

Supporting Information

Bent and Planar Structures of $\mu\text{-}\eta^2\text{:}\eta^2\text{-N}_2$ Dinuclear Early Transition Metal Complexes

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Cartesian coordinates of all stationary points optimized at B3LYP/BSI level

Table S1. Relative energies calculated at B3LYP/BSI level including potential energy (ΔE), potential energy with zero-point correction (ΔZPE) and free energy (ΔG). (unit: kcal/mol)

Complex	<i>trans</i>			Complex	<i>cis</i>		
	ΔE	ΔZPE	ΔG		ΔE	ΔZPE	ΔG
TaN_P^{trans}	0.0	0.0	0.0	TaN_{B1}^{cis}	-4.5	-2.8	-1.4
TSTaN_{B-P}^{trans}	11.7	12.0	13.5	TSTaN_{B1-B2}^{cis}	-1.4	-0.8	0.8
TaN_B^{trans}	7.7	8.7	9.9	TaN_{B2}^{cis}	-1.6	-1.0	-0.4
NbN_P^{trans}	0.0	0.0	0.0	NbN_{B1}^{cis}	-2.2	-1.8	-1.9
TSNbN_{B-P}^{trans}	10.8	11.0	12.7	TSNbN_{B1-B2}^{cis}	-1.3	-0.6	1.4
NbN_B^{trans}	0.2	2.3	5.7	NbN_{B2}^{cis}	-2.2	-1.0	0.4
MoN_P^{trans}	0.0	0.0	0.0	MoN_{B1}^{cis}	4.6	4.5	4.1
TSMoN_{B-P}^{trans}	6.8	6.9	9.4	TSMoN_{B1-B2}^{cis}	6.3	6.3	6.7
MoN_B^{trans}	-5.2	-3.7	-1.2	MoN_{B2}^{cis}	-4.4	-3.4	-1.2
WN_P^{trans}	0.0	0.0	0.0	WN_{B1}^{cis}	14.0	13.9	13.2
TSWN_{B-P}^{trans}	6.3	7.3	9.4	TSWN_{B1-B2}^{cis}	15.4	15.2	15.0
WN_B^{trans}	-3.2	-1.6	0.2	WN_{B2}^{cis}	-3.9	-2.7	-1.2

Table S2. Energies calculated at B3LYP/BSI level including potential energy (E), potential energy with zero-point correction (ZPE) and free energy (G). (unit: a.u.)

Complex	<i>trans</i>			Complex	<i>cis</i>		
	E	ZPE	G		E	ZPE	G
TaN_P^{trans}	-1068.3763	-1067.9932	-1068.0547	TaN_{B1}^{cis}	-1068.3834	-1067.9978	-1068.0569
TSTaN_{B-P}^{trans}	-1068.3577	-1067.9742	-1068.0332	TSTaN_{B1-B2}^{cis}	-1068.3785	-1067.9945	-1068.0533
TaN_B^{trans}	-1068.3640	-1067.9794	-1068.0389	TaN_{B2}^{cis}	-1068.3788	-1067.9948	-1068.0554
NbN_P^{trans}	-1065.3513	-1064.9680	-1065.0292	NbN_{B1}^{cis}	-1065.3549	-1064.9709	-1065.0322
TSNbN_{B-P}^{trans}	-1065.3341	-1064.9505	-1065.0089	TSNbN_{B1-B2}^{cis}	-1065.3534	-1064.9689	-1065.0270
NbN_B^{trans}	-1065.3510	-1064.9644	-1065.0201	NbN_{B2}^{cis}	-1065.3549	-1064.9696	-1065.0287
MoN_P^{trans}	-1087.6925	-1087.3084	-1087.3697	MoN_{B1}^{cis}	-1087.6852	-1087.3012	-1087.3631
TSMoN_{B-P}^{trans}	-1087.6817	-1087.2974	-1087.3546	TSMoN_{B1-B2}^{cis}	-1087.6825	-1087.2984	-1087.3590
MoN_B^{trans}	-1087.7008	-1087.3142	-1087.3716	MoN_{B2}^{cis}	-1087.6996	-1087.3138	-1087.3716
WN_P^{trans}	-1088.2867	-1087.9027	-1087.9627	WN_{B1}^{cis}	-1088.2644	-1087.8804	-1087.9416
TSWN_{B-P}^{trans}	-1088.2766	-1087.8910	-1087.9477	TSWN_{B1-B2}^{cis}	-1088.2621	-1087.8784	-1087.9389
WN_B^{trans}	-1088.2918	-1087.9053	-1087.9624	WN_{B2}^{cis}	-1088.2929	-1087.9070	-1087.9647

Table S3. Energy decomposition analyses for the different butterfly distortion structures of the M_2N_2 (M= Ta, Nb, Mo and W) cores from DFT/PBE calculations. (unit: eV)

	Steric Interaction			Orbital Interactions	Total Bonding Energy
	Pauli Repulsion	Electrostatic Interaction	Sum*		
ZrN_{B1}^{cis}	40.8274	-8.6470	32.1804	-42.7845	-10.6041
ZrN_{B2}^{cis}	40.8274	-8.6470	32.1804	-42.7845	-10.6041
ZrN_{B1}^{trans}	40.8401	-8.6465	32.1936	-42.7959	-10.6024
ZrN_{B2}^{trans}	40.8316	-8.6440	32.1876	-42.7900	-10.6024
HfN_{B1}^{cis}	41.3512	-8.8869	32.4643	-43.0822	-10.6180
HfN_{B2}^{cis}	41.3536	-8.8883	32.4653	-43.0831	-10.6179
HfN_{B1}^{trans}	41.3395	-8.8815	32.4581	-43.0742	-10.6161
HfN_{B2}^{trans}	41.3327	-8.8798	32.4529	-43.0690	-10.6161
NbN_{B1}^{cis}	41.2230	-8.7477	32.4753	-43.1272	-10.6519
NbN_{B2}^{cis}	41.1016	-8.7193	32.3823	-43.0211	-10.6387
NbN_P^{trans}	41.3478	-8.8123	32.5355	-43.1828	-10.6474
NbN_B^{trans}	41.0441	-8.7070	32.3371	-42.9692	-10.6320
TaN_{B1}^{cis}	42.2070	-9.2791	32.9279	-43.5944	-10.6666
TaN_{B2}^{cis}	42.0994	-9.2462	32.8532	-43.5096	-10.6564
TaN_P^{trans}	42.1802	-9.2866	32.8936	-43.5463	-10.6527
TaN_B^{trans}	41.9700	-9.2221	32.7478	-43.4005	-10.6526
MoN_{B1}^{cis}	41.4378	-8.8892	32.5486	-43.1440	-10.5954
MoN_{B2}^{cis}	41.3862	-8.8472	32.5390	-43.1122	-10.5732
MoN_P^{trans}	41.6925	-8.9285	32.7640	-43.3626	-10.5986
MoN_B^{trans}	41.2852	-8.8584	32.4268	-43.0120	-10.5852
WN_{B1}^{cis}	42.5144	-9.4846	33.0298	-43.7098	-10.6800
WN_{B2}^{cis}	42.4377	-9.4288	33.0089	-43.6579	-10.6490
WN_P^{trans}	42.7388	-9.5497	33.1891	-43.8730	-10.6840
WN_B^{trans}	42.3001	-9.4410	32.8590	-43.5251	-10.6660

* Steric interaction is the sum of the electrostatic and Pauli interaction.

Table S4. Calculated imaginary frequencies of transition states at B3LYP/BSI level.

TSTaN_{B-P}^{trans}	62.4 <i>i</i>	TSTaN_{B1-B2}^{cis}	26.2 <i>i</i>
TSNbN_{B-P}^{trans}	69.3 <i>i</i>	TSNbN_{B1-B2}^{cis}	14.8 <i>i</i>
TSMoN_{B-P}^{trans}	98.3 <i>i</i>	TSMoN_{B1-B2}^{cis}	33.5 <i>i</i>
TSWN_{B-P}^{trans}	122.8 <i>i</i>	TSWN_{B1-B2}^{cis}	23.3 <i>i</i>

Table S5. The comparison between calculated results using B3LYP and those using ω b97x-D

Method/model	Complex/ Parameters	B3LYP/BSI				ω b97x-D/BSII			
		C1	C2	C3	C4	C1	C2	C3	C4
TaN_B^{trans}	$\angle$ M ¹ -N ¹ -N ² -M ²	98.7	99.2	107.9	176.7	96.1	96.4	98.0	176.2
	M ¹ -M ² Distance	2.835	2.846	2.982	3.753	2.773	2.780	2.806	3.735
	N ¹ -N ² Distance	1.495	1.493	1.547	1.464	1.471	1.470	1.481	1.429
TaN_B^{cis}	$\angle$ M ¹ -N ¹ -N ² -M ²	144.3	149.7	155.7	173.4	101.2	103.3	146.7	171.0
	M ¹ -M ² Distance	3.557	3.613	3.669	3.786	2.869	2.907	3.574	3.751
	N ¹ -N ² Distance	1.446	1.459	1.455	1.429	1.498	1.501	1.432	1.406
NbN_B^{trans}	$\angle$ M ¹ -N ¹ -N ² -M ²	84.5	85.2	86.2	177.8	84.3	84.7	85.5	177.0
	M ¹ -M ² Distance	2.715	2.719	2.752	3.902	2.681	2.685	2.708	3.877
	N ¹ -N ² Distance	1.331	1.335	1.338	1.360	1.324	1.325	1.329	1.336
WN_B^{trans}	$\angle$ M ¹ -N ¹ -N ² -M ²	82.6	83.1	122.2	179.6	81.9	82.3	117.5	169.6
	M ¹ -M ² Distance	2.588	2.591	3.202	3.784	2.548	2.560	3.114	3.329
	N ¹ -N ² Distance	1.344	1.348	1.528	1.469	1.328	1.332	1.504	1.492
MoN_B^{trans}	$\angle$ M ¹ -N ¹ -N ² -M ²	80.3	99.2	119.3	179.1	79.1	79.8	114.5	178.9
	M ¹ -M ² Distance	2.294	2.846	3.300	3.884	2.564	2.562	3.174	3.787
	N ¹ -N ² Distance	1.278	1.493	1.394	1.357	1.258	1.265	1.385	1.385

Figure S1. The detailed geometrical parameters (unit: Å) of optimized structures.

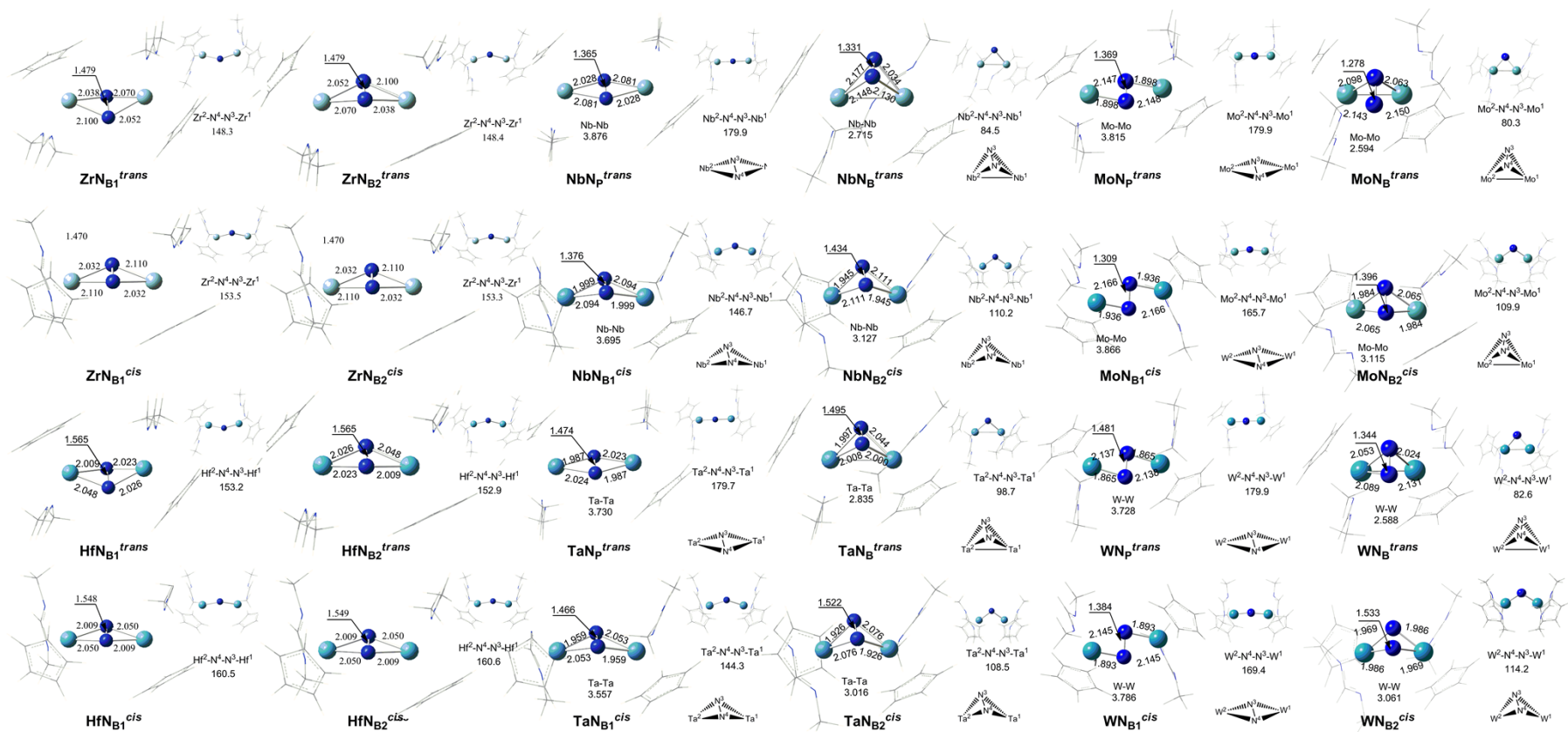


Figure S2. HOMO and LUMO of $[L_nM]_2(\mu-\eta^2:\eta^2-N_2)$ (M= Ta, Mo and W) in the different butterfly distortion structures.

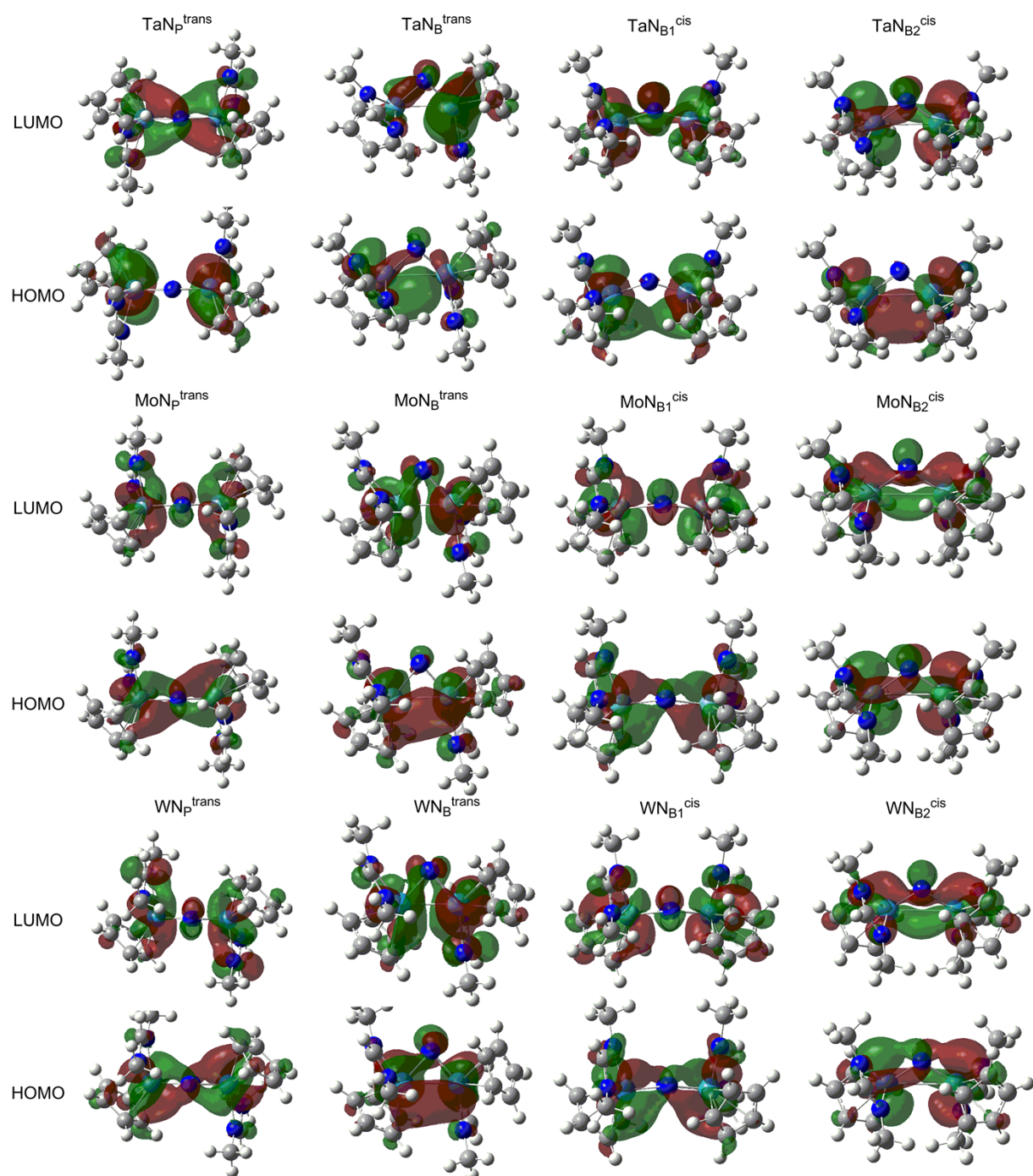
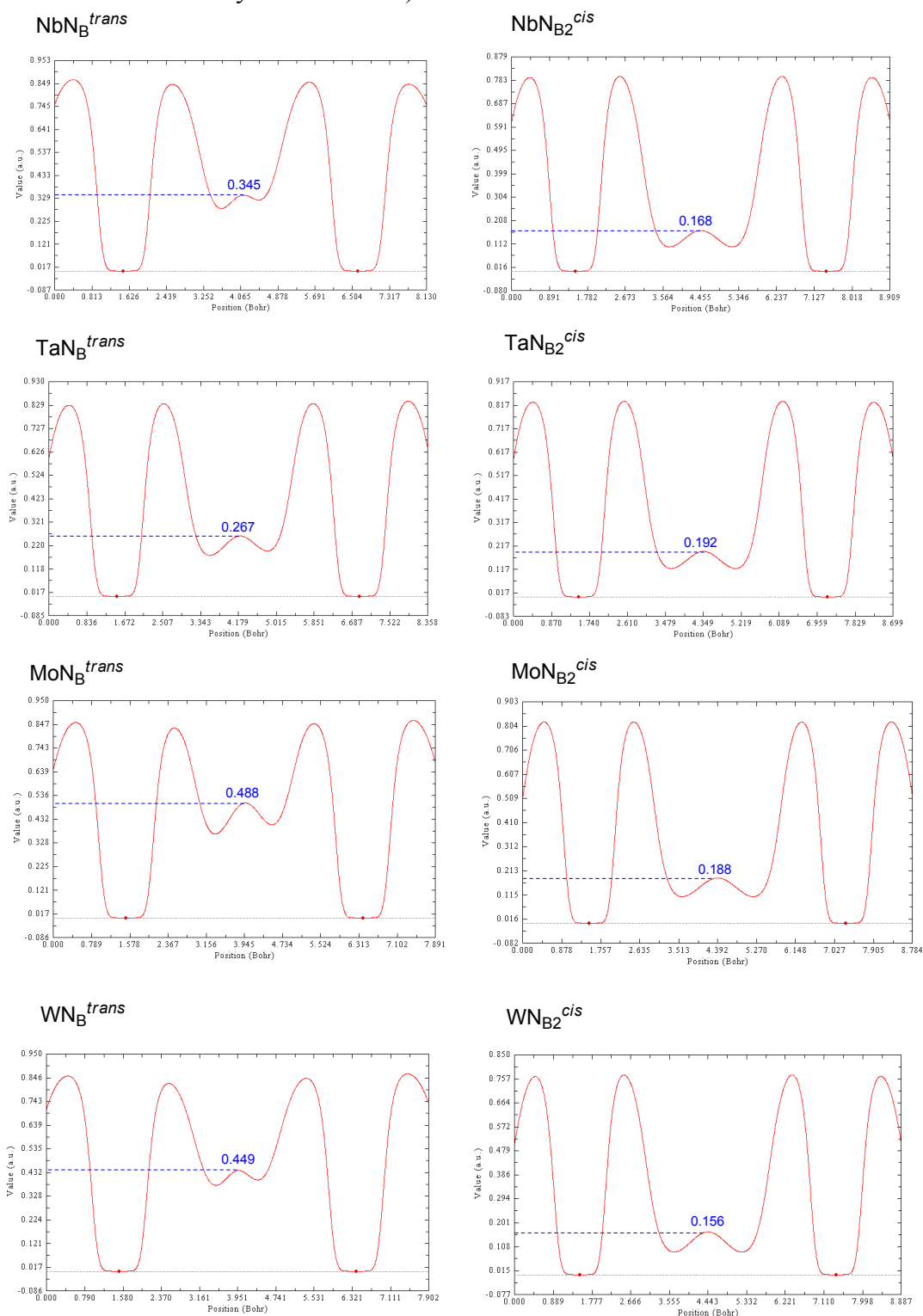


Figure S3. Global statistics ELF analysis on M^1-M^2 bond of MN_B^{trans} and MN_{B2}^{cis} ($M = Nb, Ta, Mo$ and W) in a line. (The red circle denote the position of the two metal atom nuclei, and the saddle-backing between them stand for the covalent interaction. And the strength of the covalent interaction is consistent with the results of NBO and Mayer bond order.)



