

Photochemical CO₂ Conversion on Pristine and Mg-doped Gallium Nitride (GaN): a Comprehensive DFT Study Based on Cluster Model Approach

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Supporting Information

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1. Selection of the computational protocol.

The reliability of the selected functional has been checked by performing further tests on the smaller A_GaN and using the double hybrid PBE0DH functional that combine exact HF exchange with an MP2-like correlation to a DFT calculation. Calculations performed at B3LYP gave similar adsorption energies as the more accurate double hybrid PBE0DH level of theory. Moreover, good agreement between the calculated geometric parameters using the two computational methods has been found.

Table S1. CO₂ Adsorption energy on **A_GaN** cluster model and main geometric parameters calculated using B3LYP and PBE0DH functionals.

	B3LYP/6-31G	PBE0DH/6-31G
Ads energy (eV)	-2.74	-3.35
Ga1 N1 (Å)	1.889	1.888
a2 N1(Å)	1.971	1.970
Ga2 N2 (Å)	1.850	1.845
Ga3 N2(Å)	1.861	1.856
Ga1-N1-Ga2 (°)	112.1	111.9
N1-Ga2-N2 (°)	111.9	111.9
Ga2-N2-Ga3 (°)	119.7	119.7

Mi et al. have calculated an adsorption energy of 1.76 eV for one CO₂ molecule adsorbed on pristine GaN surface by periodic boundary condition calculations. Among the tested functionals, B3LYP gives an adsorption energy whose value is closer to the one calculated by PBC approach but still the adsorption is found to be ~1 eV more favorable than PBC method. By computing the counterpoise error has implemented in Gaussian 16, the corrected adsorption energy is 2.01 eV. A similar result of 2.15 eV (see table 1 in the main text) is also computed by performing single-point calculations using more extended 6-31+G** basis sets, except for Ga, on fully optimized geometry. Based on these results we selected the B3LYP functional, LANL2DZ for Ga and 6-31G basis set for all the other atoms to perform the geometry optimization of all the stationary points. In order to obtain more

accurate energies, single point calculations on the optimized geometries using the more extended 6-31+G** basis set has been performed.

2. Comparison of the geometric parameters between Mg-doped clusters and PBC structures in ref. 21.

Table S2. Main calculated geometric parameters for clusters **A_Mg1** and **B_Mg1** along with the related values for PBC calculations taken from Ref. 21.

	A_Mg1	B_Mg1	Ref. 21
	B3LYP/ 6-31+G**	B3LYP / 6-31+G**	PBC
C-N2 (Å)	1.424	1.418	1.40
O1-Ga1 (Å)	1.986	2.335	2.23
O2-Ga3(Å)	2.490	2.053	1.98
Ga1-N2-Ga3 (°)	168.4	167.5	
O1-C-O2 (°)	125.2	126.2	

3. Stability of the selected cluster models.

The relative stabilities of the model clusters were investigated by computing the binding energies per atom, E_b , according to the following equation¹:

$$E_b = \frac{1}{N} (E_{TOT}^{cluster} - \sum_i n E_i) \quad (1)$$

where $E_{TOT}^{cluster}$ are the total energies of the pure and Mg-doped clusters, n and E_i are the number and the total energies of the free atoms, respectively. According to (1), the binding energy, E_b , is related to the energy required to add the dopant atom to GaN, characterizing the stability of the dopant-GaN systems. Therefore, the more negative the E_b value, the more stable the Mg-doped system is. All the calculated binding energies are reported in table S3.

Table S3. Binding energies (eV) calculated by eq. (1) for all the studied cluster models.

	A_GaN	A_Mg^{surf}	A_Mg^{FL}	A_Mg^{bulk}	B_GaN	B_Mg^{surf}	B_Mg^{FL}	B_Mg^{bulk}
E_b	-3.27	-3.29	-3.27	-3.29	-3.44	-3.45	-3.44	-3.46

As it can be seen from table S3, more negative binding energies are obtained by increasing the size of the cluster, which underlines the higher stabilities of bigger cluster models. However, this difference is not significant in any of the studied cases, underlines a relative stability of all the selected clusters. Moreover, doping with Mg has not influence in the relative binding energies which means that the stability of the Mg-doped clusters is essentially similar to the one of the pure cases. This behavior can be explained by considering the tiny difference between the radii of Mg^{2+} (0.65 Å) and Ga^{3+} (0.62 Å).

4. Band Gaps derived from PES/IPES process.

As mentioned in the main text, band gaps can also be derived from the gap between the photoemission (PES) and inverse-photoemission (IPES) energy levels. It is indeed possible to compute the electron affinity/ionization potential of pristine and Mg-doped GaN by the addition/removal of an electron from the neutral system. This would be analogous to the measurement of the fundamental gap arising from the photoemission/ inverse-photoemission (PES/IPES) process.

The change in the energy of a system after removal of an electron is the work function or ionization potential (IP), while the electron affinity (EA) corresponds to the change in the energy after the addition of the electron. Therefore, the IP-EA difference represents the experimental measured gap obtained from photoemission spectroscopy. Taking into account that ionization potential is defined by:

$$IP = E(N - 1) - E(N) \quad (1)$$

where $E(N - 1)$ is the energy after electron removal and $E(N)$ is the N -electron ground state, and electron affinity corresponds to:

$$EA = E(N) - E(N + 1) \quad (2)$$

where $E(N + 1)$ is the energy after electron addition, the energy gap between them can be expressed as:^{ref}

$$E_g = E(N-1) + E(N+1) - 2 E(N) \quad (3)$$

5. Simulated UV-spectra calculated by TD-DFT method.

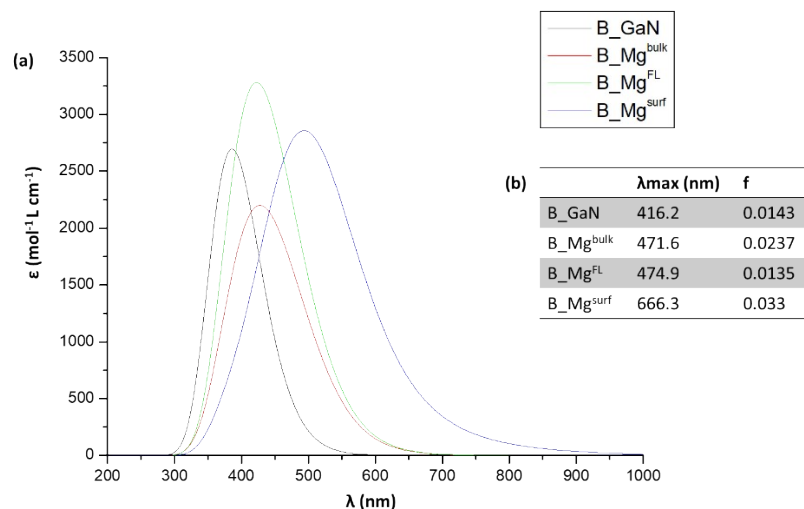


Figure S1. (a) Computed absorption spectra of pure **B_GaN** (black), and Mg-doped **B_Mg^{bulk}**(red), **B_Mg^{FL}** (green) and **B_Mg^{surf}** (blue) cluster models and their corresponding (b) λ_{max} (nm) and oscillator strengths, f .

6. Alternative reaction mechanism involving TS12'_GaN.

Figure S2 shows an alternative mechanism in which after the formation of the intermediate 12A_GaN, an additional molecule of hydrogen approaches forming 12'A_GaN. The hydrogen molecule dissociates heterolytically forming 18A_GaN, in which a Ga-H bond is formed along with an additional O-H bond, whose oxygen keeps its bond with the surface Ga atom. The following transition state, TS18_GaN involves the breaking of the uncoordinated OH group leading to 19A_GaN. The hydrogen transfer from the Ga atom to the carbon leads to the formation of 20A_GaN. As mentioned in the main text, no transition state related to the final production of methanol has been intercepted.

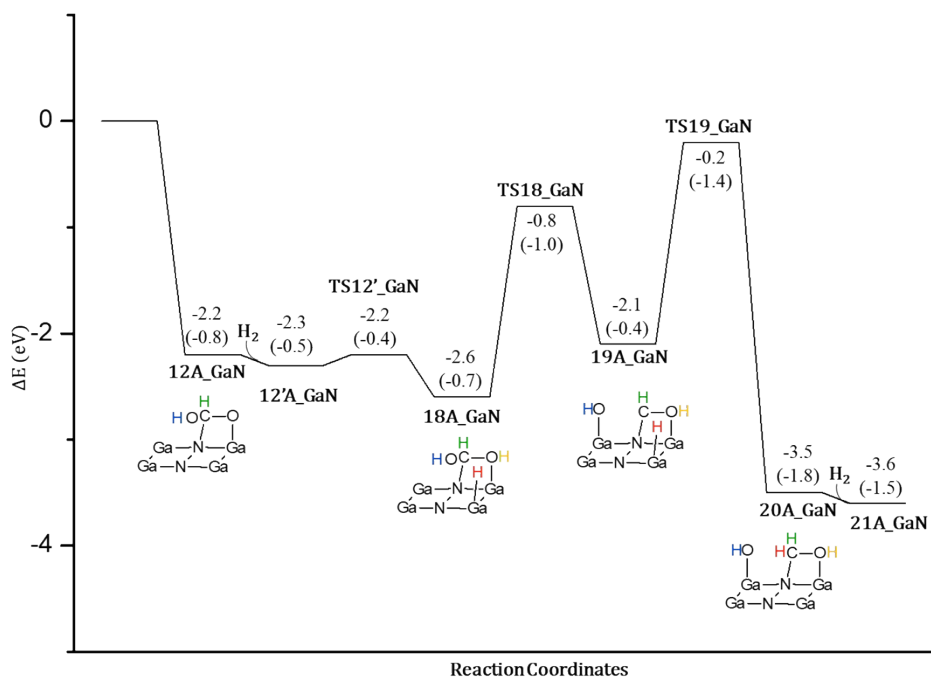


Figure S2. Alternative reaction mechanism involving TS12'_GaN.

7. Alternative reaction mechanism involving TS13'_GaN and TS13''_GaN.

Alternatively to TS13_GaN discussed in the main text, to additional transition states have been intercepted:

- TS13'_GaN, in which an uncoordinated hydrogen molecule dissociates forming a C-H and OH bonds. However the IRC of this transition state reveals once the hydrogen binds the oxygen atoms, the already bound H is transferred to the next Ga atom. However, the energy barrier involved in this step is 0.8 eV higher than the one discussed in the main text and, therefore, this mechanism can be ruled out.
- TS13''_GaN, where an uncoordinated hydrogen molecule dissociates heterolytically forming a C-H bond alongside a N-H bond, as in 22A_GaN. The adsorbed hydrogen is then transferred to the oxygen atom via TS22_GaN. A further hydrogen molecule approaches the surface and dissociates forming the already discussed intermediate 16A_GaN. By applying the ESM to this mechanism, a δE of 4.2eV is computed (TDI=10A_GaN and TDTS=TS24_GaN). Due to the higher energetic span, this mechanism can be also ruled out.

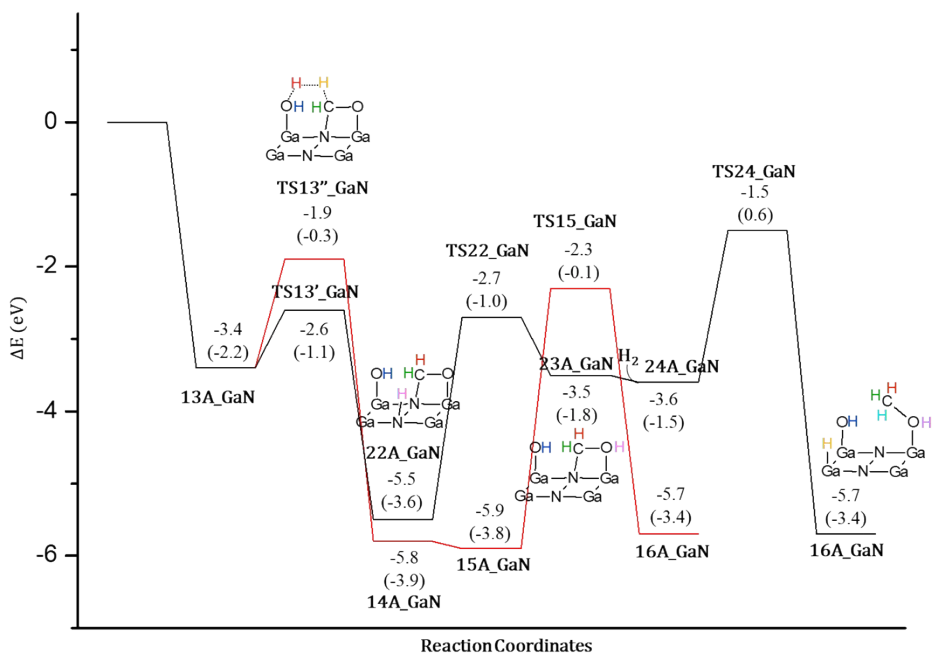


Figure S3. Alternative reaction mechanism involving TS13'_GaN and TS13''_GaN.

8. Cartesian Coordinates along with electronic energies of all the stationary points presented in the main text. The energies are given in Hartree and referred to B3LYP functional, 6-31G basis set for N, H, C, O and LAN2LDZ for Ga atoms.

A_GaN

HF=-869.7947543

Ga	1.52175000	-2.46710500	1.99682700
Ga	1.58383300	2.72585200	1.84698200
N	1.60390400	-0.64409600	1.63016900
Ga	3.16508600	0.08573600	0.95735800
N	3.22886400	-3.12907200	0.82910900
N	3.12786400	2.05781100	0.98791200
Ga	3.27331900	-2.39420100	-1.00095800
Ga	3.19448300	2.77963200	-0.93671000
N	3.18005500	-0.48015400	-0.96038500
Ga	-1.49108600	-2.48819800	1.98945600
Ga	-1.63194900	2.70134000	1.84372500
N	-1.60038400	-0.66640400	1.62481300
Ga	-0.00207400	0.03657000	0.99849600
Ga	-3.17152000	0.03969000	0.95098600
N	0.02179400	-3.15469500	0.82996700
N	-0.01801300	2.01825100	1.07192400
N	-3.18548400	-3.17807400	0.82270200
N	-3.16397700	2.01077100	0.98170200
Ga	0.03304800	-2.39313500	-0.94560000
Ga	-0.02162100	2.75509300	-0.93985400
Ga	-3.23366600	-2.44106800	-1.00175800
Ga	-3.23783100	2.73057600	-0.94295000
N	0.00804400	-0.48725900	-0.97408400
N	-3.17423700	-0.52691500	-0.96530000

Ga	1.58653500	0.17125300	-1.89968700
Ga	-1.58589100	0.14182700	-1.90190400
N	1.63099900	-3.10251600	-1.94942400
N	1.57340500	2.10349400	-1.83229200
N	-1.55484000	-3.10550400	-1.91984200
N	-1.60113400	2.07685000	-1.83590300
H	1.57334000	4.27582900	1.87184100
H	-1.64521100	4.25129100	1.86865100
H	-4.00630400	-2.85866300	1.29758000
H	-4.46720600	-0.45372500	1.59094300
H	-4.04630500	2.37339400	1.37932300
H	4.00372100	2.43488600	1.38724200
H	4.46739000	-0.38558300	1.59978000
H	4.04367200	-2.79722200	1.30561800
H	-4.44528300	-3.01766300	-1.75430900
H	-4.02389700	-0.19925300	-1.45425400
H	-4.49400700	2.19978700	-1.67976100
H	-3.26376400	4.28033900	-0.92735400
H	-0.03343900	4.30499800	-0.91909800
H	4.46004800	2.26807200	-1.67088000
H	3.19676300	4.32961000	-0.92096000
H	-1.58611600	-2.78133100	-2.89101800
H	1.63101800	-2.75671000	-2.88787000
H	-1.60556600	-0.35189100	-3.36754100
H	1.61431300	-0.32727500	-3.36435900
H	-1.62615500	2.45879600	-2.80968500
H	1.59109900	2.48356600	-2.80647600
H	-1.57488000	-4.12685000	-1.96332000
H	1.63848800	-4.10233800	-1.96016700
H	-3.17616700	-4.17803500	0.80614100
H	0.02937200	-4.15474300	0.81509600
H	3.23476300	-4.12912100	0.81248300
H	4.02621700	-0.13784900	-1.44638200
H	4.49119500	-2.94942300	-1.74541000

1A_GaN

HF=-1058.395636

Ga	1.49087500	-2.41400800	1.88738000
Ga	1.45603500	2.74994100	1.83127400
N	1.54575700	-0.61410700	1.60956500
Ga	3.16216100	0.15595200	1.08626500
N	3.28294500	-3.07908800	0.99383100
N	3.08103800	2.10062000	1.10626600
Ga	3.46316000	-2.34757100	-0.84865200
Ga	3.28221800	2.81591800	-0.81563900
N	3.32625800	-0.44489900	-0.81515400
Ga	-1.54117600	-2.60832200	1.94468200
Ga	-1.74833300	2.66509300	1.57300200
N	-1.66218400	-0.55075500	1.59077800
Ga	0.02250200	0.10112700	0.81468000
Ga	-3.22656800	0.04197400	0.51083200
N	0.08708600	-3.16530100	0.73974200
N	-0.01213400	2.02654700	0.81851100
N	-3.10827200	-3.24904600	0.47855600

N	-3.21549100	1.95747100	0.51146000
Ga	0.21662400	-2.43353600	-1.04723500
Ga	0.07718400	2.73116500	-1.07428200
Ga	-3.02971400	-2.53852500	-1.34640800
Ga	-3.12744000	2.64603300	-1.33280800
N	0.12970300	-0.53500100	-1.06432200
N	-2.99719400	-0.62121500	-1.32143500
Ga	1.79369500	0.17884700	-1.88444000
Ga	-1.36669900	0.09864100	-2.15525300
N	1.91153700	-3.10096900	-1.90258700
N	1.75186500	2.09565400	-1.83967400
N	-1.26592700	-3.16360500	-2.12640200
N	-1.40892400	2.00899900	-2.09552700
H	1.41537500	4.29968300	1.84326000
H	-1.79170500	4.21459200	1.58418100
H	-3.96991400	-2.94186600	0.88381100
H	-4.49644100	-0.54435000	1.12053800
H	-4.11160500	2.28878800	0.92053000
H	3.90977700	2.50157000	1.56800000
H	4.40638500	-0.30820200	1.83927400
H	4.05136700	-2.72931600	1.53146500
H	-4.16152000	-3.12899900	-2.19187200
H	-3.81673700	-0.30124700	-1.88168900
H	-4.31104700	2.08697900	-2.16298400
H	-3.18272100	4.19511800	-1.33173700
H	0.03569700	4.28051700	-1.06681800
H	4.61114700	2.32357100	-1.44273000
H	3.25480900	4.36584700	-0.81203200
H	-1.22569700	-2.84637500	-3.09947600
H	1.97997000	-2.76129400	-2.84076400
H	-1.25136500	-0.42089200	-3.59537500
H	1.95706700	-0.33572500	-3.33644300
H	-1.36748900	2.39247900	-3.06333600
H	1.83808800	2.47745900	-2.80462300
H	-1.26386900	-4.18541700	-2.16313800
H	1.93807100	-4.10051900	-1.90470300
H	-3.07941600	-4.24868900	0.47052300
H	0.11438600	-4.16524800	0.73448800
H	3.30893100	-4.07946900	0.98645400
H	4.20478000	-0.08877900	-1.23427500
H	4.74311500	-2.89283200	-1.47304600
C	-1.87155300	0.04934600	2.92163400
O	-2.12047900	-0.69106800	3.89210300
O	-1.79112300	1.38792500	3.00316300

B_GaN

HF=-1849.020055

Ga	3.95805700	-0.34695700	-3.27695200
Ga	0.99678900	0.95568000	-3.05348500
N	2.00170200	-0.67135700	-3.18586000
N	4.32135100	1.47926100	-3.20100000
Ga	4.24943100	-3.18054300	-1.62189100
Ga	1.38064000	-1.70751100	-1.59757000
Ga	1.71860100	-4.47638000	0.03276800

