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On the Stability of Noble Gas bound 1-Tris(pyrazolyl)borate Beryllium and Magnesium Complexes

Sudip Pan, Ranajit Saha, and Pratim K. Chattaraj*

Department of Chemistry and Centre for Theoretical Studies

Indian Institute of Technology Kharagpur, 721302, India

*Corresponding author: pkc@chem.iitkgp.ernet.in

Supporting information

Table S1. Stretching frequency of Ng-M bonds (M=Be,Mg) and their corresponding IR intensity are given for $TpMNg^+$ clusters studied at the MPW1B95/def2-TZVP level.

Clusters	Frequency (cm^{-1})	Intensity (km/mol)	Clusters	Frequency (cm^{-1})	Intensity (km/mol)
$TpBeHe^+$	318.68	0.04	$TpMgHe^+$	240.57	8.65
$TpBeNe^+$	129.07	3.14	$TpMgNe^+$	133.64	0.13
$TpBeAr^+$	125.64	3.80	$TpMgAr^+$	89.50	1.46
$TpBeKr^+$	99.41	3.22	$TpMgKr^+$	76.73	1.39
$TpBeXe^+$	86.60	3.03	$TpMgXe^+$	68.01	1.75
$TpBeRn^+$	73.05	3.39	$TpMgRn^+$	60.86	2.05

Table S2. The valence orbital population of M and Ng centers in $TpMNg^+$ clusters obtained at the MPW1B95/def2-TZVP level.

Clusters	M	Ng
$TpBe^+$	$2s^{0.26}\,2p_x^{0.22}\,2p_y^{0.22}\,2p_z^{0.03}$	
$TpBeHe^+$	$2s^{0.28}\,2p_x^{0.24}\,2p_y^{0.24}\,2p_z^{0.11}$	$1s^{1.90}$
$TpBeNe^+$	$2s^{0.27}\,2p_x^{0.23}\,2p_y^{0.23}\,2p_z^{0.08}$	$2s^{1.97}\,2p_x^{2.00}\,2p_y^{2.00}\,2p_z^{1.97}$
$TpBeAr^+$	$2s^{0.29}\,2p_x^{0.24}\,2p_y^{0.24}\,2p_z^{0.15}$	$3s^{1.93}\,3p_x^{1.99}\,3p_y^{1.99}\,3p_z^{1.90}$
$TpBeKr^+$	$2s^{0.30}\,2p_x^{0.24}\,2p_y^{0.24}\,2p_z^{0.18}$	$4s^{1.92}\,4p_x^{1.98}\,4p_y^{1.98}\,4p_z^{1.87}$
$TpBeXe^+$	$2s^{0.31}\,2p_x^{0.24}\,2p_y^{0.24}\,2p_z^{0.22}$	$5s^{1.92}\,5p_x^{1.98}\,5p_y^{1.98}\,5p_z^{1.82}$
$TpBeRn^+$	$2s^{0.32}\,2p_x^{0.24}\,2p_y^{0.24}2p_z^{0.23}$	$6s^{1.93}\,6p_x^{1.98}\,6p_y^{1.98}\,6p_z^{1.79}$
$TpMg^+$	$3s^{0.20}\,3p_x^{0.08}\,3p_y^{0.08}\,3p_z^{0.02}$	
$TpMgHe^+$	$3s^{0.22}\,3p_x^{0.09}\,3p_y^{0.09}\,3p_z^{0.05}$	$1s^{1.95}$
$TpMgNe^+$	$3s^{0.21}\,3p_x^{0.09}\,3p_y^{0.09}\,3p_z^{0.04}$	$2s^{1.98}\,2p_x^{2.00}\,2p_y^{2.00}\,2p_z^{1.98}$
$TpMgAr^+$	$3s^{0.24}\,3p_x^{0.10}\,3p_y^{0.10}\,3p_z^{0.08}$	$3s^{1.96}\,3p_x^{1.99}\,3p_y^{1.99}\,3p_z^{1.94}$
$TpMgKr^+$	$3s^{0.25}\,3p_x^{0.10}\,3p_y^{0.10}\,3p_z^{0.10}$	$4s^{1.96}\,4p_x^{1.99}\,4p_y^{1.99}\,4p_z^{1.92}$
$TpMgXe^+$	$3s^{0.26}\,3p_x^{0.10}\,3p_y^{0.10}\,3p_z^{0.12}$	$5s^{1.95}\,5p_x^{1.99}\,5p_y^{1.99}\,5p_z^{1.89}$
$TpMgRn^+$	$3s^{0.27}\,3p_x^{0.10}\,3p_y^{0.10}\,3p_z^{0.13}$	$6s^{1.96}\,6p_x^{1.98}\,6p_y^{1.98}\,6p_z^{1.87}$