Cartesian coordinates of all stationary points optimized at B3LYP/BSI level

ZrN_{B1}^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.07023500	-1.02993100	-0.03800500
N	0.00471200	0.06949400	-1.02537500
N	2.93289600	-1.54426700	1.08902800
N	3.37734500	-1.18766300	-1.10252200
C	3.52393600	-1.94744100	-0.01426100
C	2.85275200	-2.41201200	2.24210100
C	4.06540400	-1.50581700	-2.33437000
N	-2.28185600	1.37296200	1.21103800
N	-2.72683800	1.70246200	-0.98110700
C	-2.71802500	2.18172500	0.24100900
C	-2.36009400	1.76578800	2.60058400
C	-3.05717000	2.53906100	-2.11126100
H	3.52312400	-3.28033800	2.14676100
H	3.36226300	-1.53682500	-3.17507800
H	-2.58311000	2.83852500	2.70125000
H	-2.18862500	2.66338400	-2.77134200
C	3.36090400	1.75061400	1.22310800
C	1.99458800	2.11956900	1.40924600
C	1.50471100	2.61327600	0.16710900
C	2.55342600	2.51833700	-0.78548000
C	3.70226600	1.99831400	-0.12385600
C	-4.05437000	-1.38083700	0.85613100
C	-4.26044000	-1.27180700	-0.53750200
C	-3.33004100	-2.13589800	-1.18976600
C	-2.56371100	-2.78764800	-0.18419000
C	-2.99712000	-2.30828600	1.07916900
H	-3.25499600	-2.30404000	-2.25810600
H	-4.98549500	-0.63387200	-1.02723100
H	-4.59368400	-0.83594900	1.62115900
H	-2.60581200	-2.61360000	2.04194600
H	-1.76499400	-3.49744000	-0.35395600
H	0.50203100	2.97110300	-0.02390400
H	2.49343600	2.81341500	-1.82625300
H	4.66133200	1.79406000	-0.58340200
H	4.01158800	1.32638700	1.97695400
H	1.44417100	2.08040400	2.34165400
H	3.13022800	-1.86758800	3.15308800
H	1.82913800	-2.78621000	2.37778400
H	4.83212200	-0.75420900	-2.57066600
H	4.56263500	-2.48541600	-2.27354300
H	4.09981300	-2.88822800	-0.05636100
H	-3.39086500	3.53957600	-1.79476100
H	-3.86005000	2.08717500	-2.70782000
H	-3.05024200	3.20960300	0.46913200
H	-3.14240500	1.20922700	3.13716000
H	-1.40999200	1.56966000	3.11182300
Zr	-1.84952600	-0.32231400	-0.19198100
Zr	1.83554800	0.10426900	-0.13187600

ZrN_{B2}^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.00471800	0.06825000	-1.02617600
N	-0.07046600	-1.03084700	-0.03838200
N	2.72556500	1.70251800	-0.98131800
N	2.28115300	1.37308900	1.21094500
C	2.71685100	2.18190900	0.24074500
C	3.05563700	2.53901400	-2.11162300
C	2.35936500	1.76616400	2.60042100
N	-3.37833800	-1.18701600	-1.10212600
N	-2.93294300	-1.54395800	1.08918700
C	-3.52450300	-1.94694100	-0.01390300
C	-4.06751100	-1.50466200	-2.33349100
C	-2.85172200	-2.41216600	2.24185100
H	3.38856600	3.53984600	-1.79532400
H	1.40982800	1.56842000	3.11206900
H	-4.56201000	-2.48571400	-2.27378300
H	-1.82793100	-2.78624300	2.37651700
C	4.26051900	-1.27102700	-0.53676900
C	3.33074700	-2.13492800	-1.19019300
C	2.56411200	-2.78770500	-0.18553700
C	2.99673600	-2.30921700	1.07843700
C	4.05379400	-1.38125800	0.85668200
C	-3.70162300	1.99845800	-0.12042400
C	-3.35686900	1.75133300	1.22577500
C	-1.99001800	2.12010700	1.40826900
C	-1.50320100	2.61313400	0.16465400
C	-2.55435600	2.51795400	-0.78521100
H	-1.43719900	2.08120300	2.33926200
H	-4.00570200	1.32757700	1.98147800
H	-4.66190300	1.79422500	-0.57743200
H	-2.49699300	2.81251000	-1.82628300
H	-0.50091400	2.97058100	-0.02908500
H	1.76567500	-3.49758400	-0.35626200
H	2.60504400	-2.61546900	2.04076000
H	4.59254100	-0.83679600	1.62241500
H	4.98565700	-0.63251100	-1.02561900
H	3.25631900	-2.30224500	-2.25870500
H	3.85897600	2.08750500	-2.70785600
H	2.18717200	2.66253700	-2.77195500
H	3.14288700	1.21104100	3.13673600
H	2.58052200	2.83930500	2.70090700
H	3.04870900	3.20994200	0.46868300
H	-3.52202900	-3.28056400	2.14671000
H	-3.12854000	-1.86813700	3.15326900
H	-4.10034100	-2.88775700	-0.05590300
H	-4.83660600	-0.75467500	-2.56728600
H	-3.36549800	-1.53221200	-3.17523100
Zr	-1.83533400	0.10401900	-0.13220400
Zr	1.84919000	-0.32252100	-0.19182300

HfN_{B1}^{trans}

	Coordinates (Angstroms)		
	X	Y	Z

N	0.05927100	-0.95039200	0.19930300
N	-0.02003000	0.11823700	-0.94197000
N	2.93053500	-1.48867000	1.13172300
N	3.16763700	-1.29887900	-1.10386400
C	3.42042900	-1.98126200	0.01569400
C	2.98006700	-2.23815200	2.36574400
C	3.70363000	-1.71809800	-2.38019100
N	-2.26723800	1.45565400	1.23528200
N	-2.70345900	1.69061400	-0.96292200
C	-2.69856400	2.22878700	0.23521200
C	-2.31291300	1.90592500	2.60874800
C	-3.02212200	2.46569700	-2.13914700
H	3.62777900	-3.12378300	2.27960200
H	2.90038300	-1.84454700	-3.11580200
H	-2.54273300	2.97966900	2.67009500
H	-2.14605400	2.55444300	-2.79472800
C	3.46461200	1.71553000	1.10224100
C	2.12499500	2.16255300	1.31315200
C	1.61161200	2.60106800	0.05953900
C	2.61461600	2.38744500	-0.92298600
C	3.76277900	1.85440800	-0.26975100
C	-4.06375800	-1.27745900	0.85019600
C	-4.20290200	-1.18019600	-0.55239000
C	-3.23902600	-2.04531400	-1.15346700
C	-2.52207900	-2.68926000	-0.10666500
C	-3.01650400	-2.20023400	1.13090500
H	-3.11287000	-2.22261300	-2.21521100
H	-4.90355500	-0.54622400	-1.08071100
H	-4.63932500	-0.72667100	1.58394200
H	-2.66966000	-2.49687000	2.11321900
H	-1.71359400	-3.39682500	-0.23155100
H	0.62105200	2.99661300	-0.11864200
H	2.52728900	2.61640200	-1.97826400
H	4.69119500	1.57068600	-0.74960600
H	4.12429800	1.31148200	1.85924800
H	1.61386600	2.21933700	2.26668100
H	3.36649900	-1.61366100	3.18097600
H	1.97645400	-2.57713000	2.65483300
H	4.40778900	-0.97553200	-2.78059900
H	4.23786600	-2.67535800	-2.29342000
H	3.99651400	-2.92096600	-0.00904700
H	-3.35950400	3.48063300	-1.87964600
H	-3.81855700	1.98143600	-2.71861000
H	-3.02584700	3.26601300	0.41728200
H	-3.07626300	1.36543100	3.18651600
H	-1.34814900	1.73798700	3.10198900
Hf	-1.81952500	-0.25297700	-0.09615800
Hf	1.79825900	0.09194200	-0.08707000

HfN_{B2}^{trans}

Coordinates (Angstroms)			
	X	Y	Z
N	0.02029300	0.12308300	-0.93785100
N	-0.05857300	-0.94638200	0.20224400
N	2.70636300	1.69046200	-0.96299100

N	2.27296300	1.45546200	1.23577300
C	2.70337900	2.22848700	0.23521600
C	3.02251500	2.46590600	-2.13965400
C	2.32163500	1.90516000	2.60933700
N	-3.16357700	-1.30141100	-1.10470100
N	-2.93012900	-1.49027700	1.13129200
C	-3.41758100	-1.98375500	0.01459900
C	-3.69648900	-1.72171000	-2.38194800
C	-2.98233100	-2.23856200	2.36591000
H	3.36169800	3.48033200	-1.88050600
H	1.35827000	1.73600700	3.10483100
H	-4.23211000	-2.67821300	-2.29537100
H	-1.97912400	-2.57587500	2.65832100
C	4.20249100	-1.18242800	-0.55453600
C	3.23676000	-2.04549800	-1.15558100
C	2.51956600	-2.68913500	-0.10874900
C	3.01569700	-2.20186700	1.12884800
C	4.06425900	-1.28058100	0.84806100
C	-3.76525500	1.85203600	-0.28210300
C	-3.47885600	1.71156800	1.09224600
C	-2.14189200	2.16056900	1.31547300
C	-1.61834600	2.60176400	0.06703400
C	-2.61241100	2.38793500	-0.92453500
H	-1.63939300	2.21713400	2.27360600
H	-4.14447300	1.30542300	1.84291500
H	-4.68905300	1.56764300	-0.77040400
H	-2.51617200	2.61854100	-1.97866700
H	-0.62696300	2.99934300	-0.10192200
H	1.70990600	-3.39537000	-0.23355800
H	2.66916700	-2.49876400	2.11119000
H	4.64120400	-0.73126200	1.58182400
H	4.90369100	-0.54909400	-1.08289300
H	3.10951000	-2.22174200	-2.21737100
H	3.81680900	1.98112500	-2.72159500
H	2.14471300	2.55596700	-2.79274500
H	3.08697700	1.36520200	3.18499700
H	2.55050200	2.97911500	2.67058100
H	3.03139000	3.26554000	0.41697500
H	-3.62857000	-3.12516600	2.27873100
H	-3.37202700	-1.61379900	3.17939000
H	-3.99285500	-2.92393500	-0.01082400
H	-4.39868400	-0.97883600	-2.78518200
H	-2.89143000	-1.85006000	-3.11527400
Hf	-1.79921000	0.09268900	-0.08567000
Hf	1.82083300	-0.25192700	-0.09545700

NbN_P^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.02238200	0.53819800	-0.41915000
N	-0.02223500	-0.53803700	0.41915100
N	2.84839100	1.63951900	-0.98918700
N	2.75257400	1.30833600	1.20586400
C	2.99456200	2.15754000	0.20653600
C	2.87260900	2.44781900	-2.18485600
C	2.99035000	1.63428300	2.59179100

N	-2.75211000	-1.30860700	-1.20584700
N	-2.84813900	-1.63963300	0.98922700
C	-2.99483800	-2.15755800	-0.20644800
C	-2.99134500	-1.63417000	-2.59162600
C	-2.87346700	-2.44778900	2.18497900
H	3.28156000	3.45117100	-1.98817300
H	2.11309500	1.38872200	3.20086300
H	-3.20567000	-2.70598500	-2.71772400
H	-1.86457000	-2.56749300	2.60221900
C	4.11764900	-1.27213400	-0.74506800
C	3.00089200	-1.91544900	-1.36549700
C	2.24026200	-2.52917000	-0.30981100
C	2.88008400	-2.24041400	0.94031500
C	4.04371800	-1.47527600	0.64663400
C	-4.04379600	1.47514500	-0.64619900
C	-4.11722900	1.27235300	0.74557300
C	-3.00024600	1.91579000	1.36545900
C	-2.23996400	2.52919900	0.30935800
C	-2.88019300	2.24013800	-0.94048600
H	-2.82568200	2.00994500	2.42878200
H	-4.85880100	0.67261000	1.25696000
H	-4.72172900	1.05492300	-1.37846900
H	-2.56803800	2.58486000	-1.91671600
H	-1.34675000	3.12754800	0.43555400
H	1.34705400	-3.12743800	-0.43645600
H	2.56751900	-2.58530300	1.91635700
H	4.72135600	-1.05516600	1.37923800
H	4.85932000	-0.67214100	-1.25601000
H	2.82670400	-2.00932000	-2.42890700
H	3.49245000	1.97314200	-2.95536000
H	1.86342400	2.56701700	-2.60155000
H	3.84292700	1.06961300	2.99702300
H	3.20685100	2.70569900	2.71752200
H	3.26754900	3.21300000	0.38338200
H	-3.28287600	-3.45092300	1.98816900
H	-3.49344100	-1.97266600	2.95510300
H	-3.26877100	-3.21278900	-0.38321900
H	-3.84575700	-1.07113800	-2.99532700
H	-2.11547500	-1.38633900	-3.20172500
Nb	-1.92292900	0.23213300	0.06595600
Nb	1.92311000	-0.23217800	-0.06609900

NbN_B^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.35171000	1.15383700	-1.53620900
N	-0.09772000	-0.08389000	-1.95329000
N	-0.52339900	1.11370600	1.35037100
N	-2.22447100	2.04787700	0.16917000
C	-1.37921900	2.15741100	1.14420700
C	-0.14755200	0.92962700	2.75965200
C	-3.03941700	3.16018600	-0.26687300
N	1.64336900	-1.28285400	1.53386300
N	1.63542900	-1.86907200	-0.60890300
C	1.90839500	-2.21281600	0.62975400
C	2.12720300	-1.46415800	2.88519500

C	1.73197500	-2.76272700	-1.73487800
H	-0.62569200	1.68838200	3.39451300
H	-2.69649800	3.51356300	-1.24683300
H	2.58992300	-2.45474700	3.01518000
H	0.76614800	-2.84453900	-2.24632300
C	-2.41971700	-1.67831300	1.30963100
C	-1.61740500	-2.35436700	0.34343600
C	-2.29428400	-2.28380800	-0.91002900
C	-3.49469700	-1.53486300	-0.71021500
C	-3.57400900	-1.17805000	0.66662200
C	3.50247100	0.90969400	0.41665500
C	3.54929100	0.42778000	-0.91650600
C	2.74693400	1.27266500	-1.72424800
C	2.21681100	2.29966200	-0.88444600
C	2.68445300	2.07326800	0.43690900
H	2.55717200	1.16008900	-2.78276600
H	4.06544800	-0.46306900	-1.24861700
H	3.98920800	0.45966200	1.27174000
H	2.45440900	2.67575100	1.30690700
H	1.55919000	3.09426000	-1.20558600
H	-1.96643700	-2.72842300	-1.83992700
H	-4.23599400	-1.30302200	-1.46676400
H	-4.36242300	-0.59604500	1.12768200
H	-2.17183900	-1.54884100	2.35573700
H	-0.68886100	-2.86842200	0.53741700
H	-0.46942500	-0.05259200	3.11720200
H	0.93450000	0.99867600	2.89806500
H	-4.08302400	2.84225500	-0.36984700
H	-2.99610900	4.00059600	0.44135300
H	-1.36229000	3.03202900	1.81476200
H	2.05153400	-3.76774800	-1.41994700
H	2.45482600	-2.38767200	-2.47164900
H	2.33130000	-3.19680300	0.89632100
H	2.88656400	-0.71282700	3.15038300
H	1.31945400	-1.37810700	3.62286600
Nb	1.10369700	0.23667800	-0.20165600
Nb	-1.58855000	-0.02416000	-0.43263900

TaN_p^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
Ta	1.85431000	-0.19442800	-0.03317400
Ta	-1.85458700	0.19285400	0.03091000
N	0.02986200	0.55142300	-0.48689400
N	-0.03042200	-0.56085100	0.47790100
N	2.77395900	1.63243900	-0.99809600
N	2.66693200	1.37585700	1.19403400
C	2.91970300	2.19902200	0.17568200
C	2.78242300	2.38240300	-2.23146700
C	2.90266400	1.72466300	2.57550700
N	-2.67791800	-1.37324700	-1.19362700
N	-2.77663400	-1.63076500	0.99905400
C	-2.92564900	-2.19711800	-0.17454800
C	-2.91819200	-1.72229600	-2.57429200
C	-2.77714100	-2.38243700	2.23152900
H	3.19710100	3.39170700	-2.08838300

H	2.02712000	1.47824900	3.18580600
H	-3.11769300	-2.79819700	-2.68332400
H	-1.75908200	-2.48413700	2.63024000
C	4.04958100	-1.20758700	-0.75682400
C	2.91157300	-1.85531200	-1.33965700
C	2.18814800	-2.46830300	-0.25291700
C	2.85816200	-2.14940200	0.97816400
C	4.01563800	-1.39069200	0.63737300
C	-4.01438800	1.39813100	-0.62780600
C	-4.04213600	1.21441200	0.76641200
C	-2.89829200	1.85662100	1.34381500
C	-2.17756200	2.46726400	0.25384300
C	-2.85521200	2.15179300	-0.97408300
H	-2.70083400	1.97957800	2.40007500
H	-4.76608000	0.61996700	1.30835000
H	-4.71651900	0.96770800	-1.33100700
H	-2.58597800	2.49696400	-1.96269200
H	-1.28732200	3.07522800	0.34354000
H	1.30073000	-3.07979300	-0.34669900
H	2.58533300	-2.49515400	1.96558600
H	4.71230700	-0.95684700	1.34390700
H	4.77374200	-0.61045300	-1.29551500
H	2.72008000	-1.97996500	-2.39681100
H	3.38971800	1.86799200	-2.98594300
H	1.76694400	2.48330900	-2.63690300
H	3.76082600	1.17467300	2.98840300
H	3.10733900	2.79958000	2.68462800
H	3.19533400	3.25798600	0.31772800
H	-3.19299000	-3.39144700	2.08977600
H	-3.37949700	-1.86889000	2.99050200
H	-3.19899600	-3.25675000	-0.31598000
H	-3.78114800	-1.17655500	-2.98286200
H	-2.04664600	-1.47079500	-3.18814000

TaN_B^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
Ta	1.45578300	0.06998700	-0.30416900
Ta	-1.36098800	-0.22661900	-0.17232900
N	0.10407600	-1.28370100	-1.02438000
N	-0.02884500	0.06934000	-1.64500800
N	1.69025700	-1.18788400	1.54808200
N	2.97321100	-1.58130900	-0.20771400
C	2.61298600	-1.95859700	1.00142200
C	1.12570700	-1.47396300	2.84133600
C	3.96474500	-2.27996700	-0.98598300
N	-1.74474000	0.90381100	1.69958400
N	-1.87372500	1.90472500	-0.28028100
C	-2.03551800	2.00997700	1.02842600
C	-1.93600800	0.80946200	3.12756600
C	-2.13561200	2.98411900	-1.20120800
H	1.64991400	-2.30655900	3.33458600
H	3.52056900	-2.71077900	-1.89303000
H	-2.29139200	1.76276600	3.54426200
H	-1.30167900	3.09861100	-1.90162100
C	2.57576000	1.74210800	1.22883900

C	1.40551100	2.30744600	0.64643000
C	1.64421400	2.40898300	-0.76094400
C	2.94280800	1.88698700	-1.03335000
C	3.51591900	1.48650400	0.20407200
C	-3.71476900	-1.02479600	0.51501600
C	-3.86732700	-0.43666100	-0.75880800
C	-3.12006200	-1.21040100	-1.69893800
C	-2.52979900	-2.29347500	-0.99717700
C	-2.86777700	-2.16733700	0.37712900
H	-3.02664300	-1.01564200	-2.75930500
H	-4.42747200	0.46255300	-0.98077600
H	-4.14496200	-0.66125100	1.43874200
H	-2.57696300	-2.84822900	1.16846400
H	-1.87360500	-3.03762900	-1.42412800
H	0.96111200	2.80934700	-1.49603400
H	3.41601700	1.82480300	-2.00541000
H	4.47914000	1.01017000	0.33181600
H	2.70578400	1.50267000	2.27611900
H	0.53735700	2.66347400	1.18071600
H	1.19227500	-0.59855500	3.50191600
H	0.06228800	-1.74459400	2.76868900
H	4.76766600	-1.59990500	-1.30363700
H	4.42392900	-3.09872900	-0.41181800
H	3.04072800	-2.83750900	1.51382400
H	-2.27741900	3.93674800	-0.67133600
H	-3.03800500	2.78888800	-1.79774200
H	-2.37079100	2.93379300	1.52188400
H	-2.67519300	0.03631800	3.38102000
H	-0.99895000	0.54615400	3.63226700

MoN_P^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.17280100	0.32714100	-0.57534200
N	-0.17307200	-0.32801900	0.57556700
N	2.84471500	1.44901100	-1.02442700
N	2.42494200	1.55915300	1.14344300
C	2.80622600	2.20847900	0.05899100
C	3.03117200	1.98574600	-2.35000700
C	2.30419800	2.17379100	2.44126200
N	-2.42583900	-1.55931700	-1.14292200
N	-2.84532900	-1.44850400	1.02500100
C	-2.80692400	-2.20830200	-0.05817700
C	-2.30475000	-2.17456500	-2.44042800
C	-3.03138300	-1.98492300	2.35077400
H	3.40596300	3.02019000	-2.31311700
H	1.28062200	2.07514000	2.82369400
H	-2.55579400	-3.24569900	-2.40101600
H	-2.09068100	-1.98365200	2.91866800
C	4.05246900	-1.34115900	-0.43938900
C	2.94383900	-2.01191400	-1.05615600
C	2.08770500	-2.46764200	-0.00204800
C	2.66328000	-2.04071900	1.25393300
C	3.89127900	-1.38226800	0.95741000
C	-3.89076700	1.38251300	-0.95808700
C	-4.05207500	1.34196100	0.43871800

C	-2.94325400	2.01255600	1.05531200
C	-2.08688000	2.46757800	0.00109900
C	-2.66251600	2.04041000	-1.25476300
H	-2.82160800	2.20118800	2.11316900
H	-4.84790600	0.83216300	0.96577700
H	-4.53710800	0.90004000	-1.68024400
H	-2.26903000	2.24743400	-2.24054000
H	-1.18455200	3.05318200	0.11621600
H	1.18559700	-3.05355900	-0.11731300
H	2.26995900	-2.24826800	2.23966700
H	4.53751100	-0.89984900	1.67970200
H	4.84808500	-0.83088900	-0.96631900
H	2.82220000	-2.20020500	-2.11407500
H	3.75641900	1.38382500	-2.91222800
H	2.09063300	1.98473700	-2.91817400
H	2.97415800	1.69712800	3.17038800
H	2.55516300	3.24496200	2.40228000
H	3.03764800	3.28679700	0.04842600
H	-3.40606700	-3.01941900	2.31425700
H	-3.75654100	-1.38293100	2.91303100
H	-3.03819000	-3.28664900	-0.04723400
H	-2.97447700	-1.69819800	-3.16995700
H	-1.28105700	-2.07616000	-2.82261400
Mo	1.89443600	-0.22272400	0.00402100
Mo	-1.89439400	0.22256200	-0.00407700