N	2.31401100	-3.41444100	-1.54595900
N	4.66549300	-1.27261800	-1.57103700
N	5.00974900	-4.02352500	0.05909700
Ga	3.58740000	2.44499100	-1.80748700
Ga	3.19369800	5.15028400	-0.17755200
Ga	0.62008500	3.70785500	-1.47217700
N	1.65958400	2.10751800	-1.67274100
N	1.26544900	4.82501400	-0.06807500
N	3.95220300	4.25229700	-1.61539500
Ga	3.90176700	-0.40644700	-0.01461000
Ga	3.48773100	2.36315300	1.55798700
Ga	4.21888200	-3.18747800	1.69100100
Ga	3.84905400	-0.44678600	3.26295600
Ga	1.04981500	1.06116300	-0.01010200
Ga	0.66274500	3.85340300	1.59736100
Ga	1.34093200	-1.67275800	1.60744200
Ga	0.99722100	1.12570300	3.20358400
N	1.97760900	-0.68585600	-0.00387500
N	1.59413700	2.08682800	1.55313100
N	2.28622900	-3.39210600	1.60953000
N	1.92310200	-0.64801500	3.17909600
N	4.29631700	1.50103600	0.01535700
N	3.92749400	4.27471700	1.60131900
N	4.64084900	-1.25002200	1.64515400
N	4.27191600	1.52356400	3.23112300
Ga	-1.24337600	-1.08646300	-3.24899400
Ga	-4.11369900	0.39012800	-3.25863300
N	-3.19483500	-1.27471600	-3.27976500
N	-0.78425100	0.74359600	-3.10693900
Ga	-0.94285300	-3.85638600	-1.62196200
Ga	-3.76985700	-2.36176900	-1.62867700
Ga	-3.42567700	-5.11284500	0.00145300
N	-2.85247500	-4.06306800	-1.61552100
N	-0.51672600	-1.94193100	-1.58815400
N	-0.19300300	-4.65075200	0.02216700
Ga	-1.60966900	1.71448500	-1.73446100
Ga	-2.00141700	4.45397000	-0.10910100
Ga	-4.48254200	3.16284000	-1.67312500
N	-3.53130600	1.53436900	-1.87471000
N	-3.91822700	4.17959900	-0.18834200
N	-1.16030400	3.51495700	-1.51264300
Ga	-1.29640800	-1.06656800	-0.03124800
Ga	-1.69649900	1.68418900	1.54577700
Ga	-0.97601000	-3.83287900	1.64275000
Ga	-1.33737700	-1.08922300	3.20709800
Ga	-4.13910500	0.41159500	-0.04209300
Ga	-4.50793900	3.18546200	1.54354300
Ga	-3.79468500	-2.33934500	1.58749900
Ga	-4.16377500	0.43411100	3.17359500
N	-3.18979100	-1.32198300	-0.06816400
N	-3.56436700	1.43954500	1.47806700
N	-2.87571000	-4.06182300	1.59116600
N	-3.23426000	-1.32766600	3.15800800
N	-0.86403000	0.84599500	-0.02179700

N	-1.24935000	3.58830600	1.53910100
N	-0.54998100	-1.89503300	1.57535100
N	-0.90991500	0.85687900	3.14863400
H	3.49830200	6.61900200	-0.02652500
H	0.77598900	5.74349500	-0.04156000
H	-1.69849200	5.94777600	-0.06209100
H	-4.42070900	5.07249200	-0.07697600
H	-6.02057300	2.96447500	-1.68279100
H	-5.65151200	0.19067200	-3.26902800
H	-5.30708000	-2.56029600	-1.63905400
H	-5.67603900	0.21333100	-0.05308400
H	-6.04506000	2.98686400	1.53312600
H	-5.70088000	0.23569400	3.16313400
H	-5.33192400	-2.53790500	1.57708100
H	-4.96293300	-5.31150500	-0.00902800
H	5.31324900	1.60652700	-3.19411600
H	4.94434400	4.38039700	-1.60777600
H	4.91942300	4.40280800	1.60792900
H	5.28862800	1.62927600	0.02178300
H	5.65747000	-1.14427100	-1.56417900
H	5.26344000	1.65160000	3.23806000
H	5.63248700	-1.12198800	1.65192600
H	6.00150400	-3.89559600	0.06580800
H	4.82687600	-3.82627900	2.93244700
H	4.45787400	-1.05269800	4.51856000
H	1.63947800	-1.15835200	4.04756900
H	2.00849100	-3.93192200	2.46148700
H	-0.73881400	-1.72380700	4.48307900
H	-0.36982100	-4.49739100	2.89698300
H	-3.55716000	-1.82946300	4.01211500
H	-3.18816900	-4.60302100	2.42604100
H	-2.73338900	-6.49971600	0.01646500
H	4.80490600	-5.00241400	0.06427700
H	2.46335200	-5.82862800	0.05195300
H	-0.39177100	-5.67349600	0.02880100
H	3.87911600	1.95545900	4.04323400
H	1.43441000	1.90526600	4.47462500
H	-1.31747000	1.28443700	4.00773800
H	-3.76227200	1.23418600	4.43912300
H	3.53515100	4.70670800	2.41311100
H	1.09031100	4.65641700	2.84459600
H	-1.66157800	4.03567100	2.37773400
H	-4.10640200	3.98531000	2.80910500
H	4.52727000	-1.11528800	-4.44947100
H	1.70175500	-1.21458800	-4.02053800
H	-0.66954900	-1.78627700	-4.48486300
H	-3.49492900	-1.88575700	-4.05606400
H	-3.15068600	-4.63676900	-2.42597000
H	-0.32536300	-4.53739000	-2.85476000
H	2.04600200	-3.96565500	-2.39048600
H	4.87136500	-3.86628400	-2.81925200

1B_GaN

HF=-1849.020055

Ga	3.91426600	0.17323300	3.29612800
Ga	0.92907900	-1.15340400	3.13880800
N	1.93124500	0.49904200	3.19130500
N	4.25931100	-1.64687000	3.15860800
Ga	4.30587400	3.06414000	1.74070800
Ga	1.41619100	1.62493400	1.61543000
Ga	1.83419000	4.45869300	0.08270700
N	2.37305100	3.32487800	1.64224700
N	4.68500700	1.15180800	1.63163700
N	5.11087000	3.95026900	0.10467300
Ga	3.51752800	-2.55786700	1.73934500
Ga	3.12218400	-5.19121000	-0.00635400
Ga	0.52601900	-3.73872900	1.29195300
N	1.57453800	-2.16611300	1.62260800
N	1.19695800	-4.82131100	-0.13241400
N	3.87192300	-4.35696100	1.47080800
Ga	3.94206800	0.35319000	0.03119000
Ga	3.50776600	-2.35237200	-1.64156400
Ga	4.34006800	3.18548500	-1.57094800
Ga	3.95194000	0.50728400	-3.24372700
Ga	1.07128800	-1.05705100	-0.05193600
Ga	0.65530800	-3.78562200	-1.78489600
Ga	1.43734700	1.72319200	-1.59717500
Ga	1.07494400	-1.01221700	-3.28830200
N	2.02237500	0.66834800	-0.00325400
N	1.61813500	-2.03958700	-1.64781000
N	2.41089200	3.42266300	-1.51933000
N	2.02964000	0.74167600	-3.18908300
N	4.29762800	-1.55844300	-0.05628600
N	3.91035200	-4.26873000	-1.74419900
N	4.72353700	1.24001700	-1.58319400
N	4.33624400	-1.47024500	-3.27108400
Ga	-1.30473400	1.19455900	3.11143700
Ga	-4.15461200	-0.40299800	3.09201200
N	-3.22013300	1.30212600	3.14421100
N	-0.96498300	-0.72303200	2.88939900
Ga	-0.87082100	3.87327600	1.64260300
Ga	-3.72888700	2.39564200	1.56515200
Ga	-3.30308900	5.19412300	0.03818900
N	-2.77371600	4.08747700	1.62398400
N	-0.46914300	1.94284400	1.53962300
N	-0.07222300	4.67709500	0.05488900
Ga	-1.72015200	-1.66243000	1.36865500
Ga	-2.06296600	-4.39449000	-0.16427500
Ga	-4.54189100	-3.11296300	1.40430100
N	-3.60486700	-1.45762400	1.56373100
N	-3.96706100	-4.08972700	-0.10684100
N	-1.24540700	-3.46508600	1.27042600
Ga	-1.24732200	1.14243300	-0.06558700
Ga	-1.66611700	-1.57023100	-1.74327400
Ga	-0.84564100	3.93242700	-1.60714200
Ga	-1.22541700	1.24851200	-3.27235300
Ga	-4.11631000	-0.31454400	-0.12280700
Ga	-4.50360300	-3.02486700	-1.81060500

Ga	-3.69041300	2.48391200	-1.64968400
Ga	-4.07779900	-0.22628300	-3.33759300
N	-3.12707600	1.40955700	-0.02892700
N	-3.52334900	-1.29521900	-1.68047300
N	-2.73824500	4.18889500	-1.57711200
N	-3.11455600	1.51763000	-3.24410300
N	-0.83287500	-0.77273500	-0.13344200
N	-1.25139400	-3.48309800	-1.76135800
N	-0.44490900	1.99110200	-1.60729200
N	-0.82500900	-0.70520000	-3.27322000
H	3.40674300	-6.65852100	-0.20688400
H	0.70131700	-5.73381600	-0.21392300
H	-1.77666600	-5.89230600	-0.24788400
H	-4.48231300	-4.96737900	-0.25498700
H	-6.07535300	-2.88641000	1.39199900
H	-5.68800500	-0.17608500	3.07995200
H	-5.26220000	2.62239300	1.55301600
H	-5.64955800	-0.08787000	-0.13492400
H	-6.03688100	-2.79814200	-1.82282000
H	-5.61107500	0.00036600	-3.34976900
H	-5.22372700	2.71064300	-1.66187700
H	-4.83639300	5.42090200	0.02604300
H	5.24852300	-1.79294600	3.16641500
H	4.86117800	-4.50323600	1.47847800
H	4.89963600	-4.41497800	-1.73635200
H	5.28696500	-1.70471700	-0.04844400
H	5.67430500	1.00552900	1.63944000
H	5.32544200	-1.61647600	-3.26330400
H	5.71277600	1.09377400	-1.57537800
H	6.10011100	3.80404700	0.11250000
H	4.98140400	3.85489800	-2.77678800
H	4.59405800	1.14466900	-4.46465700
H	1.76935600	1.28663900	-4.04452600
H	2.15671100	3.99696600	-2.35657900
H	-0.58937200	1.91094000	-4.50562000
H	-0.20203000	4.62119800	-2.81772700
H	-3.41420200	2.05293900	-4.08545400
H	-3.02686000	4.76325600	-2.39753000
H	-2.58577900	6.56743700	0.08444600
H	4.92383200	4.93233100	0.12939800
H	2.59762700	5.80106500	0.12542700
H	-0.25962300	5.69863300	0.08842200
H	3.95214300	-1.86674500	-4.10493700
H	1.51760800	-1.75612600	-4.58107700
H	-1.23130500	-1.10039400	-4.14591800
H	-3.66582500	-0.98983000	-4.62207800
H	3.52633600	-4.66526700	-2.57800100
H	1.09176600	-4.55467700	-3.05411500
H	-1.65714500	-3.89891300	-2.61895400
H	-4.09164000	-3.78834500	-3.09513100
H	4.48678000	0.89852400	4.49947300
H	1.67295100	1.06520400	4.02044900
H	-0.69661200	1.66483500	4.45855300
H	-3.51064900	1.83163800	3.97934900

H	-3.08488800	4.63014600	2.45245000
H	-0.27082800	4.46337700	2.93166500
H	2.09867500	3.86384500	2.49347100
H	4.91261900	3.69706600	2.97266900
C	-1.35231700	-1.38920600	4.07936300
O	-2.57880700	-1.43108000	4.45403500
O	-0.26722800	-1.90810500	4.66501900

A_Mg1

HF=-1067.903909

Ga	-2.02219800	2.11273000	2.32389500
Ga	-1.03011100	-2.99508600	1.68755700
N	-1.69462900	0.28979500	1.68363200
Ga	-3.05751300	-0.65736100	0.90059100
N	-3.77225300	2.47335800	0.92663200
N	-2.65942900	-2.60581900	0.78127900
Ga	-3.62100100	1.86415100	-0.90641200
Ga	-2.52730500	-3.19646800	-1.15210600
N	-3.15868200	0.00053000	-0.99922200
Ga	2.11586600	-2.34066300	1.80476100
N	1.47772200	0.71897700	1.92803200
Ga	3.11861300	0.56398700	1.13243600
N	-0.63559800	3.12678700	1.04718500
N	0.42367700	-1.99779100	0.94606500
N	2.50106700	3.77824800	1.15998800
N	3.52706300	-1.35003700	0.99365700
Ga	-0.47343800	2.49122200	-0.71407900
Ga	0.61968700	-2.54240000	-1.03541100
Ga	2.72829100	3.17530800	-0.68632100
Ga	3.76694700	-1.88820500	-0.91850800
N	-0.03957300	0.63556200	-0.87907400
N	3.06145800	1.28835200	-0.75936600
Ga	-1.43924300	-0.25968900	-1.89178200
Ga	1.65134500	0.38235100	-1.78202000
N	-2.13191500	2.92793900	-1.78795600
N	-1.05027100	-2.16346000	-1.95384900
N	0.98867300	3.55312700	-1.64089200
N	2.06282500	-1.51492100	-1.83816800
H	-0.71440800	-4.51240300	1.62975300
H	2.43460500	-3.85781400	1.74636900
H	3.35769200	3.59809900	1.64657000
H	4.27686600	1.31671900	1.82644600
H	4.42882200	-1.51948600	1.44796600
H	-3.44751200	-3.15724000	1.15575200
H	-4.46484300	-0.50030500	1.50289900
H	-4.51883200	1.96089100	1.35479300
H	3.83431700	4.02334600	-1.37385800
H	3.97084000	1.16417700	-1.24180900
H	4.91148000	-1.07828600	-1.57894100
H	4.09795500	-3.40096200	-0.98563400
H	0.93718900	-4.05833400	-1.09770800
H	-3.84966400	-2.89959300	-1.90371400
H	-2.22333900	-4.71508900	-1.21992800
H	1.10819900	3.30032100	-2.62620600

H	-2.03958000	2.64586000	-2.74300400
H	1.61961500	0.95495800	-3.23196100
H	-1.53087500	0.29988200	-3.34884900
H	2.18119000	-1.82563100	-2.82603400
H	-0.96654000	-2.47996400	-2.94278700
H	0.80754100	4.55936600	-1.62836400
H	-2.33662600	3.90578000	-1.74500400
H	2.29621200	4.75686500	1.19713300
H	-0.84122000	4.10554000	1.08680000
H	-3.97743000	3.45285600	0.96468400
H	-3.90594800	-0.47301100	-1.53397100
H	-4.90964500	2.20566800	-1.69803900
Ga	0.01753300	-0.04456700	1.08301300
Mg	0.99094600	2.62322200	2.14141700

A_Mg2

HF=-1067.855208

Ga	1.52619700	-2.47268100	2.03384400
Ga	1.58259900	2.71541800	1.88170700
N	1.67935500	-0.66928900	1.77010000
Ga	3.15620900	0.07752100	1.00369600
N	3.23049200	-3.13321800	0.83365800
N	3.13464000	2.06213800	1.00033200
Ga	3.26290100	-2.38360900	-0.97976300
Ga	3.19314100	2.78442800	-0.90160000
N	3.18126600	-0.47466500	-0.93945800
Ga	-1.49244200	-2.49509300	2.02565400
Ga	-1.63292200	2.68911700	1.87865000
N	-1.67541800	-0.69448200	1.76667700
Ga	-3.16270700	0.02828800	0.99777600
N	0.02315000	-3.16053100	0.83450200
N	-0.01964800	2.11721700	1.08270400
N	-3.18395300	-3.18534400	0.82726900
N	-3.17272800	2.01176000	0.99436100
Ga	0.03289400	-2.37273600	-0.92111700
Ga	-0.02315200	2.75830100	-0.90471300
Ga	-3.22149800	-2.43247400	-0.98060500
Ga	-3.23927900	2.73224000	-0.90770500
N	0.00750100	-0.50514200	-1.00337200
N	-3.17433100	-0.52410300	-0.94447400
Ga	1.57210600	0.17197600	-1.86520100
Ga	-1.57034900	0.14356000	-1.86718600
N	1.63225400	-3.09320200	-1.94480500
N	1.57611000	2.11472500	-1.80369100
N	-1.55339800	-3.09843000	-1.91526200
N	-1.60935100	2.08777600	-1.80669600
H	1.57136800	4.26524600	1.91468200
H	-1.64725400	4.23912200	1.91147500
H	-4.00471200	-2.86855800	1.30378700
H	-4.46677300	-0.46567400	1.60980900
H	-4.04730200	2.36260200	1.41288300
H	4.00263400	2.42792200	1.42038400
H	4.46741700	-0.39327700	1.61819000
H	4.04502200	-2.80330900	1.31155400

H	-4.44401200	-3.01222100	-1.74865000
H	-4.02388900	-0.19518900	-1.43408200
H	-4.49525100	2.20468000	-1.64715400
H	-3.26597100	4.28192200	-0.88410200
H	-0.03568700	4.30811900	-0.87595500
H	4.45887500	2.27731900	-1.63862800
H	3.19458200	4.33432600	-0.87795000
H	-1.58506200	-2.76872200	-2.88436900
H	1.63209000	-2.74258900	-2.88134600
H	-1.60569500	-0.33678500	-3.34832200
H	1.61415300	-0.31069400	-3.34526600
H	-1.62765700	2.47093800	-2.77594600
H	1.58944500	2.49699500	-2.77293800
H	-1.57307100	-4.11900600	-1.96367400
H	1.64025900	-4.09299100	-1.96060800
H	-3.17404700	-4.18524100	0.80570500
H	0.03145000	-4.16055800	0.81458300
H	3.23671000	-4.13322500	0.81179300
H	4.02614300	-0.13003400	-1.42640100
H	4.49238800	-2.93979500	-1.74014300
Mg	-0.00269800	0.06085300	1.05926800

A_Mg3

HF=-1067.899032

Ga	1.50711300	2.60320900	-1.86266700
Ga	1.59079500	-2.59675100	-1.88426900
N	1.59886400	0.75141500	-1.60822400
Ga	3.15651000	0.03050700	-0.92595200
N	3.22367200	3.23679100	-0.73436900
N	3.13904300	-1.95198100	-0.99571300
Ga	3.22420900	2.47529000	1.10260300
Ga	3.20080300	-2.70990900	0.89770600
N	3.17870900	0.54705600	0.99680100
Ga	-1.48299400	2.61672700	-1.85025900
Ga	-1.62441700	-2.57866200	-1.88188300
N	-1.59563600	0.76676200	-1.60555300
Ga	-3.16042900	0.06317100	-0.92158600
N	0.01626300	3.25595800	-0.73571800
N	-0.01275700	-1.94394200	-1.09424200
N	-3.19086200	3.27252900	-0.72932800
N	-3.16430400	-1.91760200	-0.99137600
Ga	-0.01551300	-2.69200300	0.90022900
Ga	-3.19332500	2.50689000	1.10243000
Ga	-3.23165900	-2.67414600	0.90245800
N	0.00441300	0.37517800	0.97956100
N	-3.17354000	0.58021000	1.00005400
Ga	1.56840600	-0.14251700	1.90611100
Ga	-1.56633700	-0.12181300	1.90737300
N	1.62459900	3.14478800	2.04237800
N	1.59210600	-2.08378300	1.80660600
N	-1.56083200	3.14245700	2.01181600
N	-1.61432100	-2.06481300	1.80894100
H	1.58367100	-4.14579700	-1.94445000
H	-1.63495700	-4.12789400	-1.94191700