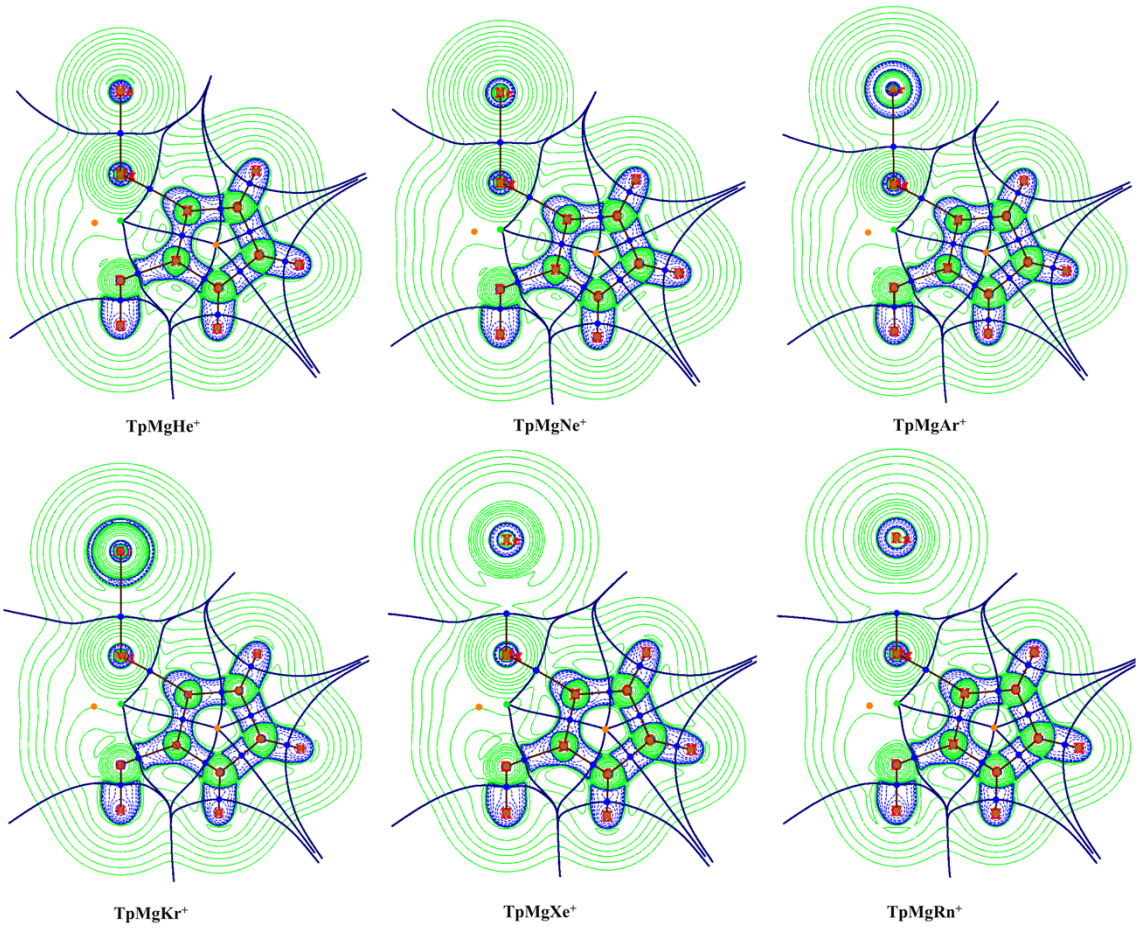
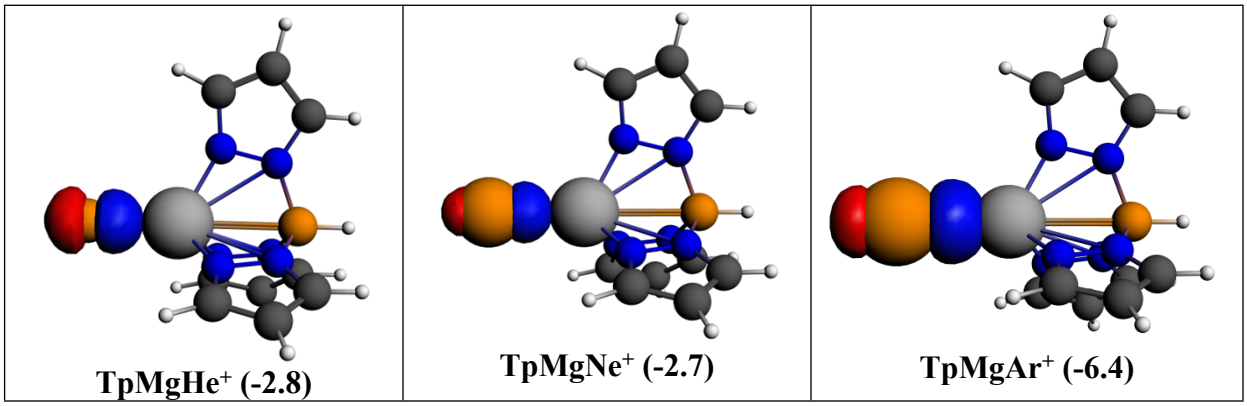