MoN_B^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.40890400	-1.49383600	-0.78529400
N	0.18444700	-0.61053500	-1.68115800
N	2.40218600	-1.19041200	1.24119100
N	3.03219800	-0.95513100	-0.85451300
C	3.19645500	-1.61137300	0.27329400
C	2.42351900	-1.72619500	2.57689300
C	3.54478400	-1.40769800	-2.12158200
N	-1.93472100	1.44035700	1.03928300
N	-2.11261600	1.27497900	-1.15646800
C	-2.46105800	1.93506700	-0.06579200
C	-2.32728200	1.90673700	2.34570400
C	-2.55036200	1.61308200	-2.48752700
H	3.20712500	-2.49186300	2.68567300
H	2.73784100	-1.80800600	-2.75031600
H	-2.87519400	2.85959300	2.28426900
H	-1.69125500	1.70157500	-3.16258900
C	2.43680300	1.96996000	1.23025300
C	1.06371200	2.31944600	1.14053000
C	0.76170000	2.51659000	-0.24138700
C	1.94568400	2.28407800	-1.00153800
C	2.97998500	1.95079200	-0.07769200
C	-3.42661100	-1.13428600	0.93097200
C	-3.60756300	-1.35940700	-0.44745300
C	-2.58433100	-2.23579900	-0.89156200
C	-1.81623000	-2.62579900	0.25682700
C	-2.31944000	-1.92757700	1.38478600
H	-2.43201500	-2.59088100	-1.90195000

H	-4.33493900	-0.86537800	-1.07913800
H	-4.01690600	-0.46943800	1.54712400
H	-1.97135500	-2.01637100	2.40482600
H	-0.98673900	-3.31704800	0.25075400
H	-0.19226800	2.80533700	-0.65071400
H	2.04640000	2.37042400	-2.07470900
H	3.98996800	1.66341800	-0.33597400
H	2.96910100	1.71343200	2.13703500
H	0.37957000	2.43742100	1.96489300
H	2.61468100	-0.94147400	3.32277700
H	1.46000600	-2.18859200	2.83009000
H	4.01395000	-0.58157900	-2.67147600
H	4.29847700	-2.19908000	-1.98646200
H	3.92000300	-2.43415500	0.39961400
H	-3.09863200	2.56713900	-2.49342900
H	-3.21077000	0.83772000	-2.89928300
H	-3.12968600	2.81189600	-0.07985100
H	-2.97424100	1.18140900	2.86144400
H	-1.45103100	2.06166300	2.98761000
Mo	-1.22365400	-0.37898500	-0.08305000
Mo	1.30238100	0.20825100	-0.03694700

WN_P^{trans}

Coordinates (Angstroms)			
	X	Y	Z
N	0.17904200	0.34784500	-0.62892700
N	-0.17908700	-0.34817900	0.62881700
N	2.85851700	1.46410100	-0.98718000
N	2.37827000	1.55351500	1.15643600
C	2.79812100	2.22340800	0.09608300
C	3.11499100	1.98516700	-2.30841200
C	2.20997300	2.13307000	2.46639500
N	-2.37864600	-1.55346200	-1.15645100
N	-2.85867900	-1.46401300	0.98722300
C	-2.79840600	-2.22332900	-0.09604300
C	-2.21042300	-2.13309000	-2.46639000
C	-3.11488800	-1.98511400	2.30849500
H	3.53156900	3.00211600	-2.26174200
H	1.17213100	2.02649200	2.80361800
H	-2.46701500	-3.20266900	-2.46553300
H	-2.19610700	-2.01826300	2.90940500
C	4.07031200	-1.27264400	-0.35738500
C	2.96295700	-1.89133700	-1.04143300
C	2.05471700	-2.37580400	-0.02370900
C	2.58778100	-1.96200100	1.26653100
C	3.84784300	-1.33325700	1.02518800
C	-3.84774000	1.33352300	-1.02506900
C	-4.07011000	1.27291200	0.35752200
C	-2.96261200	1.89143100	1.04149400
C	-2.05438000	2.37578000	0.02370800
C	-2.58760700	1.96208400	-1.26649800
H	-2.90858900	2.09513100	2.10216500
H	-4.89299300	0.76079400	0.83938800
H	-4.47045900	0.87036300	-1.78050600
H	-2.16841500	2.19968100	-2.23441200
H	-1.18429400	2.99842900	0.18102500

H	1.18474000	-2.99859000	-0.18108200
H	2.16855500	-2.19965100	2.23441700
H	4.47043600	-0.86999500	1.78066600
H	4.89315900	-0.76041700	-0.83919800
H	2.90904900	-2.09506900	-2.10210400
H	3.83437000	1.34805900	-2.83748900
H	2.19633700	2.01827500	-2.90951900
H	2.85062200	1.63134100	3.20428700
H	2.46677200	3.20259900	2.46565700
H	3.03177800	3.29935700	0.10343400
H	-3.53150400	-3.00205000	2.26188200
H	-3.83413900	-1.34800100	2.83774100
H	-3.03205700	-3.29927900	-0.10335300
H	-2.85126600	-1.63154600	-3.20424000
H	-1.17264500	-2.02634100	-2.80375200
W	-1.85411400	0.19079400	0.01173400
W	1.85412600	-0.19085100	-0.01177500

WN_B^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.31414100	-1.50588700	-0.61801200
N	0.09167400	-0.62437700	-1.60747600
N	2.41692400	-1.17179300	1.25542000
N	2.92771000	-1.10960300	-0.87680900
C	3.14767000	-1.69150600	0.28011200
C	2.55076600	-1.54836800	2.63928200
C	3.30350100	-1.68434200	-2.14357100
N	-1.89169600	1.54548000	1.00423200
N	-2.09781400	1.31921200	-1.16473800
C	-2.38420500	2.06010100	-0.10846600
C	-2.18685600	2.07774600	2.31046900
C	-2.43960200	1.64304700	-2.52726500
H	3.28185100	-2.36177000	2.75817100
H	2.42404600	-2.09992200	-2.65237700
H	-2.63193400	3.08137500	2.24163100
H	-1.54541800	1.61183900	-3.15977000
C	2.63670800	1.90509000	1.08198300
C	1.26657500	2.28306600	1.10749500
C	0.84470100	2.44627200	-0.25108000
C	1.95260900	2.14986200	-1.10924000
C	3.05721200	1.82288800	-0.26591800
C	-3.48557600	-0.93810800	1.00918400
C	-3.69189600	-1.17890700	-0.36301900
C	-2.72262400	-2.11999200	-0.80307100
C	-1.95983800	-2.52211200	0.34098100
C	-2.40703800	-1.76887900	1.46422800
H	-2.60282200	-2.50128000	-1.80790300
H	-4.40018200	-0.65919200	-0.99579400
H	-4.03335000	-0.23069300	1.61727600
H	-2.06143000	-1.87141900	2.48364400
H	-1.16923100	-3.25663000	0.34106600
H	-0.11937600	2.79254000	-0.58106900
H	1.96463000	2.21432900	-2.18822000
H	4.02958300	1.48960200	-0.60176300
H	3.23923600	1.65124200	1.94445000

H	0.66616500	2.45553400	1.98677400
H	2.88574500	-0.70355200	3.25930800
H	1.59090500	-1.89079300	3.04518600
H	3.74048300	-0.92252800	-2.80122800
H	4.04201700	-2.48994100	-2.01275700
H	3.85033600	-2.52722900	0.42728900
H	-2.88460900	2.64617200	-2.59464000
H	-3.15726900	0.92062000	-2.93852400
H	-2.96179300	2.99646000	-0.15330900
H	-2.88843900	1.43603400	2.86368500
H	-1.27588100	2.14963000	2.91598500
W	-1.25278100	-0.31186600	-0.03901000
W	1.29058500	0.16704400	-0.03285500

ZrN_{B1}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.02221600	0.43016700	-0.73458200
N	-0.02221500	0.43016800	0.73457500
C	-2.35183900	-2.48719400	-0.55080000
C	-3.65582000	-1.93197000	-0.38747500
C	-1.82017500	-1.99469800	-1.77728700
C	-2.77851200	-1.11506300	-2.34662900
C	-3.91595100	-1.08995800	-1.49015800
H	-1.87692500	-3.20340500	0.10933000
H	-4.31682500	-2.10359900	0.45251000
H	-0.85464200	-2.23956700	-2.19940200
H	-2.67053300	-0.57832400	-3.28155500
H	-4.81153100	-0.50019000	-1.64056600
N	-3.16737200	1.79580600	0.03396300
C	-3.33696400	1.60788200	1.34449800
N	-2.93494100	0.45986600	1.84547800
C	-3.64620700	2.99495500	-0.61817200
C	-2.87315600	0.26119800	3.27610400
H	-3.76982800	2.40120700	1.97810300
H	-4.03086700	3.72185600	0.11271900
H	-2.84074000	3.47893800	-1.18320900
H	-4.45714500	2.76755700	-1.32445100
H	-3.41394500	1.05017800	3.82142400
H	-1.83200500	0.25930400	3.62585900
H	-3.31679500	-0.70429200	3.54854300
N	2.93495200	0.45985300	-1.84547900
C	3.33698100	1.60786800	-1.34450200
N	3.16737800	1.79580100	-0.03396900
C	2.87317900	0.26117600	-3.27610500
C	3.64621800	2.99495000	0.61816100
H	3.76985400	2.40118700	-1.97810800
H	3.41397200	1.05015300	-3.82142500
H	3.31681900	-0.70431600	-3.54853400
H	1.83203000	0.25928100	-3.62586900
H	4.03088800	3.72184400	-0.11273100
H	4.45715100	2.76755000	1.32444600
H	2.84075200	3.47894300	1.18319300
C	1.82014300	-1.99473000	1.77724300
C	2.35187300	-2.48719200	0.55077200
C	3.65585000	-1.93193700	0.38751600

C	2.77843500	-1.11508600	2.34664600
C	3.91591300	-1.08994100	1.49022700
H	0.85459600	-2.23962600	2.19931000
H	1.87700500	-3.20340100	-0.10939300
H	4.31689600	-2.10353600	-0.45244300
H	2.67040200	-0.57836600	3.28157700
H	4.81147400	-0.50015800	1.64068700
Zr	-1.87699300	-0.01553000	-0.16738500
Zr	1.87699400	-0.01553000	0.16738100

ZrNb₂^{cis}

Coordinates (Angstroms)			
	X	Y	Z
N	0.02189300	0.42579600	-0.73453300
N	-0.02189400	0.42579800	0.73452200
C	-2.35988300	-2.48689900	-0.55133200
C	-3.66232200	-1.92764500	-0.38934500
C	-1.82527000	-1.99568700	-1.77704800
C	-2.78017300	-1.11287100	-2.34723500
C	-3.91852000	-1.08450000	-1.49207500
H	-1.88802900	-3.20489400	0.10905500
H	-4.32481100	-2.09743200	0.44984500
H	-0.86001200	-2.24345400	-2.19810500
H	-2.66940700	-0.57617500	-3.28185200
H	-4.81208200	-0.49190200	-1.64335600
N	-3.16474100	1.79676100	0.03568100
C	-3.33530300	1.60828000	1.34601000
N	-2.93484200	0.45952000	1.84651600
C	-3.64261600	2.99641500	-0.61621000
C	-2.87430400	0.25972700	3.27702700
H	-3.76780400	2.40165500	1.97980100
H	-4.02641900	3.72359200	0.11485700
H	-2.83681200	3.47968800	-1.18136200
H	-4.45393300	2.76988800	-1.32234700
H	-3.41517600	1.04854400	3.82250500
H	-1.83345100	0.25703800	3.62767800
H	-3.31862700	-0.70576100	3.54833900
N	2.93485300	0.45949300	-1.84652100
C	3.33532000	1.60825500	-1.34602600
N	3.16474000	1.79676000	-0.03570300
C	2.87433400	0.25968000	-3.27703100
C	3.64259400	2.99643000	0.61617200
H	3.76783000	2.40162000	-1.97982500
H	3.41521800	1.04848600	-3.82251200
H	3.31865800	-0.70581400	-3.54832100
H	1.83348700	0.25698900	-3.62769900
H	4.02643700	3.72358100	-0.11490000
H	4.45387800	2.76991600	1.32235200
H	2.83677000	3.47972900	1.18127500
C	1.82524200	-1.99572800	1.77699000
C	2.35996900	-2.48688700	0.55130300
C	3.66239500	-1.92756800	0.38942600
C	2.78006000	-1.11288000	2.34726900
C	3.91847000	-1.08443600	1.49219400
H	0.85996400	-2.24354800	2.19796900
H	1.88820100	-3.20489200	-0.10913300

H	4.32495500	-2.09730600	-0.44971800
H	2.66919700	-0.57620800	3.28188800
H	4.81199200	-0.49179800	1.64355600
Zr	-1.87781000	-0.01690600	-0.16666500
Zr	1.87780900	-0.01690700	0.16665800

HfN_{B1}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.03181800	0.26936100	0.77363600
N	0.03181700	0.26936100	-0.77363700
C	2.48038900	-2.46392800	0.45085800
C	3.74352400	-1.82050600	0.28656200
C	1.92947600	-2.02737800	1.69007900
C	2.83157200	-1.09304700	2.26538300
C	3.95700600	-0.97989200	1.40045500
H	2.04837700	-3.20134000	-0.21516400
H	4.40658200	-1.93380700	-0.56147500
H	0.98440100	-2.33921800	2.11358100
H	2.69569500	-0.57959800	3.20953400
H	4.81248100	-0.33364500	1.55232200
N	2.96084800	1.84808800	-0.00964800
C	3.21888700	1.68195400	-1.30870300
N	2.90058300	0.51641000	-1.82722500
C	3.32760800	3.06342600	0.68338400
C	2.94413700	0.29518700	-3.25430700
H	3.65546900	2.49528900	-1.91181400
H	3.72226100	3.81702700	-0.01363300
H	2.45900800	3.49640900	1.19338600
H	4.09841300	2.87247300	1.44319500
H	3.46480800	1.11123700	-3.77796100
H	1.92950400	0.21820500	-3.66720000
H	3.46702800	-0.64198500	-3.48231800
N	-2.90058200	0.51641000	1.82722500
C	-3.21888800	1.68195400	1.30870200
N	-2.96084900	1.84808800	0.00964700
C	-2.94413400	0.29518800	3.25430800
C	-3.32761200	3.06342400	-0.68338500
H	-3.65547000	2.49528900	1.91181400
H	-3.46480500	1.11123800	3.77796300
H	-3.46702400	-0.64198500	3.48232000
H	-1.92950000	0.21820600	3.66719900
H	-3.72226200	3.81702600	0.01363200
H	-4.09841900	2.87247000	-1.44319400
H	-2.45901300	3.49640600	-1.19339100
C	-1.92947600	-2.02737500	-1.69008400
C	-2.48038100	-2.46393000	-0.45086100
C	-3.74351800	-1.82051300	-0.28655800
C	-2.83157800	-1.09304500	-2.26538200
C	-3.95700900	-0.97989700	-1.40044800
H	-0.98440100	-2.33921000	-2.11359100
H	-2.04836300	-3.20134200	0.21515600
H	-4.40657100	-1.93381900	0.56148300
H	-2.69570700	-0.57959400	-3.20953200
H	-4.81248600	-0.33365200	-1.55230900
Hf	1.84472500	-0.04656800	0.13011500

Hf	-1.84472600	-0.04656800	-0.13011500
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HfN_{B2}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z

N	0.03159400	0.26984400	-0.77348900
N	-0.03159400	0.26984700	0.77348800
C	-2.48085700	-2.46414900	-0.45027800
C	-3.74385900	-1.82021800	-0.28698100
C	-1.92896700	-2.02817500	-1.68926700
C	-2.83033600	-1.09367400	-2.26544300
C	-3.95629900	-0.97985800	-1.40127300
H	-2.04948900	-3.20151600	0.21621500
H	-4.40743800	-1.93296500	0.56072100
H	-0.98373200	-2.34045700	-2.11209100
H	-2.69377500	-0.58058800	-3.20968800
H	-4.81147600	-0.33339700	-1.55390300
N	-2.96004200	1.84817500	0.01021000
C	-3.21663200	1.68264600	1.30963000
N	-2.89971700	0.51657300	1.82784800
C	-3.32547600	3.06410300	-0.68251500
C	-2.94033800	0.29618100	3.25518800
H	-3.65061600	2.49695000	1.91330300
H	-3.71658000	3.81900600	0.01509100
H	-2.45698200	3.49463800	-1.19474200
H	-4.09854700	2.87470700	-1.44041300
H	-3.45878700	1.11318300	3.77956200
H	-1.92486700	0.21816300	3.66580700
H	-3.46392000	-0.64018900	3.48485400
N	2.89971700	0.51656600	-1.82785000
C	3.21662700	1.68264300	-1.30963800
N	2.96004000	1.84817600	-0.01021700
C	2.94034300	0.29616500	-3.25518700
C	3.32547200	3.06410700	0.68250200
H	3.65061100	2.49694500	-1.91331400
H	3.45879200	1.11316400	-3.77956500
H	3.46392700	-0.64020600	-3.48484600
H	1.92487300	0.21814300	-3.66580900
H	3.71657600	3.81900800	-0.01510700
H	4.09854200	2.87471700	1.44040300
H	2.45697600	3.49464400	1.19472400
C	1.92896700	-2.02817400	1.68926600
C	2.48086900	-2.46414500	0.45028100
C	3.74386900	-1.82020600	0.28699300
C	2.83032700	-1.09366800	2.26544900
C	3.95629500	-0.97984500	1.40128800
H	0.98373100	-2.34046300	2.11208300
H	2.04951000	-3.20151400	-0.21621500
H	4.40745500	-1.93294800	-0.56070300
H	2.69375600	-0.58058400	3.20969300
H	4.81146800	-0.33337900	1.55392500
Hf	-1.84474700	-0.04681800	-0.12987900
Hf	1.84474700	-0.04681700	0.12987900

NbN_{B1}^{cis}

Coordinates (Angstroms)			
	X	Y	Z
N	0.02704400	0.68730700	0.54223600
N	-0.02704400	-0.68730600	0.54223500
C	-2.40473000	1.03108800	-2.18804800
C	-3.69154600	0.77370100	-1.62330100
C	-1.81772600	2.09464000	-1.42070300
C	-2.73412700	2.46364500	-0.38756300
C	-3.88903700	1.64442400	-0.53240900
H	-1.99806000	0.57788900	-3.08174500
H	-4.37431800	-0.00252900	-1.94324100
H	-0.85172600	2.54654000	-1.60174500
H	-2.58898800	3.24072200	0.35065100
H	-4.74823200	1.64296000	0.12627700
N	-3.07229900	-0.48328600	1.63756200
C	-3.22129200	-1.70736400	1.13555100
N	-2.77163400	-1.85173100	-0.08975200
C	-3.60386300	-0.09454800	2.92216800
C	-2.67809800	-3.14335200	-0.72527100
H	-3.66675500	-2.53312900	1.71764900
H	-4.05238700	-0.95353500	3.44307200
H	-2.81568700	0.31818000	3.56291300
H	-4.38052500	0.67627100	2.81454500
H	-3.25796700	-3.90567300	-0.18223100
H	-1.63521300	-3.48581500	-0.77703800
H	-3.05973700	-3.09407000	-1.75257700
N	2.77163500	1.85173200	-0.08975300
C	3.22129200	1.70736400	1.13555100
N	3.07230000	0.48328700	1.63756100
C	2.67809800	3.14335300	-0.72527200
C	3.60386100	0.09454900	2.92216800
H	3.66675300	2.53313000	1.71764900
H	3.25796200	3.90567500	-0.18222800
H	3.05974300	3.09407300	-1.75257600
H	1.63521200	3.48581300	-0.77704400
H	4.05238100	0.95353700	3.44307600
H	4.38052500	-0.67626700	2.81454600
H	2.81568500	-0.31818200	3.56291100
C	1.81772500	-2.09464000	-1.42070300
C	2.40473200	-1.03108900	-2.18804800
C	3.69154600	-0.77370300	-1.62330100
C	2.73412600	-2.46364600	-0.38756200
C	3.88903600	-1.64442600	-0.53240700
H	0.85172600	-2.54653900	-1.60174500
H	1.99806300	-0.57788900	-3.08174500
H	4.37432000	0.00252700	-1.94323900
H	2.58898700	-3.24072100	0.35065200
H	4.74823200	-1.64296300	0.12628000
Nb	-1.83523700	0.21316300	-0.00949700
Nb	1.83523700	-0.21316300	-0.00949800

NbN_{B2}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.03931900	0.71579300	1.32753300
N	-0.03929800	-0.71576600	1.32753000
C	-1.35697900	1.76710900	-1.72560200
C	-2.68848000	1.26464100	-1.78905900
C	-1.26432000	2.58239200	-0.55620900
C	-2.52940500	2.56949400	0.09375200
C	-3.40829400	1.75707400	-0.67574200
H	-0.58193900	1.60896800	-2.46070000
H	-3.07364700	0.59022000	-2.54300600
H	-0.38057600	3.09523400	-0.20483900
H	-2.77710200	3.08336300	1.01401600
H	-4.43408800	1.51849800	-0.42679300
N	-3.17914000	-0.76240700	1.24453200
C	-3.20695500	-1.74426800	0.35600200
N	-2.31261600	-1.65492500	-0.60589400
C	-4.10362900	-0.68741800	2.34965500
C	-2.27531100	-2.61255800	-1.68427300
H	-3.93778400	-2.56938400	0.41574600
H	-4.82115400	-1.52147300	2.32678300
H	-3.57417100	-0.72216700	3.31034900
H	-4.67621600	0.25034200	2.32265100
H	-3.05539900	-3.38082400	-1.56789100
H	-1.30756300	-3.12580300	-1.73783600
H	-2.43479900	-2.12069700	-2.65437700
N	2.31266700	1.65494200	-0.60585400
C	3.20703800	1.74422100	0.35601400
N	3.17922200	0.76232400	1.24450700
C	2.27528900	2.61266600	-1.68415000
C	4.10379300	0.68722400	2.34955300
H	3.93789400	2.56931200	0.41577000
H	3.05539900	3.38091100	-1.56776700
H	2.43468800	2.12088100	-2.65430700
H	1.30754300	3.12592900	-1.73759000
H	4.82132700	1.52127300	2.32670200
H	4.67636900	-0.25053900	2.32242300
H	3.57440800	0.72189500	3.31029000
C	1.26420200	-2.58233400	-0.55628200
C	1.35688100	-1.76701300	-1.72564900
C	2.68840700	-1.26461600	-1.78911600
C	2.52930100	-2.56952700	0.09365100
C	3.40821800	-1.75712800	-0.67583100
H	0.38043400	-3.09513100	-0.20490800
H	0.58182800	-1.60879400	-2.46071300
H	3.07359500	-0.59018600	-2.54304500
H	2.77698800	-3.08344000	1.01389300
H	4.43403100	-1.51861700	-0.42689500
Nb	-1.53062300	0.31908400	0.24958300
Nb	1.53063000	-0.31906600	0.24957000