H	-4.01065900	2.96210000	-1.21170700
H	-4.46644400	0.56394400	-1.55960700
H	-4.03993400	-2.26630700	-1.41165800
H	4.01012500	-2.31107500	-1.41746700
H	4.46771200	0.51435700	-1.56610700
H	4.03917100	2.91740900	-1.21778200
H	-4.45118100	3.05174700	1.84250000
H	-4.02378700	0.24165800	1.47930700
H	-4.48923300	-2.16271500	1.65055500
H	-3.25445200	-4.22329800	0.85204800
H	-0.02410000	-4.24114300	0.84454400
H	4.46505600	-2.21249100	1.64391000
H	3.20623500	-4.25920500	0.84725200
H	-1.59202000	2.79591500	2.97492800
H	1.62509300	2.77798700	2.97258200
H	-1.60637400	0.35614300	3.39652400
H	1.61295100	0.33827700	3.39414800
H	-1.62129100	-2.44123100	2.77547100
H	1.59581600	-2.45907400	2.77314100
H	-1.58329300	4.16191400	2.07770800
H	1.63021600	4.14410300	2.07532600
H	-3.18360300	4.27217800	-0.69070500
H	0.02202200	4.25576100	-0.69908300
H	3.22743700	4.23653000	-0.69544600
H	4.02615500	0.19705900	1.47332200
H	4.48517800	3.00214100	1.83587100
Ga	-0.00086000	0.04591900	-0.94615100
Mg	0.03210100	2.39004800	1.04624100

B_Mg1

HF=-2047.148989

Ga	-3.95050300	-0.24784900	3.30092900
Ga	-0.95567500	0.96682400	3.06838400
N	-2.01760700	-0.64194200	3.19529600
N	-4.28605700	1.57799400	3.26060800
Ga	-4.33182500	-3.04038200	1.59594600
Ga	-1.43110900	-1.64020000	1.58204000
Ga	-1.84797200	-4.37179800	-0.09411200
N	-2.41070500	-3.33708600	1.50552000
N	-4.70632600	-1.13354100	1.58075700
N	-5.12692300	-3.84364600	-0.09899900
Ga	-3.49406600	2.54642300	1.88788200
Ga	-3.03096200	5.27043000	0.30709500
N	-1.63193100	2.09820000	1.74493200
N	-1.16077600	4.91565700	0.15285400
N	-3.85088400	4.36944900	1.72543800
Ga	-3.90875100	-0.24496300	0.04373300
Ga	-3.43044700	2.53848500	-1.47052800
Ga	-4.31330900	-2.98599700	-1.71686700
Ga	-3.87781700	-0.22964900	-3.23506600
Ga	-1.03206400	1.19014500	0.09513400
Ga	-0.58180800	3.98393400	-1.45420200
Ga	-1.40039300	-1.54010700	-1.60885500
Ga	-0.98997600	1.28139000	-3.14038200

N	-2.00443300	-0.59245000	0.00947500
N	-1.55801200	2.20409400	-1.49041200
N	-2.39237400	-3.25353700	-1.64878100
N	-1.96451400	-0.48912100	-3.16919000
N	-4.27156500	1.65883700	0.04481500
N	-3.83713500	4.45148600	-1.49069800
N	-4.69229200	-1.05130900	-1.63451300
N	-4.25767400	1.74117500	-3.16993900
Ga	1.21662300	-1.12386700	3.23579200
Ga	4.11827500	0.27180800	3.26477500
N	3.16362100	-1.37941200	3.25279400
N	0.82697000	0.70814900	3.14803800
Ga	0.83299200	-3.84948200	1.55968100
Ga	3.69822200	-2.43939900	1.58507100
Ga	3.27787700	-5.14967300	-0.09460800
N	2.73958100	-4.12415300	1.53940800
N	0.46016100	-1.93990500	1.56354300
N	0.05809400	-4.60568100	-0.09470400
Ga	1.66714400	1.73511100	1.79657800
Ga	2.10155900	4.43283900	0.25567400
Ga	4.55298300	3.06315500	1.72960000
N	3.60004100	1.40732200	1.87074300
N	4.03829500	4.10727700	0.23472500
N	1.40652300	3.54842800	1.72717300
Ga	1.25567000	-1.03072800	0.02610900
Ga	1.71781700	1.73278900	-1.49108600
Ga	0.85505900	-3.76346400	-1.70007000
Ga	1.28000600	-1.00334900	-3.21120500
Ga	4.13305700	0.35306000	0.04907300
Ga	4.56774900	3.14553300	-1.48603300
Ga	3.71260200	-2.35735800	-1.63008500
Ga	4.14747500	0.43494500	-3.16568600
N	3.14309600	-1.37265400	0.03858300
N	3.58548800	1.41128100	-1.46602400
N	2.75131600	-4.06205000	-1.66037200
N	3.17422100	-1.30586800	-3.18041000
N	0.87621400	0.87644500	0.05651500
N	1.32658800	3.63278200	-1.45540700
N	0.48374500	-1.83139500	-1.59763300
N	0.90824200	0.93895700	-3.12014400
H	-3.34202800	6.75259600	0.17910600
H	-0.64357700	5.80807500	0.16715000
H	1.83588700	5.94807500	0.18179900
H	4.53442600	5.00333500	0.16955000
H	6.08512300	2.82555800	1.72966500
H	5.65039500	0.03287700	3.26536000
H	5.22993000	-2.67743200	1.58579500
H	5.66466600	0.11499900	0.05023700
H	6.09936600	2.90743800	-1.48539500
H	5.67898800	0.19698900	-3.16503600
H	5.24428200	-2.59546400	-1.62949000
H	4.80955300	-5.38788800	-0.09387600
H	-5.27447400	1.73041600	3.25974700
H	-4.83980700	4.52332200	1.72405200

H	-4.82525400	4.60522300	-1.49098100
H	-5.26007900	1.81275700	0.04464000
H	-5.69478500	-0.97963800	1.58018000
H	-5.24557000	1.89470000	-3.17064800
H	-5.68032400	-0.89769500	-1.63501000
H	-6.11506000	-3.69017800	-0.09945300
H	-4.94881100	-3.59730800	-2.96883400
H	-4.51406300	-0.80493800	-4.50436800
H	-1.69787500	-0.99157200	-4.04654000
H	-2.13264800	-3.78403800	-2.51094500
H	0.66366300	-1.60956100	-4.50174100
H	0.22895200	-4.40196500	-2.96617000
H	3.48004300	-1.79616000	-4.04384900
H	3.04531400	-4.58864900	-2.50828100
H	2.55012100	-6.51782600	-0.13277100
H	-4.94730500	-4.82716400	-0.12321100
H	-2.62759700	-5.71306800	-0.13541500
H	0.23045700	-5.63178900	-0.12055800
H	-3.85665800	2.17799300	-3.97541300
H	-1.41543600	2.07316500	-4.41709800
H	1.32104100	1.37335100	-3.97274500
H	3.76228500	1.26856800	-4.41455100
H	-3.43636100	4.88853200	-2.29572700
H	-0.99506200	4.78367300	-2.73750300
H	1.74140900	4.08393200	-2.29307200
H	4.18267700	3.97903600	-2.73492400
H	-4.55411400	-1.03337900	4.46055700
H	-1.73402600	-1.19686800	4.01933700
H	0.62357800	-1.83797600	4.46337700
H	3.44396000	-2.00183600	4.02179000
H	3.02363200	-4.71231900	2.34220900
H	0.20325200	-4.54853200	2.78389300
H	-2.15432700	-3.90771700	2.33964900
H	-4.97455700	-3.74383400	2.78125000
Mg	-0.52879000	3.84308000	1.74835800

B_Mg2

HF=-2047.107601

Ga	-3.93824200	-0.46331400	3.26258400
Ga	-1.00025300	0.92868500	3.10366900
N	-2.00019600	-0.74546800	3.17860800
N	-4.36797000	1.34892200	3.20046700
Ga	-4.14252800	-3.28201500	1.58007100
Ga	-1.31988100	-1.72370100	1.59850300
Ga	-1.57008500	-4.49229000	-0.06577400
N	-2.21094500	-3.47279900	1.51409900
N	-4.62206000	-1.39582200	1.54138200
N	-4.87643600	-4.13917900	-0.11765100
Ga	-3.62415200	2.35098400	1.83238700
Ga	-3.30501600	5.07385300	0.22483200
N	-1.70359100	2.06832000	1.70605000
N	-1.39090400	4.81034900	0.11451700
N	-4.06420000	4.14613800	1.64465900
Ga	-3.86100000	-0.48815300	0.00467300

Ga	-3.51378600	2.30385100	-1.53554900
Ga	-4.08891800	-3.25802200	-1.73259000
Ga	-3.78316100	-0.49685400	-3.27221300
Ga	-1.04836900	1.06231800	0.04220400
Ga	-0.73425200	3.87477900	-1.53264300
Ga	-1.25539100	-1.66191600	-1.60302200
Ga	-0.97894700	1.15960000	-3.16616700
N	-1.94787000	-0.72414400	0.00117200
N	-1.62990800	2.08336300	-1.52936300
N	-2.16101900	-3.41823300	-1.64010500
N	-1.86202200	-0.64883100	-3.18049200
N	-4.31830700	1.40242300	-0.01550900
N	-4.01504100	4.20062100	-1.57180600
N	-4.57294900	-1.34110600	-1.67407900
N	-4.26949400	1.45711900	-3.23042900
Ga	1.26527800	-1.03734200	3.29381500
Ga	4.09357100	0.49509600	3.31592800
N	3.22640500	-1.20979900	3.30283200
N	0.75204100	0.75171100	3.29506300
Ga	1.05754200	-3.80324700	1.61728800
Ga	3.83967800	-2.24932600	1.65710000
Ga	3.58551500	-4.99281800	-0.00192500
N	2.97376900	-3.98569400	1.61346200
N	0.57790400	-1.91668400	1.59529400
N	0.34208600	-4.62224400	-0.04354700
Ga	1.89062000	4.53615400	0.21517400
Ga	4.39693900	3.29229700	1.76003800
N	3.59445900	1.60846100	1.90973600
N	3.82314500	4.30397700	0.26400800
N	1.08054700	3.68238100	1.65255900
Ga	1.34304700	-0.98958900	0.05331100
Ga	1.67430600	1.76255100	-1.47872200
Ga	1.11422800	-3.75965300	-1.64790700
Ga	1.40758700	-0.99308400	-3.17767300
Ga	4.14300800	0.54871300	0.10003500
Ga	4.44691400	3.34723100	-1.45593400
Ga	3.88913400	-2.19475400	-1.55831700
Ga	4.19283500	0.60328400	-3.11486500
N	3.24534400	-1.22855300	0.08836100
N	3.55708500	1.56827400	-1.43579000
N	3.02137000	-3.94915700	-1.58463200
N	3.31401300	-1.18625600	-3.12554000
N	0.82356100	0.85971200	-0.00640900
N	1.17887200	3.65854700	-1.47294600
N	0.63408800	-1.85818900	-1.57485000
N	0.92790500	0.93223600	-3.11888800
H	-3.66436000	6.53948400	0.08190400
H	-0.91929300	5.74082000	0.11081100
H	1.54863500	6.01381000	0.15318700
H	4.29393100	5.21478100	0.18174100
H	5.93964700	3.13704700	1.78036400
H	5.63601500	0.33863300	3.33702300
H	5.38176000	-2.40489400	1.67807700
H	5.68539900	0.39333000	0.12166400

H	5.98887800	3.19146200	-1.43495100
H	5.73471200	0.44781200	-3.09390300
H	5.43117000	-2.35040800	-1.53741900
H	5.12760500	-5.14857500	0.01910300
H	-5.36312300	1.44811000	3.18670200
H	-5.05958000	4.24674000	1.62988900
H	-5.01006300	4.30119600	-1.58523700
H	-5.31371200	1.50295100	-0.02867400
H	-5.61722900	-1.29521500	1.52777800
H	-5.26411600	1.55743600	-3.24423200
H	-5.56771500	-1.24071800	-1.68766300
H	-5.87127400	-4.03894500	-0.13118400
H	-4.67653000	-3.90879000	-2.98735800
H	-4.37293800	-1.11066200	-4.54381400
H	-1.55664900	-1.14209300	-4.05109800
H	-1.86024400	-3.94028000	-2.49459500
H	0.83999000	-1.63656500	-4.47260400
H	0.53642800	-4.43472900	-2.91610600
H	3.65646900	-1.66795200	-3.97981300
H	3.35289800	-4.46617100	-2.42334100
H	2.93249700	-6.39828200	-0.03581100
H	-4.64417500	-5.11186000	-0.13050000
H	-2.28042200	-5.87222100	-0.10703800
H	0.56877700	-5.63778000	-0.05926700
H	-3.88258900	1.90772700	-4.03519300
H	-1.43401600	1.93001600	-4.44708600
H	1.33033200	1.38183700	-3.96393000
H	3.77890400	1.40413800	-4.37591600
H	-3.62856200	4.65149400	-2.37622200
H	-1.17984600	4.67378900	-2.78814400
H	1.58453300	4.12547000	-2.30504900
H	4.03307900	4.14780100	-2.71698800
H	-4.51081800	-1.26253700	4.42181900
H	-1.68069300	-1.27854000	4.01531700
H	0.70216700	-1.78846300	4.49323100
H	3.53243400	-1.80473600	4.08645300
H	3.27833000	-4.54841300	2.42752900
H	0.44804500	-4.53216300	2.83436300
H	-1.93482400	-4.02253500	2.35638300
H	-4.76497100	-4.00619300	2.76313600
Ga	-0.68508700	3.71235600	1.54728200
Mg	1.58934500	1.77794200	1.81764000

B_Mg3

HF=-2047.154615

Ga	3.97086200	-0.26516400	-3.26472600
Ga	0.99142500	1.01822300	-3.06464800
N	2.02366000	-0.61457200	-3.18621500
N	4.32134400	1.56148400	-3.19072900
Ga	4.30334500	-3.09252100	-1.62434700
Ga	1.43179200	-1.65917500	-1.57955700
Ga	1.80314500	-4.42781000	0.02376100
N	2.38211100	-3.37246200	-1.55512700
N	4.70310500	-1.19086300	-1.56882000

N	5.08504100	-3.94157100	0.05310700
Ga	3.54253500	2.52848100	-1.82831800
Ga	3.12989400	5.19345000	-0.15526900
N	1.65208200	2.22903900	-1.79665500
N	1.21004400	4.85245100	-0.05897200
N	3.91291800	4.32376000	-1.59715300
Ga	3.90549300	-0.34141000	-0.01050900
Ga	3.45060300	2.41683000	1.56917000
Ga	4.27102400	-3.10841000	1.68565600
Ga	3.86400300	-0.38448800	3.26068800
Ga	0.63607700	3.85062800	1.61638400
Ga	1.39052000	-1.63151700	1.58318500
Ga	1.00452800	1.16287700	3.19073800
N	2.04557500	-0.73335200	-0.00267300
N	1.59593000	2.16063700	1.62854400
N	2.35178300	-3.36079100	1.60627200
N	1.94912900	-0.62075900	3.18184900
N	4.29454500	1.57262600	0.02612800
N	3.88658300	4.33607900	1.62018500
N	4.67675600	-1.17840600	1.64740400
N	4.26856400	1.58511400	3.24166200
Ga	-1.18965300	-1.06633500	-3.23702300
Ga	-4.09739400	0.35488900	-3.25557000
N	-3.14443900	-1.28573700	-3.26909700
N	-0.79261100	0.76914500	-3.13087100
Ga	-0.86449900	-3.83804500	-1.62822400
Ga	-3.71611700	-2.39695500	-1.63386700
Ga	-3.33442900	-5.14796400	-0.01209700
N	-2.77771200	-4.09191600	-1.62230300
N	-0.47119800	-1.93307900	-1.59073400
N	-0.10878000	-4.64179100	0.01126000
Ga	-1.61845700	1.70118400	-1.71024900
Ga	-2.03610400	4.42927200	-0.09264100
Ga	-4.50551400	3.11717100	-1.66206600
N	-3.55331200	1.50907900	-1.88173800
N	-3.96205700	4.13547000	-0.16927400
N	-1.21666800	3.53267400	-1.52656000
Ga	-1.27330400	-1.04713900	-0.03506800
Ga	-1.70821700	1.65909100	1.53119000
Ga	-0.89882700	-3.82349500	1.63133500
Ga	-1.29426600	-1.09572800	3.19857800
Ga	-4.12463900	0.36613000	-0.03911800
Ga	-4.53283400	3.12983700	1.55475100
Ga	-3.74272700	-2.38471300	1.58221300
Ga	-4.15114000	0.37841800	3.17660200
N	-3.17192100	-1.37385400	-0.06596000
N	-3.59226900	1.39848500	1.50196700
N	-2.80184100	-4.10018800	1.57891200
N	-3.19818600	-1.37107900	3.15687900
N	-0.97361700	0.84351500	-0.04297700
N	-1.28747400	3.57776500	1.55102500
N	-0.50825400	-1.89498300	1.57062500
N	-0.90901500	0.84733900	3.15179300
H	3.42547800	6.67874100	-0.00086900

H	0.71603800	5.76581500	-0.02004500
H	-1.76134700	5.93561200	-0.04109900
H	-4.47101100	5.02248000	-0.05986500
H	-6.04072100	2.89758000	-1.67295300
H	-5.63240100	0.13398300	-3.26750400
H	-5.25046500	-2.61693500	-1.64576800
H	-5.65876000	0.14647300	-0.05146600
H	-6.06704300	2.90975800	1.54299700
H	-5.68533600	0.15868300	3.16477800
H	-5.27705900	-2.60467400	1.57045000
H	-4.86875700	-5.36799500	-0.02392000
H	5.31168400	1.70201300	-3.18280300
H	4.90339500	4.46581600	-1.58808700
H	4.87663300	4.47799200	1.62757500
H	5.28509900	1.71468600	0.03308500
H	5.69329300	-1.04859600	-1.56107800
H	5.25822500	1.72682100	3.24945800
H	5.66657200	-1.03641100	1.65506600
H	6.07485100	-3.79980000	0.06071400
H	4.89802100	-3.75557500	2.92693300
H	4.48970900	-0.99230700	4.52126300
H	1.67337400	-1.13571400	4.04860800
H	2.08173400	-3.89905100	2.45424900
H	-0.69705900	-1.73554800	4.48115400
H	-0.28876500	-4.49885500	2.88680000
H	-3.51350600	-1.87894100	4.00845800
H	-3.10519500	-4.64229600	2.41412800
H	-2.62289700	-6.52509300	-0.00093700
H	4.89376600	-4.92315900	0.05520500
H	2.56386900	-5.78176700	0.03917500
H	-0.29300400	-5.66642900	0.01508500
H	3.86945100	2.00895200	4.05486800
H	1.42541000	1.92336600	4.48481700
H	-1.31730600	1.26575200	4.01472900
H	-3.76137800	1.18016100	4.44472200
H	3.48789300	4.76012000	2.43302400
H	1.04368100	4.67452800	2.86303000
H	-1.69900900	4.01679400	2.39297400
H	-4.14305600	3.93119700	2.82295100
H	4.56400400	-1.02638300	-4.44651300
H	1.74024300	-1.16621400	-4.01959900
H	-0.62285400	-1.76959600	-4.48670900
H	-3.39565700	-1.86770100	-4.07661100
H	-3.06504400	-4.66075400	-2.43783600
H	-0.24115000	-4.52069100	-2.86495300
H	2.12190400	-3.91749700	-2.39777500
H	4.94567800	-3.77738000	-2.82483300
Mg	1.05486400	1.09860600	-0.02962300
Ga	0.57293200	3.73438800	-1.48520800

