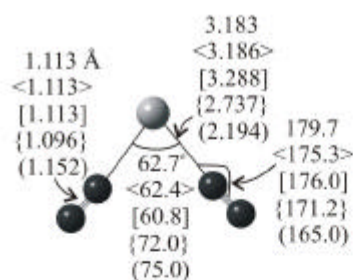
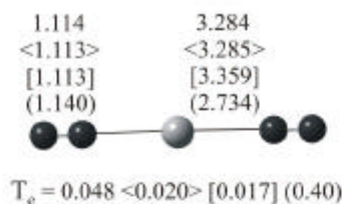


Supporting Information

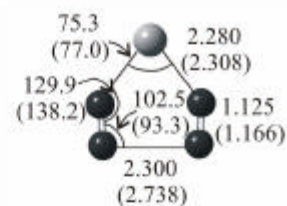
Optimized geometries of 37 isomers of doublet and quartet GaN₄ molecule at MP2/aug-cc-pVTZ <MP2/cc-pVTZ> [6-311+G(2df)] {B3LYP/aug-cc-pVTZ} (B3LYP/LANL2DZ)



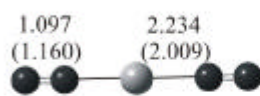
$T_e = 0.0$ eV
a. ${}^2m1 / {}^2B_1/C_{2v}$



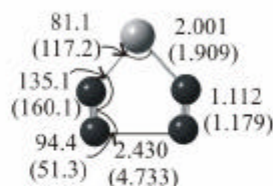
$T_e = 0.048$ <0.020> [0.017] (0.40)
b. ${}^2s2 / {}^2\Pi_u/D_{\infty h}$



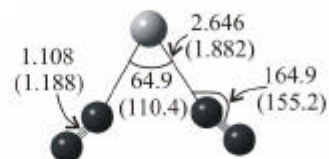
$T_e = 0.85$ (0.40)
c. ${}^2m3 / {}^2A_1/C_{2v}$



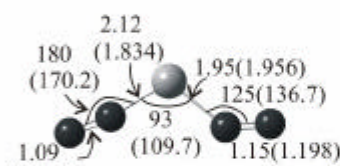
$T_e = 3.07$ (2.42)
d. ${}^4m4 / {}^4\Sigma_g^-/D_{\infty h}$



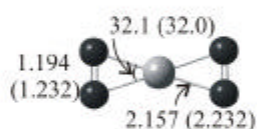
$T_e = 3.68$ (2.33)
e. ${}^4m5 / {}^4B_1/C_{2v}$



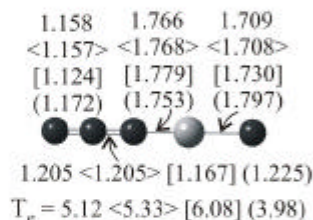
$T_e = 3.85$ (2.59)
f. ${}^4s6 / {}^4A_2/C_{2v}$



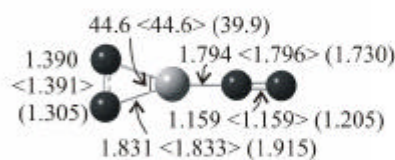
$T_e = 3.96$ (2.57)
g. ${}^4s7 / {}^4A''/C_s$



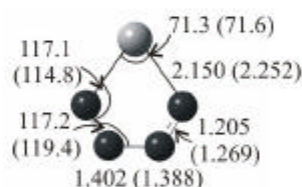
$T_e = 4.81$ (4.28)
h. ${}^4s8 / {}^4B_{1u}/D_{2h}$



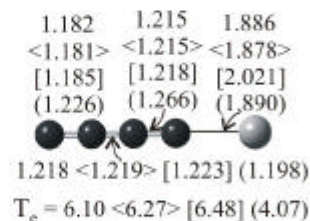
$T_e = 5.12$ <5.33> [6.08] (3.98)
i. ${}^2s9 / {}^2\Pi/C_{\infty v}$



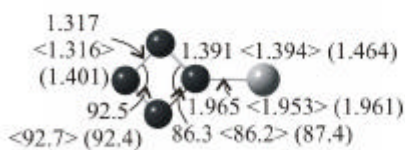
$T_e = 5.82$ <6.05> (4.08)
j. ${}^2s10 / {}^2A_2/C_{2v}$



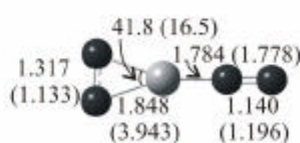
$T_e = 5.85$ (3.93)
k. ${}^4m11 / {}^4A_2/C_{2v}$



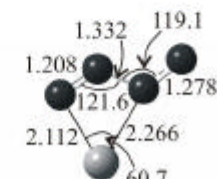
$T_e = 6.10$ <6.27> [6.48] (4.07)
l. ${}^2s12 / {}^2\Pi/C_{\infty v}$



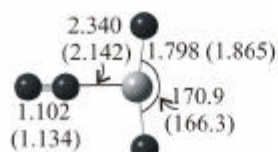
$T_e = 6.28$ <6.45> (4.63)
m. ${}^2m13 / {}^2A_2/C_{2v}$



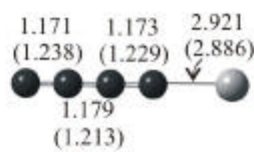
$T_e = 6.50$ (2.67)
n. ${}^4s14 / {}^4A_1/C_{2v}$



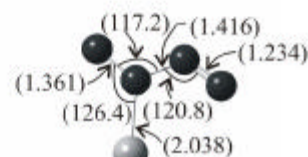
$T_e = 6.53$
o. ${}^4s15 / {}^4A''/C_s$



$T_e = 6.97$ (4.96)
p. ${}^4m16 / {}^4B_1/C_{2v}$



$T_e = 8.70$ (5.99)
q. ${}^4s17 / {}^4\Pi/C_{\infty v}$



$T_e = (4.24)$
r. ${}^4s18 / {}^4A''/C_s$

Supporting Information (continued)

