-1.8603149188\H,0,-1.0112970504,1.8003
849806,-1.0247915777\F,0,-5.9762506129,2.9303141753,-2.4174362024\F,0,
-6.2381653609,1.6000967829,-0.7225868809\F,0,-5.8743814748,0.778663241
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FHFB1=-489.4838168\HF/GFHFB2=-489.4927044\G4=-491.572628\FreqCoord=-7.
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9126082,-5.7256415189,1.5877232284,-1.8809586961,-3.9227939486,3.30099
00749,-2.265922518,-5.8624103755,7.0618258951,-4.1982212599,-5.8305645
199,-0.2989806812,-1.1098662392,-10.4775219733,3.3854414899,-3.5154857
174,-1.9110744642,3.4022345471,-1.9365754251,-11.2934769599,5.53749127
46,-4.5682923662,-11.7884241038,3.0237447059,-1.3654913121,-11.1009721
875,1.4714602759,-5.0710179804\PG=C01 [X(C5H3F3)]\NImag=0\\

cis-di(trifluoromethyl)-1,3-cyclobutadiene
\\0,1\C,0,-4.0846994844,1.941365304,-1.7039587209\C,0,-3.1693290
488,2.90333264,-1.7779015638\C,0,-3.0331749609,0.995792318,-1.01518679
78\C,0,-2.1199521623,1.9598258937,-1.0888173561\H,0,-3.1528157535,3.91
65323115,-2.1510252559\C,0,-3.0665342983,-0.4016885055,-0.5265393978\C
,0,-5.511285329,1.8007858766,-2.0753090411\H,0,-1.0836364977,2.0554568
172,-0.8007683752\F,0,-5.9497786167,2.8871666984,-2.7213732341\F,0,-6.
2821902714,1.6228994894,-0.9901167416\F,0,-5.6998068968,0.7337193648,-
2.8679877856\F,0,-4.0576372218,-0.5779495644,0.361796891\F,0,-1.911392
257,-0.7338554018,0.0610035731\F,0,-3.2847472014,-1.2645232419,-1.5322
661943\\Version=EM64L-G09RevB.01\State=1-A\MP2/GTBas1=-826.6572997\MP4
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-5.7318699892,1.8817747663,-1.9184250215,-4.0061290017,3.7035342073,-2
.0575666117,-5.9579583216,7.4011734593,-4.0648486385,-5.7949100008,-0.
7590812662,-0.99501526,-10.414819912,3.4029921308,-3.9217657288,-2.047
7762083,3.8842504625,-1.513232925,-11.2434521369,5.4559543599,-5.14265
01178,-11.8716191276,3.0668355763,-1.8710494813,-10.7710740453,1.38652
86579,-5.4197114673,-7.6678230957,-1.0921663953,0.6836970398,-3.612007
8982,-1.3867857306,0.1152800463,-6.2072726264,-2.3896026158,-2.8955634
698\PG=C01 [X(C6H2F6)]\NImag=0\\

trans-di(trifluoromethyl)-1,3-cyclobutadiene
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701,2.8803791015,-1.8934670248\C,0,-3.0641817448,0.9746552393,-1.09850
04891\C,0,-2.1479184364,1.9161279166,-1.3074935936\H,0,-3.2412339347,3
.8829701092,-2.2943620374\C,0,-5.6180972781,1.8354628044,-1.9108769609
\C,0,-0.6880913811,2.0193810694,-1.0815650384\F,0,-6.1011482526,2.9605
025736,-2.4492955024\F,0,-6.2761070065,1.6069378324,-0.7615667974\F,0,
-5.9144430509,0.8171749285,-2.7363534764\F,0,-0.2050549695,0.894368011
,-0.5430741241\F,0,-0.3916444584,3.037736962,-0.2562191322\F,0,-0.0301
446537,2.2477534504,-2.2309467651\H,0,-3.0650568175,-0.02791415,-0.697
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5.790464319,1.8418314763,-2.0758650812,-4.0589776006,3.620956998,-2.47
08048124,-6.1250444692,7.3377500885,-4.3357159003,-10.6166652435,3.468
5220274,-3.6110341298,-1.3003042646,3.8160771791,-2.0438617174,-11.529
4992935,5.5945390798,-4.6284977181,-11.860123423,3.0366724157,-1.43915
26791,-11.1766775947,1.5442368175,-5.1709586732,-0.3874977346,1.690110
6029,-1.0262613644,-0.7401007678,5.740490922,-0.4841839899,-0.05696513
98,4.2476384355,-4.2158784031,-5.7921179669,-0.0527500987,-1.318181253
5\PG=C01 [X(C6H2F6)]\NImag=0\\