2A_GaN

HF=-1059.8083879

Ga	-1.47003500	2.40922700	1.89073400
Ga	-1.48851900	-2.75126500	1.77674100

N	-1.54108700	0.61694300	1.59510400
Ga	-3.16517900	-0.13113000	1.06056200
N	-3.24989100	3.10785700	1.01255400
N	-3.10526000	-2.07422200	1.05383200
Ga	-3.43246600	2.40247900	-0.84168200
Ga	-3.30734200	-2.76197900	-0.87604900
N	-3.31627600	0.49931300	-0.83229300
Ga	1.56855300	2.57850300	1.97736400
Ga	1.71751400	-2.69764000	1.52893200
N	1.66645400	0.51737000	1.59414800
Ga	-0.02221000	-0.10713000	0.79746300
Ga	3.22682600	-0.07545200	0.50708300
N	-0.05260600	3.16275500	0.76884700
N	-0.00766000	-2.03079000	0.77249400
N	3.14426800	3.21543700	0.51801400
N	3.19485200	-1.99071400	0.48442100
Ga	-0.18360600	2.45613800	-1.02862300
Ga	-0.10080200	-2.70853300	-1.12432200
Ga	3.06379500	2.53075800	-1.31606900
Ga	3.10536700	-2.65467900	-1.37238900
N	-0.11720300	0.55813300	-1.07137400
N	3.01035500	0.61340800	-1.31701200
Ga	-1.78682100	-0.12774300	-1.90528300
Ga	1.37487600	-0.07810700	-2.16605800
N	-1.86956500	3.15377200	-1.87934500
N	-1.76591800	-2.04432900	-1.88645300
N	1.30904900	3.18497400	-2.09313500
N	1.39690000	-1.98893000	-2.13183100
H	-1.46469800	-4.30144500	1.76803800
H	1.74355500	-4.24768500	1.51951500
H	4.00135700	2.89354500	0.92161000
H	4.50129100	0.48747700	1.12758500
H	4.08648100	-2.33838200	0.88839200
H	-3.93868900	-2.47286600	1.50978700
H	-4.40574600	0.33820900	1.81741000
H	-4.02369100	2.75926700	1.54320900
H	4.20428800	3.11987200	-2.15072000
H	3.82809000	0.29217000	-1.87959300
H	4.29739300	-2.09734000	-2.19155300
H	3.14385900	-4.20410900	-1.39199200
H	-0.07609000	-4.25817100	-1.13753700
H	-4.62897400	-2.24687800	-1.50029000
H	-3.29668200	-4.31202200	-0.89320800
H	1.26834700	2.88127900	-3.07049300
H	-1.93882300	2.82747400	-2.82220400
H	1.26933100	0.46254600	-3.59891500
H	-1.94061700	0.40868800	-3.35039900
H	1.35345500	-2.35881400	-3.10441900
H	-1.85362500	-2.41252300	-2.85612000
H	1.31814000	4.20714100	-2.11611600
H	-1.88530800	4.15348900	-1.86808600
H	3.12627500	4.21539500	0.52340100
H	-0.06905700	4.16303400	0.77703500
H	-3.26506700	4.10850100	1.01856400

H	-4.19722100	0.15791100	-1.25822000
H	-4.70452100	2.97058200	-1.46081600
C	1.86005700	-0.10150300	2.91480700
O	2.12603100	0.61431300	3.89813300
O	1.73833400	-1.44242000	2.98342100
H	-1.09917200	-2.25334400	4.27127400
H	-0.40244000	-2.00285200	4.14730300

TS2A_GaN

HF=-1059.560266

Ga	-1.37744000	2.43413300	1.75376800
Ga	-1.58371400	-2.68416400	1.79815200
N	-1.49713300	0.66929400	1.58802600
Ga	-3.17297000	-0.03003600	1.09859100
N	-3.09832600	3.24664600	1.06228700
N	-3.19283200	-1.94246500	1.06105400
Ga	-3.33898200	2.54246500	-0.81385400
Ga	-3.43276200	-2.61166400	-0.83272600
N	-3.29966000	0.64923400	-0.78655500
Ga	1.76932000	2.61330000	2.07851400
Ga	1.61820400	-2.76859000	1.51225500
N	1.69182400	0.41546100	1.64693700
Ga	-0.01049700	-0.13731400	0.77940800
Ga	3.22298300	-0.19939400	0.49167800
N	0.09499300	3.16328700	0.78038800
N	-0.05752400	-2.03532400	0.69704200
N	3.28706800	3.07826200	0.49177700
N	3.10848900	-2.10994800	0.48946200
Ga	-0.07189600	2.46171700	-1.02673900
Ga	-0.23009300	-2.69654200	-1.11913700
Ga	3.16082800	2.40374100	-1.33405800
Ga	2.97232400	-2.78117700	-1.40534500
N	-0.09848000	0.57492600	-1.06544100
N	3.01938200	0.48695300	-1.33661000
Ga	-1.81014900	-0.05277400	-1.88056500
Ga	1.34763000	-0.13799400	-2.17880400
N	-1.75214600	3.23800900	-1.84581900
N	-1.87191400	-1.95637300	-1.86593700
N	1.42209000	3.13198900	-2.09744300
N	1.29404900	-2.04080000	-2.14889700
H	-1.62727000	-4.23408100	1.78730600
H	1.57716900	-4.31885900	1.50065100
H	4.13475800	2.71910400	0.88469400
H	4.53217200	0.29311900	1.08145700
H	3.99281100	-2.51140000	0.84400800
H	-4.02259700	-2.29966800	1.56083900
H	-4.36376100	0.52840900	1.87747600
H	-3.88054600	2.93118200	1.60170600
H	4.31090300	2.94169800	-2.18958400
H	3.81582900	0.13244900	-1.91744100
H	4.17750700	-2.27449800	-2.23797500
H	2.94337300	-4.33076200	-1.42730600
H	-0.27263800	-4.24585300	-1.13455700
H	-4.73815500	-2.03877700	-1.44053900

H	-3.48942700	-4.16071700	-0.85192400
H	1.35665500	2.83206200	-3.07458700
H	-1.84668000	2.91668300	-2.78817500
H	1.24663100	0.41649300	-3.60596400
H	-1.95945700	0.50115900	-3.31928300
H	1.21439600	-2.40672800	-3.11597300
H	-1.98885500	-2.32200300	-2.82953900
H	1.47512800	4.15286300	-2.11924300
H	-1.72448800	4.23748700	-1.83312800
H	3.31313800	4.07830100	0.49858200
H	0.12164300	4.16386400	0.79028000
H	-3.07054900	4.24724700	1.06967500
H	-4.19982300	0.34467300	-1.20064400
H	-4.58721500	3.17701700	-1.39374600
C	1.82191300	-0.18134300	2.92646300
O	2.31238100	0.33284300	3.92763200
O	1.32158900	-1.53609000	3.01722200
H	0.12779100	-1.73661900	3.30126300
H	-0.86720200	-2.03079000	3.31685600

3A_GaN

HF=-1059.621567

Ga	-1.36417500	2.45441800	1.68082900
Ga	-1.60636900	-2.65545000	1.82967600
N	-1.48536700	0.70649700	1.56573900
Ga	-3.17738600	-0.02092700	1.12856400
N	-3.05362100	3.28758000	1.05823100
N	-3.23668700	-1.90986100	1.04193900
Ga	-3.32361600	2.56308100	-0.81772300
Ga	-3.47468500	-2.58083300	-0.78758500
N	-3.30068500	0.68031400	-0.76896600
Ga	1.85287400	2.74704200	2.06664900
Ga	1.59162900	-2.78063100	1.51959800
N	1.74120400	0.40268500	1.66858800
Ga	-0.01957000	-0.14472700	0.79667500
Ga	3.23099100	-0.26204300	0.45832100
N	0.13608700	3.16228900	0.75255700
N	-0.02523000	-2.01999400	0.72156000
N	3.32448600	3.03581700	0.44036900
N	3.08671100	-2.15799500	0.46353200
Ga	-0.04972900	2.44134500	-1.05127900
Ga	-0.27571300	-2.70769100	-1.09768600
Ga	3.17636300	2.34704000	-1.37813600
Ga	2.92335500	-2.83406700	-1.40774300
N	-0.09469700	0.55992200	-1.05945400
N	3.01236400	0.43305900	-1.36090200
Ga	-1.83337200	-0.05340800	-1.86546100
Ga	1.32332900	-0.18224600	-2.18909300
N	-1.73022200	3.23957700	-1.85989100
N	-1.90532200	-1.95013900	-1.83917400
N	1.44041800	3.09242500	-2.13489400
N	1.25176100	-2.07888100	-2.14605400
H	-1.66906700	-4.20480200	1.83137400
H	1.53195900	-4.33163700	1.52116100

H	4.17080000	2.66956700	0.82964300
H	4.53989500	0.24024700	1.04263100
H	3.96434700	-2.55900900	0.83168600
H	-4.04209200	-2.24274800	1.60788200
H	-4.34606700	0.59170900	1.90462100
H	-3.83557400	2.98612500	1.60608000
H	4.32585700	2.86578300	-2.24757400
H	3.79855700	0.06518600	-1.94928000
H	4.12802500	-2.34849700	-2.25346500
H	2.87508000	-4.38300400	-1.41709200
H	-0.33725900	-4.25613600	-1.10050800
H	-4.77757000	-1.99661000	-1.38994500
H	-3.55047800	-4.12912000	-0.79402200
H	1.36376100	2.78563700	-3.10907100
H	-1.83599300	2.91203100	-2.79892600
H	1.21998800	0.36752500	-3.62038400
H	-1.98251300	0.49402000	-3.30993400
H	1.15687400	-2.45108500	-3.10774500
H	-2.04272800	-2.32460600	-2.79757800
H	1.50582100	4.11236300	-2.16520500
H	-1.69021600	4.23871400	-1.85537800
H	3.36299500	4.03574400	0.43905200
H	0.17507400	4.16303400	0.75447900
H	-3.01362200	4.28789200	1.05745600
H	-4.20818600	0.38181300	-1.17308600
H	-4.56227000	3.21710400	-1.38575600
C	1.84101300	-0.03456900	2.94470200
O	1.94271000	0.49666100	4.04078400
O	1.81623600	-1.59477800	3.06326400
H	1.70221000	-1.83628100	4.00420900
H	-1.36542300	-1.99968700	3.28806000

TS3A_GaN

HF= -1059.48546

Ga	-1.55211900	2.34045000	1.72460300
Ga	-1.36897200	-2.78889300	1.79083600
N	-1.58003900	0.59822400	1.50614300
Ga	-3.17382400	-0.25205400	1.08530600
N	-3.31348900	3.01768500	1.07544900
N	-3.02683800	-2.16469800	1.07438100
Ga	-3.50908700	2.30007700	-0.80471800
Ga	-3.23095800	-2.84574400	-0.83137800
N	-3.33788300	0.41424100	-0.78576300
Ga	1.60360200	2.75120100	2.11046600
Ga	1.82880800	-2.63914300	1.48953400
N	1.56735900	0.44947400	1.70877600
Ga	-0.04359200	-0.15085200	0.77551300
Ga	3.20618400	0.00035100	0.55082800
N	-0.12396900	3.16657700	0.77852400
N	0.09406000	-2.04599200	0.69016100
N	3.06436200	3.31424800	0.47506800
N	3.26517700	-1.89573700	0.41753300
Ga	-0.24015300	2.44836500	-1.02811000
Ga	-0.03206400	-2.69758200	-1.13271700

Ga	2.98608500	2.62484600	-1.34374900
Ga	3.16688400	-2.54893200	-1.43400700
N	-0.14060600	0.56369500	-1.07440300
N	2.97785800	0.70564600	-1.33447500
Ga	-1.80026100	-0.17298700	-1.88501500
Ga	1.36288500	-0.03120000	-2.18819000
N	-1.98419200	3.11250700	-1.83884400
N	-1.73233700	-2.07840900	-1.86732800
N	1.18811400	3.23768000	-2.10538300
N	1.42876400	-1.93227400	-2.16828100
H	-1.29999500	-4.33791300	1.77655100
H	1.90094400	-4.18955300	1.47510600
H	3.93781600	3.01706300	0.86324400
H	4.51121100	0.62571600	1.05262500
H	4.17571700	-2.20991900	0.81136400
H	-3.83042000	-2.58197800	1.56561800
H	-4.37445700	0.21323700	1.89026700
H	-4.06828300	2.64530300	1.61774200
H	4.08262600	3.25777300	-2.21131300
H	3.79416800	0.41958900	-1.94322600
H	4.32792200	-1.95415200	-2.27095300
H	3.25022300	-4.09620100	-1.45928900
H	0.03799500	-4.24555400	-1.15150900
H	-4.57734700	-2.36788800	-1.43183900
H	-3.17510000	-4.39472900	-0.85382800
H	1.13996700	2.93566200	-3.08287100
H	-2.05966700	2.78697100	-2.78149500
H	1.20303200	0.51952800	-3.61924500
H	-1.99934800	0.37070200	-3.31757100
H	1.37812800	-2.29946600	-3.13552000
H	-1.82136100	-2.44805900	-2.83415300
H	1.16681400	4.25975000	-2.12509500
H	-2.02911100	4.11133500	-1.82402500
H	3.01789700	4.31379700	0.48406100
H	-0.17003400	4.16694800	0.79076500
H	-3.35850300	4.01773900	1.08499200
H	-4.21230300	0.04786900	-1.18897100
H	-4.80518700	2.84497200	-1.37385100
C	1.39111700	-0.08274500	2.99875000
O	1.42896800	0.44093900	4.10366000
O	2.27335200	-1.63708900	3.03596400
H	2.21236200	-1.93056800	3.96347600
H	-0.05133500	-1.14740600	3.00331500

4A_GaN

HF= -1059.624733

Ga	-1.37477500	2.44427300	1.73975900
Ga	-1.71977100	-2.67142800	1.61729000
N	-1.52224800	0.72387000	1.46679100
Ga	-3.19583900	0.02664200	0.96062900
N	-3.00689500	3.33182200	1.05250300
N	-3.27996000	-1.85683600	0.77964400
Ga	-3.17840000	2.69946200	-0.86574800
Ga	-3.42759800	-2.43215700	-1.09792800

N	-3.19517100	0.81753100	-0.91168400
Ga	1.80358200	2.52202000	2.29316900
Ga	1.48809000	-2.85292000	1.48880500
N	1.69105400	0.32892000	1.79276000
Ga	-0.04193400	-0.15245700	0.78378300
Ga	3.24272800	-0.32919600	0.62517500
N	0.19275100	3.15274300	0.92806500
N	-0.08031600	-2.01977400	0.63932300
N	3.39203800	2.97163800	0.79637300
N	3.06039300	-2.21438800	0.53717600
Ga	0.09672400	2.51874000	-0.91681500
Ga	-0.21861400	-2.61334900	-1.22665300
Ga	3.33698600	2.37459700	-1.06191200
Ga	2.98978200	-2.79395500	-1.35517100
N	0.02199700	0.64247500	-1.03157700
N	3.13777800	0.46766100	-1.15142100
Ga	-1.68183000	0.10760500	-1.95569900
Ga	1.48903700	-0.07501300	-2.10297900
N	-1.51331100	3.39337100	-1.78225600
N	-1.78813900	-1.78746400	-2.02405200
N	1.66472000	3.19078100	-1.87857500
N	1.37837000	-1.96903600	-2.15190100
H	-1.81146000	-4.21719900	1.53987900
H	1.39959300	-4.39813200	1.41093900
H	4.20593100	2.56856600	1.21615500
H	4.51621500	0.12490400	1.33215800
H	3.90134800	-2.64840300	0.95177200
H	-4.12978200	-2.19593200	1.27386300
H	-4.39742100	0.62723800	1.68988700
H	-3.82502500	3.02139900	1.53847700
H	4.54700000	2.90729600	-1.83353400
H	3.95015300	0.10766500	-1.70320600
H	4.25175800	-2.29550300	-2.10462000
H	2.91323400	-4.33967000	-1.44272500
H	-0.30928800	-4.15834000	-1.30831100
H	-4.68126600	-1.79199600	-1.74618800
H	-3.53206000	-3.97642700	-1.18408100
H	1.64026600	2.93228600	-2.86939100
H	-1.56928900	3.11311900	-2.74070300
H	1.48156000	0.54480900	-3.50522100
H	-1.73075500	0.72578800	-3.37641200
H	1.33504200	-2.29295800	-3.13483500
H	-1.87441900	-2.11205300	-3.00610800
H	1.75101600	4.20931500	-1.85541700
H	-1.45479100	4.39003200	-1.72684600
H	3.44851500	3.96887600	0.84592400
H	0.25068200	4.15003400	0.98036500
H	-2.94752200	4.32957500	1.10273300
H	-4.08103600	0.56056500	-1.38110900
H	-4.36842100	3.40977500	-1.47586500
C	1.69473900	-0.38041400	2.96121000
O	1.73013400	-1.66718200	3.05534900
O	-1.49216600	-1.94227700	3.27019000
H	-1.55139500	-2.43557300	4.10290900

H 1.67481500 0.15711400 3.91290900

5A_GaN

HF= -1060.803005

Ga	-1.37556900	2.44531500	1.70977600
Ga	-1.74398400	-2.66468200	1.57827500
N	-1.52732100	0.72318000	1.44085800
Ga	-3.20090400	0.04230300	0.90827200
N	-2.99556200	3.34558400	1.00824300
N	-3.29005900	-1.84114300	0.72626000
Ga	-3.14984700	2.71738900	-0.91303400
Ga	-3.42137000	-2.41331100	-1.15476700
N	-3.17479100	0.83524800	-0.96174100
Ga	1.80044300	2.51276800	2.30205300
Ga	1.46414500	-2.86175000	1.48395700
N	1.67966100	0.31832100	1.79359900
Ga	-0.04324000	-0.15050700	0.76180600
Ga	3.24067800	-0.34537200	0.64295200
N	0.20432000	3.15096400	0.91788700
N	-0.09187100	-2.01878700	0.62191200
N	3.40391100	2.95432900	0.82027100
N	3.04919400	-2.22969800	0.55089500
Ga	0.12552100	2.52132400	-0.92924800
Ga	-0.21211500	-2.61008400	-1.24931300
Ga	3.36616400	2.36037200	-1.03895200
Ga	2.99655400	-2.80626900	-1.34365700
N	0.04240300	0.64525700	-1.04850800
N	3.15827100	0.45419200	-1.13367100
Ga	-1.65439600	0.11922200	-1.99087400
Ga	1.51796900	-0.07861700	-2.10431500
N	-1.47134700	3.40367600	-1.81023800
N	-1.76864500	-1.77525900	-2.06228200
N	1.70650500	3.18561300	-1.87274200
N	1.39765200	-1.97216700	-2.15623300
H	-1.84240400	-4.20987700	1.49768800
H	1.36892400	-4.40640100	1.40295000
H	4.21126800	2.54669100	1.24818800
H	4.50832000	0.10137800	1.36404000
H	3.88400200	-2.66835300	0.97313800
H	-4.14781200	-2.17688700	1.20968700
H	-4.40607600	0.64699100	1.62682700
H	-3.82037300	3.03851700	1.48497000
H	4.58671300	2.88791500	-1.79718200
H	3.97480100	0.09107300	-1.67724400
H	4.26892800	-2.31299500	-2.07881400
H	2.91338300	-4.35146800	-1.43422400
H	-0.30947000	-4.15449800	-1.33413500
H	-4.66485700	-1.76611500	-1.81553000
H	-3.53246100	-3.95693000	-1.24423100
H	1.69142400	2.92859800	-2.86412900
H	-1.51840400	3.12501500	-2.76962700
H	1.52786600	0.54280100	-3.50501800
H	-1.68472200	0.73937800	-3.41042400
H	1.36348800	-2.29471600	-3.14025900

H	-1.84624600	-2.09822800	-3.04571700
H	1.79753300	4.20367900	-1.84721100
H	-1.40854600	4.39996100	-1.75278700
H	3.46473500	3.95120900	0.87184200
H	0.26656800	4.14788600	0.97222300
H	-2.93184800	4.34296300	1.06052500
H	-4.05707000	0.58296800	-1.44068900
H	-4.32946700	3.43368200	-1.53447400
C	1.66271900	-0.39142500	2.96116800
O	1.68489700	-1.67924000	3.05468900
O	-1.57081400	-1.97346700	3.26382100
H	-1.56440200	-2.53536500	4.05577400
H	1.63384400	0.14493500	3.91325600
H	-1.79768100	0.19909400	5.45426300
H	-1.75667200	-0.23894400	4.84879700

