

8330f16, Peer Review of A04 by _____ (authors' names)

| | Beginning, 1 | Developing, 2 | Accomplished, 3 | Exemplary, 4 | Score |
|---|--|--|---|--|--------------|
| Word File Organization Counts 0.5 | Serious problems with at least one key component (text, refs., Tables, Figs.). | Contains discussion, endnotes, 2 Tables & 2 Figs. Sequencing issues. Major issues with format. | Disc. followed by endnotes, 2 Tables & 2 Figs. Minor issues w/ page numbers or headers. | Disc. in sect.1, endnotes follow, sect. 2 with 2 Tables & 2 Figs. on separate pages. Formatted as requested. | /2 |
| Citation Counts 0.5 | More than 3 sources missing. Or more than 4 issues with citation or endnotes format. | Good sources, 2 missing. Or 3-4 issues with in-text citation or endnotes format. | Good sources; 1 missing. Or 1-2 issues with in-text citation or endnotes format. | Good sources & complete. Citation mark placement & endnotes format A-OK. | /2 |
| Structures Figure 1 Counts 0.5 | <u>At least two</u> str. correct. "Ball & Stick" models are shown. | <u>At least two</u> str. correct. "Ball & Stick", white BG. Perspective & align. issues. | <u>Three</u> str. correct. "Ball & Stick", white BG. Minor issues w/ arrangement. | <u>Three</u> str. correct. "Ball & Stick", 65%, white BG. Well oriented & aligned. | /2 |
| Tables Data | More than 6 data points are incorrect in number or unit. | At least 6 data points are incorrect in number or unit. | At least 3 data points are incorrect in number or unit. | All data given w/ correct units, appear fully correct. | /4 |
| Legends Tables & Figs. Counts 0.5 | Content of Tables and Figures remains unclear to a novice reader. | Content of Tables and Figures clearly described to a novice reader. | Legends "self-contained". Relevant params. (str., rel. E, MO # or eigenvalue) given. | "Self-contained". Relevant parameters given. Perfect format. | /2 |
| Theo. Level Discussion | TL effects correctly described for at least <u>one</u> of the three criteria. | TL effects correctly described for at least <u>two</u> of the three criteria. | TL effects on structures, rxn. and act. energies described. Transparent logic. | TL effects on structures, rxn. and act. energies described. Brief, concise, clear. | /4 |
| MOs in Figure 2 Counts 0.5 | At least <u>six</u> MOs are shown of formaldehyde. | <u>Eight</u> MOs of H ₂ CO are shown and labeled. | <u>Eight</u> MOs, organized by eigenvalue, labeled. Alignments OK. | <u>Ten</u> MOs w/ $\rho=0.004$, organized by eigenvalue, labeled. Perfect alignments. | /2 |
| Discussion of MOs Counts 0.5 | Correct explanations of <u>four</u> of the seven terms. | Correct explanations of <u>five</u> of the seven terms. | Correct explanations of <u>six</u> of the seven terms. | Correct explanation of 5 MO terms plus "full active space" & "fc approximation". | /2 |
| Total (Max. 20) | | | | | |

Constructive Comments (to guide the authors' revision):