MOLECULAR PHYSICS, 1974, VOL. 28, NO. 3, 715–727

Semiempirical LCAO calculations of electronic and dynamical ...

paths [17–19]. It was suggested that the application of the ... valence electron

M.O. approach

[redacted]

methods to describe both dynamical and electronic properties of

system, thus examining the possible applicability of the MO

molecular crystals. We chose

of crystalline nitrogen,

availability of extensive experimental and

al

ato

and forms

because of the

rk on the ground state

[redacted]

...plicitly on the net atomic cha...

[redacted]

...al from the original

lations, and the charge dependent part of

work of Rien *et al.* [8]

been used previously ... in calculat...

intermolecular potential for describing reaction mechanisms

[18, 19]. Hence, we have examined to some extent the

calculated by the INDO potential. As expected, this method

ing the

[redacted]

[illegible]

1·098 (*a*)	Equilibrium $^1\Sigma_g$	1·17	1·15
	distance/Å		
1·213 (*c*)	Equilibrium $^1\Pi_u$	1·20	1·21

[illegible]

molecules was found to vary from $-15{\cdot}4\times10^{-4}$ for a unit cell dimens

ture of N_2.

anchiated accounts of the spectroscopic
[5] and IEXH, EXH and INDO theories. (a) Linear
ndicular ring-plane configuration.

Figure 2. Diatomic
potentia
conf

[redacted]

(kcal/mole)

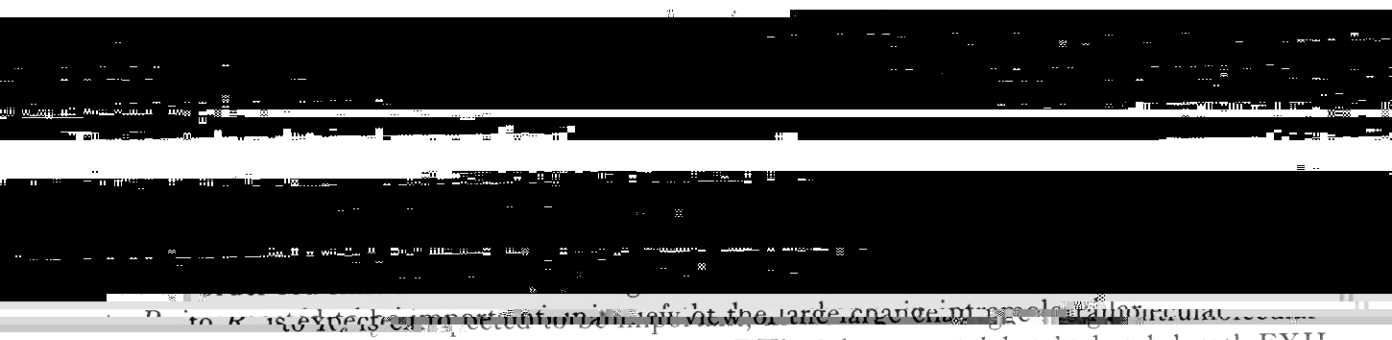
$\gamma - N_2$ form :

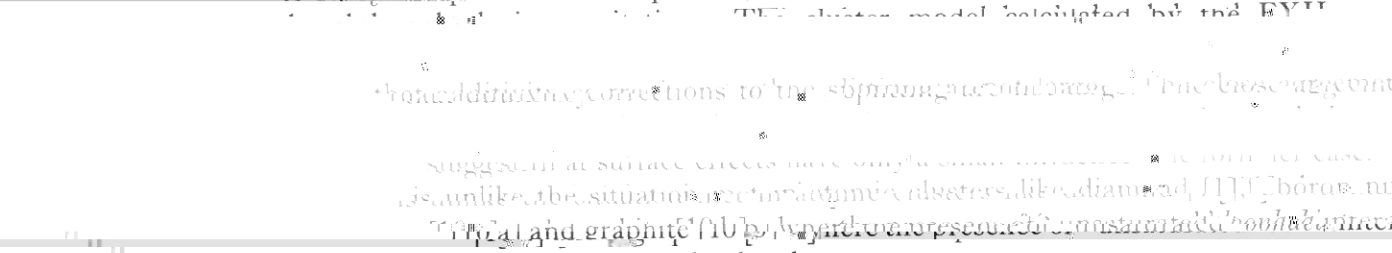
a, b, c/Å	$a = b = 4{\cdot}12$ $c = 5{\cdot}31$	$a = b = 3{\cdot}957$ $c = 5{\cdot}109$	$a = b = 4{\cdot}09$ $c = 5{\cdot}17$	$b = 4{\cdot}12$ $c = 5{\cdot}09$
E_{static}/(kcal/mole)	$-1{\cdot}76$	—	$-1{\cdot}91$	$-1{\cdot}99$