TaN_{BI}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z

Ta	1.76838300	-0.18911800	0.00795300
Ta	-1.76838600	0.18911700	0.00795400
N	0.02503000	0.73237800	0.57842400
N	-0.02503500	-0.73239000	0.57841100
C	-2.30226600	1.03516600	-2.14885200
C	-3.60443200	0.71801800	-1.64746300
C	-1.78697000	2.09646900	-1.32305300
C	-2.75174000	2.38395400	-0.30421600
C	-3.87300700	1.53291300	-0.53165200
H	-1.85632500	0.64653800	-3.05367000
H	-4.24571000	-0.06963300	-2.02102100
H	-0.83668500	2.59423200	-1.45593300
H	-2.67027700	3.14384000	0.46091400
H	-4.75457900	1.47157600	0.09391400
N	-3.00795300	-0.56993300	1.61073800
C	-3.15242600	-1.77585900	1.06741100
N	-2.67478800	-1.86265900	-0.15320500
C	-3.55487600	-0.21333500	2.89857900
C	-2.55715700	-3.11795800	-0.85398600
H	-3.61299800	-2.62189100	1.60509600
H	-4.03697300	-1.07774300	3.37740000
H	-2.76852700	0.15325400	3.56867600
H	-4.30713800	0.58238600	2.80310600
H	-3.17426400	-3.90096900	-0.38830900
H	-1.51631300	-3.47001400	-0.86716500
H	-2.87954800	-3.00387800	-1.89590700
N	2.67478200	1.86265900	-0.15318100
C	3.15243200	1.77584400	1.06742800
N	3.00794800	0.56991700	1.61074700
C	2.55717100	3.11795900	-0.85396300
C	3.55487300	0.21330200	2.89858500
H	3.61303000	2.62186500	1.60511200
H	3.17434600	3.90094200	-0.38832900
H	2.87949400	3.00385400	-1.89590100
H	1.51634400	3.47007000	-0.86708200
H	4.03710600	1.07766500	3.37734800
H	4.30702300	-0.58252300	2.80310900
H	2.76850200	-0.15315400	3.56873000
C	1.78697700	-2.09645100	-1.32307900
C	2.30227600	-1.03513500	-2.14886100
C	3.60443900	-0.71799200	-1.64746100
C	2.75174300	-2.38394800	-0.30424200
C	3.87300900	-1.53290200	-0.53165900
H	0.83669300	-2.59421200	-1.45597200
H	1.85634100	-0.64649700	-3.05367700
H	4.24571800	0.06966400	-2.02100500
H	2.67027600	-3.14384600	0.46087700
H	4.75457700	-1.47157300	0.09391300

TaN_{B2}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
Ta	1.48384200	0.26786100	-0.18621900
Ta	-1.48377100	-0.26793100	-0.18632600
N	0.03639900	-0.76024400	-1.26133500
N	-0.03610700	0.75956500	-1.26172200

C	-1.44929700	-1.72698100	1.76997200
C	-2.76032500	-1.16745800	1.80128400
C	-1.36173600	-2.53762000	0.59509000
C	-2.60265300	-2.45096800	-0.09652600
C	-3.46665200	-1.61080500	0.66030100
H	-0.69238600	-1.61235300	2.53042000
H	-3.13652000	-0.48239600	2.54987300
H	-0.49491900	-3.09163600	0.26508300
H	-2.84692900	-2.94451600	-1.02855200
H	-4.46983800	-1.31673500	0.38102700
N	-3.07577200	0.88098900	-1.17978400
C	-3.07202700	1.86041700	-0.28978500
N	-2.21159300	1.69771200	0.69427400
C	-3.89424800	0.90033700	-2.36755200
C	-2.14661200	2.62087500	1.80114900
H	-3.74255300	2.73289700	-0.36447100
H	-4.60656000	1.73819800	-2.34680800
H	-3.27840800	0.99971400	-3.27104300
H	-4.46937600	-0.03058700	-2.45964100
H	-2.88706300	3.42791200	1.69481400
H	-1.15645500	3.08460200	1.88384600
H	-2.34586800	2.10881700	2.75306000
N	2.21196400	-1.69751700	0.69474700
C	3.07200000	-1.86054200	-0.28959300
N	3.07588300	-0.88105200	-1.17953600
C	2.14660000	-2.62098000	1.80134500
C	3.89371600	-0.90081700	-2.36774000
H	3.74198500	-2.73340000	-0.36466100
H	2.88589800	-3.42896000	1.69414100
H	2.34726200	-2.10956000	2.75331200
H	1.15590700	-3.08341900	1.88458900
H	4.60495400	-1.73960600	-2.34778800
H	4.47001100	0.02940700	-2.45970500
H	3.27724800	-0.99898000	-3.27092800
C	1.36154600	2.53791800	0.59460600
C	1.44927400	1.72762900	1.76970400
C	2.76031100	1.16814500	1.80105000
C	2.60242300	2.45118000	-0.09706900
C	3.46653900	1.61128400	0.65990400
H	0.49464300	3.09175900	0.26452300
H	0.69233000	1.61300200	2.53012900
H	3.13662600	0.48334700	2.54981900
H	2.84658100	2.94446500	-1.02926500
H	4.46973700	1.31723700	0.38065200

MoN_{B1}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.05264200	0.65228500	0.14751900
N	0.05264200	-0.65228600	0.14751900
C	-2.57647000	0.91317900	-2.27080400
C	-3.79087400	0.69402300	-1.54940500
C	-1.89818300	1.98463200	-1.60933200
C	-2.68409600	2.41401500	-0.49166600
C	-3.85780200	1.60377000	-0.46781300
H	-2.27270300	0.41777000	-3.18280800

H	-4.51653700	-0.08096000	-1.76227100
H	-0.94546100	2.40467600	-1.90480000
H	-2.45429200	3.22723300	0.18342400
H	-4.64870600	1.65370400	0.26994300
N	-2.61747400	-0.48207700	1.86442000
C	-3.04495400	-1.63495600	1.38941900
N	-2.79999000	-1.76457600	0.09501700
C	-2.92826800	-0.00641300	3.18860100
C	-2.95587300	-2.99504200	-0.63418900
H	-3.56550600	-2.39667200	1.99389300
H	-3.38251400	-0.79943600	3.80241800
H	-2.01867800	0.33948400	3.69399100
H	-3.62874500	0.84108900	3.16005900
H	-3.50919600	-3.74096200	-0.04330200
H	-1.98062300	-3.42864500	-0.89872400
H	-3.50524200	-2.82822200	-1.56974300
N	2.79999000	1.76457600	0.09501600
C	3.04496100	1.63495400	1.38941700
N	2.61747400	0.48207800	1.86442000
C	2.95586900	2.99504400	-0.63418800
C	2.92826300	0.00641500	3.18860300
H	3.56551400	2.39666900	1.99389000
H	3.50919600	3.74096300	-0.04330200
H	3.50523400	2.82822400	-1.56974400
H	1.98061800	3.42864800	-0.89871800
H	3.38251200	0.79943800	3.80241900
H	3.62873700	-0.84109000	3.16006300
H	2.01867100	-0.33947600	3.69399300
C	1.89818300	-1.98463200	-1.60933100
C	2.57647100	-0.91318000	-2.27080300
C	3.79087500	-0.69402400	-1.54940400
C	2.68409600	-2.41401600	-0.49166400
C	3.85780200	-1.60377000	-0.46781100
H	0.94546100	-2.40467600	-1.90479900
H	2.27270500	-0.41777100	-3.18280800
H	4.51653800	0.08095900	-1.76227000
H	2.45429200	-3.22723300	0.18342600
H	4.64870600	-1.65370500	0.26994500
Mo	-1.92170300	0.20632700	-0.09094500
Mo	1.92170400	-0.20632700	-0.09094400

MoN_{B2}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.07676300	0.69353600	-1.32731400
N	0.07672700	-0.69354200	-1.32730500
C	1.71319800	1.77315700	1.54577400
C	3.04730800	1.29748500	1.34156900
C	1.36202600	2.52629600	0.37817400
C	2.46407100	2.50477300	-0.52789300
C	3.49805300	1.74229800	0.07602600
H	1.12905800	1.65813000	2.44686400
H	3.60347000	0.66680300	2.02279700
H	0.40939000	3.00469700	0.19765300
H	2.49803800	2.96831900	-1.50465700
H	4.44945100	1.49543700	-0.37733300

N	2.97783700	-1.10697700	-1.03087000
C	2.94414000	-1.91511200	0.01002700
N	2.02082800	-1.57086000	0.88712600
C	3.84139400	-1.28341600	-2.16919200
C	1.95493300	-2.16869600	2.19756100
H	3.63217800	-2.76705000	0.14652700
H	4.52571900	-2.13276300	-2.02252800
H	3.25566800	-1.46784100	-3.07914000
H	4.44737700	-0.38444500	-2.34460900
H	2.65424200	-3.01452100	2.28654400
H	0.94794700	-2.54362300	2.41410000
H	2.20781900	-1.44297000	2.98456800
N	-2.02084900	1.57090000	0.88711700
C	-2.94418400	1.91509800	0.01002200
N	-2.97789100	1.10691600	-1.03083700
C	-1.95494000	2.16880100	2.19752100
C	-3.84149100	1.28327800	-2.16913800
H	-3.63223900	2.76702600	0.14650100
H	-2.65426800	3.01461200	2.28647700
H	-2.20779100	1.44310700	2.98456900
H	-0.94796000	2.54376600	2.41402000
H	-4.52583500	2.13261300	-2.02249000
H	-4.44745500	0.38428300	-2.34449400
H	-3.25580000	1.46767700	-3.07911300
C	-1.36196100	-2.52626700	0.37831300
C	-1.71311400	-1.77308600	1.54589200
C	-3.04723800	-1.29744800	1.34170700
C	-2.46403000	-2.50480400	-0.52772400
C	-3.49801500	-1.74233600	0.07620100
H	-0.40931900	-3.00465600	0.19778500
H	-1.12894600	-1.65800700	2.44695700
H	-3.60339200	-0.66674700	2.02292500
H	-2.49801500	-2.96838900	-1.50446900
H	-4.44943400	-1.49552000	-0.37713600
Mo	1.53068000	0.28838400	-0.23784600
Mo	-1.53068000	-0.28838100	-0.23779200

WN_{B1}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.06870700	-0.68867700	0.09055200
N	-0.06870600	0.68867500	0.09055200
C	2.62568800	-0.98348500	-2.15963300
C	3.82732200	-0.62910600	-1.46289200
C	2.03102700	-2.04610300	-1.39247000
C	2.83518400	-2.31018700	-0.23141300
C	3.95066600	-1.41665200	-0.29855500
H	2.32173800	-0.63599700	-3.13716900
H	4.49072300	0.18218900	-1.73563000
H	1.11499400	-2.56203000	-1.64816000
H	2.68083800	-3.08746500	0.50419700
H	4.73083000	-1.32457200	0.44674400
N	2.40242200	0.71564500	1.84028200
C	2.82063300	1.84259700	1.30252700
N	2.70088100	1.82016100	-0.01894500
C	2.59820300	0.36395500	3.22410400

C	2.76578800	2.99119700	-0.85459600
H	3.24004200	2.68787700	1.87130700
H	2.96446900	1.22254100	3.80624800
H	1.65405300	0.02562900	3.66694200
H	3.32335400	-0.45529900	3.33191500
H	3.24286100	3.83048200	-0.32713600
H	1.76208700	3.31157600	-1.16930700
H	3.34516400	2.78537600	-1.76286100
N	-2.70088100	-1.82015900	-0.01894000
C	-2.82057800	-1.84261600	1.30253700
N	-2.40241900	-0.71564300	1.84028600
C	-2.76582000	-2.99118300	-0.85460400
C	-2.59823200	-0.36394400	3.22410200
H	-3.23998000	-2.68789800	1.87132000
H	-3.24287000	-3.83047600	-0.32713700
H	-3.34522500	-2.78535700	-1.76285000
H	-1.76212600	-3.31155200	-1.16934700
H	-2.96447500	-1.22253800	3.80625000
H	-3.32340800	0.45528900	3.33190400
H	-1.65409500	-0.02558800	3.66694100
C	-2.03102800	2.04610300	-1.39246900
C	-2.62568900	0.98348200	-2.15962900
C	-3.82732300	0.62910500	-1.46288700
C	-2.83518100	2.31018600	-0.23141000
C	-3.95066400	1.41665200	-0.29855000
H	-1.11499600	2.56203000	-1.64816200
H	-2.32174000	0.63599300	-3.13716500
H	-4.49072500	-0.18218900	-1.73562300
H	-2.68083400	3.08746500	0.50419900
H	-4.73082700	1.32457300	0.44675000
W	1.88445700	-0.18097000	-0.08098600
W	-1.88445500	0.18096900	-0.08098300

WN_{B2}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.11148800	0.75857500	-1.16483300
N	0.11144600	-0.75862800	-1.16480300
C	1.83549200	1.76523300	1.54395700
C	3.13905700	1.18752200	1.41483900
C	1.57325300	2.45105600	0.30378000
C	2.69107500	2.25818900	-0.57818600
C	3.64960200	1.48404900	0.13485100
H	1.24157200	1.79123900	2.44495000
H	3.62239200	0.55935400	2.15161400
H	0.68157100	3.01600800	0.07270700
H	2.80867900	2.66793300	-1.57153800
H	4.58101500	1.11043400	-0.27032000
N	2.92652600	-1.20616000	-0.96899300
C	2.84784600	-2.02578600	0.05827300
N	2.02140900	-1.56911100	0.98115500
C	3.57473900	-1.50704800	-2.21871300
C	1.90505600	-2.15522000	2.29171000
H	3.40999200	-2.97047200	0.14401400
H	4.19560900	-2.41150400	-2.13763600
H	2.83341300	-1.66604600	-3.01290600

H	4.21980400	-0.67508000	-2.52865700
H	2.47557900	-3.09352800	2.35785200
H	0.85999100	-2.37745200	2.53279500
H	2.28223300	-1.47773300	3.07190800
N	-2.02138000	1.56915300	0.98114900
C	-2.84784500	2.02578700	0.05827200
N	-2.92655600	1.20611700	-0.96895600
C	-1.90498200	2.15532000	2.29167400
C	-3.57478000	1.50696200	-2.21868000
H	-3.40997900	2.97048300	0.14398500
H	-2.47547300	3.09364900	2.35778400
H	-2.28216400	1.47788200	3.07191200
H	-0.85990400	2.37752900	2.53272700
H	-4.19565000	2.41142100	-2.13762800
H	-4.21984800	0.67498400	-2.52858900
H	-2.83346200	1.66593400	-3.01288700
C	-1.57324000	-2.45104000	0.30394800
C	-1.83544500	-1.76515300	1.54409700
C	-3.13901700	-1.18745400	1.41498700
C	-2.69108900	-2.25822400	-0.57799500
C	-3.64959800	-1.48405000	0.13503000
H	-0.68156200	-3.01599900	0.07287600
H	-1.24149800	-1.79110900	2.44507300
H	-3.62233300	-0.55924900	2.15174200
H	-2.80871900	-2.66801700	-1.57132400
H	-4.58102400	-1.11046100	-0.27013400
W	1.51081500	0.24311300	-0.17424800
W	-1.51082500	-0.24312200	-0.17418900

TSTaNB-P^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
Ta	1.60582500	0.07760600	-0.24206000
Ta	-1.59056200	-0.19207500	-0.21858000
N	0.00203100	-1.25077200	-0.58384700
N	-0.00009500	0.07853800	-1.36776200
N	2.05862500	-1.20148500	1.54069600
N	3.09407700	-1.53933200	-0.38152500
C	2.81691200	-2.00829600	0.82367600
C	1.48889700	-1.60404500	2.80071500
C	3.91962000	-2.24485800	-1.33092600
N	-1.69143600	0.80870900	1.69802900
N	-2.00569700	2.00029300	-0.14949700
C	-2.09497000	1.96660300	1.16516800
C	-1.78269100	0.54666300	3.11694800
C	-2.39978300	3.14819000	-0.93120100
H	1.98071700	-2.50437800	3.19955800
H	3.34457500	-2.52216700	-2.22346200
H	-2.08145100	1.45110300	3.66523200
H	-1.58274100	3.46163200	-1.59221400
C	3.00984100	1.70839900	1.05960200
C	1.72512200	2.24076700	0.74332100
C	1.66675500	2.36465100	-0.68817500
C	2.89736700	1.87455600	-1.23408400
C	3.71937900	1.48445600	-0.14097500
C	-3.84702200	-1.12145800	0.54703500

C	-4.05170400	-0.42050700	-0.66205400
C	-3.32631200	-1.09239400	-1.69760600
C	-2.68955700	-2.21993000	-1.10314600
C	-2.99059000	-2.23213000	0.28653100
H	-3.31298600	-0.82920800	-2.74737500
H	-4.63772200	0.48169000	-0.78287000
H	-4.24663400	-0.84135400	1.51366000
H	-2.65378900	-2.96803400	1.00504000
H	-2.03870200	-2.91717900	-1.61234700
H	0.83667100	2.75934700	-1.25640400
H	3.17193300	1.85044200	-2.28013500
H	4.69486700	1.02215300	-0.21830300
H	3.35627500	1.44720600	2.05094800
H	0.97607900	2.56924800	1.45098600
H	1.59636200	-0.80430300	3.54523000
H	0.41520300	-1.82055500	2.70127500
H	4.76012100	-1.61871900	-1.66099000
H	4.33539500	-3.16485300	-0.89403200
H	3.15987600	-2.99475500	1.18158000
H	-2.66559600	4.00001300	-0.28853900
H	-3.26464100	2.91864600	-1.56849800
H	-2.49844400	2.78880400	1.77355800
H	-2.51631300	-0.24133000	3.33682200
H	-0.81336800	0.21719800	3.50637900

TSTaN_{B1-B2}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
Ta	1.70009300	-0.21337400	0.05763200
Ta	-1.70009400	0.21337000	0.05763100
N	0.02455800	0.74025200	0.78103300
N	-0.02455800	-0.74026300	0.78103500
C	-2.05766000	1.27873700	-2.06511400
C	-3.37714200	0.84627100	-1.73092900
C	-1.67995700	2.26286200	-1.08899600
C	-2.74807500	2.39537600	-0.14854800
C	-3.79493100	1.52281200	-0.56726100
H	-1.49920800	0.99718400	-2.94617000
H	-3.93598100	0.07647900	-2.24697100
H	-0.75015100	2.81243500	-1.07072600
H	-2.77599200	3.06763300	0.69841200
H	-4.72715800	1.35796300	-0.04239700
N	-3.05737200	-0.67407500	1.49937600
C	-3.17271200	-1.82422700	0.84476900
N	-2.57982700	-1.82655000	-0.32828200
C	-3.68993500	-0.41828500	2.77107900
C	-2.48397800	-3.01288900	-1.14259100
H	-3.70802000	-2.69565100	1.25813600
H	-4.23088300	-1.30525400	3.13113400
H	-2.94628500	-0.14173500	3.52785400
H	-4.40970100	0.40910600	2.69601000
H	-3.14998700	-3.80881100	-0.77686700
H	-1.45994200	-3.41004300	-1.15390000
H	-2.75931300	-2.79011500	-2.18094000
N	2.57982000	1.82654900	-0.32829400
C	3.17270800	1.82423100	0.84475500

N	3.05737600	0.67408100	1.49936800
C	2.48393600	3.01290200	-1.14258000
C	3.68993800	0.41830200	2.77107300
H	3.70801700	2.69565700	1.25811500
H	3.14993800	3.80882800	-0.77685400
H	2.75925500	2.79015300	-2.18093800
H	1.45989300	3.41003900	-1.15386200
H	4.23098000	1.30523800	3.13106700
H	4.40962300	-0.40916200	2.69603100
H	2.94628000	0.14186300	3.52788100
C	1.67997300	-2.26286600	-1.08899700
C	2.05767300	-1.27873700	-2.06511100
C	3.37715100	-0.84626200	-1.73092000
C	2.74808900	-2.39537600	-0.14854600
C	3.79494300	-1.52280900	-0.56725700
H	0.75017000	-2.81244600	-1.07073100
H	1.49922400	-0.99718800	-2.94616900
H	3.93598600	-0.07646300	-2.24695700
H	2.77600700	-3.06763500	0.69841300
H	4.72716800	-1.35795700	-0.04239000