TS5A_GaN

HF= -1060.756031

Ga	-1.36070000	2.45569200	1.76578900
Ga	-1.74330500	-2.66949500	1.57626500
N	-1.47929100	0.66665600	1.62768000
Ga	-3.18061500	0.02564900	0.95539100
N	-2.99614500	3.34339900	1.02708600
N	-3.29021900	-1.84418800	0.72036600
Ga	-3.15079800	2.72240400	-0.89967600
Ga	-3.41934200	-2.40862000	-1.15710500
N	-3.16866100	0.83791600	-0.93625000
Ga	1.76507500	2.43085500	2.24730300
Ga	1.46419500	-2.86309600	1.48218000
N	1.62338400	0.34084100	1.74763600
Ga	3.21235400	-0.33962000	0.69880600
N	0.20315800	3.14897600	0.93702900
N	-0.10705600	-2.00995000	0.60774500
N	3.40298600	2.95400300	0.84040900
N	3.04911700	-2.22987100	0.54852800
Ga	0.12592900	2.54329300	-0.92688700
Ga	-0.21026700	-2.60381100	-1.25056100
Ga	3.37167700	2.35811500	-1.01946400
Ga	2.99904400	-2.79949000	-1.34404500
N	0.01844900	0.67188100	-1.05915300
N	3.15709600	0.45802400	-1.11652100
Ga	-1.66217300	0.12308500	-1.99397700
Ga	1.52543200	-0.06893400	-2.09679500
N	-1.47073800	3.41147200	-1.79103300
N	-1.76821900	-1.76607300	-2.06371700
N	1.70710600	3.19497600	-1.85295200
N	1.39668000	-1.95928400	-2.15541000
H	-1.84151900	-4.21389700	1.48916600
H	1.37017600	-4.40973100	1.39583700
H	4.21051500	2.54523100	1.26743400
H	4.50821500	0.09952400	1.37471900
H	3.88486400	-2.66916000	0.97370800
H	-4.14708700	-2.18036000	1.20767600
H	-4.40613200	0.64175200	1.63428700

H	-3.82154800	3.03358500	1.50138200
H	4.58751700	2.89729100	-1.77655600
H	3.97637400	0.09992600	-1.66685600
H	4.27125400	-2.30242500	-2.07677900
H	2.91606500	-4.34366200	-1.44017700
H	-0.30687900	-4.14822100	-1.34125800
H	-4.66279400	-1.75922800	-1.81652700
H	-3.53005500	-3.95174000	-1.25239300
H	1.69693000	2.89305200	-2.83269200
H	-1.52634700	3.12682300	-2.77387700
H	1.53029200	0.55735100	-3.49432300
H	-1.68241100	0.75273700	-3.40075000
H	1.36651000	-2.28145600	-3.13977700
H	-1.84329200	-2.08622900	-3.04630900
H	1.79801000	4.21244600	-1.82342100
H	-1.40817400	4.40746100	-1.73006600
H	3.46386000	3.95085300	0.89566800
H	0.26559700	4.14630700	0.99500500
H	-2.93288400	4.33986700	1.08168400
H	-4.05572600	0.58843400	-1.43290600
H	-4.32901000	3.43956100	-1.51679100
C	1.47887100	-0.38703900	2.98743500
O	-1.78772400	-1.93120800	3.23926100
O	1.61405100	-1.70595000	3.02567700
H	1.79017000	0.12895700	3.89843200
H	-1.48848900	-2.37530500	4.04769200
H	-0.00291600	-0.12069000	3.33601300
H	-0.77287700	0.06611300	2.90861400
Ga	-0.00442800	-0.13819100	0.70277400

6A_GaN

HF= -1060.862915

Ga	-1.50369500	2.42991800	2.02212500
Ga	-1.57255300	-2.77188000	1.57981100
N	-1.58165000	0.55019300	1.69405200
Ga	-3.22647700	-0.15950300	0.84655400
N	-3.22043600	3.13992900	0.98318600
N	-3.16768100	-2.05030500	0.71356700
Ga	-3.31551500	2.51986400	-0.91091900
Ga	-3.24195600	-2.64014900	-1.16688500
N	-3.21189100	0.62666300	-0.97522600
Ga	1.52525700	2.44551300	2.00172200
Ga	1.64137400	-2.75067700	1.50927200
N	1.62592200	0.48679300	1.72209700
Ga	3.22832100	-0.12566500	0.70405000
N	-0.01543800	3.15955900	0.91673200
N	0.01083900	-2.02085800	0.59339900
N	3.19081500	3.17890900	0.84390100
N	3.19432200	-2.01698400	0.56915600
Ga	-0.06470400	2.53984900	-0.93579300
Ga	-0.02648400	-2.62048900	-1.23664700
Ga	3.20740300	2.56215500	-1.04094700
Ga	3.18945500	-2.60142300	-1.30642900
N	-0.03373300	0.66240800	-1.01680000

N	3.12733300	0.66476800	-1.10862300
Ga	-1.64305100	-0.00103500	-2.00262900
Ga	1.52472500	0.01937700	-2.07432300
N	-1.68268800	3.29346700	-1.82452200
N	-1.63534400	-1.89304200	-2.06736600
N	1.50293500	3.28993500	-1.86282900
N	1.53779300	-1.87333100	-2.13594200
H	-1.56647500	-4.32006100	1.50186100
H	1.65168900	-4.30087900	1.43229100
H	4.02109900	2.82788600	1.27911200
H	4.48097100	0.40825200	1.40414800
H	4.04728800	-2.39826600	1.01662500
H	-4.00084500	-2.44711700	1.19126000
H	-4.45125800	0.35371800	1.59788900
H	-4.02726400	2.77857300	1.45379300
H	4.39619000	3.18630800	-1.76437200
H	3.97284000	0.35499900	-1.64100500
H	4.43088200	-2.02460900	-2.03342700
H	3.21067900	-4.14822600	-1.39323700
H	-0.01874900	-4.16850900	-1.31810300
H	-4.52117300	-2.07949000	-1.83914500
H	-3.24842500	-4.18782700	-1.25305700
H	1.52027100	2.98220200	-2.84062500
H	-1.71178300	2.99990200	-2.80584500
H	1.51522800	0.63670600	-3.48842000
H	-1.70395300	0.61703100	-3.41855900
H	1.53920600	-2.20454200	-3.11680400
H	-1.67706200	-2.22418200	-3.04703700
H	1.52534200	4.31137400	-1.83915900
H	-1.68732700	4.29176000	-1.76947200
H	3.18486100	4.17811400	0.89313700
H	-0.01998400	4.15952400	0.96893900
H	-3.22497900	4.13892400	1.03193100
H	-4.07543100	0.30583300	-1.46639800
H	-4.53834900	3.13167200	-1.57044300
C	1.72918100	-0.25989200	3.10143100
O	-1.54712800	-1.78463400	3.15197500
O	1.58089400	-1.65887700	3.02410100
H	2.70966200	0.00498700	3.52816500
H	-0.82041000	-1.93776200	3.78444500
H	0.94784200	0.15613000	3.75249800
H	-1.58788900	-0.05735400	2.55630000
Ga	0.00675100	-0.15567300	0.78142600

7A_GaN

HF= -1062.039794

Ga	-1.52586900	2.37584700	2.06544900
Ga	-1.53223100	-2.81600200	1.50930600
N	-1.58148300	0.50176700	1.69630800
Ga	-3.22230200	-0.21039200	0.84159600
N	-3.25630900	3.08650600	1.04877900
N	-3.14118900	-2.09646100	0.66426800
Ga	-3.35380700	2.50597400	-0.85728600
Ga	-3.21779100	-2.64595000	-1.22540400

N	-3.22687700	0.61589100	-0.96335200
Ga	1.50400600	2.42978500	2.02516600
Ga	1.68057500	-2.75293600	1.42275400
N	1.62295400	0.47847700	1.70382800
Ga	3.23023900	-0.09567300	0.67113900
N	-0.05167500	3.14737900	0.96652200
N	0.03447300	-2.02263100	0.53847500
N	3.15365700	3.20811900	0.87777100
N	3.22041100	-1.98279700	0.48554600
Ga	-0.10352400	2.56709900	-0.89957600
Ga	-0.00324100	-2.58498000	-1.31102600
Ga	3.16805800	2.63076800	-1.02040800
Ga	3.21187400	-2.52441200	-1.39669900
N	-0.05064500	0.69172000	-1.02130400
N	3.11053200	0.73481900	-1.12680500
Ga	-1.65642100	0.03030600	-2.01265800
Ga	1.51187000	0.09165700	-2.09892300
N	-1.73522800	3.31942900	-1.76276900
N	-1.62492600	-1.85988800	-2.11735400
N	1.44990800	3.35631100	-1.81728500
N	1.54568600	-1.79908100	-2.20157800
H	-1.50754400	-4.36186600	1.39795700
H	1.70985600	-4.30132000	1.31260000
H	3.99028000	2.85815200	1.30112700
H	4.48060000	0.44213200	1.37163100
H	4.07949200	-2.36041200	0.92589800
H	-3.96640100	-2.51312900	1.14016300
H	-4.44920100	0.27255700	1.60941800
H	-4.05579800	2.70502500	1.51546100
H	4.34468400	3.28656200	-1.73576300
H	3.95696900	0.44825800	-1.67132100
H	4.44211500	-1.91647600	-2.11731900
H	3.25162100	-4.06839300	-1.51692300
H	0.02316000	-4.13045200	-1.42587800
H	-4.50736500	-2.08683900	-1.87891800
H	-3.20564600	-4.19131300	-1.34489400
H	1.46580500	3.06990500	-2.80157900
H	-1.76598100	3.04667400	-2.75005400
H	1.48622000	0.73900900	-3.49976600
H	-1.73205500	0.67782200	-3.41404400
H	1.54717100	-2.10902100	-3.18967400
H	-1.66816300	-2.17015500	-3.10405600
H	1.45984000	4.37720300	-1.77172600
H	-1.75191200	4.31615900	-1.68621000
H	3.13540600	4.20585600	0.94864100
H	-0.06852500	4.14581700	1.04020600
H	-3.27258000	4.08398400	1.11901000
H	-4.08909900	0.29523500	-1.45702100
H	-4.58731500	3.11671100	-1.49778800
C	1.72511500	-0.28993600	3.07054600
O	-1.55716000	-1.86131800	3.09962300
O	1.68816900	-1.69407800	2.96276300
H	2.66645500	0.03187600	3.54294000
H	-0.95647000	-2.08498700	3.83122100

H	0.89100900	0.05683100	3.69725400
H	-1.57935100	-0.11989100	2.54672700
Ga	0.00797400	-0.16053300	0.75755400
H	1.08348000	-2.56045500	5.29080800
H	0.78377800	-2.73250000	5.95168000

TS7A_GaN

HF= -1061.91236

Ga	-1.56798300	2.37265200	2.11654200
Ga	-1.46808300	-2.84007100	1.52887400
N	-1.58838500	0.47712700	1.69468800
Ga	-3.20893700	-0.26560500	0.85212900
N	-3.31721500	3.02182800	1.03612000
N	-3.09290100	-2.16070600	0.68575800
Ga	-3.41093000	2.43064800	-0.85332600
Ga	-3.16797700	-2.72382600	-1.19984100
N	-3.24558300	0.53875400	-0.95927400
Ga	1.45522800	2.42673600	1.91992500
Ga	1.74222500	-2.71017900	1.42854300
N	1.60849100	0.53282200	1.65639600
Ga	3.20883700	-0.01910400	0.68460600
N	-0.11491400	3.14901500	0.94029200
N	0.09244800	-2.02059300	0.57979300
N	3.08776100	3.27635800	0.83780700
N	3.25102200	-1.91823200	0.49937700
Ga	-0.17070800	2.55314200	-0.91784900
Ga	0.04415600	-2.59615300	-1.29923600
Ga	3.10530500	2.68150800	-1.06219100
Ga	3.25696200	-2.46890500	-1.39863300
N	-0.08101700	0.67492600	-1.03840900
N	3.08994600	0.78390600	-1.14709100
Ga	-1.67071400	-0.01713300	-2.01101000
Ga	1.49740100	0.10952500	-2.10647500
N	-1.81291900	3.26738900	-1.78317100
N	-1.59440400	-1.91229500	-2.10108100
N	1.37049800	3.37058100	-1.85118300
N	1.57308100	-1.78676400	-2.19927000
H	-1.41160700	-4.38573800	1.42776200
H	1.80345000	-4.25845000	1.32858000
H	3.93332900	2.94677000	1.25986000
H	4.47430800	0.54218400	1.34444500
H	4.13030100	-2.27115700	0.91912700
H	-3.90965800	-2.59066300	1.16788200
H	-4.44881800	0.18734300	1.62055500
H	-4.10674300	2.62681500	1.50876800
H	4.26645700	3.36202100	-1.78125000
H	3.93850400	0.51668100	-1.69625900
H	4.47136800	-1.84031500	-2.12849900
H	3.32863200	-4.01255600	-1.50879900
H	0.10254900	-4.14149800	-1.40388900
H	-4.47159300	-2.19624200	-1.85169500
H	-3.12392000	-4.26936200	-1.30905100
H	1.37101700	3.07955600	-2.83493200
H	-1.85739400	2.98556600	-2.76639600

H	1.45490000	0.74335700	-3.51631500
H	-1.76101200	0.61543200	-3.41679300
H	1.57679100	-2.10063300	-3.18747100
H	-1.63621900	-2.22842500	-3.08806400
H	1.35929400	4.39180600	-1.81245000
H	-1.85010400	4.26416400	-1.71316800
H	3.04900600	4.27389500	0.90196000
H	-0.15273700	4.14736100	1.00730700
H	-3.35411200	4.01914600	1.09978600
H	-4.10162400	0.19686100	-1.44745200
H	-4.65894700	3.00696900	-1.50496000
C	1.66419000	-0.25812600	3.45489400
O	-1.44817300	-1.89823400	3.12391000
O	1.89093100	-1.69052900	3.07410500
H	0.66246200	0.02899800	3.72020700
H	-1.56448800	-0.11444100	2.55918100
H	2.52997100	0.29699900	3.76802000
H	-1.34716600	-2.26319200	4.01613300
H	1.89060200	-1.94577200	4.09700900
H	1.72550100	-1.01243100	5.05957800
Ga	0.01906100	-0.13971800	0.76608900

8A_GaN

HF= -1062.081205

Ga	-1.78388200	2.19289000	2.36729000
Ga	-1.21828600	-3.00680200	1.38216400
N	-1.61688400	0.27719600	1.71664100
Ga	-3.16238300	-0.52424800	0.83243100
N	-3.56005400	2.69382600	1.17122300
N	-2.88895100	-2.41739100	0.61288900
Ga	-3.61061000	2.19856600	-0.72759600
Ga	-2.93298800	-2.90504800	-1.33782500
N	-3.28833300	0.32407300	-0.94047400
Ga	1.26285400	2.45672500	1.85474400
Ga	1.96915100	-2.60103900	1.28832700
N	1.54592700	0.74120300	1.44440300
Ga	3.18633000	0.26782500	0.67025200
N	-0.38048600	3.09718500	1.08130700
N	0.25137300	-2.00950900	0.49404800
N	2.80002800	3.50057600	0.98508200
N	3.39168900	-1.62573800	0.44253100
Ga	-0.40473200	2.57509700	-0.79615600
Ga	0.25647600	-2.50038700	-1.43108900
Ga	2.85565200	2.99381600	-0.95192200
Ga	3.44627800	-2.09626500	-1.52434000
N	-0.17257800	0.72053000	-1.04106300
N	3.00878000	1.11478000	-1.13154400
Ga	-1.68332300	-0.04370200	-2.02277100
Ga	1.45973400	0.35917100	-2.10175200
N	-2.09316100	3.20066300	-1.63310800
N	-1.44228600	-1.92602300	-2.19772800
N	1.06967000	3.57685200	-1.69621100
N	1.70928800	-1.52416000	-2.28877000
H	-1.03125000	-4.53553100	1.20705100

H	2.16087900	-4.13092000	1.11383400
H	3.67182000	3.22379600	1.39089400
H	4.41530100	0.87273000	1.36005900
H	4.30931600	-1.93621000	0.80016200
H	-3.67359100	-2.94865400	1.03356400
H	-4.44452000	-0.25120400	1.61899200
H	-4.31099400	2.21094900	1.62429800
H	3.95618000	3.81076200	-1.62680900
H	3.87104400	0.94706200	-1.67841300
H	4.60010100	-1.33285400	-2.22319000
H	3.64816500	-3.62136800	-1.70835700
H	0.44509900	-4.02859300	-1.60968600
H	-4.27930300	-2.45946600	-1.96358800
H	-2.75849300	-4.43426300	-1.52104300
H	1.10839300	3.33409000	-2.69153300
H	-2.10237300	2.96667800	-2.63074700
H	1.36974100	1.04881600	-3.48542600
H	-1.82330300	0.64372200	-3.39208800
H	1.73366000	-1.78704000	-3.29336200
H	-1.45651600	-2.19174900	-3.20012500
H	0.97206200	4.59034700	-1.60853300
H	-2.21451600	4.18612000	-1.51542100
H	2.67662400	4.48667600	1.09703700
H	-0.50203600	4.08400700	1.19627200
H	-3.68086300	3.68014900	1.28262600
H	-4.11192400	-0.06566800	-1.44502900
H	-4.90578600	2.68649200	-1.36767500
C	2.32743400	-1.42294900	4.14239900
O	-0.90964700	-2.36122400	3.15509300
O	1.55858500	-2.15698600	3.14362100
H	1.89757000	-1.61566100	5.12863800
H	-1.39559300	-2.70004600	3.92564700
H	2.29994100	-0.35601500	3.91008900
H	-1.51753600	-0.26927700	2.58806700
Ga	0.02830200	-0.12923500	0.75270700
H	0.49757200	-2.19968800	3.29458700
H	3.35507500	-1.79152400	4.12209300

9A_GaN

HF= -871.04826

Ga	1.63516300	-2.54702400	2.12995200
Ga	1.52942900	2.76397700	1.81808200
N	1.63075400	-0.56016500	1.74104700
Ga	3.21112700	0.22218800	0.87462700
N	3.30058200	-3.05533100	0.81194400
N	3.11130800	2.13313700	0.85290000
Ga	3.31815500	-2.33648000	-1.01615400
Ga	3.10643700	2.84049700	-0.98420300
N	3.16618700	-0.43262400	-0.98934400
Ga	-1.43499700	-2.47680000	1.82803800
Ga	-1.68471900	2.66339500	1.85317900
N	-1.57302800	-0.69179200	1.62778100
Ga	-0.01402500	0.09258200	0.93763700
Ga	-3.18781400	-0.00740100	0.98305600

N	0.09557300	-3.15705500	0.85030200
N	-0.12378500	2.00638700	0.93286800
N	-3.10956800	-3.25652100	0.88151600
N	-3.21745100	1.92697200	1.01501300
Ga	0.08800800	-2.41692600	-0.95005300
Ga	-0.10834700	2.74004600	-0.94963100
Ga	-3.19933400	-2.51666600	-0.97475500
Ga	-3.32286500	2.63925800	-0.91486600
N	0.02586600	-0.52815700	-0.95578800
N	-3.17911400	-0.61679900	-0.92084300
Ga	1.56399800	0.20542600	-1.92970800
Ga	-1.60632500	0.10047700	-1.88310900
N	1.67113700	-3.08251200	-1.94732100
N	1.48236400	2.10968700	-1.86771200
N	-1.51314400	-3.16070600	-1.88051000
N	-1.68955700	2.01255200	-1.83245700
H	1.48263500	4.31362900	1.83532600
H	-1.73390000	4.21289600	1.86976700
H	-3.93233000	-2.95385000	1.36397900
H	-4.44659200	-0.55891900	1.64976900
H	-4.09555400	2.27586000	1.41850200
H	3.95022200	2.52800900	1.33197100
H	4.48308800	-0.27930500	1.55424200
H	4.11325600	-2.70207400	1.27768700
H	-4.40279200	-3.14031300	-1.68161300
H	-4.04494900	-0.31111800	-1.40140400
H	-4.57443400	2.07479300	-1.63420900
H	-3.38524700	4.18804600	-0.90726500
H	-0.15654900	4.28917000	-0.93685700
H	4.37502900	2.35501600	-1.73032100
H	3.07193700	4.39026500	-0.97659100
H	-1.56336700	-2.84279600	-2.85289300
H	1.65208700	-2.74203200	-2.88751000
H	-1.64595200	-0.41723000	-3.34205700
H	1.57229200	-0.31635400	-3.37669300
H	-1.72676000	2.39528300	-2.79891200
H	1.48862600	2.49593400	-2.83351600
H	-1.50948700	-4.18248400	-1.91824700
H	1.70223000	-4.08193800	-1.95280100
H	-3.07687400	-4.25607600	0.86994700
H	0.12718200	-4.15701300	0.84171000
H	3.33076300	-4.05562200	0.80128700
H	4.00112000	-0.05945900	-1.48795500
H	4.52903100	-2.86064500	-1.77755400
H	1.64514400	-0.13872300	2.68296700
H	1.51267300	2.04454300	3.27861400

