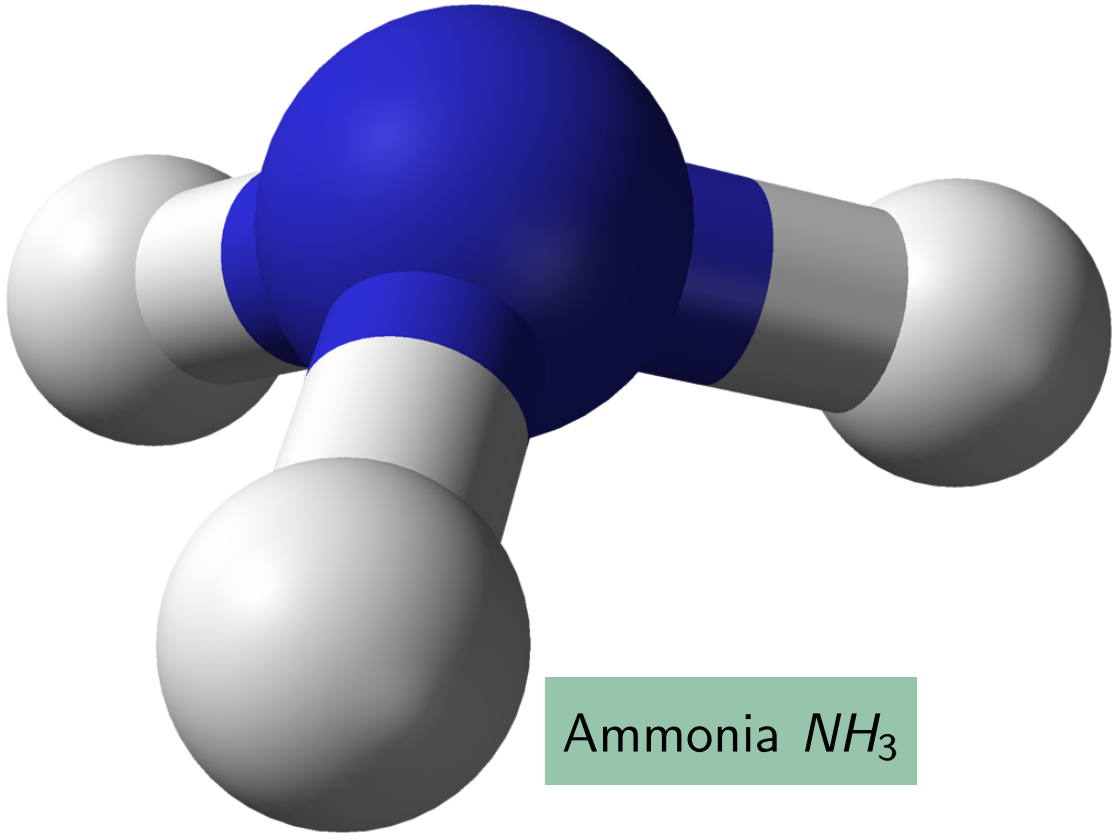
What is...chemical representation theory?

Or: Applications (rep theory in chemistry)

Symmetry groups of molecules

D_3 acts on



Ammonia NH_3

- Molecular symmetry describes the symmetry of molecules
- The main players are point set groups and their characters
- These can be used predict or explain many chemical properties

Characters of point set groups

D_3 :

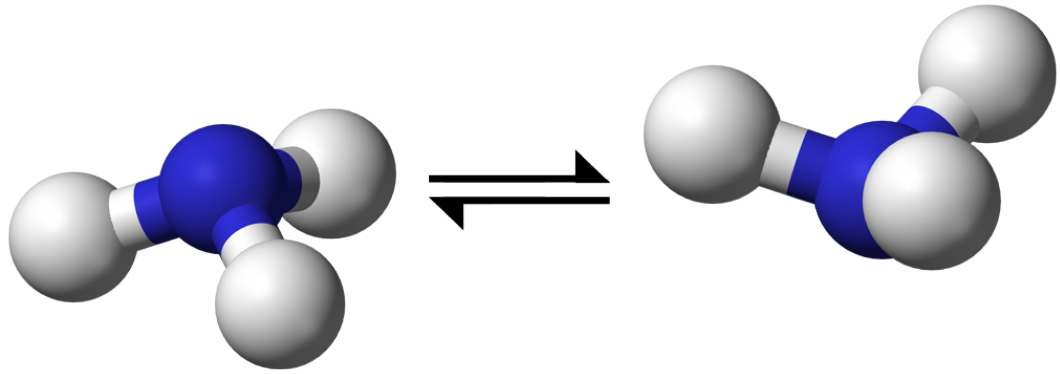
```
----------------
Class |   1  2  3
Size  |   1  3  2
Order |   1  2  3
----------------
p  =  2   1  1  3
p  =  3   1  2  1
----------------
X.1   +   1  1  1
X.2   +   1 -1  1
X.3   +   2  0 -1
```

