Here is a detailed **peer review** of the article entitled "**Electrical and Optical Properties of Molecules: A Comprehensive Theoretical and Computational Investigation**", authored by Richard Murdoch Montgo and submitted to the *Scottish Science Society* periodical. This review is crafted for a **mid-tier scientific periodical**, balancing accessibility with technical depth.

✦ General Assessment

Overall Recommendation: ✅ *Accept with Minor Revisions*

This article presents a comprehensive and didactically rich examination of the electrical and optical properties of molecules, focusing on polarisability, conductance, and photophysical behaviour from a theoretical and computational chemistry standpoint. It is well suited to an audience familiar with quant chemistry, and presents advanced concepts with pedagogical clarity, rigorous derivations, and illustrati figures.

✦ Strengths

1. Clarity and Depth of Theoretical Derivations

The article excels in its clear and rigorous presentation of foundational quantum mechanical concepts:

- The derivations of key equations such as the time-independent Schrödinger equation (Eq. 1), the Landauer formula for conductance (Eq. 6), the polarisability-conductance relationship (Eq. 8), and transition dipole moments (Eq. 10) are precise and well contextualised.
- Use of boxed derivations (e.g., for Eq. 6 and Eq. 8) effectively guides the reader through complex material.

2. Integration of Theory and Computation

- The author skilfully bridges theoretical foundations with computational methods, especially **density functional theory (DFT)** and **time-dependent DFT (TDDFT)**.
- The presentation of the **Casida equations** (Eq. 19) and vibrational coupling via the **Herzberg-Teller expansion** (Eq. 20) shows the author's fluency in contemporary quantum chemistry modelling.

3. Novel Insights and Interpretative Value

- The central thesis—an **inverse relationship between polarisability and conductance**—is both counterintuitive and well-argued. It is supported by empirical fits and theoretical reasoning (pp. 10
- The use of the **Clausius-Mossotti relation** to bridge microscopic polarisability and macroscopic dielectric constant is particularly insightful.

4. Figures and Visuals

- The article is visually rich, featuring well-annotated and highly informative figures:
  - *Figure 1 (p. 12)*: Shows empirical fit of polarisability vs conductance.
  - *Figure 2 & 3*: Link spectral features to electronic transitions and emission properties.
  - *Figure 4 (p. 21)*: Electronically annotated MO diagram provides a visually intuitive depiction of transitions.

✦ Weaknesses and Points for Revision

1. Stylistic Redundancy and Pedagogical Tone

While the article is commendably pedagogical, some passages are overly explanatory for an average periodical readership:

- **Example**: The detailed breakdown of the molecular Hamiltonian (p. 4–5) and polarisability derivatio 6–7) might be condensed or partially moved to supplementary material.
- The tone occasionally shifts from scholarly to didactic textbook style—acceptable but perhaps too expansive for some editorial lines.

Recommendation: Consider tightening some theoretical passages, focusing on the *novelty and implica* rather than fully re-deriving standard equations.

2. Data Limitations and Model Scope

- While *Figure 1* and *Table 1* demonstrate the polarisability-conductance trend, the number of molec studied appears limited. No specific molecular names or experimental methods are given for valida

Recommendation: Add a supplementary section with:

- Molecular identities used in the fit.
- Basis for the polarisability values (e.g., experimental vs DFT-predicted).
- Error bars or statistical treatment of G/G_0 variations.

3. TDDFT Functional Limitations

- The choice of CAM-B3LYP and aug-cc-pVDZ is sensible, but no justification is offered for avoiding popular functionals like ωB97X-D or basis sets like def2-TZVP.
- Likewise, the discussion does not address **known TDDFT failures** (e.g., charge-transfer states or multireference character).

Recommendation: Add a brief note acknowledging the scope and known limitations of CAM-B3LYP/au pVDZ for excited state predictions.

4. Referencing Style

- The reference list is adequate and draws on solid literature (Heath & Ratner, 2003; Mazinani et al., However, several key recent works (post-2020) are absent.
- The APA format is followed inconsistently (e.g., missing DOIs, page numbers).

Recommendation:

- Update the reference list to include more recent articles (e.g., post-2020 works on polarisability an machine learning).
- Ensure APA referencing is fully consistent throughout.

✦ Contribution to the Field

This article contributes meaningfully to the **ongoing discourse in molecular electronics and photophys** particularly by:

- Challenging established assumptions about π-conjugation and conductance.
- Providing a tractable and physically meaningful descriptor (α_iso) for predicting electrical behaviou
- Clarifying the quantum mechanical underpinnings of optical response and fluorescence.

The final sections (Discussion & Conclusion) are particularly effective in linking theory to real-world des principles for optoelectronic molecules.

✦ Final Verdict

Criterion	Evaluation
Originality	★★★★☆ (Strong theoretical synthesis)
Scientific Rigor	★★★★★ (Equational and analytical depth)
Clarity and Pedagogical Quality	★★★★☆ (Strong, sometimes excessive)
Relevance to Average Periodical	★★★★☆ (May require modest condensation)
Visual and Structural Presentation	★★★★★ (Clear and professional)

> ✅ **Accept with Minor Revisions**