G3 archive entries

monofluorotetrahedrane
\\0,1\C,0,0.0164425637,0.0099717654,0.0069730969\C,0,1.474367207
8,-0.0053389571,-0.00357638\C,0,0.7166151952,1.288858041,-0.0041282363
\C,0,0.7163322834,0.4202993455,1.2184564168\F,0,-1.0689825165,-0.62573
05552,-0.4449025601\H,0,2.3846374347,-0.4675596751,-0.3317296105\H,0,0
.759137615,2.3086525005,-0.3329679224\H,0,0.7585502167,0.445447535,2.2
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20934\MP4/GTBas2=-253.1737405\MP2/GTBas3=-253.2796947\MP4/GTBas3=-253.
3401592\MP2/GTLarge=-253.6066165\G3=-253.6983133\FreqCoord=0.046695933
7,0.0279695017,0.0196540564,2.775076861,0.0009954193,0.0011067931,1.35
84552399,2.4205475576,0.0001131196,1.3578719144,0.7967887236,2.2857339
064,-1.965448235,-1.1502871922,-0.8179352423,4.4685555854,-0.879409873
3,-0.6238396147,1.4195361631,4.3276818947,-0.6265104235,1.4185988571,0
.8327837767,4.2928627266\PG=C01 [X(C4H3F1)]\NImag=0\\

trifluorotetrahedrane
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23,0.0088795377,-0.0095755834\C,0,0.7533739117,1.2864245212,-0.0099468
91\C,0,0.7531666612,0.4349669058,1.2313924624\F,0,0.753244267,2.561939
0592,-0.3964958183\F,0,2.595713179,-0.6291004099,-0.3955033497\F,0,-1.
0888262986,-0.6290304076,-0.3962212367\H,0,0.7532714851,0.4353001767,2
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.1147425\MP4/GTBas2=-451.1786235\MP2/GTBas3=-451.3624868\MP4/GTBas3=-4
51.4392869\MP2/GTLarge=-451.893443\G3=-452.0508704\FreqCoord=0.0500779
326,0.0283957945,-0.0012428532,2.7972643057,0.0285032691,-0.0009997827
,1.4236628685,2.4075499041,-0.0016857123,1.423283068,0.8219617768,2.31
17142863,1.423346128,4.7625308195,-0.7497731894,4.8368882827,-1.149475
5891,-0.747907006,-1.9892887002,-1.1492491237,-0.7493814306,1.42357859
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tetrafluorotetrahedrane
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-0.5701684666,0.6534923479\C,0,-0.7053754082,0.2612896277,-0.525722032
5\C,0,0.6244249665,-0.4293945259,-0.5176117152\F,0,1.531823461,-1.0528
325934,-1.2685007569\F,0,-1.730210748,0.6408511591,-1.2883011491\F,0,-
0.7363183881,-1.3986094073,1.6017763987\F,0,0.9347158901,1.8106159573,
0.9549856871\\Version=EM64L-G09RevB.01\State=1-A\MP2/G3Bas1=-550.06280
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550.4833243\MP2/GTLarge=-551.0311628\G3=-551.221897\FreqCoord=0.708018
8869,1.3718420791,0.7241424648,-0.5576154385,-1.0594950605,1.214127572
3,-1.3107324494,0.4855185871,-0.9767089675,1.160322505,-0.7978342892,-
0.9616589011,2.8413391736,-1.9533477573,-2.3540086148,-3.2094890027,1.
1888220194,-2.3908334202,-1.3655622078,-2.5943351802,2.9722953043,1.73
37563273,3.3589240882,1.7724933841\PG=C01 [X(C4F4)]\NImag=0\\