C_{3v} :

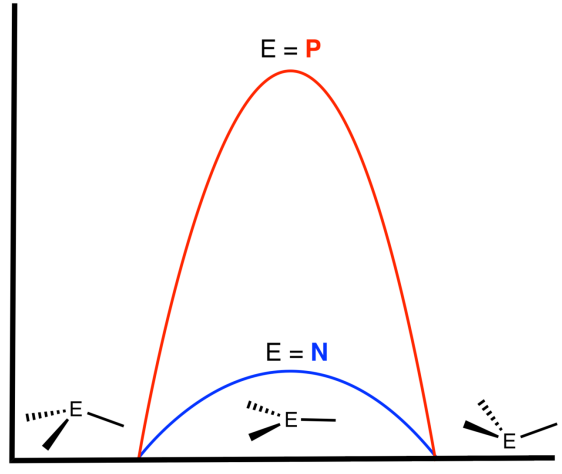
C_{3v}	$\hat{E}$	$2\hat{C}_3$ Rot	$3\hat{\sigma}_v$ Rfl	$\langle\chi\|\chi\rangle$
A_1	1	1	1	6
A_2	1	1	-1	6
E	2	-1	0	6
$\chi(1s)$	3	0	1	12
$\chi(\Delta\phi)$	3	0	-1	12

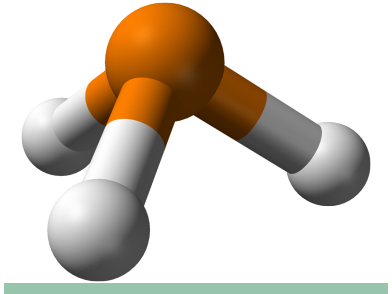
- Up to notation, chemist like the same character tables as rep theorists
- Example The character table for $D_3 = C_{3v}$ for ammonia

Predicting chemical behavior



Qualitative reaction for inversion of an amine and a phosphine : The y-axis is energy





Phosphine PH_3

- $1s$ and $\Delta\Phi$ both appear for molecules with D_3 symmetry
- We have $1s \cong A_1 \oplus E$ and $\Delta\Phi \cong A_2 \oplus E \Rightarrow$ should be related by reflection
- Indeed molecules such as ammonia show inverse phenomena

For completeness: A formal statement

Molecular symmetry group = group that leave the Hamiltonian invariant

(i) Space symmetries — We have seen these

(ii) Time symmetries

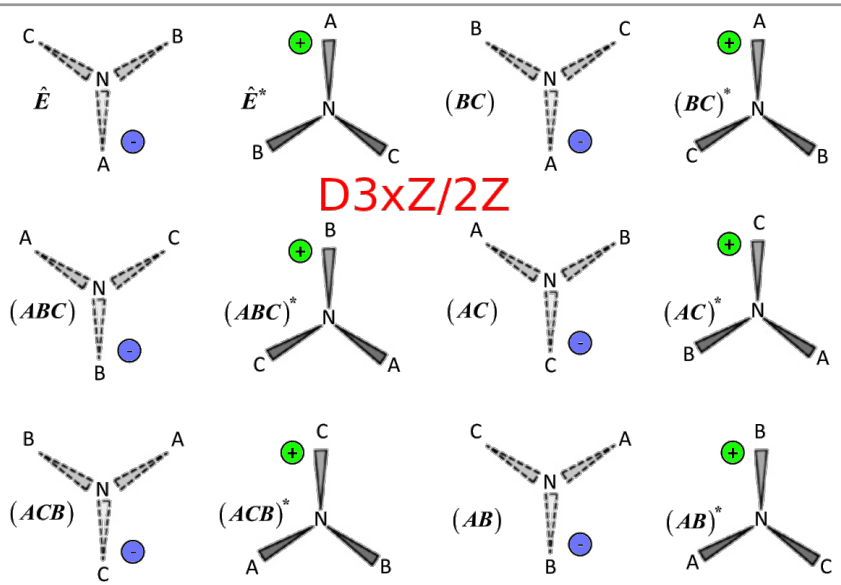
(iii) Permutational symmetry of a set of particles

