

Interactive 3D structure renders for:

Homochiral *vs.* heterochiral preference in chiral self-recognition of cyclic diols

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1 How to use

The interactive 3d structures of the 1-phenyl-*cis*-1,2-cyclohexanediol dimers can be enabled by clicking on them. Flash player is required. Online PDF viewers are often not capable of displaying the structures. If problems arise with other PDF viewers Adobe Acrobat always worked in our testing. By holding left click the render can be rotated, while the mouse-wheel can be used to zoom in and out (holding right click has the same effect). Holding the control key allows to move the structure within the render box. In the static images intermolecular OH \cdots O hydrogen bonds are highlighted by blue dotted lines and intramolecular ones by red dotted lines. Similar images of the most stable dimers of *trans*-cyclohexane-1,2-diol are available in the ESI of Ref. [1].

2 Homo dimers

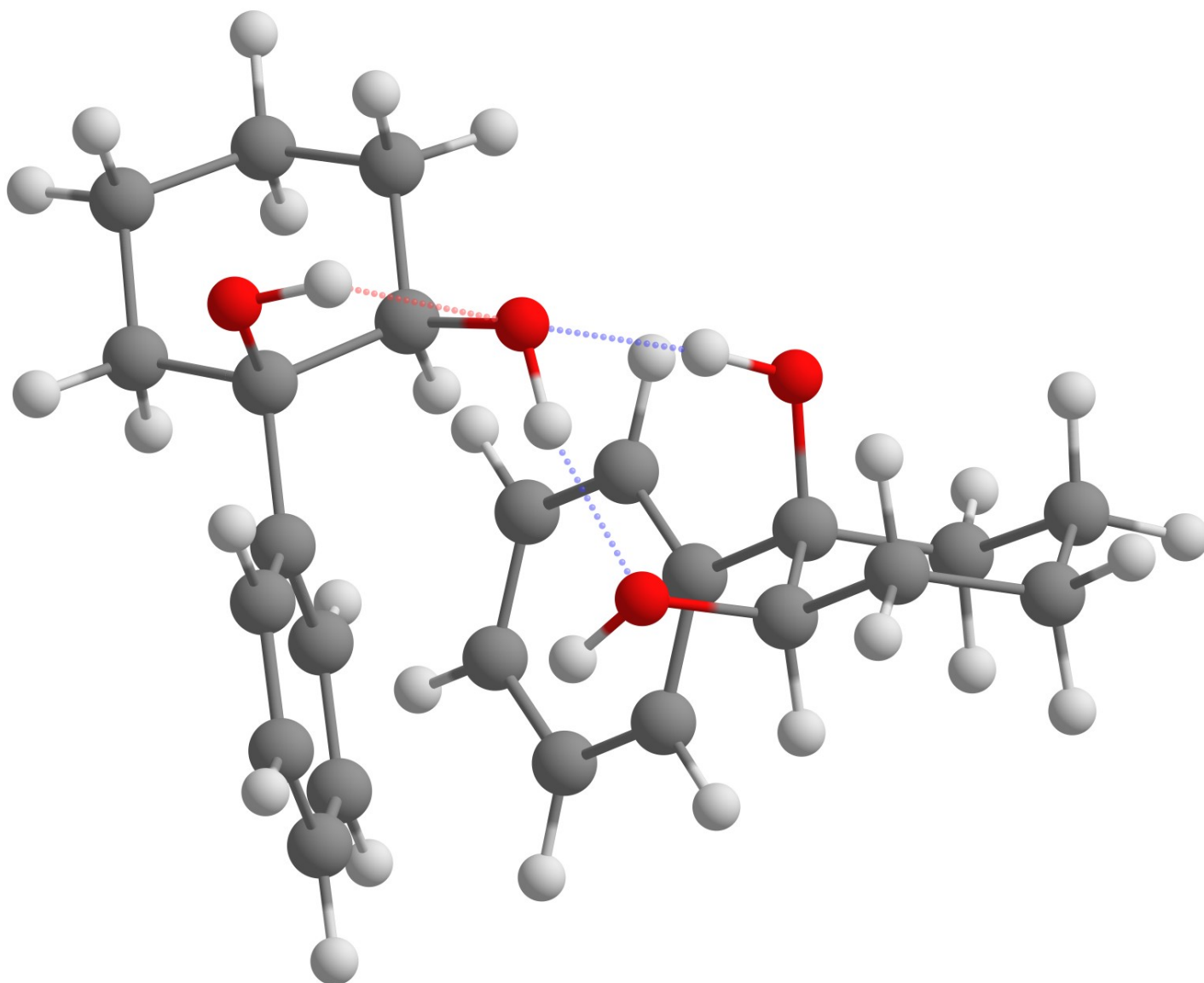


Fig. S1: Interactive 3d representation of the Insertion M_1+M_1 homo-dimer.