tetrafluoro-1,3-cyclobutadiene
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8219,0.\C,0,-1.9316305911,2.6088516692,0.\C,0,-1.8741913596,1.28011358
05,0.\F,0,-1.1122121028,3.6497871352,0.\F,0,-0.9680015252,0.3137734296
,0.\F,0,-4.414393474,3.5070390905,0.\F,0,-4.270182885,0.171025342,0.\\
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/GTBas2=-550.3058028\MP2/GTBas3=-550.5180224\MP4/GTBas3=-550.6068669\M
P2/GTLarge=-551.1563578\G3=-551.3499086\FreqCoord=-6.621027215,4.77345
39071,0.,-6.5149118,2.3186762236,0.,-3.6563411714,4.9016120154,0.,-3.5
502244704,2.4468355195,0.,-2.1273909837,6.8240080964,0.,-1.8610828837,
0.6635532871,0.,-8.3101683674,6.5567368814,0.,-8.0438630643,0.39628098
99,0.\PG=CS [SG(C4F4)]\NImag=0\\

B3LYP/6-31G(d) optimized geometries

tri-t-butyltetrahedrane
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86,0.630848758,-0.4602825698\C,-0.4856701634,0.5234156343,0.6219585693
\C,0.6199589226,-0.4763647301,0.5378861073\C,1.5178620327,-1.414421834
5,1.2923534483\C,-1.4397607898,1.25900462,1.5188093426\C,1.2957782758,
1.5484849831,-1.3760854108\C,2.4707282443,-0.620482773,2.2103387645\C,
2.3481105825,-2.2505089176,0.2947194424\C,0.6626476249,-2.3722364962,2
.1497628769\C,-2.2973976279,0.2442274844,2.3053382325\C,-2.37565469,2.
1422701557,0.6659485459\C,-0.6621986261,2.1487705362,2.5111344735\C,2.
1933910273,0.7156829564,-2.3165858388\C,2.1748918329,2.5157952955,-0.5
561065667\C,0.3014076878,2.3620833785,-2.2321777279\H,1.6962695588,-2.
8183151938,-0.3785513693\H,2.9876546032,-2.9626352672,0.8306836122\H,2
.994024418,-1.6125040163,-0.3175416609\H,-0.045020081,-2.9305328154,1.
5266940128\H,0.0901041554,-1.8249239176,2.9059329098\H,1.3025550562,-3
.0956096626,2.6697887141\H,3.1085659927,0.0540917029,1.6283096782\H,3.
1221758092,-1.3020262545,2.7711005316\H,1.9113601366,-0.0160099935,2.9
330813105\H,2.7171449163,1.3693726453,-3.0248450883\H,1.5990041213,-0.
0025471068,-2.8924089281\H,2.9484539026,0.1569046768,-1.753630854\H,0.
8409486006,3.0148054237,-2.929446777\H,-0.3384635052,2.9928828492,-1.6
06291276\H,-0.3452408109,1.6990770385,-2.8177739399\H,2.7372598984,3.1
828177895,-1.2211085409\H,2.8953656917,1.9679822871,0.0614940761\H,1.5
645181586,3.1374837734,0.1083896108\H,-0.0447801116,2.8838321409,1.982
8374678\H,-0.0022344423,1.5477941494,3.1467068971\H,-1.3548873322,2.69
47122111,3.1634269318\H,-2.9210655599,1.5402944431,-0.0695355563\H,-1.
8128134123,2.9105324335,0.1253877473\H,-3.1104890018,2.6486741289,1.30
36650744\H,-2.8543209458,-0.4088475639,1.6241659665\H,-3.0205221511,0.
7672379237,2.9432770954\H,-1.6764028862,-0.3882416727,2.9483272835\H,-
1.0670724032,-1.0881940289,-1.1179904932\\Version=EM64L-G09RevB.01\Sta
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65\C,0.8082461617,-0.9753145323,-0.0234761674\C,1.9398770307,-1.979587
3224,0.0645281559\C,1.7712249173,1.8363155721,-0.1033054142\C,1.515540
1959,-3.4146778706,-0.3010846948\C,2.4914805721,-1.993947523,1.5139188
995\C,3.0793800718,-1.5909126865,-0.9067209925\C,-1.830740122,-1.72418
50409,0.028450679\C,0.9666834323,3.1292849119,0.1542131772\C,2.4133580
149,1.9484713484,-1.5093324345\C,2.8776060588,1.738293187,0.9707508014
\C,-2.6448884324,-1.2166876017,1.2480648673\C,-1.7065927492,-3.2500627
144,0.1499036976\C,-2.6200298069,-1.3988501354,-1.2665738819\H,-1.2946
341062,1.3847631059,-0.0590776838\H,0.178193902,3.2623671214,-0.594647
7518\H,1.6280674745,4.0019707381,0.1014994466\H,0.4977483674,3.1136499
726,1.1440263209\H,1.6404017052,2.0904208876,-2.2725863868\H,2.9869934
088,1.0575769758,-1.7770017263\H,3.0931878624,2.8092652605,-1.54692664
99\H,2.7179137749,-1.5427860304,-1.9404227317\H,3.8781327255,-2.341163
6072,-0.8627704255\H,3.5230238856,-0.6252572253,-0.6567654579\H,1.0572
742858,-3.4556363042,-1.2951317184\H,0.8135358408,-3.8308006656,0.4222
192436\H,2.3990944401,-4.0642921438,-0.3114549945\H,-1.186268008,-3.69
02719722,-0.7042979244\H,-2.7097579305,-3.6916852,0.1907620805\H,-1.18
23978354,-3.5401061076,1.0662623594\H,-2.0911819865,-1.775470327,-2.14
92126511\H,-2.7608814493,-0.3199846103,-1.3941370707\H,-3.6121476591,-
1.8663036321,-1.2358131192\H,3.5042784443,2.6384126969,0.9470079012\H,
3.5337753973,0.8775362502,0.8136648771\H,2.4445906385,1.6553477361,1.9
74183084\H,2.8111256914,-0.9988543828,1.8373000209\H,3.3553434769,-2.6

