Exploiting Multiple Symmetry-Broken SCF Solutions to Describe Ground and Excited States of Transition–Metal Complexes

Bang C. Huynh[1] Alex J. W. Thom[1]

[1]Department of Chemistry, University of Cambridge, United Kingdom

UNIVERSITY OF CAMBRIDGE

CAMBRIDGE COMMONWEALTH EUROPEAN AND INTERNATIONAL TRUST

Low-Lying UHF Solutions and NOCI Wavefunctions in Model Octahedral $[VF_6]^{3-}$

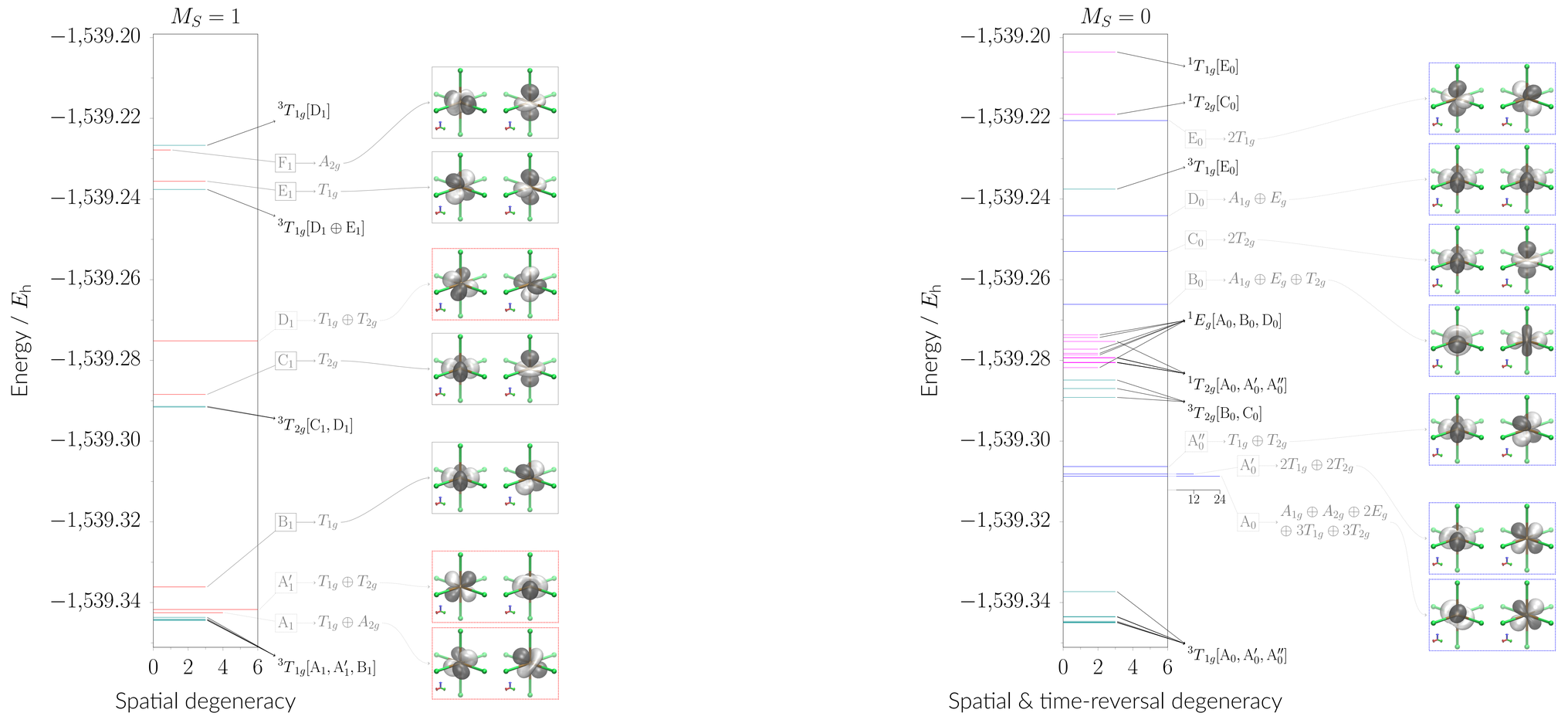

Figure 1. Energy and symmetry of low-lying UHF solutions and NOCI wavefunctions constructed from them in octahedral $[VF_6]^{3-}$. $\boxed{S_{M_S}}$: symmetry-conserved solution S with $\hat{S}_z$ eigenvalue M_S. S_{M_S}: spatial or spin symmetry-broken solution S with $\hat{S}_z$ eigenvalue M_S. $\Gamma[A \oplus B \oplus C]$: a specific NOCI set of symmetry Γ constructed from all of A, B, and C. $\Gamma[A, B, C]$: multiple NOCI sets of symmetry Γ constructed from all non-trivial combinations of A, B, and C.

Symmetry Breaking in SCF Methods

Nam vulputate nunc felis, non condimentum lacus porta ultrices. Nullam sed sagittis metus. Etiam consectetur gravida urna quis suscipit.

- **Mauris tempor** risus nulla, sed ornare
- **Libero tincidunt** a duis congue vitae
- **Dui ac pretium** morbi justo neque, ullamcorper

Eget augue porta, bibendum venenatis tortor.

A highlighted block

This block catches your eye, so **important stuff** should probably go here.

Curabitur eu libero vehicula, cursus est fringilla, luctus est. Morbi consectetur mauris quam, at finibus elit auctor ac. Aliquam erat volutpat. Aenean at nisl ut ex ullamcorper eleifend et eu augue. Aenean quis velit tristique odio convallis ultrices a ac odio.

- **Fusce dapibus tellus** vel tellus semper finibus. In consequat, nibh sed mattis luctus, augue diam fermentum lectus.
- **In euismod erat metus** non ex. Vestibulum luctus augue in mi condimentum, at sollicitudin lorem viverra.
- **Suspendisse vulputate** mauris vel placerat consectetur. Mauris semper, purus ac hendrerit molestie, elit mi dignissim odio, in suscipit felis sapien vel ex.