TSNbN_{B-P}^{trans}

Coordinates (Angstroms)			
	X	Y	Z
N	0.01107000	-1.26261400	-0.75181400
N	0.02453400	-0.00489000	-1.45527300
N	2.06636500	-1.24913300	1.46242000
N	3.18106200	-1.49526000	-0.44393100
C	2.85679900	-2.01076100	0.73158400
C	1.44516000	-1.73921100	2.66759200
C	4.05658900	-2.16515400	-1.37502600
N	-1.68925900	0.84914100	1.61369900
N	-1.99231000	2.00701800	-0.26914900
C	-2.09550700	1.98747400	1.03978100
C	-1.82990600	0.62641100	3.03529400
C	-2.43065500	3.13235600	-1.05981900
H	1.92743000	-2.66215800	3.02551800
H	3.53508600	-2.38921500	-2.31403400
H	-2.12295400	1.55153900	3.55288800
H	-1.62330300	3.48350600	-1.71448500
C	2.93081200	1.75433100	1.06301700
C	1.63850200	2.25056100	0.73224400
C	1.59869400	2.40627800	-0.69263600
C	2.86112000	1.99834800	-1.22353300
C	3.67565900	1.60015200	-0.12995000
C	-3.82082400	-1.22112900	0.53234000
C	-4.05578000	-0.54722300	-0.68755100
C	-3.34254200	-1.23388400	-1.72025100
C	-2.68297900	-2.34101100	-1.11590100
C	-2.95919300	-2.32846800	0.27607500
H	-3.34590900	-0.98772600	-2.77447100
H	-4.66042000	0.34160200	-0.81805300
H	-4.21250600	-0.93116600	1.49941100
H	-2.59938000	-3.04442700	1.00379600
H	-2.03089400	-3.03919400	-1.62287900
H	0.75740900	2.77024500	-1.26527400

H	3.14995700	2.00227500	-2.26634700
H	4.67339400	1.18704900	-0.20121300
H	3.26672300	1.47914200	2.05416400
H	0.84764000	2.49622800	1.42732700
H	1.51261900	-0.99143800	3.46835100
H	0.37926600	-1.95513800	2.50522600
H	4.92487500	-1.53789800	-1.62050400
H	4.43194700	-3.11287200	-0.96029500
H	3.19283400	-3.01146900	1.05632900
H	-2.74668200	3.97454800	-0.42560800
H	-3.27501100	2.85768100	-1.70654200
H	-2.51793200	2.81776700	1.62797500
H	-2.58859500	-0.13791900	3.25516900
H	-0.88157000	0.28307400	3.46453500
Nb	-1.59929200	-0.23631500	-0.27789800
Nb	1.64124400	0.08099100	-0.30215600

TSNbN_{B1-B2}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.03552500	0.70325500	1.01603600
N	-0.03552600	-0.70325200	1.01604600
C	-1.76389000	1.49372800	-1.96710500
C	-3.10574700	1.04592400	-1.79620700
C	-1.48995200	2.42064900	-0.91076900
C	-2.65385400	2.52567300	-0.09507200
C	-3.64934100	1.67469500	-0.65419600
H	-1.10005400	1.22605100	-2.77680200
H	-3.60645800	0.30649900	-2.40766600
H	-0.56134900	2.94985900	-0.75385400
H	-2.76523600	3.14954900	0.78203100
H	-4.63516100	1.49806600	-0.24392800
N	-3.18252300	-0.64271200	1.43466000
C	-3.28214000	-1.74236200	0.69737000
N	-2.56602700	-1.73351700	-0.40491200
C	-3.93018700	-0.44848000	2.65339600
C	-2.53129700	-2.86445500	-1.29835100
H	-3.91705100	-2.59547500	0.99404500
H	-4.57681700	-1.31309000	2.86545600
H	-3.25879200	-0.30914200	3.50994800
H	-4.56998600	0.44261000	2.58655500
H	-3.24109500	-3.64659100	-0.98764100
H	-1.53174100	-3.31678500	-1.33821100
H	-2.79014000	-2.56215000	-2.32196200
N	2.56602400	1.73352000	-0.40489900
C	3.28215700	1.74234700	0.69737000
N	3.18252200	0.64270200	1.43466400
C	2.53130400	2.86445700	-1.29833900
C	3.93018900	0.44846000	2.65339600
H	3.91709900	2.59544200	0.99403100
H	3.24120000	3.64653400	-0.98770100
H	2.79002500	2.56212300	-2.32197100
H	1.53178400	3.31687600	-1.33810800
H	4.57690500	1.31302000	2.86540200
H	4.56990300	-0.44269200	2.58658500
H	3.25879900	0.30922600	3.50997000

C	1.48997100	-2.42066400	-0.91075100
C	1.76386700	-1.49374900	-1.96710100
C	3.10571600	-1.04591000	-1.79623400
C	2.65389100	-2.52565500	-0.09507600
C	3.64934800	-1.67465800	-0.65422700
H	0.56138000	-2.94989100	-0.75381200
H	1.10000700	-1.22609100	-2.77678400
H	3.60639700	-0.30648000	-2.40771100
H	2.76530400	-3.14951700	0.78203300
H	4.63517200	-1.49800500	-0.24398200
Nb	-1.67402000	0.28622300	0.14627100
Nb	1.67401400	-0.28622100	0.14627200

TSMoNb-P^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.21724900	-1.17037100	-0.45428700
N	-0.09728900	-0.05193000	-1.13874500
N	2.54678000	-1.51972900	1.14502100
N	3.15295100	-1.17314700	-0.94951500
C	3.16360500	-2.00122600	0.08943800
C	2.25312500	-2.32572000	2.30437700
C	3.67210600	-1.50342500	-2.25320900
N	-1.52180600	1.01844900	1.39700200
N	-2.25135300	1.86523100	-0.50305300
C	-1.98824800	2.09258100	0.76626200
C	-1.32703100	0.98032100	2.82622000
C	-2.78230300	2.87294600	-1.38647900
H	2.83817600	-3.25841500	2.30418300
H	2.86147800	-1.63871300	-2.98103200
H	-1.33927000	1.99268200	3.25898700
H	-2.12648000	3.01785500	-2.25481100
C	3.38707500	1.52250900	0.97864100
C	2.03935700	1.92097400	1.24696200
C	1.47276700	2.33852200	-0.00694400
C	2.47208000	2.18138000	-1.02485100
C	3.65095100	1.70985600	-0.39407600
C	-3.81128200	-1.18015000	0.97344400
C	-4.28397500	-0.57780100	-0.20756700
C	-3.66858700	-1.22925600	-1.33072700
C	-2.80893700	-2.26573100	-0.81319000
C	-2.87771100	-2.19901700	0.62512700
H	-3.89432800	-1.03916700	-2.37201900
H	-4.96007000	0.26604700	-0.26082200
H	-4.04902800	-0.86292700	1.98138400
H	-2.35888600	-2.84754900	1.31830500
H	-2.25987300	-2.99899500	-1.38976300
H	0.47568800	2.72623300	-0.16044500
H	2.35308000	2.41181000	-2.07473400
H	4.56663900	1.43037100	-0.89905500
H	4.07341600	1.10321700	1.70233500
H	1.57125200	1.98009800	2.22008900
H	2.48739700	-1.77840100	3.22605000
H	1.18827700	-2.59223100	2.33503000
H	4.32555000	-0.70370900	-2.62557600
H	4.25968800	-2.43227800	-2.21609800

H	3.61859300	-3.00444900	0.04729500
H	-2.89347700	3.84204200	-0.87531300
H	-3.76917500	2.57979300	-1.77061600
H	-2.14186700	3.06690900	1.26013300
H	-2.11043100	0.39410700	3.32921700
H	-0.36509800	0.51319600	3.06994600
Mo	-1.86363700	-0.30764000	-0.29456300
Mo	1.67185200	0.09412500	-0.11039400

TSMoN_{B1-B2}^{cis}

Coordinates (Angstroms)			
	X	Y	Z
N	0.07278300	-0.65923500	0.75151500
N	-0.07273000	0.65930900	0.75144300
C	2.34201900	-1.38153200	-1.92078400
C	3.54943400	-1.27782600	-1.14588100
C	1.48556400	-2.27892500	-1.22475900
C	2.14375700	-2.70910300	-0.03819900
C	3.42172000	-2.09565900	0.01291900
H	2.15883500	-0.93595700	-2.88912200
H	4.41008300	-0.67114500	-1.39798200
H	0.47806200	-2.54716200	-1.51211800
H	1.71844500	-3.35296200	0.72052300
H	4.16442800	-2.22806800	0.78865400
N	3.00223500	0.91615200	1.49166500
C	3.26763200	1.85168600	0.60040500
N	2.63036900	1.64412900	-0.53986100
C	3.66250400	0.83040300	2.77058100
C	2.73669700	2.51861100	-1.67786400
H	3.96493400	2.68885100	0.77201800
H	4.31561700	1.69924600	2.94354400
H	2.92663800	0.78971800	3.58300900
H	4.27887000	-0.07689200	2.84064800
H	3.40780200	3.36557100	-1.46921500
H	1.75777900	2.93001600	-1.95993700
H	3.12873200	1.98547700	-2.55523000
N	-2.63023100	-1.64409000	-0.53999500
C	-3.26739500	-1.85186900	0.60029300
N	-3.00204200	-0.91642700	1.49165100
C	-2.73693700	-2.51816700	-1.67827600
C	-3.66205100	-0.83102700	2.77072200
H	-3.96458100	-2.68914200	0.77184900
H	-3.40714900	-3.36576100	-1.46934200
H	-3.13023600	-1.98501600	-2.55507900
H	-1.75794300	-2.92862700	-1.96142300
H	-4.31513700	-1.69991200	2.94357900
H	-4.27839300	0.07625500	2.84114400
H	-2.92603100	-0.79056000	3.58302200
C	-1.48590600	2.27887500	-1.22510100
C	-2.34285600	1.38153400	-1.92055600
C	-3.54984500	1.27799100	-1.14497000
C	-2.14337300	2.70918000	-0.03819200
C	-3.42138000	2.09589200	0.01372500
H	-0.47853400	2.54696400	-1.51305800
H	-2.16023100	0.93581000	-2.88893200
H	-4.41072100	0.67142800	-1.39657800

H	-1.71752500	3.35299300	0.72027100
H	-4.16365000	2.22850800	0.78984100
Mo	1.85043500	-0.28124200	0.09401900
Mo	-1.85044100	0.28126900	0.09409000

TSWN_{B-P}^{trans}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.25591800	1.07908300	0.98129700
N	-0.13828500	-0.22074900	1.57081600
N	2.52424300	1.57217400	-0.62083900
N	2.93091600	0.58754700	1.29403700
C	3.16628000	1.63888800	0.53176000
C	2.63511000	2.57050400	-1.65259500
C	3.28708400	0.50057100	2.68734400
N	-2.01300600	-1.48817500	-0.92342600
N	-2.72445100	-1.22529600	1.13601300
C	-2.70706900	-2.00673700	0.07899400
C	-2.05396000	-2.03241600	-2.25874500
C	-3.16009600	-1.62998500	2.44942100
H	3.36457700	3.34794400	-1.38014500
H	2.40208100	0.63132700	3.32333400
H	-2.29983000	-3.10431300	-2.24122500
H	-2.30263100	-1.69960100	3.13049900
C	2.95981400	-1.27157200	-1.59317400
C	1.58632700	-1.49577200	-1.91582400
C	1.00721400	-2.23231500	-0.80900300
C	2.03350800	-2.39386200	0.19947000
C	3.23055200	-1.81900000	-0.32553400
C	-2.90097600	1.23099500	-1.72550000
C	-3.62545900	1.30172500	-0.52056600
C	-2.88967200	2.11182800	0.40253000
C	-1.69844800	2.53624300	-0.26540500
C	-1.68367400	1.94612100	-1.56871800
H	-3.21688200	2.41564900	1.38834600
H	-4.55952900	0.79865400	-0.30775400
H	-3.17921600	0.64858100	-2.59361700
H	-0.91917500	2.08194000	-2.31994500
H	-0.93540400	3.17748300	0.14960100
H	0.02285900	-2.66834100	-0.77309800
H	1.94133800	-2.94178700	1.12690100
H	4.16463200	-1.71712400	0.21080900
H	3.65505000	-0.69015300	-2.18479300
H	1.11919900	-1.26324800	-2.86221900
H	2.95950500	2.12415300	-2.60329400
H	1.67054200	3.06304200	-1.83569000
H	3.71883200	-0.48254500	2.91397600
H	4.02767400	1.26884300	2.95515200
H	3.80615600	2.48344300	0.83289800
H	-3.66378600	-2.60692600	2.41791400
H	-3.86014100	-0.89571000	2.86706400
H	-3.20644100	-2.98737300	0.02980000
H	-2.80276500	-1.53075500	-2.89035800
H	-1.08253100	-1.91270000	-2.74578300
W	-1.41831700	0.29216900	0.25058100
W	1.39411900	-0.20303200	-0.02031600

TSWN_{B1-B2}^{cis}

	Coordinates (Angstroms)		
	X	Y	Z
N	0.08367800	-0.78916100	0.16485000
N	-0.07930900	0.61392700	0.30491700
C	2.64952200	-1.35292700	-1.89117600
C	3.84585700	-0.76076000	-1.36686300
C	2.19107200	-2.26609000	-0.86887000
C	3.06273100	-2.18739900	0.27758500
C	4.08789100	-1.24899700	-0.07064700
H	2.28009000	-1.26294600	-2.90291100
H	4.41219600	0.02740600	-1.84684400
H	1.32244600	-2.90513700	-0.94736500
H	3.03358300	-2.80416100	1.16487900
H	4.87008500	-0.90227800	0.59315900
N	2.54682700	1.08652000	1.59719500
C	2.75358000	2.11276300	0.79777200
N	2.54131800	1.79607900	-0.46862700
C	2.77561000	1.10773300	3.01964900
C	2.48638900	2.75306800	-1.54413300
H	3.06355300	3.11430800	1.13802100
H	3.15105000	2.08743000	3.35044500
H	1.84679000	0.89597800	3.56356600
H	3.50993200	0.34480100	3.31201600
H	2.86812600	3.73380400	-1.22426500
H	1.45749300	2.88676700	-1.90487400
H	3.09032200	2.41437400	-2.39576500
N	-2.67794400	-1.74391600	-0.54415800
C	-2.86866600	-2.12563400	0.71037400
N	-2.55890900	-1.16730400	1.55830100
C	-2.63700800	-2.64924400	-1.66465300
C	-2.80277100	-1.22852800	2.97718700
H	-3.24699900	-3.11889200	1.00156200
H	-3.07653100	-3.62321900	-1.40380100
H	-3.19800000	-2.23855000	-2.51339800
H	-1.60469500	-2.81655800	-2.00107400
H	-3.21197800	-2.20630000	3.27124500
H	-3.51428400	-0.45206400	3.29074900
H	-1.87167600	-1.06524800	3.53295100
C	-2.03213600	2.32224500	-0.72422500
C	-2.48259500	1.52295300	-1.83842900
C	-3.72705000	0.95367400	-1.42193000
C	-2.96632300	2.21013600	0.36703000
C	-4.01410200	1.35207100	-0.10129300
H	-1.12732200	2.91463900	-0.70903900
H	-2.05860600	1.48576800	-2.83204200
H	-4.30698100	0.23825400	-1.99160900
H	-2.95511300	2.75926800	1.29827000
H	-4.85218300	1.00481500	0.49012900
W	1.87036900	-0.22681900	-0.02024700
W	-1.88121900	0.19741800	-0.00091000

TaNB^{trans} (C2)

	Coordinates (Angstroms)		
	X	Y	Z
Ta	-1.40440000	0.17410000	-0.43010000
Ta	1.41490000	0.01050000	-0.07810000
N	0.17730000	1.45410000	-0.65780000
N	0.18380000	0.32680000	-1.63740000
N	-1.62320000	0.94270000	1.67940000
N	-2.71100000	1.93930000	0.02960000
C	-2.38710000	1.95490000	1.30540000
C	-1.04180000	0.89480000	2.99780000
C	-3.57430000	2.92460000	-0.57200000
N	1.48600000	-1.63700000	1.41050000
N	1.67920000	-2.05970000	-0.76230000
C	1.69630000	-2.54570000	0.46800000
C	1.56380000	-1.96570000	2.81370000
C	1.87220000	-2.87290000	-1.93820000
H	-1.51000000	1.62990000	3.67020000
H	-3.04310000	3.48960000	-1.34910000
H	1.73280000	-3.04210000	2.96090000
H	1.09450000	-2.66240000	-2.68000000
C	-2.86350000	-1.70350000	0.51760000
C	-1.71500000	-2.21800000	-0.15590000
C	-1.83130000	-1.88040000	-1.54260000
C	-3.02730000	-1.12490000	-1.71390000
C	-3.65580000	-1.02520000	-0.44210000
C	3.11700000	1.45190000	1.12580000
C	3.76510000	0.20030000	0.88820000
C	3.92580000	0.05800000	-0.50660000
C	3.37940000	1.21930000	-1.13340000
C	2.92950000	2.11440000	-0.12000000
H	-1.17170000	-0.09750000	3.44610000
H	0.03850000	1.10590000	2.97650000
H	-4.44510000	2.45060000	-1.04670000
H	-3.94670000	3.64270000	0.17390000
H	-2.71700000	2.74510000	2.00230000
H	1.83860000	-3.94420000	-1.69420000
H	2.84100000	-2.66280000	-2.41310000
H	1.85820000	-3.60980000	0.69330000
H	2.38620000	-1.42670000	3.30610000
H	0.63670000	-1.69300000	3.33190000
C	-3.19820000	-1.90040000	1.96870000
H	-3.68070000	-1.01570000	2.39600000
H	-3.88210000	-2.75040000	2.09530000
H	-2.29870000	-2.11120000	2.55560000
H	3.35140000	1.41470000	-2.19820000
H	-0.94950000	-2.83160000	0.29580000
H	-1.12840000	-2.13760000	-2.32150000
C	2.36230000	3.48470000	-0.33240000
H	2.26280000	4.01930000	0.61830000
H	3.01060000	4.07680000	-0.98880000
H	1.36750000	3.40450000	-0.79000000
H	4.36220000	-0.79180000	-1.01550000
H	4.06380000	-0.51520000	1.64230000
H	2.88350000	1.87300000	2.09800000
H	-4.56710000	-0.48000000	-0.22880000
H	-3.40140000	-0.71600000	-2.64430000

TaN_B^{trans} (C3)

	Coordinates (Angstroms)		
	X	Y	Z
Ta	1.50540000	-0.20990000	-0.24700000
Ta	-1.45630000	0.13870000	-0.20130000
N	-0.08440000	-1.04910000	-1.07100000
N	0.01040000	0.44160000	-1.47350000
N	1.60470000	-1.69740000	1.43900000
N	2.49550000	-2.23130000	-0.51140000
C	2.14900000	-2.63970000	0.68970000
C	1.12700000	-1.96870000	2.77140000
C	2.93440000	-3.13610000	-1.54240000
N	-1.60340000	1.53650000	1.50110000
N	-2.03570000	2.26690000	-0.55800000
C	-1.84940000	2.57210000	0.71400000
C	-1.40800000	1.69010000	2.92130000
C	-2.09430000	3.26680000	-1.59800000
H	1.42560000	-2.97390000	3.10710000
H	2.17600000	-3.22740000	-2.33240000
H	-1.34200000	2.75110000	3.20240000
H	-1.23900000	3.16640000	-2.27690000
C	3.28840000	0.95130000	1.24870000
C	2.34320000	1.92040000	0.79100000
C	2.45030000	1.97710000	-0.64260000
C	3.43850000	1.02370000	-1.05710000
C	3.96610000	0.40730000	0.12350000
C	-3.13150000	-1.35700000	1.13120000
C	-3.90360000	-0.28010000	0.58570000
C	-3.84780000	-0.37350000	-0.83690000
C	-3.03330000	-1.49680000	-1.17760000
C	-2.59070000	-2.10480000	0.04590000
H	1.52920000	-1.24470000	3.49070000
H	0.03250000	-1.90460000	2.82410000
H	3.86130000	-2.78160000	-2.01340000
H	3.12640000	-4.14200000	-1.13860000
H	2.28700000	-3.67840000	1.03860000
H	-2.08530000	4.28380000	-1.17820000
H	-3.00750000	3.15600000	-2.19600000
H	-1.85450000	3.60890000	1.08670000
H	-2.23420000	1.24660000	3.49340000
H	-0.48330000	1.19240000	3.23440000
C	1.78670000	2.98010000	-1.54460000
H	2.47130000	3.80830000	-1.77750000
H	1.46780000	2.52480000	-2.48680000
H	0.89660000	3.40840000	-1.07700000
C	5.09980000	-0.57690000	0.18690000
H	6.03810000	-0.07240000	0.45810000
H	4.92090000	-1.35850000	0.93280000
H	5.26140000	-1.07210000	-0.77450000
C	3.60220000	0.63690000	2.68380000
H	3.86560000	-0.41670000	2.81930000
H	4.45290000	1.23600000	3.03880000
H	2.75490000	0.85590000	3.34070000
C	-4.72320000	0.71330000	1.35910000
H	-5.79190000	0.45950000	1.32610000
H	-4.42970000	0.74600000	2.41210000
H	-4.61850000	1.72720000	0.95540000
C	-1.78990000	-3.37230000	0.11350000

H	-2.40530000	-4.23820000	-0.16790000
H	-0.93940000	-3.32180000	-0.57470000
H	-1.40110000	-3.55610000	1.11920000
C	-2.75260000	-2.03690000	-2.55290000
H	-1.68730000	-2.26400000	-2.66580000
H	-3.32460000	-2.95690000	-2.73690000
H	-3.02750000	-1.31960000	-3.33280000
C	1.63240000	2.91820000	1.66080000
H	1.32380000	2.48030000	2.61400000
H	2.28620000	3.77440000	1.88640000
H	0.73730000	3.31330000	1.17490000
C	3.94280000	0.84250000	-2.46510000
H	4.74240000	1.56170000	-2.69560000
H	4.35060000	-0.16060000	-2.62500000
H	3.14580000	0.99470000	-3.20000000
C	-3.04880000	-1.72650000	2.58720000
H	-3.00930000	-0.84830000	3.23780000
H	-3.92950000	-2.31180000	2.88880000
H	-2.16710000	-2.33640000	2.80250000
C	-4.59770000	0.50460000	-1.80060000
H	-4.07180000	0.60400000	-2.75550000
H	-5.59070000	0.08670000	-2.01660000
H	-4.74340000	1.50960000	-1.39440000

TaN_B^{trans} (C4)