Figure S1. The plots of Laplacian of electron density ($\nabla^2\rho(r)$) of $TpMgNg^+$ complexes at the MPW1B95/def2-TZVP level.



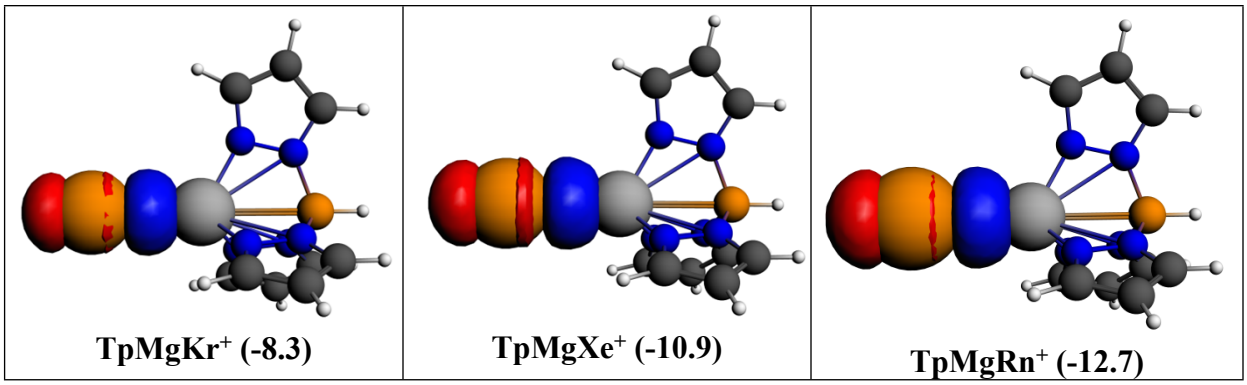


Figure S2. The plot of deformation densities (Δρ) of the pair-wise orbital interactions and the associated ΔE^{orb} energies obtained from the EDA-NOCV. ΔE^{orb} is given within the parentheses in kcal/mol.

The Cartesian coordinates of the studied complexes

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TpBeF

0 1

B	0.00000000	0.00000000	-1.36659300
H	0.00000000	0.00000000	-2.55982400
Be	0.00000000	0.00000000	1.41002200
N	0.00000000	1.53378700	0.55617200
N	0.00000000	1.42379100	-0.77753800
N	1.32829900	-0.76689400	0.55617200
N	1.23304000	-0.71189600	-0.77753800
N	-1.32829900	-0.76689400	0.55617200
N	-1.23304000	-0.71189600	-0.77753800
C	0.00000000	2.82174900	0.85025400
H	0.00000000	3.13814600	1.87756400
C	0.00000000	3.57316700	-0.32021200
H	0.00000000	4.64159500	-0.41744200
C	0.00000000	2.63757700	-1.33114100
H	0.00000000	2.75301400	-2.39933000
C	2.44370600	-1.41087500	0.85025400
H	2.71771400	-1.56907300	1.87756400
C	3.09445300	-1.78658400	-0.32021200
H	4.01974000	-2.32079800	-0.41744200
C	2.28420800	-1.31878800	-1.33114100

H	2.38418000	-1.37650700	-2.39933000
C	-2.44370600	-1.41087500	0.85025400
H	-2.71771400	-1.56907300	1.87756400
C	-3.09445300	-1.78658400	-0.32021200
H	-4.01974000	-2.32079800	-0.41744200
C	-2.28420800	-1.31878800	-1.33114100
H	-2.38418000	-1.37650700	-2.39933000
F	0.00000000	0.00000000	2.84875600