10A_GaN

HF= -1059.629119

Ga	-1.66040300	2.59425200	2.14650000
Ga	-1.46530400	-2.74345700	1.85090200
N	-1.57448600	0.56708800	1.68771900
Ga	-3.22268000	-0.23858600	0.95229900
N	-3.34039500	3.03943600	0.82511600

N	-3.10679000	-2.14517600	0.95607800
Ga	-3.45867500	2.28637700	-0.97251500
Ga	-3.19183100	-2.89053900	-0.85893700
N	-3.27988200	0.38238700	-0.92825900
Ga	1.44973300	2.53867800	1.62919600
Ga	1.74479500	-2.61671700	1.70827200
N	1.60219700	0.61761300	1.36380100
Ga	-0.07756500	-0.14870900	0.71847000
Ga	3.26921200	-0.02930800	0.56373700
N	-0.13912100	3.16678600	0.68606200
N	0.11208400	-2.01706000	0.81121300
N	3.06133200	3.29215600	0.54031600
N	3.24266200	-1.91136900	0.70662200
Ga	-0.23670300	2.40227000	-1.09719600
Ga	0.01907000	-2.76421700	-1.00203000
Ga	3.04916300	2.53038800	-1.31831500
Ga	3.22969500	-2.63766100	-1.14494100
N	-0.13343500	0.51770900	-1.09351400
N	3.05167300	0.62991600	-1.23254500
Ga	-1.74498000	-0.26686500	-1.95404800
Ga	1.43159500	-0.14350800	-2.09454200
N	-1.86411100	3.02221400	-2.01911400
N	-1.62402500	-2.16021900	-1.84881900
N	1.31827300	3.12671000	-2.12791600
N	1.54307400	-2.03678600	-1.98888100
H	-1.40382800	-4.29211800	1.89700600
H	1.80884300	-4.16558200	1.75374400
H	3.91227800	3.00626300	0.98316300
H	4.46268900	0.62182100	1.28900800
H	4.12495400	-2.21979800	1.13489800
H	-3.91101300	-2.53664300	1.49306900
H	-4.45610100	0.27048300	1.68695600
H	-4.12361700	2.68977700	1.34150700
H	4.21451300	3.13306400	-2.08674400
H	3.89775300	0.30756500	-1.73000500
H	4.43510400	-2.07841200	-1.94287200
H	3.30621800	-4.18537200	-1.10930800
H	0.08172500	-4.31236400	-0.96046900
H	-4.50344500	-2.43063200	-1.54438700
H	-3.14309300	-4.43953600	-0.82177300
H	1.31828500	2.78906800	-3.09489400
H	-1.89326300	2.66244400	-2.95181900
H	1.39580400	0.35459700	-3.53848800
H	-1.81850300	0.22783600	-3.39526700
H	1.53124100	-2.44529900	-2.94355800
H	-1.68023100	-2.57181500	-2.80046000
H	1.30338300	4.14742700	-2.18611800
H	-1.90444500	4.02105200	-2.04317800
H	3.01965000	4.29123800	0.51028600
H	-0.18040500	4.16655200	0.65911900
H	-3.38044100	4.03921700	0.79572000
H	-4.13848900	-0.00880600	-1.37189700
H	-4.70644900	2.78159800	-1.68907400
H	-1.52663900	0.14837600	2.63103100

H	-1.39145100	-1.96812000	3.26854800
C	1.76873900	0.34986700	2.75874000
O	1.82488400	1.50236400	3.42234200
O	1.85816800	-0.85077300	3.19219600

TS10_GaN

HF= -1059.562951

Ga	1.50573700	-2.39894100	1.67844400
Ga	1.52604100	2.74094600	1.74677800
N	1.49693400	-0.60025600	1.70557400
Ga	3.16906000	0.17642100	1.05176400
N	3.20975900	-3.14136500	0.98944300
N	3.15900600	2.05468200	0.89464400
Ga	3.37198800	-2.43277400	-0.91256800
Ga	3.28731700	2.71325800	-0.94448500
N	3.25739400	-0.55202600	-0.86439800
Ga	-1.65365400	-2.64363500	2.16881200
Ga	-1.68469900	2.71868800	1.56845100
N	-1.59787900	-0.47642800	1.69107900
Ga	0.04824700	0.12609700	0.66906900
Ga	-3.22258700	0.12474400	0.65516400
N	0.00777700	-3.16438400	0.81482800
N	-0.05118400	1.99565300	0.69801600
N	-3.19324000	-3.18573900	0.63345400
N	-3.19260400	2.02481500	0.56285400
Ga	0.08564100	-2.48473600	-1.02541900
Ga	0.07579700	2.69142500	-1.12330200
Ga	-3.16055900	-2.50670800	-1.19384700
Ga	-3.13545900	2.66935600	-1.30192400
N	0.08750500	-0.60814000	-1.09162900
N	-3.07054000	-0.59344500	-1.20588400
Ga	1.74262100	0.10727300	-1.94873000
Ga	-1.46248300	0.08129900	-2.12495900
N	1.76737700	-3.19432800	-1.87169000
N	1.70990200	1.99632600	-1.92384800
N	-1.41527400	-3.19389000	-2.01680300
N	-1.45561100	1.97567100	-2.10077900
H	1.51811400	4.29136500	1.72686300
H	-1.69518100	4.26937100	1.54786300
H	-4.03866800	-2.85219400	1.05292500
H	-4.50899100	-0.43939500	1.25105000
H	-4.07059000	2.37981200	0.98181300
H	3.96695200	2.43515300	1.42936300
H	4.41153100	-0.37827200	1.74820800
H	3.99878700	-2.79720300	1.50066100
H	-4.31025300	-3.09891900	-2.01254800
H	-3.89917800	-0.27337000	-1.77102100
H	-4.35050400	2.11846200	-2.09100200
H	-3.15833600	4.21889800	-1.33245300
H	0.06672600	4.24117700	-1.14774900
H	4.58978800	2.17981000	-1.59309100
H	3.29223400	4.26319400	-0.97318100
H	-1.39252200	-2.89785900	-2.99705600
H	1.81965600	-2.87574800	-2.81826100

H	-1.38001300	-0.48322200	-3.54368500
H	1.83492600	-0.46106200	-3.36471500
H	-1.42442900	2.34243300	-3.06892000
H	1.78766900	2.36444100	-2.89009800
H	-1.43534500	-4.21606700	-2.03179400
H	1.77310800	-4.19408200	-1.85317100
H	-3.18610200	-4.18603600	0.64604000
H	0.01445800	-4.16522000	0.83052200
H	3.21523000	-4.14227700	1.00267200
H	4.13862200	-0.21851500	-1.32351100
H	4.61244700	-3.03775400	-1.51564500
H	0.65617600	-0.30469000	2.96632200
H	1.46518100	2.07190700	3.19671300
C	-1.28106100	0.28422400	2.82904600
O	-0.25104500	-0.09362600	3.57751200
O	-1.86691000	1.42067000	3.07347700

TS10'_GaN

HF= -1059.519041

Ga	-1.85936300	2.48841700	2.12795000
Ga	-1.22263700	-2.85582700	1.83728000
N	-1.67167700	0.49782600	1.62222700
Ga	-3.19481400	-0.44696900	0.94749200
N	-3.57015900	2.75920400	0.85207600
N	-2.88379100	-2.36775500	1.03758000
Ga	-3.62748100	2.01699400	-0.95442500
Ga	-2.94501200	-3.12997900	-0.86531500
N	-3.30359500	0.12059900	-0.92172100
Ga	1.21853700	2.53723300	1.71193800
Ga	1.96553800	-2.46582700	1.68050800
N	1.49713900	0.64653500	1.36387800
Ga	-0.09994300	-0.15344500	0.71976800
Ga	3.24143600	0.22350100	0.59409100
N	-0.39081000	3.14907100	0.69892400
N	0.21427900	-2.03504200	0.81313600
N	2.78784900	3.53693000	0.53907300
N	3.40124000	-1.66228300	0.63661200
Ga	-0.42248700	2.38665200	-1.08039500
Ga	0.24399500	-2.74032700	-1.02255600
Ga	2.83399700	2.78408000	-1.30516200
Ga	3.43270900	-2.35046600	-1.17961300
N	-0.18438900	0.50578400	-1.10506500
N	2.98824200	0.88586300	-1.23412200
Ga	-1.71345400	-0.38472300	-1.95617800
Ga	1.44408600	0.00072600	-2.09918500
N	-2.11183400	2.87752200	-1.99900200
N	-1.46148800	-2.27633800	-1.85330900
N	1.05071300	3.24291000	-2.12194100
N	1.68582600	-1.88828300	-2.00948100
H	-1.03431500	-4.39446300	1.87456100
H	2.15643700	-4.00445300	1.71714300
H	3.66157900	3.31944200	0.97639700
H	4.40694400	0.98656700	1.26654200
H	4.30226800	-1.87234200	1.09833100

H	-3.67884700	-2.84822200	1.49190700
H	-4.45099200	-0.09621000	1.70378700
H	-4.31949300	2.34392400	1.37014800
H	3.93687600	3.48628000	-2.09412900
H	3.85436900	0.64254000	-1.75151300
H	4.58421900	-1.69028000	-1.98001500
H	3.63589600	-3.88687000	-1.15286800
H	0.43342700	-4.27833100	-0.98982200
H	-4.29333400	-2.77555800	-1.54214600
H	-2.76940300	-4.66994700	-0.83691800
H	1.07348100	2.91135600	-3.09075600
H	-2.11614700	2.52135000	-2.93353200
H	1.34785300	0.49371700	-3.54812000
H	-1.84451200	0.10334900	-3.39073700
H	1.71512700	-2.28868200	-2.96926800
H	-1.47443300	-2.67857300	-2.81202100
H	0.95199200	4.25926100	-2.17444600
H	-2.23394900	3.86980900	-2.01737200
H	2.66434100	4.52938100	0.51474500
H	-0.51396200	4.14222000	0.67768400
H	-3.69209000	3.75248200	0.82837900
H	-4.12705900	-0.33289000	-1.35799500
H	-4.92321600	2.40319700	-1.65715400
H	-0.03405300	-0.63462600	3.10335500
C	1.57084900	0.23710900	2.78829600
O	1.57651500	1.39096200	3.48924800
O	2.21762500	-0.89399500	3.04838700
H	-1.47833400	0.12916500	2.57083900

18A_GaN

HF= -1059.585006

Ga	-1.74647400	2.60053900	2.18708500
Ga	-1.35842700	-2.78541400	1.87127100
N	-1.61995700	0.48322200	1.69109300
Ga	-3.21451700	-0.29912600	0.96900100
N	-3.43979000	2.92236000	0.83586600
N	-2.99448000	-2.23163700	1.08646500
Ga	-3.53945100	2.17379200	-0.95918900
Ga	-3.10150200	-3.00628700	-0.82278900
N	-3.30579200	0.25419900	-0.90458800
Ga	1.44856800	2.50563800	1.60834400
Ga	1.84311000	-2.54705200	1.69992500
N	1.47797000	0.61650000	1.28633400
Ga	-0.10638000	-0.12471800	0.68154100
Ga	3.21730800	0.05887400	0.64378800
N	-0.25053800	3.15916300	0.66788600
N	0.08563200	-2.02534300	0.89954800
N	2.94368600	3.39735200	0.49433000
N	3.30948400	-1.84126000	0.63266700
Ga	-0.32207300	2.38977400	-1.09678400
Ga	0.10194900	-2.76885000	-0.99414000
Ga	2.95723000	2.61425900	-1.34013100
Ga	3.30492700	-2.53136800	-1.16527500
N	-0.19828600	0.49298800	-1.13103800

N	3.01297800	0.71513900	-1.24466600
Ga	-1.75331500	-0.33208600	-1.95422500
Ga	1.43632900	-0.09016600	-2.09965300
N	-1.99081700	2.94328400	-2.02151900
N	-1.58576100	-2.23580900	-1.82059700
N	1.18499500	3.15797200	-2.15807300
N	1.56994900	-1.99531600	-1.99033600
H	-1.24224400	-4.33146100	1.92421500
H	1.96271800	-4.09377100	1.75278200
H	3.80796200	3.14341700	0.93116700
H	4.44292900	0.78128500	1.24274600
H	4.20383400	-2.07102300	1.10536900
H	-3.81242300	-2.66613700	1.53390900
H	-4.45331800	0.12136900	1.71892100
H	-4.20892800	2.54882100	1.35999500
H	4.07960500	3.26570600	-2.14171900
H	3.86449400	0.43295800	-1.76951200
H	4.48304500	-1.93407200	-1.97612300
H	3.43560400	-4.07511100	-1.12327600
H	0.21902500	-4.31360000	-0.94593100
H	-4.43398500	-2.59572600	-1.49895800
H	-2.99831300	-4.55247200	-0.77896900
H	1.18876900	2.81613600	-3.12335600
H	-2.01514900	2.57839800	-2.95206800
H	1.34738500	0.38368900	-3.55651200
H	-1.85935700	0.14574700	-3.38502300
H	1.58543100	-2.40680800	-2.94996700
H	-1.61831700	-2.64452200	-2.77858100
H	1.13419000	4.17754500	-2.22065100
H	-2.06611000	3.94012800	-2.04954800
H	2.86714200	4.39421000	0.46011600
H	-0.32515200	4.15897600	0.63789500
H	-3.51812800	3.92085400	0.80196300
H	-4.15220000	-0.16172300	-1.34093400
H	-4.82018600	2.60525600	-1.66564600
C	1.50239300	0.30973300	2.77463100
O	2.00212100	1.64600900	3.25473500
O	2.16714100	-0.91427600	2.98413400
H	-1.53528200	0.19789800	2.67491700
H	0.48782400	0.24000300	3.19865800

11A_GaN

HF= -1059.581354

Ga	-1.38792600	2.45148400	1.67435400
Ga	-1.59022800	-2.66397000	1.82985700
N	-1.49887200	0.70320900	1.54937000
Ga	-3.18106800	-0.04557600	1.11184100
N	-3.08179200	3.26503600	1.03569900
N	-3.22440600	-1.93398100	1.02728100
Ga	-3.33481300	2.53382500	-0.83881900
Ga	-3.44416500	-2.61102600	-0.79808900
N	-3.29733400	0.65165400	-0.78764400
Ga	1.81811800	2.72312000	2.08453900
Ga	1.61054000	-2.76437700	1.53829900

N	1.73138900	0.43580300	1.68346500
Ga	-0.03518300	-0.13728000	0.77185700
Ga	3.23639400	-0.23750000	0.46916800
N	0.11042000	3.16545100	0.74846900
N	-0.01000400	-2.01084800	0.72782000
N	3.30156300	3.06446200	0.45450200
N	3.11025900	-2.13210700	0.47776600
Ga	-0.06028800	2.44263500	-1.05580800
Ga	-0.24245300	-2.71211900	-1.08978600
Ga	3.16914300	2.37191100	-1.36278600
Ga	2.95901400	-2.81287600	-1.38144300
N	-0.09183000	0.56119500	-1.07048100
N	3.02048400	0.45695000	-1.34560300
Ga	-1.82177800	-0.07309600	-1.87712700
Ga	1.34274200	-0.17664700	-2.18171900
N	-1.74156500	3.22091700	-1.87477300
N	-1.87433700	-1.96951600	-1.84263300
N	1.43169200	3.09918600	-2.13148700
N	1.28462200	-2.07268300	-2.13138700
H	-1.64011600	-4.21378600	1.83504900
H	1.56351600	-4.31474300	1.54308000
H	4.14860100	2.70589700	0.84944200
H	4.53646600	0.28047700	1.07042100
H	3.98514900	-2.52411700	0.86301100
H	-4.02789800	-2.27193100	1.59326300
H	-4.35680600	0.56065200	1.88137000
H	-3.86431600	2.95839200	1.57989200
H	4.31950500	2.89607000	-2.22731800
H	3.81344500	0.09181200	-1.92520500
H	4.16461000	-2.31975100	-2.22162100
H	2.92365700	-4.36245600	-1.38735900
H	-0.29137300	-4.26126100	-1.08920300
H	-4.74840700	-2.03904100	-1.40922100
H	-3.50722200	-4.15994900	-0.80117600
H	1.36307100	2.78949400	-3.10536000
H	-1.83931900	2.89028400	-2.81358800
H	1.24208000	0.36906600	-3.61156400
H	-1.96306300	0.46989200	-3.31950600
H	1.19922500	-2.44880100	-3.09239400
H	-2.00306600	-2.34791900	-2.80058300
H	1.48887100	4.11958100	-2.16392700
H	-1.70980300	4.22035800	-1.87244400
H	3.33178500	4.06443400	0.45093800
H	0.14125100	4.16616000	0.74801200
H	-3.05000100	4.26559300	1.03274700
H	-4.19980100	0.34451600	-1.19498800
H	-4.57597300	3.17627200	-1.41654700
C	1.76493200	-0.22875900	2.86819100
O	1.68598000	0.49824300	4.01051400
O	1.85742900	-1.51547500	3.03369200
H	1.64284900	-0.09047700	4.79616400
H	-1.39537200	-1.98116100	3.27882200

TS11_GaN

HF= -1059.498255

Ga	1.55720300	-2.35621500	1.72865500
Ga	1.37220400	2.78410400	1.79387600
N	1.59075300	-0.61407200	1.48609600
Ga	3.17524300	0.24847000	1.06552000
N	3.31876000	-3.01738200	1.04305100
N	3.02625300	2.16386500	1.06624000
Ga	3.50074100	-2.29296400	-0.83136200
Ga	3.21862800	2.85380800	-0.83892000
N	3.32969200	-0.40613300	-0.80831800
Ga	-1.55867600	-2.69921900	2.11863800
Ga	-1.82755100	2.63305900	1.51122100
N	-1.56673800	-0.46198900	1.71574800
Ga	0.04983500	0.14027900	0.77661000
Ga	-3.20549800	-0.00954500	0.55118800
N	0.12766200	-3.16886600	0.76438300
N	-0.09408800	2.04248700	0.70256500
N	-3.06232300	-3.31858200	0.47900600
N	-3.27175800	1.89249700	0.44251100
Ga	0.23506700	-2.44517100	-1.03727900
Ga	0.01809000	2.70316100	-1.12208700
Ga	-2.99382900	-2.62468000	-1.33667000
Ga	-3.18217900	2.55228800	-1.40505200
N	0.13062400	-0.55900600	-1.07925800
N	-2.98889200	-0.70423500	-1.32532900
Ga	1.78510700	0.18269900	-1.89489100
Ga	-1.37824400	0.03858100	-2.18087500
N	1.97235100	-3.10152800	-1.86374500
N	1.71470100	2.08930700	-1.86907800
N	-1.20135000	-3.22907300	-2.11210400
N	-1.44771100	1.94069800	-2.15186900
H	1.30145800	4.33303800	1.78652100
H	-1.90083900	4.18216100	1.50311200
H	-3.93372800	-3.02371200	0.87354800
H	-4.50854700	-0.63403300	1.07621900
H	-4.17750700	2.20311400	0.84465100
H	3.83251800	2.58083700	1.55336400
H	4.38143300	-0.21511500	1.86322900
H	4.07621900	-2.64634200	1.58244200
H	-4.09643300	-3.25190300	-2.20106000
H	-3.80933800	-0.41442200	-1.92298600
H	-4.34769500	1.96004200	-2.23768700
H	-3.26747900	4.09984100	-1.42350800
H	-0.05362600	4.25142700	-1.13401500
H	4.56199500	2.37998100	-1.44928000
H	3.16100900	4.40286600	-0.85464000
H	-1.15927800	-2.92298800	-3.08862400
H	2.04190600	-2.77203600	-2.80545600
H	-1.22808500	-0.50471300	-3.61459700
H	1.97584700	-0.35360300	-3.33116300
H	-1.40335700	2.31212500	-3.11820300
H	1.79775000	2.46296900	-2.83501200
H	-1.17906700	-4.25103000	-2.13618100
H	2.01840700	-4.10035400	-1.85330700

