



Everything need to calculate a specific molecule should be in .mol file, since best for simplicity.



Problems arising in parsing molecule list  
(ie. html  $\rightarrow$  dat)

Be S

l which should be ( $B^l \Sigma^+$ )

HBr

missing superscript

( $1 \Sigma^+, 1 \underline{\pi}$ )

also need to deal with these double  
labels.

For BeS, a hard fix was put in parse-mol.

For HBr,

specifically in relabel routine



Following molecules not in NIST, but in disort.

HeH <sup>+</sup> (SET)	TiC	CS <sup>-</sup> (SET)	TiF
CH <sup>+</sup> (SET)	FeC		VF
ScH <sup>+</sup>	NiC	FeS	CoF
TiH <sup>+</sup>		CoS	
VH <sup>+</sup>	ScN	NiS	TiCl
CrH <sup>+</sup>	CrN	ZnS	VCl
MnH <sup>+</sup>			
FeH <sup>+</sup>	TiO <sup>+</sup>		CuSe (SET)
CoH <sup>+</sup>	ZrO <sup>+</sup>		
NiH <sup>+</sup>			
CuH <sup>+</sup>			

These have no states:

ScH	CN <sup>-</sup>	CoO	ClF
TiH		ZnO	CrF
VH	CS <sup>-</sup>	LaO	
FeH			AuSi
PdH	VN	Bo <sup>-</sup>	
			Vs
HS <sup>-</sup>		CrCl	
		CoCl	