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$TpBe^{+}$

1 1

B	0.00000000	0.00000000	1.14832300
H	0.00000000	0.00000000	2.33427200
Be	0.00000000	0.00000000	-1.34623600
N	0.00000000	1.55256900	-0.79713200
N	0.00000000	1.43081600	0.54982400
N	-1.34456400	-0.77628500	-0.79713200
N	-1.23912300	-0.71540800	0.54982400
N	1.34456400	-0.77628500	-0.79713200
N	1.23912300	-0.71540800	0.54982400
C	0.00000000	2.84908800	-1.08502500
H	0.00000000	3.18740600	-2.10563400
C	0.00000000	3.58425500	0.08673700
H	0.00000000	4.65211800	0.18825100
C	0.00000000	2.64463900	1.09615600
H	0.00000000	2.76310600	2.16435600
C	-2.46738300	-1.42454400	-1.08502500
H	-2.76037500	-1.59370300	-2.10563400
C	-3.10405600	-1.79212800	0.08673700
H	-4.02885200	-2.32605900	0.18825100
C	-2.29032500	-1.32232000	1.09615600
H	-2.39292000	-1.38155300	2.16435600
C	2.46738300	-1.42454400	-1.08502500
H	2.76037500	-1.59370300	-2.10563400
C	3.10405600	-1.79212800	0.08673700
H	4.02885200	-2.32605900	0.18825100
C	2.29032500	-1.32232000	1.09615600
H	2.39292000	-1.38155300	2.16435600

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$TpBeHe^{+}$

1 1

B	0.00000000	0.00000000	1.20231300
H	0.00000000	0.00000000	2.38856600

Be	0.00000000	0.00000000	-1.32139000
N	-1.52208000	-0.28442400	-0.74128700
N	-1.40503200	-0.26281700	0.60405600
N	1.00735800	-1.17594700	-0.74128700
N	0.93012200	-1.08538500	0.60405600
N	0.51472200	1.46037100	-0.74128700
N	0.47490900	1.34820200	0.60405600
C	-2.79658500	-0.52285600	-1.03055000
H	-3.12891700	-0.58504300	-2.05130700
C	-3.52096300	-0.65894000	0.14002700
H	-4.57065300	-0.85565800	0.24039400
C	-2.59796400	-0.48660000	1.15019500
H	-2.71490700	-0.50938100	2.21826500
C	1.85109900	-2.16048500	-1.03055000
H	2.07112000	-2.41720000	-2.05130700
C	2.33114000	-2.71977300	0.14002700
H	3.02634700	-3.53047200	0.24039400
C	1.72039000	-2.00660300	1.15019500
H	1.79859000	-2.09648800	2.21826500
C	0.94548500	2.68334100	-1.03055000
H	1.05779700	3.00224300	-2.05130700
C	1.18982300	3.37871300	0.14002700
H	1.54430500	4.38613000	0.24039400
C	0.87757400	2.49320300	1.15019500
H	0.91631700	2.60586900	2.21826500
He	0.00000000	0.00000000	-3.06443100

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$TpBeNe^{+}$

1 1

B	0.00000000	0.00000000	-1.42037200
H	0.00000000	0.00000000	-2.60661900
Be	0.00000000	0.00000000	1.10347900
N	-1.54902200	-0.00102100	0.52352200
N	-1.42949500	-0.00044000	-0.82216000
N	0.77362700	1.34200300	0.52352200
N	0.71436600	1.23819900	-0.82216000
N	0.77539500	-1.34098200	0.52352200
N	0.71512900	-1.23775900	-0.82216000
C	-2.84552300	-0.00092200	0.81222100
H	-3.18415100	-0.00106000	1.83278800
C	-3.58239700	0.00000000	-0.35858400
H	-4.65031400	0.00047800	-0.45932400
C	-2.64320600	0.00012200	-1.36838200
H	-2.76207300	0.00106300	-2.43650000
C	1.42196300	2.46475600	0.81222100

H	1.59115800	2.75808600	1.83278800
C	1.79119900	3.10244700	-0.35858400
H	2.32557100	4.02705100	-0.45932400
C	1.32170900	2.28902300	-1.36838200
H	1.38195700	2.39149400	-2.43650000
C	1.42356000	-2.46383400	0.81222100
H	1.59299400	-2.75702600	1.83278800
C	1.79119900	-3.10244700	-0.35858400
H	2.32474300	-4.02752900	-0.45932400
C	1.32149700	-2.28914500	-1.36838200
H	1.38011600	-2.39255700	-2.43650000
Ne	0.00000000	0.00000000	3.12204900