671567315,1.5888024973\H,1.7239822146,-2.342295443,2.2137565161\H,-2.8
071449561,-0.1344457045,1.2108163036\H,-2.1265520126,-1.4466446156,2.1
858057195\H,-3.6280702685,-1.7025238518,1.2734361468\\Version=EM64L-G0
9RevB.01\State=1-A\HF=-626.453693\PG=C01 [X(C16H28)]\

tri-t-butylmono(trimethylsilyl)tetrahedrane
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.7989230129,-0.30096185\C,0.5881982783,-0.1506227564,0.8335203987\C,1.
0082466568,-1.761604968,-1.4825466146\C,1.0303245751,2.1467449241,-0.7
977123281\C,1.0369386568,-0.4047179988,2.2459372812\Si,-2.5023149247,0
.0144916836,0.0192528162\C,0.3135326296,-1.5994885264,-2.8514252387\C,
0.6226617548,-3.1309172383,-0.8835583038\C,2.5385341686,-1.7103126202,
-1.6833516688\H,-0.452626337,-3.1856260988,-0.6812250406\H,1.154344895
7,-3.3152373746,0.0562667565\H,0.8792266236,-3.9390983959,-1.579542588
5\H,-0.7748484465,-1.672809924,-2.751591035\H,0.6445386844,-2.38364086
39,-3.5434561831\H,0.5466304272,-0.6297392649,-3.3036689418\H,2.843308
0834,-0.770776359,-2.157388595\H,2.8679781444,-2.5358039351,-2.3262551
719\H,3.0674876882,-1.79417225,-0.7275568431\C,2.5682229631,-0.5994619
914,2.2831937037\C,0.3518074332,-1.674600537,2.7944845454\C,0.65868038
27,0.7947319932,3.1409278023\H,0.5882702625,-2.5513921183,2.1824176302
\H,-0.7372997255,-1.5581981738,2.810831575\H,0.6867860912,-1.877251339
4,3.8192184311\H,1.1798270499,1.7044260214,2.8237380796\H,0.933667027,
0.5954470857,4.1839833418\H,-0.4184467286,0.9911865039,3.1058665821\H,
2.8701421636,-1.4703096712,1.6908975645\H,2.9098000591,-0.7567925791,3
.3136865017\H,3.0894377453,0.2780215066,1.8847087124\C,2.5654739374,2.
2687424597,-0.6843423509\C,0.3707402796,3.2607936678,0.0429599215\C,0.
6179766088,2.3242460145,-2.2746116687\H,2.893122313,2.1897267675,0.358
1292513\H,2.9017951404,3.238629609,-1.0711450619\H,3.0691439493,1.4830
412989,-1.2581854337\H,0.630034761,3.1669911497,1.1027764694\H,-0.7208
062754,3.224011914,-0.0421768766\H,0.7053454202,4.2471334084,-0.301155
2369\H,1.1152626816,1.5883883316,-2.9158222454\H,0.8956180151,3.323683
517,-2.6315961482\H,-0.4640118858,2.2077255603,-2.4000724294\C,-3.1765
270815,0.5511009285,-1.670202605\C,-3.141264457,1.2213197675,1.3358648
502\C,-3.1658441177,-1.7184370606,0.4121601547\H,-2.8951547666,-2.4388
097832,-0.368911573\H,-4.2606402274,-1.7086830558,0.4868582761\H,-2.77
21998353,-2.0974018207,1.3625366413\H,-2.8715164118,1.5746403972,-1.91
80980792\H,-4.2734834664,0.522191451,-1.6783763104\H,-2.822111644,-0.1
042126799,-2.4743503291\H,-2.7637555778,2.2376257257,1.1730173527\H,-2
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1 [X(C19H36Si1)]\\