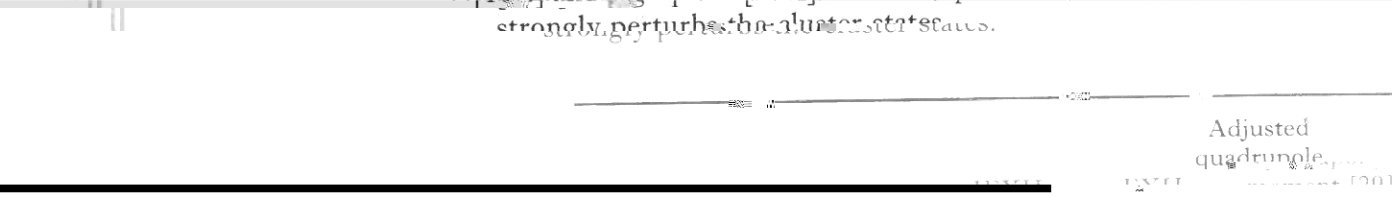
(a) Ref. 3 (e) Ref. 24.
(b) Ref. 21 (f) Ref. 23
(c) Ref. 28 (g) Ref. 22 at 5900 atm
(d) Ref. 22 (h) Calculated for internal pressure f

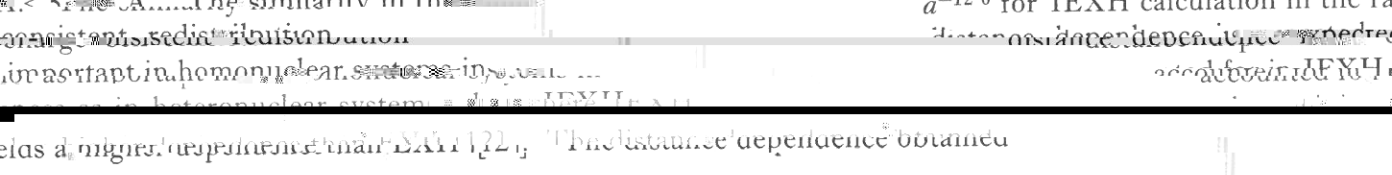
5. LATTICE MODE FREQUENCIES

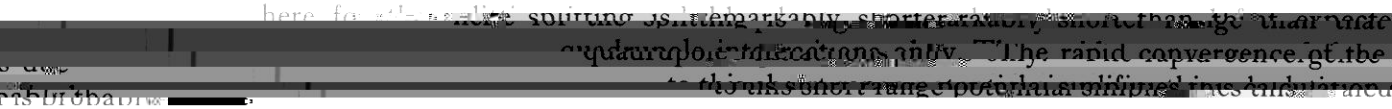
[redacted]

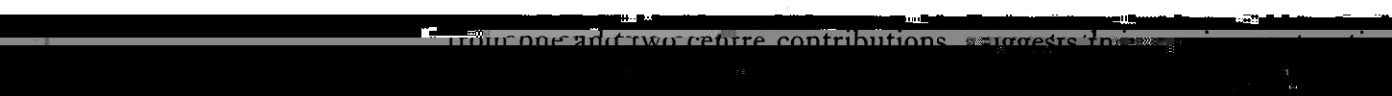


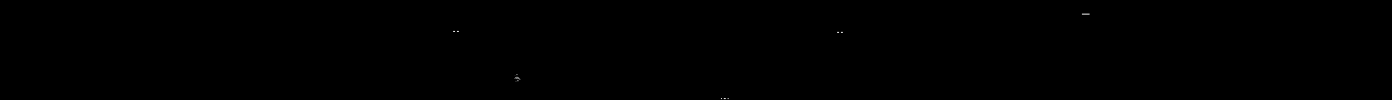












R_{min}/Å

Configuration EXH EXH

9. SUMMARY AND CONCLUSIONS

[redacted]

[redacted]

[redacted]

[7] Herman, R., 1963, *J. chem. Phys.*, 39, 1307

and B. Pullman (N.Y. : Academic Press).

[20] SALEM, L., 1968, *J. Am. chem. Soc.* **90**, 543;