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$TpBeAr^{+}$

1 1

B	0.00000000	0.00000000	-1.64505600
H	0.00000000	0.00000000	-2.83177300
Be	0.00000000	0.00000000	0.91169000
N	0.00000000	1.54539700	0.29656900
N	0.00000000	1.42801300	-1.04750700
N	1.33835300	-0.77269900	0.29656900
N	1.23669600	-0.71400700	-1.04750700
N	-1.33835300	-0.77269800	0.29656900
N	-1.23669600	-0.71400600	-1.04750700
C	0.00000000	2.84159600	0.58596300
H	0.00000000	3.17967600	1.60672700
C	0.00000000	3.58037600	-0.58393800
H	0.00000000	4.64835500	-0.68390300
C	0.00000000	2.64161200	-1.59407900
H	0.00000000	2.76056300	-2.66214700
C	2.46089400	-1.42079800	0.58596300
H	2.75368000	-1.58983800	1.60672700
C	3.10069700	-1.79018800	-0.58393800
H	4.02559400	-2.32417800	-0.68390300
C	2.28770300	-1.32080600	-1.59407900
H	2.39071800	-1.38028200	-2.66214700
C	-2.46089400	-1.42079800	0.58596300
H	-2.75368000	-1.58983800	1.60672700
C	-3.10069700	-1.79018800	-0.58393800
H	-4.02559400	-2.32417700	-0.68390300
C	-2.28770300	-1.32080600	-1.59407900
H	-2.39071800	-1.38028100	-2.66214700
Ar	0.00000000	0.00000000	3.16971900

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$TpBeKr^+$

1 1

B	0.00000000	0.00000000	-2.05735400
H	0.00000000	0.00000000	-3.24423100
Be	0.00000000	0.00000000	0.50945000
N	1.54465100	0.00000000	-0.11638000
N	1.42752000	-0.00001400	-1.46000300
N	-0.77232500	-1.33770700	-0.11638000
N	-0.71377200	-1.23626200	-1.46000300
N	-0.77232600	1.33770700	-0.11638000
N	-0.71374800	1.23627600	-1.46000300
C	2.84084200	-0.00082600	0.17275800
H	3.17926500	-0.00134400	1.19339100
C	3.57983500	-0.00134200	-0.99709600
H	4.64780100	-0.00202100	-1.09713500
C	2.64091900	-0.00114500	-2.00704900
H	2.75951400	-0.00192000	-3.07514200
C	-1.42113600	-2.45982800	0.17275800
H	-1.59079600	-2.75265200	1.19339100
C	-1.79108000	-3.09955700	-0.99709600
H	-2.32565100	-4.02410300	-1.09713500
C	-1.32145100	-2.28653000	-2.00704900
H	-1.38142000	-2.38884900	-3.07514200
C	-1.41970600	2.46065400	0.17275800
H	-1.58846900	2.75399600	1.19339100
C	-1.78875500	3.10089900	-0.99709600
H	-2.32215000	4.02612400	-1.09713500
C	-1.31946800	2.28767500	-2.00704900
H	-1.37809400	2.39076900	-3.07514200
Kr	0.00000000	0.00000000	2.90274600

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$TpBeXe^+$

1 1

B	0.02145500	-2.42599300	0.00000000
H	0.03316600	-3.61293200	0.00000000
Be	-0.00417000	0.15332800	0.00000000
N	1.54301900	-0.47034500	0.00000000
N	1.44201400	-1.81445800	0.00000000
N	-0.77292900	-0.49352300	1.33635400
N	-0.69944600	-1.83594100	1.23533300
N	-0.77292900	-0.49352300	-1.33635400
N	-0.69944600	-1.83594100	-1.23533300
C	2.83542800	-0.16560800	0.00000000
H	3.15912600	0.85983000	0.00000000

C	3.58845000	-1.32627500	0.00000000
H	4.65751700	-1.41368700	0.00000000
C	2.66178300	-2.34736800	0.00000000
H	2.79319400	-3.41394500	0.00000000
C	-1.42934900	-0.21212700	2.45578300
H	-1.61039800	0.80673900	2.74782100
C	-1.78930100	-1.38601300	3.09422200
H	-2.32638400	-1.49215100	4.01662500
C	-1.30504300	-2.39040900	2.28295500
H	-1.35286700	-3.45913700	2.38497400
C	-1.42934900	-0.21212700	-2.45578300
H	-1.61039800	0.80673900	-2.74782100
C	-1.78930100	-1.38601300	-3.09422200
H	-2.32638400	-1.49215100	-4.01662500
C	-1.30504300	-2.39040900	-2.28295500
H	-1.35286700	-3.45913700	-2.38497400
Xe	-0.01233200	2.72019800	0.00000000