Symmetry of the Hamiltonian $\leftrightsquigarrow$ chemical properties

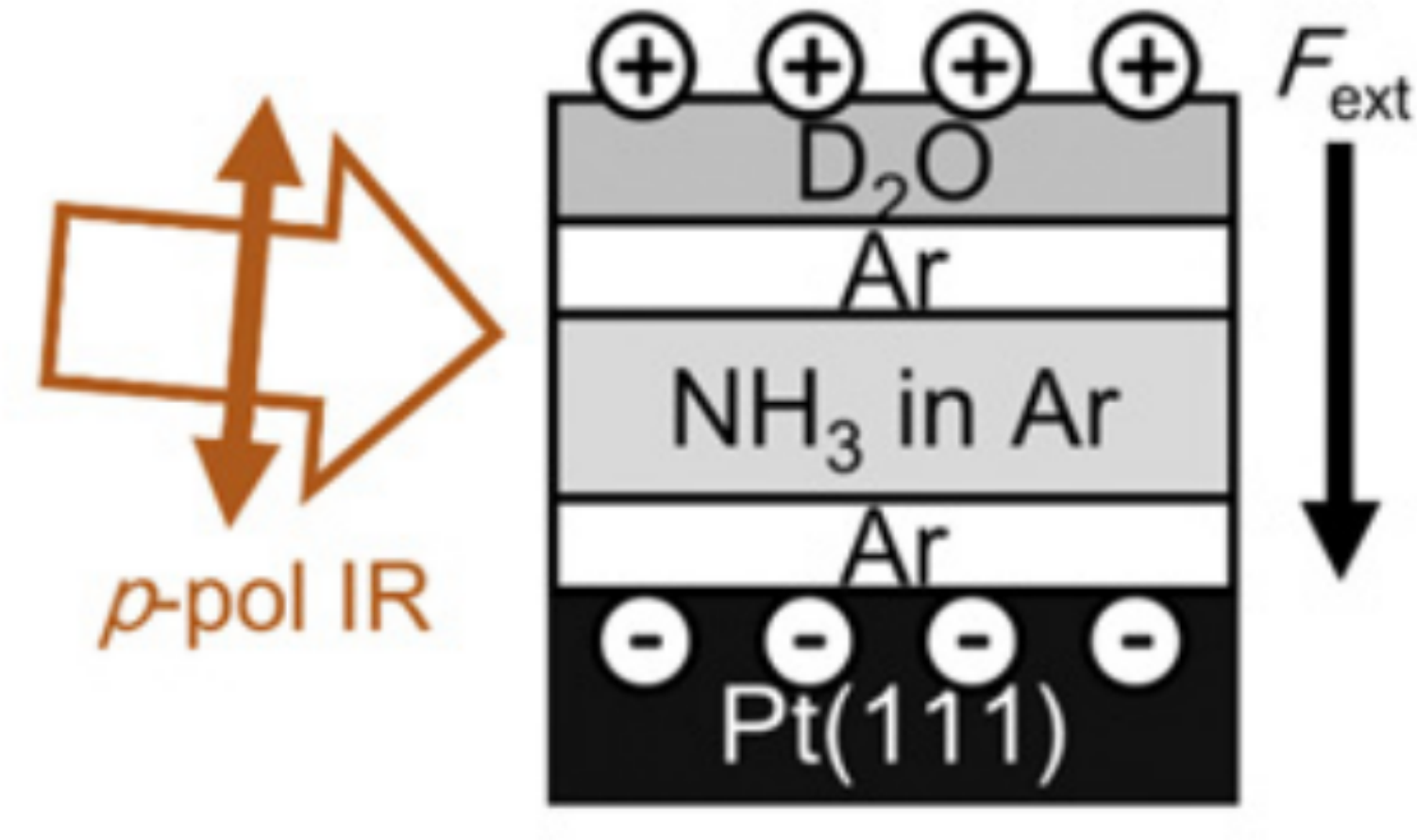
Linear symmetry $\leftrightsquigarrow$ representations

Rep theory in chemistry: put both together!

NH_3 :



Ammonia and Frobenius reciprocity



- $1s \cong A_1 \oplus E$ and $\Delta\Phi \cong A_2 \oplus E$ both restrict to the reg rep of $\mathbb{Z}/3\mathbb{Z} \subset D_3$
- Prediction Breaking the reflection symmetry of NH_3 stops it from turning out
- Experiment Put NH_3 in a magnetic field works!

Thank you for your attention!

I hope that was of some help.