tri-t-butylmono(trimethylsilyl)-1,3-cyclobutadiene
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5,1.9216124378,-0.063854952\C,-1.8911649455,0.3199043621,-0.0452424343
\C,-4.4865815478,2.7053610574,-0.5547212813\Si,-4.5108217608,-1.135327
4256,0.2588996241\C,-0.8820873682,2.9939444519,0.1623711258\C,-0.78859
56357,-0.7354417535,-0.1206990037\C,-1.4711135429,4.3516863695,0.60899
60364\C,-0.0405499146,3.2545717428,-1.1121278022\C,0.0400527589,2.5468
154695,1.3263002209\C,-5.3171012407,1.9362576576,-1.6156343191\C,-4.13
73691598,4.0636411784,-1.2019919353\C,-5.3487697555,2.979314882,0.7015
807811\C,0.4391561896,-0.2442696901,-0.9226074748\C,-1.297231757,-1.98
30944758,-0.8787377894\C,-0.3347841421,-1.1567977229,1.3003665558\C,-6
.1383815807,-0.5052893791,1.0190336938\C,-3.930961916,-2.3717142971,1.
5891903195\C,-4.9771281466,-2.0760715693,-1.327110514\H,-5.6473966946,

2.058674861,1.2057893275\H,-6.2607494544,3.5247893845,0.4260246689\H,-
4.7927127335,3.5911465154,1.4206173867\H,-4.7361629358,1.8000733736,-2
.535235329\H,-6.2186155836,2.5075085767,-1.8674560343\H,-5.6348728964,
0.9512653947,-1.2731111697\H,-1.8962183843,4.9097937155,-0.2244874475\
H,-0.6704833087,4.9707700834,1.0310553476\H,-2.2388718092,4.2260440845
,1.3800226867\H,-0.5370397997,2.4290743964,2.2509827169\H,0.809299035,
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1470368394,0.1018813781,-1.9202978114\H,1.1412350878,-1.0764353504,-1.
0528189395\H,0.9824095659,0.5609733944,-0.4267720067\H,0.0391191139,-0
.3061459422,1.8775038843\H,0.4717576784,-1.8984888376,1.2350859741\H,-
1.1622432456,-1.6006483708,1.8608797208\H,-3.6908591024,-1.8432097093,
2.5197502317\H,-3.0669759245,-2.986814006,1.3251039942\H,-4.7608063535
,-3.0559491668,1.809798713\H,-5.9711634588,-0.0093498522,1.9822548641\
H,-6.7666052769,-1.3839017483,1.2170126603\H,-6.7203246151,0.170395750
3,0.3869346224\H,-0.6785240257,3.6263156549,-1.9217947587\H,0.46621141
17,2.3576565383,-1.4727317777\H,0.7260122234,4.0142974781,-0.910980178
6\H,-3.3527874934,3.9586854713,-1.9590700757\H,-3.8202411407,4.8019231
72,-0.4660757618\H,-5.0286904406,4.4679403159,-1.6963872927\H,-5.38669
76493,-1.3990445337,-2.0857240746\H,-5.7436797507,-2.8311222197,-1.109
9727426\H,-4.1201444025,-2.5898062,-1.7744865019\H,-1.5899783815,-1.72
27804374,-1.9014845827\H,-2.1508812425,-2.4529875505,-0.3931275305\H,-
0.4989991244,-2.7335536831,-0.9330148475\\Version=EM64L-G09RevB.01\Sta
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