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$TpBeRn^{+}$

1 1

B	0.00000000	0.00000000	-2.89578900
H	0.00000000	0.00000000	-4.08296800
Be	0.00000000	0.00000000	-0.31139400
N	-1.54281800	-0.00026300	-0.95612200
N	-1.42672900	-0.00051700	-2.29888200
N	0.77118100	1.33625100	-0.95612200
N	0.71291700	1.23584200	-2.29888200
N	0.77163700	-1.33598800	-0.95612200
N	0.71381200	-1.23532500	-2.29888200
C	-2.83864700	0.00000000	-0.66674500
H	-3.17484700	0.00071300	0.35456600
C	-3.57880800	-0.00008800	-1.83614600
H	-4.64681000	0.00011200	-1.93582900
C	-2.64012600	-0.00019900	-2.84630700
H	-2.75870800	0.00022600	-3.91439400
C	1.41932300	2.45834000	-0.66674500
H	1.58804100	2.74914200	0.35456600
C	1.78932800	3.09938300	-1.83614600
H	2.32350200	4.02419900	-1.93582900
C	1.31989100	2.28651600	-2.84630700
H	1.37955000	2.38899800	-3.91439400
C	1.41932400	-2.45834000	-0.66674500
H	1.58680600	-2.74985500	0.35456600
C	1.78948000	-3.09929500	-1.83614600
H	2.32330800	-4.02431100	-1.93582900

C	1.32023500	-2.28631700	-2.84630700
H	1.37915800	-2.38922400	-3.91439400
Rn	0.00000000	0.00000000	2.33645500

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TpMgF

0 1

B	0.00000000	0.00000000	-1.36930100
H	0.00000000	0.00000000	-2.56502800
Mg	0.00000000	0.00000000	1.69390200
N	0.00000000	1.71326700	0.47064600
N	0.00000000	1.44940300	-0.84541100
N	1.48373300	-0.85663300	0.47064600
N	1.25522000	-0.72470200	-0.84541100
N	-1.48373300	-0.85663300	0.47064600
N	-1.25522000	-0.72470200	-0.84541100
C	0.00000000	3.03122400	0.60017000
H	0.00000000	3.47663200	1.57928100
C	0.00000000	3.64107400	-0.64812200
H	0.00000000	4.69041400	-0.87143000
C	0.00000000	2.59130200	-1.53741500
H	0.00000000	2.57735700	-2.61171100
C	2.62511700	-1.51561200	0.60017000
H	3.01085200	-1.73831600	1.57928100
C	3.15326300	-1.82053700	-0.64812200
H	4.06201800	-2.34520700	-0.87143000
C	2.24413300	-1.29565100	-1.53741500
H	2.23205600	-1.28867800	-2.61171100
C	-2.62511700	-1.51561200	0.60017000
H	-3.01085200	-1.73831600	1.57928100
C	-3.15326300	-1.82053700	-0.64812200
H	-4.06201800	-2.34520700	-0.87143000
C	-2.24413300	-1.29565100	-1.53741500
H	-2.23205600	-1.28867800	-2.61171100
F	0.00000000	0.00000000	3.46699700

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$TpMg^{+}$

1 1

B	0.00000000	0.00000000	-1.07338000
H	0.00000000	0.00000000	-2.26331000

N	0.00000000	1.77168700	0.77318900
N	0.00000000	1.46470400	-0.54693400
N	1.53432600	-0.88584300	0.77318900
N	1.26847100	-0.73235200	-0.54693400
N	-1.53432600	-0.88584300	0.77318900
N	-1.26847100	-0.73235200	-0.54693400
C	0.00000000	3.10163300	0.86580700
H	0.00000000	3.58504500	1.82612700
C	0.00000000	3.67026200	-0.40024800
H	0.00000000	4.71229700	-0.65309700
C	0.00000000	2.59095800	-1.26440300
H	0.00000000	2.55287000	-2.33822400
C	2.68609300	-1.55081600	0.86580700
H	3.10474000	-1.79252200	1.82612700
C	3.17854000	-1.83513100	-0.40024800
H	4.08096900	-2.35614800	-0.65309700
C	2.24383500	-1.29547900	-1.26440300
H	2.21085000	-1.27643500	-2.33822400
C	-2.68609300	-1.55081600	0.86580700
H	-3.10474000	-1.79252200	1.82612700
C	-3.17854000	-1.83513100	-0.40024800
H	-4.08096900	-2.35614800	-0.65309700
C	-2.24383500	-1.29547900	-1.26440300
H	-2.21085000	-1.27643500	-2.33822400
Mg	0.00000000	0.00000000	1.72946900

