

Table 1: Selected bond distances ( $\text{\AA}$ ) for the complex  $[\text{Et}_8\text{N}_4(\Delta)\text{Ni}]$ , experimentally synthesized, and the corresponding model system  $[\text{H}_8\text{N}_4(\Delta)\text{Ni}](\mathbf{6a})$ . For the numbering of the atoms, see Scheme 1.

| Parameter | Calculated | Experimental | Parameter | Calculated | Experimental |
|-----------|------------|--------------|-----------|------------|--------------|
| Ni-N1     | 1.877      | 1.849        | C5-C6     | 1.497      | 1.529        |
| Ni-N2     | 1.877      | 1.856        | C6-C7     | 1.392      | 1.368        |
| Ni-N3     | 1.906      | 1.870        | C7-C8     | 1.413      | 1.417        |
| Ni-N4     | 1.906      | 1.861        | C8-C9     | 1.395      | 1.381        |
| N1-C1     | 1.374      | 1.401        | C9-C10    | 1.489      | 1.526        |
| N1-C4     | 1.371      | 1.386        | C10-C11   | 1.481      | 1.476        |
| N2-C6     | 1.371      | 1.373        | C11-C12   | 1.450      | 1.450        |
| N2-C9     | 1.374      | 1.381        | C12-C13   | 1.362      | 1.338        |
| N3-C11    | 1.319      | 1.311        | C13-C14   | 1.459      | 1.463        |
| N3-C14    | 1.433      | 1.438        | C14-C15   | 1.492      | 1.527        |
| N4-C16    | 1.433      | 1.444        | C14-C16   | 1.614      | 1.567        |
| N4-C19    | 1.319      | 1.309        | C15-C16   | 1.492      | 1.521        |
| C1-C2     | 1.395      | 1.368        | C16-C17   | 1.459      | 1.467        |
| C1-C20    | 1.489      | 1.518        | C17-C18   | 1.362      | 1.304        |
| C2-C3     | 1.413      | 1.412        | C18-C19   | 1.450      | 1.474        |
| C3-C4     | 1.392      | 1.389        | C19-C20   | 1.481      | 1.504        |
| C4-C5     | 1.497      | 1.493        |           |            |              |
| C1-C19    | 2.537      | 2.541        | C4-C6     | 2.483      | 2.469        |
| C9-C11    | 2.537      | 2.507        | C14-C16   | 1.614      | 1.567        |