H	-3.01465000	-4.31783700	0.48355600
H	0.17480100	-4.16870700	0.77201900
H	3.36477300	-4.01732500	1.04818300
H	4.20096600	-0.03717300	-1.21430700
H	4.79572900	-2.83285200	-1.41423400
H	0.13782700	1.08131600	2.99087100
C	-1.47356100	0.31659000	2.91606300
O	-1.41557600	-0.44058600	4.06290800
O	-2.11888300	1.48620100	3.01537800
H	-1.42184700	0.14576000	4.84887900

12A_GaN

HF= -1059.576019

Ga	-1.47733500	2.37484800	1.90561700
Ga	-1.42468100	-2.77238100	1.81164900
N	-1.53812400	0.58487200	1.65236700
Ga	-3.16022200	-0.18067900	1.14141700
N	-3.28410200	3.06321600	1.10624200
N	-3.06955800	-2.11756100	1.13261000
Ga	-3.50328900	2.35652700	-0.75054600
Ga	-3.30911900	-2.80258900	-0.79485300
N	-3.36161200	0.45765000	-0.74233100
Ga	1.58148400	2.58358000	1.92618700
Ga	1.77261000	-2.67374600	1.48369900
N	1.65092600	0.53004500	1.58535900
Ga	-0.01791800	-0.11165700	0.81104200
Ga	3.21091100	-0.02930800	0.49171900
N	-0.09529700	3.16213400	0.78267200
N	0.00332200	-2.03227400	0.75337300
N	3.09240800	3.25963000	0.45235700
N	3.21231500	-1.94803900	0.40304200
Ga	-0.25622700	2.45430600	-1.01808800
Ga	-0.11083700	-2.70456400	-1.12301500
Ga	2.98259600	2.56585600	-1.37925300
Ga	3.08715900	-2.60621300	-1.45111700
N	-0.17453700	0.56206200	-1.05728500
N	2.94814100	0.65503200	-1.37565600
Ga	-1.84564800	-0.14860900	-1.85566200
Ga	1.31011200	-0.05319800	-2.18892500
N	-1.97789400	3.13444700	-1.81914800
N	-1.80715900	-2.06250700	-1.84242300
N	1.19365300	3.20973100	-2.11225900
N	1.34905400	-1.96295100	-2.16676500
H	-1.37996200	-4.32228800	1.79850600
H	1.82024500	-4.22401400	1.47008200
H	3.96428400	2.94895300	0.83354800
H	4.50182900	0.54936700	1.02071000
H	4.12006600	-2.28111500	0.78524200
H	-3.88434600	-2.52725800	1.60674500
H	-4.38187100	0.27644800	1.93290600
H	-4.04001700	2.70311300	1.65523700
H	4.08715300	3.18450400	-2.24236000
H	3.75653300	0.35128400	-1.96885300
H	4.25051600	-2.03075800	-2.29845700

H	3.14625500	-4.15488900	-1.47551400
H	-0.06524200	-4.25370400	-1.14075300
H	-4.65287900	-2.30436300	-1.38457600
H	-3.27768800	-4.35233100	-0.81611000
H	1.13260800	2.90762300	-3.08901500
H	-2.06632600	2.80925400	-2.76077700
H	1.15343100	0.49029700	-3.62328200
H	-2.04824700	0.39178900	-3.29473100
H	1.28849900	-2.33069700	-3.13802700
H	-1.91033700	-2.42897200	-2.80975500
H	1.18814700	4.23201700	-2.13290700
H	-2.00708000	4.13386200	-1.80500400
H	3.06156600	4.25953500	0.46062900
H	-0.12553500	4.16276800	0.79403200
H	-3.31336800	4.06379800	1.11511000
H	-4.24810000	0.10563800	-1.14739400
H	-4.79873900	2.91148800	-1.33030600
C	1.79928600	-0.12343000	2.94116700
O	3.11769000	0.29614900	3.40195100
O	1.69548700	-1.52727200	2.96932500
H	3.36586800	-0.25496100	4.17274500
H	1.04344300	0.28736800	3.62400900

TS12_GaN

HF= -1059.557017

Ga	-1.42821300	2.51089000	2.04522400
Ga	-1.52808100	-2.68890800	1.88256600
N	-1.54336000	0.66833600	1.61312500
Ga	-3.16546000	-0.05542800	1.08087800
N	-3.21986200	3.15915200	0.90845600
N	-3.13332900	-2.02327700	1.13017400
Ga	-3.40952400	2.40277300	-0.88666100
Ga	-3.34152000	-2.77223100	-0.77273600
N	-3.31487300	0.48757000	-0.84360200
Ga	1.59937700	2.49903600	1.71801000
Ga	1.67835600	-2.68093900	1.64072600
N	1.56791600	0.52934200	1.42725400
Ga	-0.12727900	-0.09032700	0.72402900
Ga	3.20794700	-0.13272500	0.54465000
N	-0.02136000	3.16882000	0.67135300
N	-0.02489600	-2.02159900	0.88373200
N	3.17521000	3.17584600	0.42646400
N	3.16386600	-2.04691200	0.56724200
Ga	-0.18644600	2.40647300	-1.09694100
Ga	-0.13406300	-2.76427600	-1.01471800
Ga	3.08070700	2.41580500	-1.40581900
Ga	3.07301700	-2.75608300	-1.25660700
N	-0.14134200	0.50232500	-1.12828100
N	3.01411900	0.50768900	-1.31641400
Ga	-1.81821500	-0.18979000	-1.90489700
Ga	1.36466900	-0.18886700	-2.14932300
N	-1.83342400	3.08752000	-1.97967400
N	-1.78909200	-2.10962200	-1.80197900
N	1.34581700	3.07486900	-2.18661100

N	1.37400200	-2.09943100	-2.04145100
H	-1.52229700	-4.23882200	1.92836000
H	1.68699900	-4.23072700	1.68613900
H	4.02827400	2.85877600	0.84322000
H	4.49974900	0.45572100	1.13466500
H	4.05295600	-2.37150900	0.99408600
H	-3.97440100	-2.39217300	1.59987200
H	-4.40949400	0.43312100	1.80742200
H	-3.99894900	2.83855300	1.44921500
H	4.24025900	2.97448200	-2.23468300
H	3.83075800	0.16251400	-1.86524100
H	4.27311000	-2.24160400	-2.09191600
H	3.09361300	-4.30556300	-1.22165400
H	-0.12725300	-4.31367500	-0.97346500
H	-4.65584300	-2.26429500	-1.41798500
H	-3.34877200	-4.32198000	-0.73538700
H	1.30361200	2.73742000	-3.15278800
H	-1.90447600	2.72922000	-2.91076400
H	1.27774400	0.30177100	-3.59586300
H	-1.93310500	0.29350700	-3.35360100
H	1.32824400	-2.50122000	-3.00229600
H	-1.87977700	-2.50935400	-2.76024700
H	1.36673700	4.09538200	-2.24550300
H	-1.83760600	4.08729800	-2.00370300
H	3.16941600	4.17578200	0.39663700
H	-0.02704800	4.16904000	0.64360400
H	-3.22372200	4.15970500	0.87929200
H	-4.19679100	0.14243500	-1.25947400
H	-4.67112200	2.95190100	-1.56208700
C	1.54938400	0.05130500	2.79824100
O	2.51795900	1.45321700	3.30368800
O	1.96477400	-1.19893300	3.03150200
H	2.57121200	1.63825200	4.26443200
H	0.67067400	0.34209100	3.38040000

13A_GaN

HF= -1059.621567

Ga	1.44865800	-2.68756300	2.13522200
Ga	1.72127500	2.53132300	1.95717900
N	1.52550400	-0.76378700	1.61661200
Ga	3.16798400	-0.14798700	0.99383300
N	3.03357300	-3.34638900	0.64238600
N	3.26430300	1.82360500	1.11943600
Ga	3.23336200	-2.52392500	-1.09294500
Ga	3.46977600	2.64654500	-0.74011800
N	3.24451700	-0.59885600	-0.96857100
Ga	-1.71106500	-2.57406500	1.50345300
Ga	-1.48493000	2.72280000	1.80506100
N	-1.70290800	-0.54221600	1.62774900
Ga	0.16330200	0.07134300	0.77074300
Ga	-3.23014100	0.33255200	0.57676700
N	-0.16207800	-3.15601800	0.49367300
N	0.12660800	1.99914500	0.96599800
N	-3.35926900	-2.96394300	0.33914600

N	-3.03328300	2.21227100	0.76571900
Ga	0.02595700	-2.32906100	-1.20776600
Ga	0.26260100	2.83891100	-0.89232600
Ga	-3.26168100	-2.13868700	-1.46272900
Ga	-2.94437700	3.03123300	-1.04464600
N	0.04612800	-0.41814400	-1.11595400
N	-3.08358900	-0.22993200	-1.27031900
Ga	1.76914200	0.21215100	-1.94225000
Ga	-1.40055200	0.41230800	-2.10998500
N	1.58364600	-3.04417400	-2.19885600
N	1.84764700	2.12861800	-1.75823500
N	-1.59332700	-2.83440100	-2.31576900
N	-1.31426600	2.31665200	-1.90827000
H	1.80955500	4.07471400	2.08143000
H	-1.39961800	4.26719200	1.92903000
H	-4.18174300	-2.61993600	0.79491700
H	-4.50076000	-0.21161300	1.22035000
H	-3.88916300	2.58810100	1.21034400
H	4.13761900	2.10714100	1.59173800
H	4.40776600	-0.74578400	1.64393800
H	3.84536300	-3.10135100	1.17643400
H	-4.47673100	-2.56252200	-2.27777600
H	-3.89050400	0.19759400	-1.77835900
H	-4.19349800	2.63200600	-1.87092700
H	-2.87119800	4.57532600	-0.93091600
H	0.34955100	4.38200900	-0.77279000
H	4.73475100	2.09687200	-1.44668400
H	3.57072600	4.18924800	-0.62478800
H	-1.55494700	-2.45033500	-3.26444700
H	1.65291600	-2.64246500	-3.11207900
H	-1.39428600	-0.00060700	-3.58453200
H	1.81634100	-0.19292300	-3.43202400
H	-1.26199700	2.76586100	-2.84903300
H	1.94575200	2.57355900	-2.69667200
H	-1.67669500	-3.84767900	-2.42548100
H	1.52747800	-4.03973900	-2.27329100
H	-3.41472700	-3.95986800	0.25857700
H	-0.21859500	-4.15334900	0.41678600
H	2.97868400	-4.34335200	0.56252100
H	4.13647100	-0.28384100	-1.39716600
H	4.43410000	-3.09666200	-1.85438800
C	-1.67006000	-0.02199000	2.89186900
O	-2.14231900	-3.26519400	3.08202700
O	-1.65183000	1.24597900	3.16061900
H	-1.46906600	-3.62856200	3.68469500
H	-1.65111000	-0.69463700	3.75077200

TS14_GaN

HF= -1060.775409

Ga	1.11984800	-2.64842300	1.95365800
Ga	1.92026800	2.39763700	1.95137600
N	1.46154400	-0.87018600	1.50636500
Ga	3.16392200	-0.39217600	1.01607300
N	2.73217200	-3.59504500	0.75345300

N	3.41075100	1.54288700	1.15088000
Ga	3.02360300	-2.80481100	-1.01585200
Ga	3.70955800	2.31203500	-0.72025500
N	3.20698100	-0.90393200	-0.91263600
Ga	-1.98307600	-2.35321300	1.51465600
Ga	-1.25399300	2.86538100	1.74612700
N	-1.71387500	-0.38178300	1.56680100
Ga	0.09410300	0.09132800	0.78361300
Ga	-3.16158000	0.59701800	0.56463200
N	-0.43406700	-3.12883600	0.55197500
N	0.32322900	2.00392300	0.91758900
N	-3.59888200	-2.66102500	0.34520600
N	-2.82750500	2.47176600	0.68665700
Ga	-0.16148000	-2.32471000	-1.17955900
Ga	0.53407800	2.78115800	-0.92521900
Ga	-3.41369900	-1.86650000	-1.46488400
Ga	-2.64151800	3.25009000	-1.12984000
N	0.02873100	-0.43886900	-1.12056600
N	-3.06395100	0.01053600	-1.30379100
Ga	1.80224900	0.02473300	-1.90934000
Ga	-1.33324700	0.49695400	-2.13298500
N	1.35296800	-3.21714600	-2.11456400
N	2.06765800	1.92076400	-1.75581200
N	-1.79140900	-2.73300700	-2.28390400
N	-1.06709000	2.38183800	-1.95825700
H	2.14171300	3.92909600	2.05158100
H	-1.03584200	4.39835100	1.84673400
H	-4.39410200	-2.23833900	0.78260700
H	-4.50700500	0.19582200	1.16358300
H	-3.65262600	2.93049300	1.11744000
H	4.29520300	1.75756200	1.63002400
H	4.31371700	-1.10666500	1.73322100
H	3.55361600	-3.41186400	1.29554600
H	-4.64021300	-2.20969000	-2.29476300
H	-3.82165600	0.49693000	-1.83165400
H	-3.90892800	2.94654000	-1.96870300
H	-2.43479300	4.78329600	-1.04034700
H	0.75411500	4.31232300	-0.82939900
H	4.93136800	1.64158100	-1.39820000
H	3.94366500	3.84174500	-0.62868400
H	-1.70640700	-2.37046100	-3.23799500
H	1.46986200	-2.83926800	-3.03312300
H	-1.32742400	0.04983800	-3.59560800
H	1.85157400	-0.41937400	-3.39053400
H	-0.96365700	2.80667300	-2.90354000
H	2.21246800	2.33779900	-2.69864200
H	-1.96170300	-3.73680800	-2.37823000
H	1.21090600	-4.20519200	-2.17358700
H	-3.74003100	-3.64944600	0.28021000
H	-0.57541300	-4.11834100	0.49083600
H	2.58992800	-4.58409100	0.68869500
H	4.12629300	-0.67655700	-1.31887800
H	4.18273300	-3.51225600	-1.72544900
C	-1.69700600	0.14618800	2.92849100

O	-2.57426800	-3.19965000	2.96433200
O	-1.45330800	1.45733100	3.11069000
H	-2.04481700	-3.40122200	3.75208100
H	-0.54713600	-0.93552100	3.51406100
H	-2.40899700	-0.28867900	3.63436600
H	-0.10461600	-1.69762300	3.47127300

14A_GaN

HF= -1060.901469

Ga	1.36098800	-2.62658000	1.81164600
Ga	1.74457000	2.54421400	1.93110900
N	1.49395600	-0.80387100	1.57958900
Ga	3.16144900	-0.16701000	1.04702100
N	2.97731800	-3.38734000	0.78935500
N	3.28952300	1.77609800	1.14722900
Ga	3.21718800	-2.58816300	-1.00452300
Ga	3.53562300	2.55981600	-0.74057600
N	3.25869800	-0.68585100	-0.89234700
Ga	-1.82619300	-2.41596800	1.53912600
Ga	-1.45528600	2.78519500	1.72402000
N	-1.69439200	-0.46268600	1.57472900
Ga	0.05917300	0.09967700	0.84272900
Ga	-3.18583600	0.38462900	0.57651700
N	-0.21417200	-3.14763800	0.58596200
N	0.20668800	2.01933200	0.88310500
N	-3.40410400	-2.90606200	0.37625700
N	-3.00237600	2.27821800	0.64924600
Ga	-0.01013200	-2.33269500	-1.16343400
Ga	0.33490600	2.80177000	-0.94799500
Ga	-3.28152700	-2.10656200	-1.44109300
Ga	-2.86573700	3.04343400	-1.15518700
N	0.06433600	-0.45008200	-1.09008300
N	-3.05871700	-0.21899600	-1.29924600
Ga	1.78568000	0.13899000	-1.90227700
Ga	-1.36660700	0.38291300	-2.12463600
N	1.57495900	-3.13480200	-2.08109900
N	1.92976400	2.04398100	-1.77313600
N	-1.59573800	-2.87528100	-2.25308200
N	-1.22990800	2.27932800	-1.97797400
H	1.85732200	4.08845000	2.01682300
H	-1.34526400	4.33030100	1.80927100
H	-4.22701900	-2.53645900	0.81028500
H	-4.51134400	-0.11277300	1.16816500
H	-3.85197000	2.67486500	1.09551700
H	4.15864500	2.07032500	1.61457600
H	4.37919400	-0.78433700	1.74474700
H	3.78356000	-3.14140600	1.32950100
H	-4.47437900	-2.55433000	-2.26714900
H	-3.84880800	0.20760900	-1.83018800
H	-4.10870200	2.64355200	-1.99034700
H	-2.76783900	4.58839900	-1.08029000
H	0.44636400	4.34551600	-0.86685600
H	4.80162600	1.97080100	-1.41283800
H	3.66113000	4.10300900	-0.66357200

H	-1.53649500	-2.51672100	-3.21065400
H	1.66495100	-2.75834000	-3.00325300
H	-1.32913200	-0.07922500	-3.59136900
H	1.87505600	-0.32102800	-3.38377600
H	-1.16081700	2.70289800	-2.92561800
H	2.04051400	2.46116300	-2.71819600
H	-1.69482100	-3.88944300	-2.33782500
H	1.50290600	-4.13089900	-2.13067000
H	-3.47482100	-3.90250000	0.32061100
H	-0.28526600	-4.14496000	0.53381300
H	2.90497800	-4.38440300	0.73432100
H	4.16212500	-0.39751000	-1.31113900
H	4.41839800	-3.22589300	-1.69086400
C	-1.79943100	0.13599400	3.01991100
O	-2.19233100	-3.34186000	3.00811100
O	-1.49253000	1.51749800	3.09478600
H	1.21802300	-3.48931800	3.13797900
H	-1.09824100	-0.41556700	3.65862800
H	-2.82261100	-0.05618400	3.37558800
H	-1.68859400	-3.45059700	3.82679000

15A_GaN

HF= -1062.078128

Ga	-1.32993600	2.63631800	1.80731000
Ga	-1.79330800	-2.52761100	1.88370600
N	-1.48926700	0.81604200	1.56910400
Ga	-3.16158100	0.21057200	1.00740300
N	-2.92560700	3.43106500	0.77851200
N	-3.32072300	-1.73059400	1.08934000
Ga	-3.16304400	2.64978700	-1.02374200
Ga	-3.56258300	-2.49494600	-0.80244300
N	-3.23449200	0.74799100	-0.92691900
Ga	1.85643800	2.38046000	1.55888300
Ga	1.40309900	-2.81616000	1.70051700
N	1.69462600	0.42983300	1.57771500
Ga	-0.06250900	-0.09956600	0.82757800
Ga	3.18066300	-0.43453500	0.58570600
N	0.26325600	3.14360300	0.59919000
N	-0.23825500	-2.01673600	0.85295400
N	3.45096300	2.85465800	0.41325700
N	2.96742500	-2.32543000	0.64127500
Ga	0.06133700	2.34585500	-1.15862700
Ga	-0.36440400	-2.78461100	-0.98587300
Ga	3.33099400	2.07087400	-1.41125700
Ga	2.83372000	-3.07384000	-1.16921000
N	-0.04366000	0.46452000	-1.09981200
N	3.07793300	0.18621700	-1.28605500
Ga	-1.76665900	-0.09288900	-1.93140900
Ga	1.38317400	-0.38328600	-2.12949000
N	-1.50387500	3.17902000	-2.08227900
N	-1.94004200	-1.99576000	-1.81826300
N	1.66377300	2.87203300	-2.23073500
N	1.21658900	-2.27827500	-1.99913800
H	-1.93083600	-4.07041100	1.95618800