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TpMgHe$^+$

1 1

B	0.00000000	0.00000000	-1.13052100
H	0.00000000	0.00000000	-2.32021700
N	-0.00085900	1.76406400	0.70703800
N	0.00048200	1.46011500	-0.61232000
N	1.52815400	-0.88128800	0.70703800
N	1.26425600	-0.73047500	-0.61232000
N	-1.52729500	-0.88277600	0.70703800
N	-1.26473800	-0.72964000	-0.61232000
C	-0.00137100	3.09028600	0.79989600
H	-0.00239600	3.57260600	1.76148800
C	0.00000000	3.65993900	-0.46028900
H	0.00008700	4.70287700	-0.71109400
C	0.00039700	2.58733000	-1.32396200
H	0.00098000	2.55290200	-2.39801500
C	2.67695200	-1.54395600	0.79989600
H	3.09516500	-1.78422800	1.76148800
C	3.16960000	-1.82997000	-0.46028900

H	4.07276700	-2.35151400	-0.71109400
C	2.24049500	-1.29400900	-1.32396200
H	2.21038800	-1.27730000	-2.39801500
C	-2.67558100	-1.54633000	0.79989600
H	-3.09277000	-1.78837800	1.76148800
C	-3.16960000	-1.82996900	-0.46028900
H	-4.07285400	-2.35136300	-0.71109400
C	-2.24089200	-1.29332100	-1.32396200
H	-2.21136800	-1.27560200	-2.39801500
Mg	0.00000000	0.00000000	1.66876600
He	0.00000000	0.00000000	3.85990000

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$TpMgNe^+$

1 1

B	0.00000000	0.00000000	-1.37618900
H	0.00000000	0.00000000	-2.56589700
N	0.00000000	1.76362700	0.46105000
N	0.00000000	1.45994400	-0.85806400
N	1.52734600	-0.88181300	0.46105000
N	1.26434900	-0.72997200	-0.85806400
N	-1.52734600	-0.88181300	0.46105000
N	-1.26434900	-0.72997200	-0.85806400
C	0.00000000	3.08985600	0.55392300
H	0.00000000	3.57197600	1.51559900
C	0.00000000	3.65966700	-0.70621300
H	0.00000000	4.70263800	-0.95694500
C	0.00000000	2.58711900	-1.56991200
H	0.00000000	2.55268400	-2.64395900
C	2.67589400	-1.54492800	0.55392300
H	3.09342200	-1.78598800	1.51559900
C	3.16936500	-1.82983300	-0.70621300
H	4.07260400	-2.35131900	-0.95694500
C	2.24051100	-1.29355900	-1.56991200
H	2.21068900	-1.27634200	-2.64395900
C	-2.67589400	-1.54492800	0.55392300
H	-3.09342200	-1.78598800	1.51559900
C	-3.16936500	-1.82983300	-0.70621300
H	-4.07260400	-2.35131900	-0.95694500
C	-2.24051100	-1.29355900	-1.56991200
H	-2.21068900	-1.27634200	-2.64395900
Mg	0.00000000	0.00000000	1.42547400
Ne	0.00000000	0.00000000	3.79340100

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$TpMgAr^+$

1 1

B	0.01147800	-1.62613400	0.00000000
H	0.02120400	-2.81607300	0.00000000
N	1.75785200	0.22321100	0.00000000
N	1.46650100	-1.09733900	0.00000000
N	-0.88504200	0.20534100	1.52106300
N	-0.72158300	-1.11244700	1.26329000
N	-0.88504200	0.20534100	-1.52106300
N	-0.72158300	-1.11244700	-1.26329000
C	3.08334200	0.32785300	0.00000000
H	3.55647000	1.29398500	0.00000000
C	3.66469900	-0.92713500	0.00000000
H	4.70981200	-1.16875600	0.00000000
C	2.59927400	-1.79981300	0.00000000
H	2.57377800	-2.87407100	0.00000000
C	-1.55012700	0.29558400	2.66842200
H	-1.80015200	1.25631100	3.08285900
C	-1.82487300	-0.96551400	3.16623400
H	-2.34527000	-1.21808900	4.06957900
C	-1.28008300	-1.82702000	2.24051600
H	-1.25346700	-2.90093000	2.21335500
C	-1.55012700	0.29558400	-2.66842200
H	-1.80015200	1.25631100	-3.08285900
C	-1.82487300	-0.96551400	-3.16623400
H	-2.34527000	-1.21808900	-4.06957900
C	-1.28008300	-1.82702000	-2.24051600
H	-1.25346700	-2.90093000	-2.21335500
Mg	-0.00294800	1.19896100	0.00000000
Ar	-0.02145000	3.78943300	0.00000000