Aenean tincidunt risus eros, at gravida lorem sagittis vel. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae.

A block containing some math

Nullam non est elit. In eu ornare justo. Maecenas porttitor sodales lacus, ut cursus augue sodales ac.

$$\int_{-\infty}^{\infty} e^{-x^2}\,dx = \sqrt{\pi}$$

Interdum et malesuada fames $\{1, 4, 9, \ldots\}$ ac ante ipsum primis in faucibus. Cras eleifend dolor eu nulla suscipit suscipit. Sed lobortis non felis id vulputate.

A heading inside a block

Praesent consectetur mi $x^2 + y^2$ metus, nec vestibulum justo viverra nec. Proin eget nulla pretium, egestas magna aliquam, mollis neque. Vivamus dictum $\mathbf{u}^\intercal\mathbf{v}$ sagittis odio, vel porta erat congue sed. Maecenas ut dolor quis arcu auctor porttitor.

Another heading inside a block

Sed augue erat, scelerisque a purus ultricies, placerat porttitor neque. Donec $P(y \mid x)$ fermentum consectetur $\nabla_x P(y \mid x)$ sapien sagittis egestas. Duis eget leo euismod nunc viverra imperdiet nec id justo.

Nullam vel erat at velit convallis laoreet

Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos himenaeos. Phasellus libero enim, gravida sed erat sit amet, scelerisque congue diam. Fusce dapibus dui ut augue pulvinar iaculis.

First column	Second column	Third column	Fourth
Foo	13.37	384,394	α
Bar	2.17	1,392	β
Baz	3.14	83,742	δ
Qux	7.59	974	γ

Table 1. A table caption.

Donec quis posuere ligula. Nunc feugiat elit a mi malesuada consequat. Sed imperdiet augue ac nibh aliquet tristique. Aenean eu tortor vulputate, eleifend lorem in, dictum urna. Proin auctor ante in augue tincidunt tempor. Proin pellentesque vulputate odio, ac gravida nulla posuere efficitur. Aenean at velit vel dolor blandit molestie. Mauris laoreet commodo quam, non luctus nibh ullamcorper in. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per

https://www.ch.cam.ac.uk/person/cbh31 cbh31@cam.ac.uk