	Coordinates (Angstroms)		
	X	Y	Z
Ta	1.85550000	0.26860000	0.07120000
Ta	-1.85910000	-0.26180000	-0.00200000
N	0.04350000	-0.56480000	0.51650000
N	-0.06070000	0.61430000	-0.34440000
N	2.85760000	-1.56360000	0.95650000
N	2.62610000	-1.30300000	-1.22970000
C	2.87240000	-2.16840000	-0.22380000
C	2.89730000	-2.32300000	2.21020000
C	2.55230000	-1.72950000	-2.63210000
N	-2.75890000	1.09140000	1.43300000
N	-2.82700000	1.67960000	-0.70280000
C	-2.93310000	2.09840000	0.55230000
C	-2.73520000	1.32160000	2.88390000
C	-2.79460000	2.61510000	-1.83260000
H	3.49760000	-3.23130000	2.05270000
H	-3.37880000	2.18420000	3.10700000
C	2.90350000	2.01600000	1.32460000
C	2.06240000	2.58110000	0.28940000
C	2.66780000	2.31610000	-0.99190000
C	3.90770000	1.64900000	-0.73830000
C	4.05290000	1.46170000	0.65590000
C	-3.99220000	-1.73110000	0.27420000
C	-3.92160000	-1.33740000	-1.08150000
C	-2.67830000	-1.79510000	-1.63920000
C	-1.98950000	-2.50570000	-0.58310000
C	-2.78980000	-2.43290000	0.61960000
H	1.98180000	-2.67100000	-2.68370000
H	-2.23540000	3.51820000	-1.54010000
C	2.22190000	2.92080000	-2.29540000

H	2.55180000	3.96790000	-2.37600000
H	2.63310000	2.38700000	-3.15730000
H	1.13270000	2.91260000	-2.39440000
C	5.27700000	0.87300000	1.30120000
H	6.16090000	1.48350000	1.07090000
H	5.18130000	0.83610000	2.38830000
H	5.48040000	-0.14520000	0.95080000
C	2.79490000	2.32510000	2.79570000
H	3.32770000	1.59070000	3.40540000
H	3.22490000	3.31300000	3.02360000
H	1.75510000	2.33730000	3.13680000
C	-5.02420000	-0.64310000	-1.82850000
H	-5.80400000	-1.36140000	-2.12060000
H	-5.50190000	0.13280000	-1.22250000
H	-4.65870000	-0.17130000	-2.74410000
C	-2.55460000	-3.24260000	1.86700000
H	-2.90320000	-4.27890000	1.73740000
H	-1.49410000	-3.28600000	2.13000000
H	-3.08670000	-2.82820000	2.72800000
C	-0.79130000	-3.39230000	-0.78360000
H	-0.24270000	-3.53710000	0.14930000
H	-1.09950000	-4.38230000	-1.15150000
H	-0.09080000	-2.97160000	-1.51090000
C	0.90320000	3.51470000	0.50670000
H	0.14690000	3.40700000	-0.27560000
H	0.41100000	3.33230000	1.46550000
H	1.24550000	4.56030000	0.50790000
C	4.94800000	1.27730000	-1.75550000
H	5.76120000	2.01730000	-1.76060000
H	5.39640000	0.30230000	-1.54070000
H	4.53760000	1.24270000	-2.76840000
C	-5.19200000	-1.50100000	1.15060000
H	-5.45890000	-0.43970000	1.21280000
H	-6.06490000	-2.03340000	0.74900000
H	-5.02850000	-1.86500000	2.16710000
C	-2.34270000	-1.87840000	-3.10480000
H	-1.26250000	-1.88570000	-3.27750000
H	-2.74990000	-2.80030000	-3.54840000
H	-2.75720000	-1.03780000	-3.66790000
C	1.49170000	-2.75280000	2.66520000
H	1.54170000	-3.28720000	3.62220000
H	0.84860000	-1.87470000	2.77760000
H	1.01990000	-3.41510000	1.93220000
C	3.58340000	-1.52100000	3.31890000
H	3.03810000	-0.59090000	3.50740000
H	3.60230000	-2.10170000	4.24860000
H	4.61340000	-1.27230000	3.05010000
C	3.09910000	-3.65860000	-0.40260000
H	4.12980000	-3.91510000	-0.13090000
H	2.43600000	-4.23320000	0.24990000
H	2.93050000	-3.98330000	-1.42890000
C	3.93900000	-1.99720000	-3.24580000
H	3.83670000	-2.39610000	-4.26270000
H	4.52290000	-1.07370000	-3.29980000
H	4.51250000	-2.72160000	-2.65760000
C	1.78030000	-0.70890000	-3.47070000
H	2.31330000	0.24480000	-3.51340000
H	1.66060000	-1.08120000	-4.49520000
H	0.79190000	-0.51450000	-3.04530000
C	-1.31760000	1.64300000	3.38840000
H	-1.31550000	1.78600000	4.47620000
H	-0.63440000	0.82370000	3.13930000
H	-0.92810000	2.55650000	2.92820000

C	-3.30580000	0.12780000	3.65250000
H	-2.71680000	-0.77210000	3.45190000
H	-3.27340000	0.32560000	4.73030000
H	-4.34390000	-0.06450000	3.37140000
C	-3.18410000	3.52940000	0.98760000
H	-4.16600000	3.60580000	1.46940000
H	-2.43580000	3.85260000	1.71710000
H	-3.16600000	4.22400000	0.14830000
C	-4.20770000	3.05530000	-2.25600000
H	-4.15480000	3.79200000	-3.06720000
H	-4.78640000	2.19680000	-2.61130000
H	-4.75940000	3.50810000	-1.42490000
C	-2.04290000	2.00330000	-3.01710000
H	-1.04790000	1.66870000	-2.71340000
H	-2.58190000	1.13820000	-3.41540000
H	-1.94400000	2.74200000	-3.82160000

NbN_B^{trans}(C2)

	Coordinates (Angstroms)		
	X	Y	Z
N	0.12690000	1.45880000	-1.24950000
N	0.11490000	0.32630000	-1.95710000
N	-0.33270000	0.86890000	1.52830000
N	-1.67770000	2.39560000	0.49830000
C	-0.91780000	2.09980000	1.50580000
C	-0.07960000	0.38130000	2.89130000
C	-2.17380000	3.73700000	0.28400000
N	1.08660000	-2.01210000	1.21550000
N	1.20700000	-2.09620000	-1.00100000
C	1.21230000	-2.76220000	0.13110000
C	1.33810000	-2.60780000	2.51000000
C	1.19760000	-2.71440000	-2.30210000
H	-0.14900000	1.20920000	3.61250000
H	-1.67680000	4.18740000	-0.58400000
H	1.48240000	-3.69640000	2.42820000
H	0.32420000	-2.38640000	-2.87690000
C	-2.89880000	-1.44220000	0.56760000
C	-2.22530000	-1.94200000	-0.58740000
C	-2.71810000	-1.25290000	-1.73440000
C	-3.66690000	-0.28680000	-1.27660000
C	-3.77560000	-0.41480000	0.14030000
C	3.09190000	1.06230000	1.01770000
C	3.55260000	-0.24870000	0.71090000
C	3.61280000	-0.36750000	-0.70120000
C	3.16780000	0.85380000	-1.26490000
C	2.86520000	1.76300000	-0.19910000
H	-0.81260000	-0.37550000	3.18950000
H	0.91460000	-0.05670000	2.97690000
H	-3.25020000	3.71100000	0.07970000
H	-1.99840000	4.38130000	1.15800000
H	-0.76330000	2.79830000	2.34480000
H	1.17830000	-3.81200000	-2.22210000
H	2.08790000	-2.42930000	-2.87890000
H	1.31970000	-3.85960000	0.17740000
H	2.24320000	-2.19470000	2.98180000
H	0.50700000	-2.43580000	3.20540000

C	-2.76460000	-1.97550000	1.96570000
H	-3.02500000	-1.21900000	2.71390000
H	-3.44000000	-2.82860000	2.11650000
H	-1.74590000	-2.32230000	2.16310000
H	3.07430000	1.07370000	-2.32040000
H	-1.50910000	-2.75130000	-0.59240000
H	-2.43260000	-1.43600000	-2.76170000
C	2.49230000	3.20820000	-0.34830000
H	2.13390000	3.62210000	0.60080000
H	3.36160000	3.80030000	-0.66400000
H	1.69790000	3.32200000	-1.09230000
H	3.89370000	-1.25480000	-1.25220000
H	3.79810000	-1.02160000	1.42670000
H	2.94960000	1.47120000	2.01120000
H	-4.41540000	0.17690000	0.78450000
H	-4.23690000	0.39650000	-1.89590000
Nb	-1.47960000	0.42600000	-0.55040000
Nb	1.16140000	-0.06510000	-0.13090000

NbN_B^{trans}(C3)

	Coordinates (Angstroms)		
	X	Y	Z
N	0.01990000	1.15560000	-1.44170000
N	-0.02420000	-0.12150000	-1.83410000
N	-0.25250000	1.21250000	1.45400000
N	-1.59710000	2.54620000	0.19290000
C	-0.78830000	2.44080000	1.19890000
C	0.00300000	0.99450000	2.88370000
C	-2.04990000	3.83220000	-0.28820000
N	1.26600000	-1.69450000	1.63570000
N	1.30950000	-2.22530000	-0.52730000
C	1.31780000	-2.64640000	0.71790000
C	1.38940000	-2.06170000	3.02950000
C	1.15070000	-3.10130000	-1.66060000
H	0.12820000	1.95740000	3.40160000
H	-1.58400000	4.05750000	-1.25540000
H	1.54090000	-3.14640000	3.14490000
H	0.26260000	-2.81740000	-2.23570000
C	-3.04260000	-1.05900000	1.16900000
C	-2.56650000	-1.89380000	0.10980000
C	-3.04100000	-1.35020000	-1.12870000
C	-3.80360000	-0.16920000	-0.81890000
C	-3.80890000	-0.00090000	0.60700000
C	3.16580000	1.29040000	0.71240000
C	3.70850000	-0.01280000	0.48370000
C	3.63580000	-0.28530000	-0.91810000
C	3.01470000	0.82070000	-1.55610000
C	2.73040000	1.80720000	-0.54540000
H	-0.82860000	0.46810000	3.36730000
H	0.90830000	0.41280000	3.03570000
H	-3.13610000	3.81920000	-0.43400000
H	-1.80230000	4.64200000	0.41400000
H	-0.55250000	3.29570000	1.85590000
H	1.05100000	-4.15100000	-1.34410000
H	2.00860000	-3.03400000	-2.34070000
H	1.35110000	-3.71780000	0.98060000

H	2.24420000	-1.56360000	3.50890000
H	0.49370000	-1.79190000	3.60510000
C	-2.93380000	-1.99600000	-2.48460000
H	-3.80380000	-2.63730000	-2.68860000
H	-2.87770000	-1.25450000	-3.28830000
H	-2.03720000	-2.61640000	-2.56270000
C	-4.57850000	1.04520000	1.36760000
H	-5.60220000	0.70660000	1.58200000
H	-4.10880000	1.28140000	2.32820000
H	-4.65980000	1.98130000	0.80560000
C	-2.86760000	-1.34320000	2.63440000
H	-2.96620000	-0.43840000	3.24250000
H	-3.62930000	-2.05260000	2.98890000
H	-1.88940000	-1.78610000	2.84570000
C	4.41000000	-0.88190000	1.48780000
H	5.50130000	-0.80070000	1.38110000
H	4.16370000	-0.59850000	2.51510000
H	4.14890000	-1.93850000	1.36380000
C	2.23730000	3.19690000	-0.82840000
H	3.03080000	3.80680000	-1.28340000
H	1.38630000	3.16540000	-1.51540000
H	1.91700000	3.70710000	0.08600000
C	2.80410000	1.02480000	-3.02870000
H	1.81110000	1.44090000	-3.22330000
H	3.55200000	1.71870000	-3.43840000
H	2.88200000	0.08530000	-3.58300000
C	-1.94800000	-3.25050000	0.29480000
H	-1.28450000	-3.28270000	1.16300000
H	-2.72920000	-4.00990000	0.45120000
H	-1.36960000	-3.55650000	-0.57930000
C	-4.58210000	0.65700000	-1.81110000
H	-5.58340000	0.23400000	-1.97780000
H	-4.71910000	1.68720000	-1.46600000
H	-4.08660000	0.69850000	-2.78730000
C	3.21720000	2.04910000	2.01110000
H	3.14200000	1.38580000	2.87850000
H	4.16560000	2.59710000	2.10540000
H	2.41060000	2.78400000	2.08620000
C	4.24060000	-1.48670000	-1.58350000
H	3.86450000	-1.61900000	-2.60130000
H	5.33270000	-1.37880000	-1.64960000
H	4.03570000	-2.40560000	-1.02510000
Nb	1.18910000	-0.05780000	-0.07070000
Nb	-1.51160000	0.37080000	-0.38160000

NbN_B^{trans}(C4)

	Coordinates (Angstroms)		
	X	Y	Z
N	0.03090000	-0.56300000	0.46690000
N	-0.05110000	0.57010000	-0.28080000
N	2.93690000	-1.57280000	0.94260000
N	2.69240000	-1.25090000	-1.24480000
C	2.92390000	-2.14050000	-0.25690000
C	2.98350000	-2.36920000	2.17060000
C	2.59190000	-1.65140000	-2.65250000
N	-2.84370000	1.06310000	1.44560000

N	-2.86980000	1.69410000	-0.68710000
C	-2.97130000	2.08690000	0.57660000
C	-2.82880000	1.27250000	2.89840000
C	-2.82680000	2.64380000	-1.80140000
H	3.53280000	-3.30140000	1.97220000
H	-3.41220000	2.17580000	3.12630000
C	2.99150000	2.04170000	1.37090000
C	2.10460000	2.62000000	0.38570000
C	2.67050000	2.41110000	-0.92100000
C	3.91760000	1.73910000	-0.73540000
C	4.11380000	1.50790000	0.64850000
C	-2.83350000	-2.51020000	0.57980000
C	-4.03200000	-1.80010000	0.25010000
C	-3.96140000	-1.38530000	-1.10260000
C	-2.72460000	-1.84460000	-1.66540000
C	-2.03150000	-2.55570000	-0.61820000
H	2.01670000	-2.58940000	-2.71580000
H	-2.25720000	3.53940000	-1.50410000
Nb	-1.92800000	-0.28530000	-0.01330000
Nb	1.92780000	0.29690000	0.11100000
C	2.91290000	2.27440000	2.85720000
H	1.88080000	2.25380000	3.22180000
H	3.47060000	1.51850000	3.41650000
H	3.33310000	3.25600000	3.12600000
C	0.92650000	3.50990000	0.67670000
H	0.47180000	3.27610000	1.64320000
H	1.23930000	4.56410000	0.71070000
H	0.14820000	3.41320000	-0.08530000
C	2.16150000	3.03330000	-2.19240000
H	2.54740000	2.52400000	-3.08020000
H	1.06920000	3.00800000	-2.24920000
H	2.46970000	4.08750000	-2.26500000
C	4.92330000	1.40760000	-1.79970000
H	4.47460000	1.38150000	-2.79650000
H	5.72130000	2.16370000	-1.82240000
H	5.39790000	0.43820000	-1.61910000
C	5.35570000	0.89910000	1.23760000
H	5.59760000	-0.06520000	0.77700000
H	6.21890000	1.56280000	1.08800000
H	5.25210000	0.73410000	2.31170000
C	-2.08720000	2.03290000	-2.99450000
H	-2.63990000	1.17810000	-3.39700000
H	-1.97960000	2.77580000	-3.79410000
H	-1.09560000	1.68160000	-2.69710000
C	-4.23830000	3.09910000	-2.21470000
H	-4.18650000	3.83390000	-3.02780000
H	-4.82760000	2.24400000	-2.56230000
H	-4.77740000	3.55800000	-1.37860000
C	-3.17270000	3.52070000	1.03480000
H	-4.14780000	3.62410000	1.52530000
H	-2.40810000	3.80890000	1.76230000
H	-3.13750000	4.22610000	0.20500000
C	-3.49890000	0.11160000	3.63760000
H	-2.97570000	-0.82630000	3.42730000
H	-3.46870000	0.28580000	4.71960000
H	-4.54390000	0.00250000	3.33700000
C	-1.40170000	1.48330000	3.43310000
H	-1.41020000	1.62430000	4.52120000
H	-0.77960000	0.61280000	3.19740000
H	-0.93330000	2.36430000	2.98240000
C	1.81070000	-0.61200000	-3.45980000
H	2.34390000	0.34240000	-3.48920000
H	1.67770000	-0.96170000	-4.49070000

H	0.82720000	-0.42670000	-3.01880000
C	3.96930000	-1.91070000	-3.29090000
H	3.85390000	-2.28480000	-4.31600000
H	4.55640000	-0.98830000	-3.32890000
H	4.54570000	-2.65100000	-2.72580000
C	3.10570000	-3.63370000	-0.47230000
H	4.11140000	-3.93740000	-0.15950000
H	2.39050000	-4.20120000	0.13030000
H	2.97610000	-3.92420000	-1.51430000
C	1.57530000	-2.74580000	2.66330000
H	1.63160000	-3.32390000	3.59430000
H	0.98280000	-1.84240000	2.83990000
H	1.04160000	-3.34730000	1.92010000
C	3.74780000	-1.62830000	3.27190000
H	3.25200000	-0.68110000	3.50800000
H	3.78190000	-2.23390000	4.18530000
H	4.77520000	-1.41450000	2.96350000
C	-5.06390000	-0.68010000	-1.84030000
H	-4.69670000	-0.18870000	-2.74490000
H	-5.84140000	-1.39430000	-2.14870000
H	-5.54460000	0.08290000	-1.22040000
C	-2.36810000	-1.87880000	-3.12780000
H	-2.75160000	-2.79460000	-3.60390000
H	-2.79190000	-1.02970000	-3.67090000
H	-1.28550000	-1.86110000	-3.28730000
C	-5.23640000	-1.59370000	1.12530000
H	-5.53140000	-0.53960000	1.17450000
H	-6.09470000	-2.15450000	0.73010000
H	-5.06290000	-1.94010000	2.14620000
C	-2.57830000	-3.31140000	1.82830000
H	-3.11620000	-2.90480000	2.68960000
H	-2.90680000	-4.35470000	1.70420000
H	-1.51610000	-3.33310000	2.08870000
C	-0.80820000	-3.40810000	-0.81930000
H	-0.10930000	-2.95990000	-1.53190000
H	-0.26680000	-3.55690000	0.11760000
H	-1.08840000	-4.39880000	-1.20700000

WN_B^{trans}(C2)

	Coordinates (Angstroms)		
	X	Y	Z
N	-0.00740000	1.46110000	-0.68980000
N	0.15160000	0.55980000	-1.68020000
N	-2.26440000	1.40240000	1.04970000
N	-2.64410000	1.41360000	-1.11230000
C	-2.83510000	2.03010000	0.02830000
C	-2.22590000	1.95340000	2.38200000
C	-2.94620000	1.98800000	-2.39740000
N	1.64720000	-1.83540000	1.02000000
N	2.03260000	-1.64350000	-1.12450000
C	2.11790000	-2.42690000	-0.06280000
C	1.78070000	-2.38130000	2.34530000
C	2.35320000	-2.03000000	-2.47550000
H	-2.98460000	2.74050000	2.50760000
H	-2.01960000	2.23880000	-2.92940000
H	1.95090000	-3.46780000	2.31750000

H	1.49650000	-1.85000000	-3.13510000
C	-2.84730000	-1.66910000	0.86420000
C	-1.53050000	-2.20690000	0.89540000
C	-1.08360000	-2.36980000	-0.45620000
C	-2.11460000	-1.90190000	-1.32920000
C	-3.19310000	-1.46790000	-0.49700000
C	2.64740000	1.28720000	1.58000000
C	3.58380000	0.34180000	1.04030000
C	3.83800000	0.69060000	-0.30310000
C	3.03480000	1.81130000	-0.62690000
C	2.33910000	2.23140000	0.55940000
H	-2.42020000	1.17730000	3.13190000
H	-1.24340000	2.39240000	2.60830000
H	-3.50710000	1.28040000	-3.02200000
H	-3.54750000	2.90430000	-2.29490000
H	-3.39420000	2.97390000	0.13270000
H	2.62200000	-3.09480000	-2.52820000
H	3.19590000	-1.44460000	-2.86680000
H	2.52450000	-3.44980000	-0.08420000
H	2.61650000	-1.92470000	2.89810000
H	0.87140000	-2.18690000	2.92470000
C	-3.71880000	-1.38280000	2.05260000
H	-4.28780000	-0.45810000	1.91680000
H	-4.43450000	-2.20050000	2.20850000
H	-3.12320000	-1.28540000	2.96580000
H	2.97670000	2.30260000	-1.58960000
H	-0.98810000	-2.49070000	1.78470000
H	-0.15760000	-2.81780000	-0.77240000
C	1.54640000	3.49230000	0.71930000
H	1.03270000	3.51160000	1.68620000
H	2.21080000	4.36470000	0.67100000
H	0.79220000	3.57200000	-0.06930000
H	4.45680000	0.13510000	-0.99630000
H	4.01440000	-0.49430000	1.57360000
H	2.30930000	1.33750000	2.60710000
H	-4.10800000	-1.00510000	-0.84310000
H	-2.10170000	-1.91950000	-2.41000000
W	-1.23460000	-0.06790000	-0.18310000
W	1.34750000	0.09110000	-0.04050000

$WN_B^{trans}(C3)$

	Coordinates (Angstroms)		
	X	Y	Z
N	0.09120000	0.81870000	-1.01990000
N	-0.06570000	-0.69850000	-1.11460000
N	-1.69050000	1.68320000	1.32940000
N	-2.37170000	2.13350000	-0.69770000
C	-2.08830000	2.62370000	0.48980000
C	-1.37910000	1.92690000	2.71460000
C	-2.53150000	2.94130000	-1.87870000
N	1.65850000	-1.78470000	1.21610000
N	2.37430000	-2.09350000	-0.82310000
C	2.08170000	-2.66550000	0.32630000
C	1.44190000	-2.08430000	2.60770000
C	2.50470000	-2.82420000	-2.05930000
H	-1.24380000	3.00160000	2.91080000