****

$TpMgKr^{+}$

1 1

B	-2.08867500	0.00000000	0.00000000
H	-3.27888000	0.00000000	0.00000000
N	-0.25118700	1.75772100	0.00000000
N	-1.56989600	1.45846300	0.00000000
N	-0.25118700	-0.87886000	-1.52223100
N	-1.56989600	-0.72923100	-1.26306600
N	-0.25118700	-0.87886000	1.52223100
N	-1.56989600	-0.72923100	1.26306600
C	-0.15529600	3.08346300	0.00000000
H	0.80760300	3.56313300	0.00000000
C	-1.41403300	3.65739900	0.00000000
H	-1.66221700	4.70096800	0.00000000
C	-2.27999800	2.58682900	0.00000000

H	-3.35407000	2.55425400	0.00000000
C	-0.15529600	-1.54173100	-2.67035700
H	0.80760300	-1.78156600	-3.08576300
C	-1.41403300	-1.82870000	-3.16740000
H	-1.66221700	-2.35048400	-4.07115800
C	-2.27999800	-1.29341500	-2.24026000
H	-3.35407000	-1.27712700	-2.21204800
C	-0.15529600	-1.54173100	2.67035700
H	0.80760300	-1.78156600	3.08576300
C	-1.41403300	-1.82870000	3.16740000
H	-1.66221700	-2.35048400	4.07115800
C	-2.27999800	-1.29341500	2.24026000
H	-3.35407000	-1.27712700	2.21204800
Mg	0.74598800	0.00000000	0.00000000
Kr	3.47019700	0.00000000	0.00000000

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$TpMgXe^{+}$

1 1

B	0.00000000	0.00000000	-2.50457800
H	0.00000000	0.00000000	-3.69502200
N	1.75538900	0.00000000	-0.66688700
N	1.45787400	-0.00175600	-1.98548500
N	-0.87769500	-1.52021100	-0.66688700
N	-0.73045800	-1.26167800	-1.98548500
N	-0.87769400	1.52021200	-0.66688700
N	-0.72741600	1.26343400	-1.98548500
C	3.08087800	-0.00082500	-0.56947500
H	3.55926800	0.00012800	0.39404200
C	3.65653500	-0.00322800	-1.82762400
H	4.70036600	-0.00434300	-2.07466400
C	2.58686900	-0.00340900	-2.69465900
H	2.55518100	-0.00466200	-3.76873900
C	-1.54115400	-2.66770600	-0.56947500
H	-1.77952300	-3.08248100	0.39404200
C	-1.83106300	-3.16503800	-1.82762400
H	-2.35394400	-4.06846500	-2.07466400
C	-1.29638700	-2.23859000	-2.69465900
H	-1.28162800	-2.21052100	-3.76873900
C	-1.53972400	2.66853100	-0.56947500
H	-1.77974500	3.08235300	0.39404200
C	-1.82547200	3.16826600	-1.82762400
H	-2.34642200	4.07280800	-2.07466400
C	-1.29048200	2.24199900	-2.69465900
H	-1.27355300	2.21518300	-3.76873900
Mg	0.00000000	0.00000000	0.34291800

Xe	0.00000000	0.00000000	3.25560100

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$TpMgRn^{+}$

1 1

B	0.00000000	0.00000000	-3.03794200
H	0.00000000	0.00000000	-4.22847600
N	1.75416700	0.00000000	-1.20014900
N	1.45757600	-0.00179100	-2.51863300
N	-0.87708300	-1.51915300	-1.20014900
N	-0.73033900	-1.26140200	-2.51863300
N	-0.87708300	1.51915300	-1.20014900
N	-0.72723700	1.26319300	-2.51863300
C	3.07953000	-0.00093000	-1.10194500
H	3.55720600	-0.00001300	-0.13808300
C	3.65608600	-0.00350200	-2.35980500
H	4.70005600	-0.00477300	-2.60625100
C	2.58687800	-0.00351100	-3.22739600
H	2.55563200	-0.00477200	-4.30148300
C	-1.54057000	-2.66648600	-1.10194500
H	-1.77861400	-3.08062400	-0.13808300
C	-1.83107600	-3.16451200	-2.35980500
H	-2.35416200	-4.06798100	-2.60625100
C	-1.29648000	-2.23854700	-3.22739600
H	-1.28194900	-2.21085600	-4.30148300
C	-1.53896000	2.66741600	-1.10194500
H	-1.77859200	3.08063700	-0.13808300
C	-1.82501000	3.16801400	-2.35980500
H	-2.34589400	4.07275400	-2.60625100
C	-1.29039800	2.24205800	-3.22739600
H	-1.27368300	2.21562800	-4.30148300
Mg	0.00000000	0.00000000	-0.18352900
Rn	0.00000000	0.00000000	2.80531400

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