H	1.26982800	-4.36009200	1.77269400
H	4.26435700	2.46896600	0.85094200
H	4.50870500	0.03862800	1.19214800
H	3.80711800	-2.73795200	1.09218000
H	-4.19728700	-2.01412100	1.55137100
H	-4.37504900	0.84249400	1.70224700
H	-3.73998000	3.19324100	1.31025700
H	4.53718600	2.50690900	-2.22414500
H	3.86575300	-0.24838000	-1.81390700
H	4.08955400	-2.68676300	-1.99111000
H	2.71154800	-4.61768800	-1.10720500
H	-0.50017100	-4.32696400	-0.91782500
H	-4.81387800	-1.88126100	-1.48025500
H	-3.71239600	-4.03653900	-0.73859400
H	1.60687900	2.52182400	-3.19154800
H	-1.59205900	2.81115300	-3.00812100
H	1.36529500	0.09083300	-3.59308100
H	-1.83640300	0.38039700	-3.40944300
H	1.14883900	-2.69341400	-2.95056500
H	-2.04999300	-2.40398100	-2.76710400
H	1.77908800	3.88516300	-2.30672600
H	-1.41613300	4.17428400	-2.12347800
H	3.53730900	3.85026400	0.36611500
H	0.35017600	4.14016500	0.55524200
H	-2.83761500	4.42720800	0.73204400
H	-4.13891500	0.47605500	-1.35477600
H	-4.34871800	3.31087700	-1.71431600
C	1.78167000	-0.18115600	3.01866400
O	2.22404600	3.29027200	3.03774300
O	1.46450200	-1.56019100	3.08056300
H	-1.18461300	3.48738400	3.14153200
H	1.07924700	0.37245200	3.65520600
H	2.80272500	0.00069800	3.38569400
H	1.71415600	3.40202000	3.85219200
H	-1.75156300	-1.01948900	4.04200700
H	-1.88847500	-1.66405300	4.39807400

TS15_GaN

HF= -1061.945423

Ga	1.36631100	-2.59698600	1.83212300
Ga	1.68644600	2.58192700	1.91381800
N	1.48424800	-0.76530900	1.60329900
Ga	3.15003700	-0.12135400	1.07908300
N	3.01505700	-3.34276000	0.84526600
N	3.25196900	1.82989800	1.16261100
Ga	3.27298500	-2.55781700	-0.95217800
Ga	3.52222000	2.59796000	-0.72734700
N	3.29034700	-0.65157700	-0.85407000
Ga	-1.81509300	-2.40438100	1.50288400
Ga	-1.51222800	2.77931200	1.65064700
N	-1.69314300	-0.48286600	1.48597600
Ga	0.02909500	0.07972400	0.82560200
Ga	-3.16662800	0.32739400	0.53096400
N	-0.17516300	-3.14650800	0.58615600

N	0.14825400	2.02059600	0.89746400
N	-3.36424400	-2.94861000	0.32041300
N	-3.02325800	2.24377900	0.57593700
Ga	0.04375400	-2.34399000	-1.16467500
Ga	0.32263700	2.79619800	-0.99085300
Ga	-3.22352700	-2.15968400	-1.49460600
Ga	-2.87685700	2.99411500	-1.25412000
N	0.11131600	-0.45543800	-1.11612800
N	-3.02662300	-0.26615000	-1.36894400
Ga	1.82505800	0.14075500	-1.89839600
Ga	-1.33015700	0.33918200	-2.16926500
N	1.65854100	-3.13316000	-2.05046200
N	1.93959800	2.05404300	-1.77855300
N	-1.51188100	-2.91668100	-2.27820100
N	-1.21629400	2.24637300	-2.03946200
H	1.77769500	4.12812400	1.98776900
H	-1.42378600	4.32624500	1.72407700
H	-4.19896400	-2.58592000	0.73715900
H	-4.52073500	-0.16330200	1.06890900
H	-3.89635400	2.63204400	0.98278700
H	4.11147200	2.13693100	1.64217800
H	4.36670800	-0.71336600	1.80128400
H	3.80876500	-3.08148800	1.39679600
H	-4.39380700	-2.63359100	-2.34367300
H	-3.81153100	0.13996400	-1.92058400
H	-4.10020700	2.57084800	-2.10657300
H	-2.80028200	4.54083200	-1.19120900
H	0.41270100	4.34190100	-0.92146000
H	4.80699600	2.01981400	-1.37293400
H	3.62643100	4.14326700	-0.66184400
H	-1.44105100	-2.56560100	-3.23776700
H	1.75925700	-2.76350500	-2.97427200
H	-1.25883500	-0.12895500	-3.63641600
H	1.94421900	-0.32700500	-3.37267300
H	-1.13787400	2.66073600	-2.99247300
H	2.06232800	2.46273400	-2.72896000
H	-1.59638600	-3.93272500	-2.35567600
H	1.60020500	-4.13050800	-2.09246900
H	-3.42104900	-3.94625000	0.27249000
H	-0.23262800	-4.14504500	0.54131100
H	2.95661400	-4.34098900	0.79789500
H	4.19655100	-0.35569900	-1.26114800
H	4.49588100	-3.18361400	-1.61152000
C	-1.81056400	0.06480600	3.36862600
O	-2.19583200	-3.33545400	2.97000000
O	-1.71212700	1.56937400	3.17237000
H	1.22186400	-3.44359100	3.16830700
H	-0.90697100	-0.44729700	3.64839800
H	-2.78944800	-0.35674700	3.50984700
H	-1.70873200	-3.43970900	3.79926100
H	-1.91008000	0.60127000	5.01148700
H	-1.80859100	1.69758100	4.20774500

16A_GaN

HF= -1062.072738

Ga	1.50565000	-2.43558400	1.94044300
Ga	1.47132700	2.75388200	1.81392000
N	1.51858500	-0.60657200	1.64676400
Ga	3.13367700	0.12589700	1.11156900
N	3.23184000	-3.09973200	1.01344100
N	3.09850200	2.08888700	1.11670700
Ga	3.46062400	-2.37401100	-0.81204500
Ga	3.34882500	2.79335300	-0.79737500
N	3.34989900	-0.46612700	-0.79254300
Ga	-1.66974000	-2.48021700	1.56304000
Ga	-1.72866000	2.71385600	1.49559600
N	-1.66249000	-0.64402600	1.34017100
Ga	-0.01095400	0.05730300	0.82495700
Ga	-3.15773000	0.06037000	0.46922100
N	0.04008100	-3.14082900	0.69816100
N	-0.02550900	2.03009100	0.85059000
N	-3.14847300	-3.18025200	0.37682600
N	-3.17017600	2.01345600	0.45717900
Ga	0.22550500	-2.38957200	-1.07223100
Ga	0.14830100	2.75311000	-1.11720200
Ga	-3.02990500	-2.45480200	-1.45742500
Ga	-3.05175400	2.71297700	-1.43642900
N	0.19211200	-0.49807300	-1.12399300
N	-2.97209600	-0.54881500	-1.42668200
Ga	1.85155500	0.17335700	-1.89169200
Ga	-1.30346400	0.13089700	-2.20798400
N	1.91607900	-3.10431100	-1.90854400
N	1.82798100	2.10035600	-1.84546700
N	-1.25713500	-3.12251900	-2.19272000
N	-1.33035000	2.05742700	-2.16182700
H	1.45275300	4.30469000	1.82521900
H	-1.74912300	4.26445200	1.50545800
H	-4.01450700	-2.86152000	0.76565600
H	-4.51095900	-0.45600600	0.99102000
H	-4.08319400	2.37022600	0.79798900
H	3.92634100	2.47157600	1.59796100
H	4.37809900	-0.34463000	1.87930000
H	3.99523500	-2.76089100	1.56554600
H	-4.15017800	-3.04730400	-2.31322800
H	-3.77178000	-0.22461300	-1.99719900
H	-4.22706700	2.17024300	-2.28864700
H	-3.08518100	4.26278300	-1.43669300
H	0.12849700	4.30316600	-1.11061600
H	4.68231800	2.28204700	-1.39893700
H	3.34304700	4.34353000	-0.79470000
H	-1.19389700	-2.80645200	-3.16487700
H	2.00719600	-2.76614700	-2.84530700
H	-1.17610600	-0.38117300	-3.66184400
H	2.02772300	-0.34077200	-3.34197600
H	-1.26289200	2.43392600	-3.13289300
H	1.93811700	2.47410000	-2.81328900
H	-1.26864200	-4.14433100	-2.22906500
H	1.92872700	-4.10418700	-1.90985100

H	-3.13460600	-4.18076400	0.36951200
H	0.05464300	-4.14206200	0.69477600
H	3.24448700	-4.10083200	1.00685700
H	4.23832100	-0.12431500	-1.19751200
H	4.74166000	-2.93572000	-1.42527900
C	-2.11248600	0.95053400	4.12436800
O	-1.97919300	-3.45589700	3.03580600
O	-1.95429900	2.27368700	3.44137400
H	1.41857100	-3.23362000	3.31652800
H	-1.36097100	0.88018800	4.91281900
H	-3.12528800	0.88710800	4.52697000
H	-1.43023000	-3.49896800	3.83322800
H	-1.94823700	0.20582800	3.33293800
H	-2.12297300	3.03689100	4.02282400

TS15'_GaN

HF= -1062.075069

Ga	-1.41725100	2.59912300	1.83112200
Ga	-1.70398400	-2.58124800	1.88638400
N	-1.50602500	0.78402600	1.54393100
Ga	-3.16153200	0.11123500	1.01593700
N	-3.03116300	3.33810600	0.78643200
N	-3.26018000	-1.83221400	1.08894700
Ga	-3.24858100	2.54962400	-1.00974800
Ga	-3.47815500	-2.60474200	-0.79643500
N	-3.25643400	0.64748000	-0.92129800
Ga	1.76273400	2.42997100	1.56096900
Ga	1.50089000	-2.76615000	1.69733300
N	1.68280300	0.47950400	1.57387200
Ga	-0.06443300	-0.10651300	0.81472100
Ga	3.19325200	-0.32139600	0.57580900
N	0.16504000	3.15471700	0.60106800
N	-0.15614100	-2.02698500	0.83120500
N	3.36013500	2.96932900	0.40905900
N	3.04347000	-2.21701700	0.65307800
Ga	-0.02224500	2.34896500	-1.15421500
Ga	-0.27253000	-2.79014400	-0.98595300
Ga	3.25640200	2.18160400	-1.42275200
Ga	2.93284500	-2.97528500	-1.17528800
N	-0.05395800	0.46763400	-1.10653800
N	3.07110600	0.29107500	-1.29142500
Ga	-1.76758300	-0.14574500	-1.92765500
Ga	1.38918800	-0.33584100	-2.13443300
N	-1.60728800	3.13364800	-2.07715500
N	-1.87303900	-2.05220800	-1.81673200
N	1.56838800	2.92981300	-2.23161800
N	1.29423200	-2.23368400	-2.00332600
H	-1.79067100	-4.12771000	1.95848300
H	1.41673200	-4.31307200	1.76876700
H	4.18643900	2.61000600	0.84502200
H	4.51018400	0.18885500	1.18454800
H	3.89904300	-2.60919700	1.08440300
H	-4.12378400	-2.14587900	1.55877400
H	-4.39398700	0.70339200	1.71145400

H	-3.83627900	3.07367600	1.31955800
H	4.45216600	2.65821500	-2.23049800
H	3.87130900	-0.11767000	-1.82048700
H	4.17392500	-2.54735800	-1.99934000
H	2.86106300	-4.52241500	-1.11388300
H	-0.35806600	-4.33627900	-0.91842300
H	-4.74998600	-2.03178900	-1.47160800
H	-3.57769000	-4.15045400	-0.73309500
H	1.52112500	2.57837100	-3.19250400
H	-1.68517300	2.76353400	-3.00299100
H	1.35788100	0.14097200	-3.59484700
H	-1.85117400	0.32626800	-3.40514600
H	1.23320400	-2.64913300	-2.95338200
H	-1.97300800	-2.46386700	-2.76384900
H	1.65060300	3.94617200	-2.30729900
H	-1.55197100	4.13122300	-2.11797500
H	3.41404100	3.96718200	0.36228800
H	0.21945700	4.15326200	0.55736600
H	-2.97555100	4.33650700	0.74026200
H	-4.15174700	0.34614300	-1.34618400
H	-4.45418200	3.17282900	-1.70383600
C	1.78176000	-0.10636400	3.00844700
O	1.38012000	-1.48324200	3.09472500
H	-0.27904200	-1.73317600	3.61188700
H	-1.04863000	-1.90624400	3.73349000
H	-1.36616700	3.47850900	3.14285700
O	1.91653500	3.14328600	3.15308900
H	2.42390500	3.72996200	3.71738900
H	2.82040800	-0.00009100	3.35013900
H	1.13561300	0.47737100	3.66931400

17A_GaN

HF= -1062.088148

Ga	-1.31517500	2.64765500	1.79843100
Ga	-1.80222800	-2.50996300	1.90501900
N	-1.46808000	0.85494300	1.51091900
Ga	-3.16155400	0.20596200	1.03066600
N	-2.89201000	3.45415900	0.78737100
N	-3.34622200	-1.71000500	1.05478500
Ga	-3.14799600	2.66148900	-1.00826500
Ga	-3.57916800	-2.47068200	-0.77603300
N	-3.22704800	0.77167800	-0.91429700
Ga	1.86511900	2.40033900	1.53813900
Ga	1.39234500	-2.82232900	1.71207100
N	1.70873500	0.43668000	1.59762400
Ga	-0.08605500	-0.11005600	0.78180800
Ga	3.18549700	-0.44098400	0.57295200
N	0.29514000	3.14194800	0.59872700
N	-0.16312900	-2.01323300	0.80896100
N	3.47702700	2.82699300	0.40426900
N	2.95032300	-2.32405700	0.70484700
Ga	0.06796400	2.34076900	-1.16337900
Ga	-0.38402400	-2.78556700	-0.96815700
Ga	3.34013700	2.04313500	-1.42910300

Ga	2.81152100	-3.10001200	-1.16057500
N	-0.02833800	0.46812200	-1.11366100
N	3.08010100	0.15871100	-1.28538300
Ga	-1.78350000	-0.08906000	-1.92172300
Ga	1.36881400	-0.40951200	-2.13303000
N	-1.48124600	3.18415900	-2.07704100
N	-1.94531200	-1.98311000	-1.80312200
N	1.68356500	2.85258200	-2.23419200
N	1.21319000	-2.29733300	-1.99266000
H	-1.95083300	-4.05150400	1.98181100
H	1.24639800	-4.36656900	1.78956300
H	4.29090500	2.43834000	0.84045900
H	4.51719300	0.00634400	1.18736300
H	3.79417900	-2.76529400	1.09695000
H	-4.20301900	-1.97889100	1.57841700
H	-4.35856200	0.87939200	1.72232200
H	-3.70679700	3.22429700	1.32223000
H	4.55418500	2.46542400	-2.23550700
H	3.86289000	-0.28358900	-1.81595500
H	4.06747400	-2.72380200	-1.98742800
H	2.67763000	-4.64188600	-1.09422300
H	-0.53115200	-4.32624900	-0.89590500
H	-4.82782200	-1.84931500	-1.45162400
H	-3.74054100	-4.01095700	-0.70761600
H	1.62103400	2.50002800	-3.19398500
H	-1.57499600	2.81432200	-3.00161400
H	1.35968900	0.07003000	-3.58839000
H	-1.83913600	0.38450000	-3.39580800
H	1.12398300	-2.71068100	-2.93793400
H	-2.07190400	-2.39641700	-2.74553000
H	1.80636100	3.86443500	-2.31344100
H	-1.38598700	4.17838000	-2.12114600
H	3.57314800	3.82335200	0.35436100
H	0.38735300	4.13801900	0.55249400
H	-2.79689100	4.44968100	0.73805500
H	-4.13454600	0.50309500	-1.33442700
H	-4.32380600	3.33851400	-1.70079200
C	1.77174700	-0.04451500	3.00853400
O	1.22313000	-1.43574800	3.16874700
H	-1.31411700	-1.83927400	3.36196800
H	-1.11364500	3.50305400	3.12802900
O	2.22594100	3.17861400	3.09071200
H	1.62986700	3.52961000	3.76761600
H	2.79777400	-0.11327300	3.37724500
H	1.17843100	0.57295700	3.68499100
H	0.24271200	-1.45424700	3.43709000

TS17_GaN

HF= -1061.950735

Ga	-1.25068300	2.61690600	1.82312800
Ga	-1.84299500	-2.51530100	1.82635700
N	-1.43743400	0.79444300	1.55102500
Ga	-3.14464200	0.24269000	0.99724400
N	-2.83323100	3.48760900	0.82868200

N	-3.36328400	-1.67907700	0.99220900
Ga	-3.08003500	2.74314800	-0.98974200
Ga	-3.59846600	-2.39151600	-0.86622300
N	-3.19562500	0.84648900	-0.93007600
Ga	1.91128800	2.30862500	1.62133500
Ga	1.34724900	-2.87308400	1.65097500
N	1.65609900	0.45301900	1.47000200
Ga	-0.01730200	-0.07151000	0.69661300
Ga	3.13484400	-0.45287200	0.65791200
N	0.34888400	3.13023800	0.65743200
N	-0.18773900	-2.00653300	0.80860700
N	3.52923600	2.77133400	0.47947700
N	2.91103300	-2.37511800	0.68931900
Ga	0.14337800	2.37949000	-1.12315900
Ga	-0.40704100	-2.75120500	-1.04147900
Ga	3.39927200	2.02021300	-1.34861700
Ga	2.78465600	-3.11055200	-1.21664800
N	-0.03359000	0.50444200	-1.16755000
N	3.10441100	0.13569700	-1.26421500
Ga	-1.76115600	-0.01021800	-1.95910800
Ga	1.40805000	-0.36849400	-2.14031200
N	-1.40435900	3.25657300	-2.03031100
N	-1.95372600	-1.91053900	-1.86595200
N	1.75610900	2.87965000	-2.17108200
N	1.19983000	-2.26754000	-2.03888700
H	-2.01599800	-4.05554300	1.86929600
H	1.17768100	-4.41540200	1.69403200
H	4.33261000	2.35960500	0.91346500
H	4.51923200	-0.08204600	1.20992300
H	3.75481300	-2.83938300	1.05488300
H	-4.23296700	-1.94027100	1.49353000
H	-4.34598600	0.91630900	1.69733000
H	-3.65540400	3.25875400	1.35237200
H	4.62032100	2.44850700	-2.15913600
H	3.88406400	-0.29773400	-1.80365700
H	4.05267900	-2.73683700	-2.02576600
H	2.62675600	-4.65181300	-1.18419500
H	-0.57829000	-4.29092300	-1.00302900
H	-4.83216800	-1.73665900	-1.53766200
H	-3.78383100	-3.93017400	-0.83199100
H	1.69566800	2.54888600	-3.13851500
H	-1.49662600	2.90819600	-2.96326500
H	1.40033300	0.13201500	-3.58673300
H	-1.79470500	0.49163700	-3.41129100
H	1.11717000	-2.65799300	-2.99765400
H	-2.07496900	-2.29859400	-2.82237200
H	1.89492500	3.89113000	-2.22749600
H	-1.29365700	4.25013200	-2.05241300
H	3.63980300	3.76582500	0.45182100
H	0.45879700	4.12541500	0.63268600
H	-2.72233100	4.48220800	0.80128000
H	-4.10399500	0.60174300	-1.36499400
H	-4.24712900	3.44686700	-1.67202700
C	0.39189900	-0.71803500	3.53401600

O	1.21653100	-1.82730300	3.42110600
H	1.73633100	-2.03776900	4.22154200
H	-1.36326500	-1.83923900	3.40065500
H	-1.10500100	3.39515400	3.20808600
H	-0.32048000	-0.35349100	2.80006800
H	0.47006200	-0.20463500	4.48806500
O	2.28822500	3.24199100	3.09750800
H	1.70081100	3.43609500	3.84280500

ⁱ F. O. Morais, K. F. Andriani, and J. L. F. Da Silva. Investigation of the Stability Mechanisms of Eight-Atom Binary Metal Clusters Using DFT Calculations and k-means Clustering Algorithm *J. Chem. Inf. Model.* **2021**, 61, 3411–3420.