H	-1.65590000	2.83700000	-2.53370000
H	1.28650000	-3.16230000	2.76640000
H	1.60600000	-2.69400000	-2.67720000
C	-3.60480000	-0.68020000	1.08890000
C	-2.58440000	-1.68290000	1.00230000
C	-2.41850000	-1.98420000	-0.40400000
C	-3.28470000	-1.11210000	-1.17190000
C	-4.02830000	-0.33310000	-0.21750000
C	2.73910000	1.32170000	1.29210000
C	3.74170000	0.37020000	0.87010000
C	3.96430000	0.52070000	-0.52950000
C	3.11330000	1.55400000	-1.01270000
C	2.37040000	2.06470000	0.10980000
H	-2.16910000	1.56520000	3.38770000
H	-0.45430000	1.40760000	2.98320000
H	-3.41420000	2.62810000	-2.45050000
H	-2.65110000	4.00550000	-1.62480000
H	-2.14730000	3.69450000	0.74910000
H	2.64680000	-3.90020000	-1.87630000
H	3.36320000	-2.46210000	-2.63720000
H	2.15620000	-3.75000000	0.51760000
H	2.29190000	-1.77820000	3.23530000
H	0.55610000	-1.55150000	2.96500000
C	-1.63940000	-3.13360000	-0.97560000
H	-2.30010000	-3.98990000	-1.17070000
H	-1.14970000	-2.85030000	-1.91120000
H	-0.85450000	-3.46340000	-0.28940000
C	-5.12040000	0.64530000	-0.54090000
H	-6.10470000	0.16880000	-0.43020000
H	-5.09720000	1.51660000	0.12060000
H	-5.04610000	1.00750000	-1.56950000
C	-4.19030000	-0.12960000	2.35680000
H	-4.37990000	0.94630000	2.28660000
H	-5.15010000	-0.61760000	2.57650000
H	-3.53450000	-0.30160000	3.21440000
C	4.53130000	-0.54840000	1.76030000
H	5.57600000	-0.21580000	1.82990000
H	4.12920000	-0.56720000	2.77640000
H	4.54100000	-1.57830000	1.38550000
C	1.47870000	3.27100000	0.05500000
H	2.07560000	4.18980000	-0.02880000
H	0.80370000	3.22030000	-0.80500000
H	0.86250000	3.35230000	0.95380000
C	3.05000000	2.09990000	-2.41070000
H	2.01860000	2.32740000	-2.69470000
H	3.63740000	3.02600000	-2.49510000
H	3.44630000	1.38760000	-3.14050000
C	-2.07630000	-2.50530000	2.15230000
H	-1.89200000	-1.89310000	3.04060000
H	-2.80390000	-3.28280000	2.43120000
H	-1.14120000	-3.00830000	1.89830000
C	-3.56810000	-1.22420000	-2.64490000
H	-4.33930000	-1.98370000	-2.84520000
H	-3.92330000	-0.27590000	-3.06010000
H	-2.66920000	-1.50790000	-3.19910000
C	2.46440000	1.70940000	2.71900000
H	2.33370000	0.83480000	3.36370000
H	3.29390000	2.30300000	3.13290000
H	1.55910000	2.31450000	2.80130000
C	4.96420000	-0.25470000	-1.33530000
H	4.69320000	-0.28190000	-2.39460000
H	5.95890000	0.20580000	-1.25790000
H	5.04430000	-1.28650000	-0.98260000

W	1.60150000	-0.10980000	-0.17730000
W	-1.59230000	0.11970000	-0.19660000

WN_B^{trans}(C4)

Coordinates (Angstroms)			
	X	Y	Z
N	-0.14250000	0.76380000	-0.86920000
N	0.13510000	-0.71230000	-0.89740000
N	-2.40000000	0.89550000	1.32070000
N	-2.96000000	1.24750000	-0.73720000
C	-2.98380000	1.76470000	0.48470000
C	-2.28540000	0.96970000	2.77750000
C	-3.40270000	1.84040000	-1.99730000
N	2.37420000	-0.96060000	1.30470000
N	2.89600000	-1.32570000	-0.77810000
C	2.87890000	-1.85030000	0.44580000
C	2.31340000	-1.03480000	2.76590000
C	3.08500000	-2.13450000	-1.98670000
H	2.53730000	-3.08540000	-1.87100000
C	-3.61140000	-1.72130000	0.21770000
C	-2.53980000	-2.34210000	0.96030000
C	-1.62110000	-2.86670000	-0.00980000
C	-2.11550000	-2.57920000	-1.31880000
C	-3.33490000	-1.85960000	-1.18740000
C	2.43280000	2.33370000	1.03190000
C	3.62290000	1.70370000	0.51660000
C	3.60530000	1.77110000	-0.90550000
C	2.40780000	2.42240000	-1.31270000
C	1.68680000	2.78110000	-0.11980000
H	-2.01730000	-0.04980000	3.07110000
H	-3.34760000	1.01130000	-2.70990000
H	2.18610000	0.00750000	3.07450000
C	-0.39050000	-3.68050000	0.26000000
H	-0.56600000	-4.73830000	0.01780000
H	0.44870000	-3.33160000	-0.34960000
H	-0.09230000	-3.62350000	1.30840000
C	-4.28810000	-1.52460000	-2.29730000
H	-4.95880000	-2.37470000	-2.48980000
H	-4.91510000	-0.66700000	-2.04310000
H	-3.76790000	-1.29780000	-3.23270000
C	-4.89970000	-1.19030000	0.78250000
H	-5.14780000	-0.20380000	0.37690000
H	-5.73620000	-1.86440000	0.55000000
H	-4.85120000	-1.09810000	1.87010000
C	4.78600000	1.20300000	1.32430000
H	5.63500000	1.89780000	1.25290000
H	4.52990000	1.11140000	2.38220000
H	5.13440000	0.22410000	0.97710000
C	0.45600000	3.63840000	-0.08220000
H	0.72060000	4.70220000	-0.16740000
H	-0.22150000	3.38870000	-0.90000000
H	-0.09500000	3.50160000	0.85170000
C	2.01730000	2.77960000	-2.71780000
H	0.93350000	2.73270000	-2.84890000
H	2.34460000	3.79980000	-2.96720000
H	2.46660000	2.09830000	-3.44690000

C	-2.58830000	-2.70940000	2.41790000
H	-3.10700000	-1.95310000	3.01330000
H	-3.13090000	-3.65660000	2.55730000
H	-1.59030000	-2.83800000	2.84360000
C	-1.45610000	-2.99320000	-2.60080000
H	-1.63340000	-4.06020000	-2.79760000
H	-1.84370000	-2.42840000	-3.45360000
H	-0.37660000	-2.82800000	-2.55670000
C	2.28190000	2.85010000	2.43770000
H	2.55260000	2.10480000	3.19190000
H	2.93660000	3.72100000	2.59420000
H	1.26010000	3.17230000	2.64480000
C	4.73560000	1.34330000	-1.79250000
H	4.41420000	1.18550000	-2.82490000
H	5.51280000	2.12070000	-1.80550000
H	5.19740000	0.41990000	-1.43510000
C	2.48450000	-1.43380000	-3.20980000
H	2.56520000	-2.08490000	-4.08910000
H	1.43510000	-1.18930000	-3.03230000
H	3.01760000	-0.50310000	-3.42810000
C	4.56430000	-2.48420000	-2.23660000
H	5.14660000	-1.57810000	-2.43390000
H	5.01740000	-2.99470000	-1.38040000
H	4.65880000	-3.14340000	-3.10870000
C	3.59040000	-1.55090000	3.45840000
H	4.48910000	-1.08150000	3.04820000
H	3.54380000	-1.31450000	4.52830000
H	3.70410000	-2.63600000	3.37530000
C	1.07260000	-1.78330000	3.27780000
H	0.17730000	-1.39370000	2.78540000
H	1.13860000	-2.85990000	3.07940000
H	0.96690000	-1.65220000	4.36230000
C	-2.45160000	2.92140000	-2.54030000
H	-1.43800000	2.51710000	-2.59140000
H	-2.76310000	3.22890000	-3.54670000
H	-2.43830000	3.81800000	-1.90950000
C	-4.86860000	2.31850000	-1.99380000
H	-5.18960000	2.53530000	-3.01980000
H	-5.53400000	1.54880000	-1.58700000
H	-5.01360000	3.23200000	-1.40840000
C	-3.59260000	1.30930000	3.51950000
H	-3.87100000	2.36350000	3.42550000
H	-4.42670000	0.70460000	3.15000000
H	-3.47080000	1.10200000	4.58950000
C	-1.12260000	1.86000000	3.23860000
H	-0.97530000	1.77360000	4.32280000
H	-0.20660000	1.54490000	2.73240000
H	-1.29970000	2.91850000	3.01110000
W	1.64800000	0.45050000	-0.16240000
W	-1.65670000	-0.45650000	-0.19070000
C	-3.54280000	3.12000000	0.86880000
H	-4.60400000	3.04780000	1.13350000
H	-3.00880000	3.53180000	1.72680000
H	-3.44930000	3.82500000	0.04160000
C	3.31480000	-3.25960000	0.79320000
H	2.72690000	-3.65890000	1.62150000
H	3.19710000	-3.92850000	-0.06270000
H	4.37040000	-3.27840000	1.08760000

	Coordinates (Angstroms)		
	X	Y	Z
N	0.20660000	1.46630000	-0.73000000
N	0.21690000	0.32890000	-1.69770000
N	-1.63800000	0.99880000	1.58200000
N	-2.68720000	1.98980000	-0.09590000
C	-2.38440000	2.01530000	1.18500000
C	-1.07900000	0.95840000	2.91030000
C	-3.52960000	2.97800000	-0.72180000
N	1.44680000	-1.61690000	1.39150000
N	1.67140000	-2.06430000	-0.77330000
C	1.66280000	-2.53760000	0.46200000
C	1.49780000	-1.93170000	2.79910000
C	1.87500000	-2.89180000	-1.93750000
H	-1.55020000	1.70550000	3.56730000
H	-2.97950000	3.52910000	-1.49570000
H	1.65260000	-3.00830000	2.96020000
H	1.11200000	-2.68060000	-2.69430000
C	-2.88770000	-1.64590000	0.42690000
C	-1.73390000	-2.17970000	-0.22210000
C	-1.82350000	-1.85530000	-1.61390000
C	-3.00810000	-1.08890000	-1.81290000
C	-3.65650000	-0.96910000	-0.55280000
C	3.11610000	1.45120000	1.10240000
C	3.75430000	0.19020000	0.88850000
C	3.93650000	0.03160000	-0.50190000
C	3.41340000	1.19210000	-1.14950000
C	2.95650000	2.10250000	-0.15310000
H	-1.22720000	-0.02770000	3.36660000
H	0.00370000	1.15760000	2.90500000
H	-4.39760000	2.50850000	-1.20620000
H	-3.90640000	3.70790000	0.01030000
H	-2.71720000	2.81610000	1.86810000
H	1.82560000	-3.96000000	-1.68310000
H	2.85380000	-2.69710000	-2.39820000
H	1.80940000	-3.60090000	0.70090000
H	2.31770000	-1.39660000	3.29960000
H	0.56530000	-1.64370000	3.29890000
C	-3.24850000	-1.82400000	1.87410000
H	-3.72830000	-0.92970000	2.28420000
H	-3.94370000	-2.66520000	1.99800000
H	-2.36120000	-2.03840000	2.47810000
H	3.40510000	1.37660000	-2.21670000
H	-0.98270000	-2.79680000	0.24860000
H	-1.11060000	-2.12830000	-2.37830000
C	2.40790000	3.47660000	-0.38900000
H	2.29860000	4.02210000	0.55440000
H	3.07350000	4.05480000	-1.04040000
H	1.42000000	3.40230000	-0.86230000
H	4.37200000	-0.82810000	-0.99460000
H	4.03260000	-0.52050000	1.65480000
H	2.87120000	1.88480000	2.06620000
H	-4.56510000	-0.41190000	-0.36040000
H	-3.36220000	-0.68570000	-2.75350000
Mo	-1.39260000	0.20590000	-0.51550000
Mo	1.41860000	0.01560000	-0.11490000

	Coordinates (Angstroms)		
	X	Y	Z
N	0.16350000	0.79210000	-1.09630000
N	-0.12680000	-0.56300000	-1.24560000
N	-1.61870000	1.73240000	1.35260000
N	-2.28030000	2.23980000	-0.67990000
C	-2.02460000	2.68470000	0.52900000
C	-1.31780000	1.98680000	2.73890000
C	-2.57100000	3.08910000	-1.80310000
N	1.55920000	-1.77060000	1.27350000
N	2.21330000	-2.23300000	-0.76940000
C	1.94230000	-2.71120000	0.42300000
C	1.37180000	-2.02330000	2.67890000
C	2.36530000	-3.05650000	-1.94110000
H	-1.32410000	3.06690000	2.95460000
H	-1.77820000	3.01270000	-2.55940000
H	1.21920000	-3.09590000	2.87420000
H	1.47820000	-2.98010000	-2.58470000
C	-3.39250000	-0.90500000	1.14900000
C	-2.52200000	-1.93190000	0.68310000
C	-2.56040000	-1.91260000	-0.75040000
C	-3.45190000	-0.86340000	-1.17630000
C	-3.96890000	-0.24840000	0.02120000
C	2.93120000	1.23840000	1.24510000
C	3.80410000	0.26490000	0.63460000
C	3.86510000	0.53020000	-0.77520000
C	3.03400000	1.65720000	-1.03740000
C	2.46340000	2.09530000	0.20200000
H	-2.04220000	1.51190000	3.41460000
H	-0.32820000	1.59460000	3.00100000
H	-3.51530000	2.80320000	-2.28670000
H	-2.65520000	4.14400000	-1.49830000
H	-2.12360000	3.74370000	0.82670000
H	2.50720000	-4.11550000	-1.67350000
H	3.23040000	-2.73740000	-2.53480000
H	2.01070000	-3.78120000	0.68970000
H	2.23420000	-1.70160000	3.28240000
H	0.49340000	-1.48120000	3.04550000
C	-1.90000000	-2.90560000	-1.66150000
H	-2.62170000	-3.66570000	-1.99230000
H	-1.48260000	-2.41500000	-2.54520000
H	-1.07540000	-3.41950000	-1.16040000
C	-5.02740000	0.81680000	0.08380000
H	-6.01520000	0.37230000	0.27120000
H	-4.83350000	1.53780000	0.88460000
H	-5.08960000	1.37660000	-0.85270000
C	-3.73630000	-0.62780000	2.58400000
H	-4.01340000	0.41880000	2.73660000
H	-4.59120000	-1.24250000	2.89980000
H	-2.90290000	-0.85680000	3.25490000
C	4.65440000	-0.74130000	1.35890000
H	5.68080000	-0.36810000	1.48460000
H	4.26220000	-0.95800000	2.35620000
H	4.71360000	-1.68850000	0.81270000
C	1.57820000	3.29930000	0.33650000
H	2.15160000	4.22190000	0.16890000
H	0.76750000	3.26820000	-0.39860000

H	1.12740000	3.36290000	1.32990000
C	2.78340000	2.30730000	-2.36710000
H	1.71160000	2.46390000	-2.52440000
H	3.28470000	3.28370000	-2.42340000
H	3.15610000	1.69390000	-3.19240000
C	-1.83280000	-2.96220000	1.52890000
H	-1.70400000	-2.61510000	2.55760000
H	-2.41930000	-3.89190000	1.56680000
H	-0.84330000	-3.20700000	1.13580000
C	-3.94080000	-0.64420000	-2.58150000
H	-4.78470000	-1.31070000	-2.81590000
H	-4.28270000	0.38370000	-2.73450000
H	-3.15060000	-0.84100000	-3.31220000
C	2.76160000	1.46050000	2.72220000
H	2.67160000	0.51930000	3.27060000
H	3.62440000	2.00170000	3.13820000
H	1.86880000	2.05310000	2.93880000
C	4.76190000	-0.17410000	-1.75250000
H	4.39230000	-0.09040000	-2.77870000
H	5.77400000	0.25460000	-1.72880000
H	4.84900000	-1.23790000	-1.51360000
Mo	1.64800000	-0.16100000	-0.21080000
Mo	-1.63430000	0.18220000	-0.21940000

MoN_B^{trans}(C4)

Coordinates (Angstroms)			
	X	Y	Z
N	0.26470000	-0.36590000	0.69670000
N	-0.15990000	0.21710000	-0.45230000
N	3.02370000	-1.13620000	1.24550000
N	2.68990000	-1.50660000	-0.91530000
C	3.06110000	-2.03310000	0.25750000
C	3.12040000	-1.54800000	2.64780000
C	2.54650000	-2.30270000	-2.13690000
N	-2.57140000	1.28710000	1.36700000
N	-2.89920000	1.46330000	-0.81300000
C	-2.92480000	2.09460000	0.36950000
C	-2.47110000	1.73770000	2.75410000
C	-3.02180000	2.18480000	-2.08320000
H	3.82180000	-2.39360000	2.71810000
H	-3.15500000	2.58710000	2.90230000
C	2.83390000	2.36060000	0.68740000
C	1.87200000	2.56290000	-0.36370000
C	2.42220000	2.01370000	-1.58900000
C	3.73970000	1.54970000	-1.29280000
C	3.98370000	1.72360000	0.08910000
C	-3.92450000	-1.74110000	0.66880000
C	-3.96650000	-1.58180000	-0.73550000
C	-2.75020000	-2.09750000	-1.30980000
C	-1.94330000	-2.57290000	-0.21820000
C	-2.66020000	-2.31610000	1.02270000
H	2.07000000	-3.26390000	-1.88660000
H	-2.46830000	3.13580000	-2.01220000
C	1.82070000	2.21020000	-2.95240000
H	2.00860000	3.23100000	-3.31820000
H	2.24060000	1.52020000	-3.68990000

H	0.73760000	2.06090000	-2.93980000
C	5.28180000	1.38530000	0.76670000
H	6.11130000	1.94650000	0.31570000
H	5.25720000	1.63520000	1.82950000
H	5.51740000	0.31840000	0.68300000
C	2.78290000	2.98990000	2.05400000
H	3.42540000	2.46690000	2.76650000
H	3.12320000	4.03550000	2.01380000
H	1.77010000	2.98970000	2.46660000
C	-5.15530000	-1.06490000	-1.49170000
H	-5.93420000	-1.83840000	-1.55530000
H	-5.59840000	-0.19230000	-1.00170000
H	-4.89730000	-0.78010000	-2.51480000
C	-2.26340000	-2.87290000	2.36260000
H	-2.48240000	-3.95000000	2.41790000
H	-1.19330000	-2.74590000	2.55050000
H	-2.80230000	-2.38910000	3.18140000
C	-0.70360000	-3.41660000	-0.32650000
H	0.04350000	-3.12790000	0.41890000
H	-0.94200000	-4.47990000	-0.17670000
H	-0.24030000	-3.31770000	-1.31150000
C	0.63430000	3.41480000	-0.30190000
H	-0.22720000	2.90890000	-0.74850000
H	0.37560000	3.66540000	0.72950000
H	0.79250000	4.36060000	-0.84000000
C	4.73960000	1.00200000	-2.26790000
H	5.48260000	1.77020000	-2.52620000
H	5.28320000	0.14820000	-1.85200000
H	4.26770000	0.68040000	-3.19980000
C	-5.05720000	-1.39270000	1.59340000
H	-5.35470000	-0.34170000	1.50060000
H	-5.94200000	-2.00340000	1.36670000
H	-4.79590000	-1.57340000	2.63840000
C	-2.51690000	-2.38750000	-2.76760000
H	-1.45460000	-2.35930000	-3.02570000
H	-2.89420000	-3.38700000	-3.03230000
H	-3.02760000	-1.66940000	-3.41500000
C	1.76260000	-2.00900000	3.20970000
H	1.86210000	-2.31640000	4.25840000
H	1.03400000	-1.19570000	3.14460000
H	1.36080000	-2.85680000	2.64420000
C	3.68870000	-0.42260000	3.51580000
H	3.02930000	0.45030000	3.48390000
H	3.77030000	-0.75170000	4.55840000
H	4.68260000	-0.12120000	3.17320000
C	3.43730000	-3.48880000	0.46970000
H	4.46430000	-3.56200000	0.84530000
H	2.78460000	-3.95610000	1.21370000
H	3.37170000	-4.06990000	-0.44940000
C	3.90040000	-2.61440000	-2.80300000
H	3.75790000	-3.27340000	-3.66860000
H	4.37910000	-1.69430000	-3.15100000
H	4.59160000	-3.10980000	-2.11290000
C	1.61940000	-1.59400000	-3.12740000
H	2.06930000	-0.65980000	-3.47640000
H	1.44060000	-2.23370000	-4.00010000
H	0.66130000	-1.34500000	-2.66300000
C	-1.04650000	2.20890000	3.09600000
H	-0.97570000	2.50340000	4.15090000
H	-0.32750000	1.40590000	2.90230000
H	-0.75880000	3.07120000	2.48580000
C	-2.90720000	0.63780000	3.72660000
H	-2.26880000	-0.24360000	3.61580000

H	-2.82780000	0.99220000	4.76130000
H	-3.94360000	0.34050000	3.54530000
C	-3.27320000	3.55980000	0.56500000
H	-4.26670000	3.65700000	1.01970000
H	-2.55750000	4.04680000	1.23310000
H	-3.28360000	4.10710000	-0.37770000
C	-4.48330000	2.52530000	-2.43220000
H	-4.53010000	3.11510000	-3.35640000
H	-5.06640000	1.61120000	-2.58140000
H	-4.96760000	3.10450000	-1.63900000
C	-2.37330000	1.39080000	-3.21910000
H	-1.34720000	1.11360000	-2.96470000
H	-2.92740000	0.46860000	-3.41600000
H	-2.36550000	1.98640000	-4.13990000
Mo	-1.92670000	-0.33260000	0.02940000
Mo	1.90230000	0.32020000	-0.00600000

TaN_{BI}^{cis}(C4)

	Coordinates (Angstroms)		
	X	Y	Z
Ta	-1.84655000	0.24152800	-0.09284500
Ta	1.84934400	-0.22698000	-0.11043100
N	-0.05003200	-0.72054700	0.19491600
N	0.04904000	0.70978000	0.26204200
C	2.75407500	-0.75854800	-2.21822600
C	3.94181400	-0.77480000	-1.39636000
C	1.92558400	-1.85713800	-1.76388100
C	2.58020800	-2.49292000	-0.64630800
C	3.83580300	-1.83474700	-0.46246500
N	2.88651700	0.15510800	1.73599400
C	2.99177700	1.46847900	1.51736200
N	2.82575600	1.81813500	0.25698000
C	3.10255600	-0.45694900	3.04901500
C	2.63261800	3.21746300	-0.13355500
H	3.15235200	2.18558500	2.33172600
H	3.19472500	-1.53151800	2.85428500
H	1.56260000	3.45598000	-0.02055600
N	-2.80956200	-1.83971900	0.08589600
C	-3.00383700	-1.59762800	1.36661800
N	-2.90070100	-0.30825600	1.70031200
C	-2.59432900	-3.19853900	-0.41914800
C	-3.13421200	0.18864300	3.05870000
H	-3.18949000	-2.37992500	2.11142000
H	-1.50696200	-3.36710700	-0.44600200
H	-3.28626700	1.26842200	2.95069000
C	-1.94098600	2.01288100	-1.60453700
C	-2.77123300	0.95542100	-2.14384400
C	-3.95013300	0.89616500	-1.31140900
C	-2.58867800	2.55085000	-0.43374100
C	-3.84010500	1.87654500	-0.29426800
C	2.60989400	-0.05704200	-3.54357200
H	3.08030100	0.93010500	-3.53762500
H	3.08300600	-0.63971900	-4.34981600
H	1.55894900	0.07912200	-3.81739900
C	-2.63983900	0.35325700	-3.51860400
H	-3.11340400	-0.63093300	-3.57721100

H	-3.12000500	0.99264000	-4.27610200
H	-1.59270700	0.23324700	-3.81268700
C	0.71018600	-2.36127100	-2.49157100
H	0.00638000	-1.55615000	-2.73324600
H	0.99908900	-2.84741600	-3.43431700
H	0.16332600	-3.09390600	-1.89380100
C	5.13754400	0.12134200	-1.56189500
H	4.87429200	1.04992100	-2.07342700
H	5.58158800	0.39303000	-0.59855300
H	5.91815900	-0.37416600	-2.15700900
C	-5.14511600	0.01225800	-1.53756700
H	-4.88118400	-0.88411800	-2.10320500
H	-5.59245600	-0.31721400	-0.59385300
H	-5.92394900	0.54394900	-2.10321900
C	-0.73768000	2.59526800	-2.29152300
H	-0.14013900	1.82692800	-2.79280100
H	-1.04525400	3.32346500	-3.05619400
H	-0.07848100	3.10697000	-1.58713600
C	2.11701700	-3.74973200	0.03846700
H	1.02772300	-3.77266100	0.14000300
H	2.41511000	-4.64546300	-0.52725700
H	2.53943200	-3.84198000	1.04402800
C	4.89411500	-2.21707200	0.53115400
H	5.64957300	-2.86051000	0.05906600
H	5.41372600	-1.33906600	0.92612000
H	4.48049000	-2.77251300	1.37791000
C	-4.89245700	2.17538400	0.73374800
H	-5.68201000	2.80595100	0.30202500
H	-5.36969600	1.26322300	1.10443600
H	-4.48256000	2.71385400	1.59305300
C	-2.11914700	3.74634500	0.34984900
H	-2.41830300	4.68577800	-0.13908100
H	-2.53483100	3.75708400	1.36240200
H	-1.02912300	3.75953600	0.44562300
C	-4.40406500	-0.39834100	3.69661100
H	-5.27188300	-0.26710700	3.04141800
H	-4.29662900	-1.46889000	3.90895400
H	-4.61417200	0.10165200	4.64894200
C	-1.90702200	-0.01324400	3.95984700
H	-1.02546700	0.44220600	3.50084400
H	-2.06424300	0.44441000	4.94457000
H	-1.70133800	-1.08048900	4.11055000
C	-3.21131500	-4.30436600	0.45384800
H	-2.74957300	-4.36686500	1.44518000
H	-4.28979100	-4.14899700	0.58408700
H	-3.06724100	-5.27623000	-0.03051100
C	-3.11211100	-3.31458400	-1.85695900
H	-2.65921800	-2.55231500	-2.49623400
H	-2.86628800	-4.29862400	-2.27330900
H	-4.20149500	-3.19275800	-1.88900600
C	4.40776600	0.01389200	3.71211700
H	5.26225000	-0.12026700	3.04066100
H	4.36031100	1.07262400	3.99472900
H	4.59674200	-0.55867400	4.62742600
C	1.89724700	-0.26078600	3.98063300
H	0.98783300	-0.63348300	3.50233400
H	2.04114000	-0.79964100	4.92543000
H	1.75019600	0.80091700	4.21584400
C	2.98787200	3.38902100	-1.61282700
H	2.44090200	2.66348400	-2.22013800
H	2.72955700	4.39697300	-1.95796800
H	4.06193000	3.23724700	-1.77330200
C	3.42650800	4.21897800	0.72247000

H	3.09751000	4.23972500	1.76695900
H	4.49776000	3.98331500	0.70352800
H	3.29425400	5.23096600	0.32388100

NbN_P^{cis}(C4)

Coordinates (Angstroms)			
	X	Y	Z
C	-1.76488900	4.03326100	0.16838800
C	-4.72486000	2.79323900	0.46396800
C	3.20080800	2.47833500	-2.39365900
C	5.01086700	2.97319600	-0.74188900
C	-1.52692800	1.38995700	3.14012700
C	-2.35594200	2.91370300	-0.64334200
C	-3.98265100	0.95375300	3.47375000
C	-3.68245100	2.39242900	-0.53958100
C	3.52259200	2.60028200	-0.90209500
C	-2.65687200	0.37695300	2.94066300
C	3.18781600	2.53224700	2.04172400
C	-1.77641600	2.35771600	-1.83835400
C	-3.91338600	1.50722600	-1.62228900
C	-0.50144700	2.82361900	-2.48221700
C	-5.22779100	0.83632700	-1.90439000
C	-2.73790100	1.46657700	-2.44436800
C	3.08817400	1.28776000	1.13765000
C	2.63634900	-0.90150000	-3.83489800
C	-3.08832300	-1.28688300	1.13855200
C	-2.63566000	0.89916400	-3.83563800
C	-3.18819700	-2.53064200	2.04359400
C	5.22797500	-0.83792500	-1.90305900
C	2.65736100	-0.37502000	2.94093000
C	2.73812900	-1.46808500	-2.44325700
C	3.91342600	-1.50851900	-1.62087200
C	3.98378000	-0.95006700	3.47435700
C	0.50147800	-2.82475000	-2.48099600
C	1.77637500	-2.35879000	-1.83703800
C	-5.01111400	-2.97351000	-0.73990000
C	1.52854700	-1.38915500	3.14103600
C	-3.52278000	-2.60088700	-0.90022500
C	3.68208400	-2.39319800	-0.53780700
C	-3.20081600	-2.48022200	-2.39186000
C	2.35551000	-2.91428300	-0.64162000
C	4.72410800	-2.79379100	0.46621800
C	1.76398200	-4.03324800	0.17057700
H	-1.96260500	5.00982800	-0.29947500
H	-2.18185700	4.06950800	1.17938100
H	-5.45366300	3.47576600	0.00372400
H	-4.28821700	3.31723700	1.31816400
H	3.29971600	3.45639800	-2.87978800
H	5.23440600	3.90477000	-1.27659900
H	-0.67977500	3.93246800	0.26443500
H	-1.72253700	2.30800600	2.57817700
H	-1.43712600	1.64893200	4.20258800
H	-4.19964700	1.91970300	3.01137000
H	-3.92145200	1.10573700	4.55904500
H	-5.28158700	1.93197800	0.84595900
H	2.91192200	3.43287300	-0.51578200

H	2.18656400	2.10846800	-2.54955600
H	3.47090300	3.34845800	1.37650300
H	5.30037900	3.10981800	0.30463600
H	3.89441200	1.78931900	-2.88471100
H	5.63988600	2.17942300	-1.15927100
H	-0.57249900	0.98866900	2.79247200
H	-0.69287700	3.67956900	-3.14626500
H	-4.82537100	0.28649100	3.27049000
H	-5.93988100	1.55170900	-2.34083300
H	0.23562700	3.13446700	-1.73816600
H	-2.41154000	-0.49591400	3.55580800
H	-5.68249900	0.43415200	-0.99360400
H	-0.04085600	2.03788100	-3.08878900
H	3.27554300	-0.02550300	-3.96810300
H	1.61282700	-0.59864200	-4.07904700
H	-5.12095900	0.01137900	-2.61261700
H	-2.94018100	1.64432000	-4.58671500
H	5.12130200	-0.01310700	-2.61146500
H	2.41110600	0.49797100	3.55553300
H	2.94060900	-1.64728800	-4.58545200
H	5.68273500	-0.43560100	-0.99236500
H	-3.27439300	0.02275500	-3.96837000
H	4.82579500	-0.28210000	3.27051300
H	-1.61195000	0.59667300	-4.07944800
H	0.04092600	-2.03906800	-3.08767400
H	5.93995800	-1.55352300	-2.33932400
H	-3.47121400	-3.34739100	1.37899900
H	-5.30078000	-3.10922400	0.30670000
H	-5.64000300	-2.18003300	-1.15803500
H	0.57364000	-0.98915900	2.79320400
H	3.92284100	-1.10130600	4.55977000
H	-0.23565500	-3.13556400	-1.73699300
H	4.20171100	-1.91612700	3.01266200
H	-3.89434000	-1.79161000	-2.88358700
H	1.43909300	-1.64762900	4.20364700
H	5.28172800	-1.93259800	0.84704300
H	-2.91226100	-3.43324600	-0.51318000
H	0.69299100	-3.68074900	-3.14495800
H	-2.18653600	-2.11055800	-2.54799900
H	1.72520200	-2.30729500	2.57959400
H	-5.23467000	-3.90551200	-1.27385500
H	0.67889900	-3.93199200	0.26648800
H	4.28693100	-3.31618900	1.32112100
H	-3.29973000	-3.45869800	-2.87715700
H	5.45218800	-3.47767900	0.00684800
H	2.18085100	-4.06919400	1.18162200
H	1.96137800	-5.01009900	-0.29682500
N	3.20087400	1.35829400	-0.19142300
N	-2.75274100	-0.03748600	1.53710600
N	0.12431300	0.65810600	-0.19471900
N	2.75278200	0.03858700	1.53709600
N	-3.20096700	-1.35838600	-0.19047200
N	-0.12432100	-0.65830600	-0.19425600
Nb	1.89892900	-0.50348500	-0.40077100
Nb	-1.89892800	0.50317500	-0.40114500
C	4.28948300	2.48561400	3.11888000
H	4.04988700	1.81215500	3.94517500
H	5.25184600	2.17433200	2.69719800
H	4.42038100	3.48906500	3.54185000
C	1.82119700	2.94201600	2.62905000
H	1.47083400	2.25755300	3.40623400
H	1.90197700	3.93911900	3.07932700
H	1.05392000	2.97658200	1.85002400

C	-1.82172700	-2.94002200	2.63154900
H	-1.47144900	-2.25495300	3.40824600
H	-1.90267500	-3.93674600	3.08263400
H	-1.05430900	-2.97531000	1.85269500
C	-4.29010100	-2.48292200	3.12045000
H	-4.05068000	-1.80866900	3.94614900
H	-5.25233600	-2.17198600	2.69821900
H	-4.42116400	-3.48595200	3.54436500

WN_P^{cis}(C4)

	Coordinates (Angstroms)		
	X	Y	Z
C	-1.89722400	-0.73860700	-3.61873500
C	-4.65929700	0.49393300	-2.50626100
C	2.65859600	-0.98989900	-3.35730000
C	4.51276500	0.72292900	-3.38518100
C	-1.05058700	2.62753000	-2.24087800
C	-2.53846800	-1.02199300	-2.28845800
C	-3.08871300	3.86507700	-1.42076800
C	-3.82231800	-0.55779600	-1.83754200
C	3.06103500	0.43190800	-2.96356600
C	-1.86627400	3.02398500	-1.00899800
C	2.76588400	3.16983400	-1.83827700
C	-2.13828400	-2.11651900	-1.40330600
C	-4.17221300	-1.24988200	-0.66198200
C	-1.07787400	-3.13659800	-1.71634700
C	-5.44421200	-1.05831300	0.11238100
C	-3.13304600	-2.21358700	-0.34849100
C	2.63652900	1.89106900	-1.03830200
C	3.27144200	-3.38067600	-0.59318500
C	-2.63657000	1.89099300	1.03839700
C	-3.27132200	-3.38079700	0.59288800
C	-2.76588400	3.16970000	1.83847000
C	5.44426100	-1.05822500	-0.11229100
C	1.86629200	3.02392200	1.00919500
C	3.13307400	-2.21356300	0.34830300
C	4.17221600	-1.24988300	0.66197100
C	3.08874200	3.86500600	1.42094800
C	1.07786400	-3.13677300	1.71597300
C	2.13826700	-2.11663700	1.40309400
C	-4.51274000	0.72263300	3.38525000
C	1.05067200	2.62738000	2.24109200
C	-3.06099300	0.43175200	2.96359600
C	3.82226200	-0.55796000	1.83760900
C	-2.65841800	-0.99002400	3.35730300
C	2.53838600	-1.02220400	2.28838600
C	4.65921900	0.49366500	2.50652100
C	1.89703500	-0.73895400	3.61864000
H	-2.13807000	-1.52719500	-4.34736700
H	-2.24068400	0.20926200	-4.04382900
H	-5.38657300	0.03091400	-3.18813700
H	-4.05080800	1.18114500	-3.10048900
H	2.72992200	-1.10922700	-4.44508000
H	4.63365100	0.58417500	-4.46663300
H	-0.80753900	-0.68834400	-3.53348500
H	-1.66443000	2.06216900	-2.94812100

H	-0.68314100	3.52642300	-2.75093800
H	-3.74550100	3.28737700	-2.07907600
H	-2.77042300	4.76601600	-1.95983200
H	-5.22511000	1.08812800	-1.78168700
H	2.40696800	1.10774900	-3.53712200
H	1.63347700	-1.20308100	-3.04336100
H	2.50355600	3.01270900	-2.88682700
H	4.81068000	1.74904400	-3.14482300
H	3.31505000	-1.72889300	-2.89024400
H	5.20484000	0.04562100	-2.87455200
H	-0.20342400	1.99709000	-1.96029200
H	-1.43172900	-3.84886600	-2.47612300
H	-3.67828800	4.18533600	-0.55558700
H	-6.27912200	-1.58206000	-0.37427700
H	-0.16351700	-2.66609600	-2.08914800
H	2.12304700	3.95722300	-1.43988600
H	3.79895600	3.53534100	-1.80868200
H	-1.21509800	3.66241700	-0.38870300
H	-5.72004300	-0.00195500	0.19294700
H	-0.80778400	-3.71241300	-0.82622000
H	3.93030800	-3.15132900	-1.43551000
H	2.30535300	-3.68404500	-1.00742900
H	-5.35925500	-1.45567500	1.12696200
H	-3.69949200	-4.25246900	0.07506900
H	5.35933000	-1.45536100	-1.12696200
H	-3.79893400	3.53526800	1.80886200
H	1.21508000	3.66238600	0.38897200
H	-2.12298500	3.95708200	1.44016600
H	3.69961600	-4.25238400	-0.07542800
H	5.72016300	-0.00186700	-0.19261300
H	-3.93014700	-3.15155900	1.43527300
H	3.67827100	4.18530800	0.55575100
H	-2.30519800	-3.68417200	1.00704600
H	0.80787000	-3.71253100	0.82578000
H	6.27911300	-1.58213300	0.37429200
H	-2.50360600	3.01247400	2.88701800
H	-4.81074800	1.74873500	3.14495500
H	-5.20475900	0.04529100	2.87459200
H	0.20351300	1.99693200	1.96051300
H	2.77046800	4.76591900	1.96006700
H	0.16345800	-2.66632800	2.08873100
H	3.74556600	3.28728300	2.07919800
H	-3.31483800	-1.72906500	2.89027700
H	0.68322700	3.52623600	2.75121700
H	5.22501900	1.08800300	1.78205500
H	-2.40696500	1.10763900	3.53714400
H	1.43167600	-3.84908600	2.47572600
H	-1.63329500	-1.20312200	3.04331700
H	1.66456100	2.06199700	2.94827800
H	-4.63359800	0.58380900	4.46669700
H	0.80735400	-0.68873900	3.53331200
H	4.05071700	1.18075400	3.10087700
H	-2.72968600	-1.10936200	4.44508500
H	5.38650500	0.03053400	3.18830900
H	2.24041500	0.20889800	4.04383700
H	2.13786600	-1.52759000	4.34722600
N	2.84401500	0.66293800	-1.52974000
N	-2.24004900	1.83575600	-0.23883100
N	0.22637600	-0.37741900	-0.69542600
N	2.24003900	1.83574500	0.23893300
N	-2.84403100	0.66283200	1.52976900
N	-0.22639800	-0.37746400	0.69539700
W	1.87981600	-0.30797100	0.18627600

W	-1.87983100	-0.30796200	-0.18631200
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MoN_p^{cis}(C4)

	Coordinates (Angstroms)		
	X	Y	Z
C	2.01042300	-0.83397000	3.65799200
C	4.71438600	0.45383900	2.44869100
C	-2.57495500	-1.01029600	3.38027900
C	-4.41181000	0.71656700	3.46348700
C	1.08663500	2.57828000	2.26071200
C	2.63737300	-1.13319100	2.32440500
C	3.10224400	3.83402400	1.41257700
C	3.87463300	-0.61981600	1.81963500
C	-2.97562500	0.41549800	2.99585600
C	1.87813400	2.98718700	1.01614600
C	-2.70905400	3.13963500	1.84577900
C	2.22611400	-2.21796700	1.44957600
C	4.19543100	-1.30859200	0.62601100
C	1.13512700	-3.20785900	1.75370700
C	5.43368600	-1.08575800	-0.19357900
C	3.18410500	-2.30980500	0.37725900
C	-2.60136800	1.85426700	1.04804700
C	-3.27911200	-3.44491200	0.60596800
C	2.60140300	1.85425300	-1.04788700
C	3.27898300	-3.44486000	-0.60629000
C	2.70900600	3.13966900	-1.84555300
C	-5.43395200	-1.08602300	0.19327100
C	-1.87806100	2.98730900	-1.01592000
C	-3.18419000	-2.30976600	-0.37747100
C	-4.19557000	-1.30858900	-0.62620200
C	-3.10213600	3.83420900	-1.41232800
C	-1.13505200	-3.20753400	-1.75390500
C	-2.22610200	-2.21774100	-1.44968500
C	4.41183900	0.71675600	-3.46341600
C	-1.08657000	2.57841600	-2.26050100
C	2.97566700	0.41560600	-2.99578700
C	-3.87476900	-0.61974100	-1.81977700
C	2.57512700	-1.01021800	-3.38023800
C	-2.63733800	-1.13285700	-2.32438500
C	-4.71463500	0.45375800	-2.44894900
C	-2.01018000	-0.83332300	-3.65779800
H	2.29530600	-1.59249500	4.40224300
H	2.32621200	0.13731200	4.04920100
H	5.51172300	0.01256200	3.06360400
H	4.12376300	1.10396500	3.09983200
H	-2.60084900	-1.12655700	4.47049500
H	-4.50310500	0.57307600	4.54746800
H	0.91802500	-0.82715000	3.59632200
H	1.71443400	2.00092300	2.94651700
H	0.73134200	3.46987300	2.79173800
H	3.77412300	3.25478300	2.05430600
H	2.78935800	4.72976200	1.96366000
H	5.19503800	1.08474500	1.69444000
H	-2.29825100	1.08618600	3.54918800
H	-1.56720400	-1.23739000	3.02261000
H	-2.43422800	2.98674400	2.89168000

H	-4.70779200	1.74619200	3.23642700
H	-3.26159000	-1.74262100	2.94540500
H	-5.12318900	0.04715800	2.96854800
H	0.23087000	1.95467600	1.98984300
H	1.46106000	-3.92428900	2.52169600
H	3.67368300	4.16259000	0.53834600
H	6.30544600	-1.56032600	0.27882700
H	0.22897700	-2.71357300	2.11677700
H	-2.06540600	3.92053900	1.43567800
H	-3.73927700	3.51409400	1.82746800
H	1.21169300	3.62653000	0.41267600
H	5.65809200	-0.02057200	-0.30874900
H	0.86005300	-3.78226600	0.86409300
H	-3.88436700	-3.18087300	1.47730700
H	-2.29405400	-3.74938300	0.97223300
H	5.33328500	-1.51054200	-1.19551200
H	3.74629700	-4.32626800	-0.14201800
H	-5.33354400	-1.51078700	1.19520900
H	3.73923700	3.51410700	-1.82737500
H	-1.21160200	3.62660900	-0.41242300
H	2.06543400	3.92056000	-1.43531100
H	-3.74650700	-4.32624500	0.14163500
H	-5.65861800	-0.02088900	0.30842000
H	3.88428300	-3.18078100	-1.47758600
H	-3.67357100	4.16276500	-0.53809200
H	2.29391600	-3.74923200	-0.97261400
H	-0.86044000	-3.78248700	-0.86450100
H	-6.30556000	-1.56079200	-0.27921600
H	2.43401600	2.98684200	-2.89142200
H	4.70777800	1.74639800	-3.23639100
H	5.12324000	0.04738500	-2.96845400
H	-0.23081200	1.95479500	-1.98964500
H	-2.78920800	4.72995900	-1.96337000
H	-0.22869600	-2.71310700	-2.11628000
H	-3.77403000	3.25502500	-2.05408900
H	3.26186500	-1.74248100	-2.94541400
H	-0.73126500	3.47001400	-2.79151000
H	-5.19573200	1.08440200	-1.69476700
H	2.29823500	1.08625600	-3.54909700
H	-1.46069600	-3.92349300	-2.52245500
H	1.56741200	-1.23743500	-3.02254200
H	-1.71437200	2.00107500	-2.94632300
H	4.50314300	0.57323900	-4.54739200
H	-0.91779300	-0.82632000	-3.59591700
H	-4.12399400	1.10415700	-3.09980000
H	2.60099300	-1.12644700	-4.47045700
H	-5.51163000	0.01232800	-3.06419600
H	-2.32606900	0.13796300	-4.04892400
H	-2.29479000	-1.59179200	-4.40220900
N	-2.80537400	0.63413100	1.55687200
N	2.24562800	1.80375000	0.24056000
N	-0.21402000	-0.43140400	0.63911700
N	-2.24557100	1.80384100	-0.24039500
N	2.80541500	0.63415100	-1.55679400
N	0.21402600	-0.43135500	-0.63911600
Mo	-1.92516400	-0.35745500	-0.21991500
Mo	1.92516700	-0.35753400	0.21991600