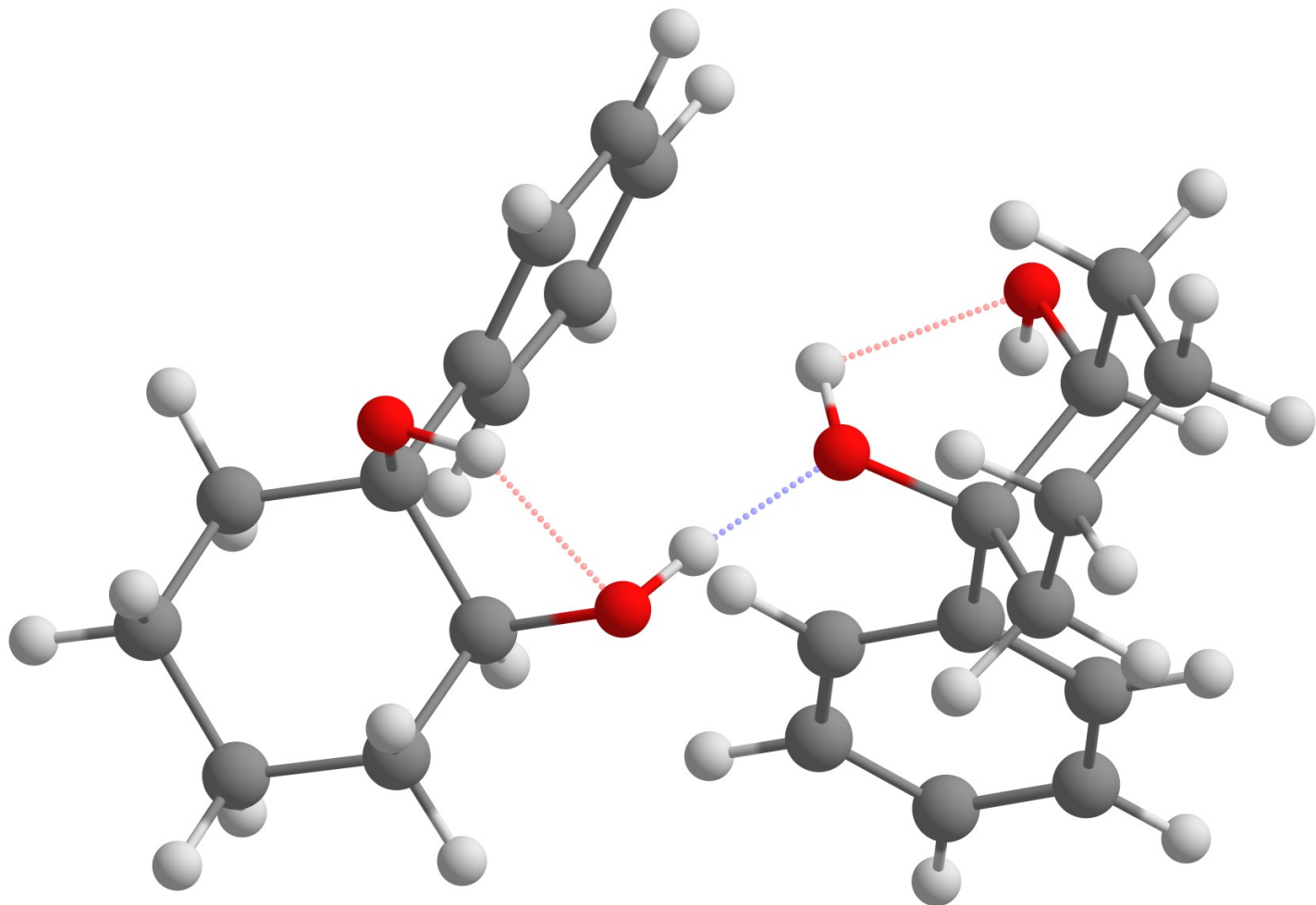


Fig. S2: Interactive 3d representation of the Addition $O_2H_2 \rightarrow O_1(M_1+M_1)$ homo-dimer.

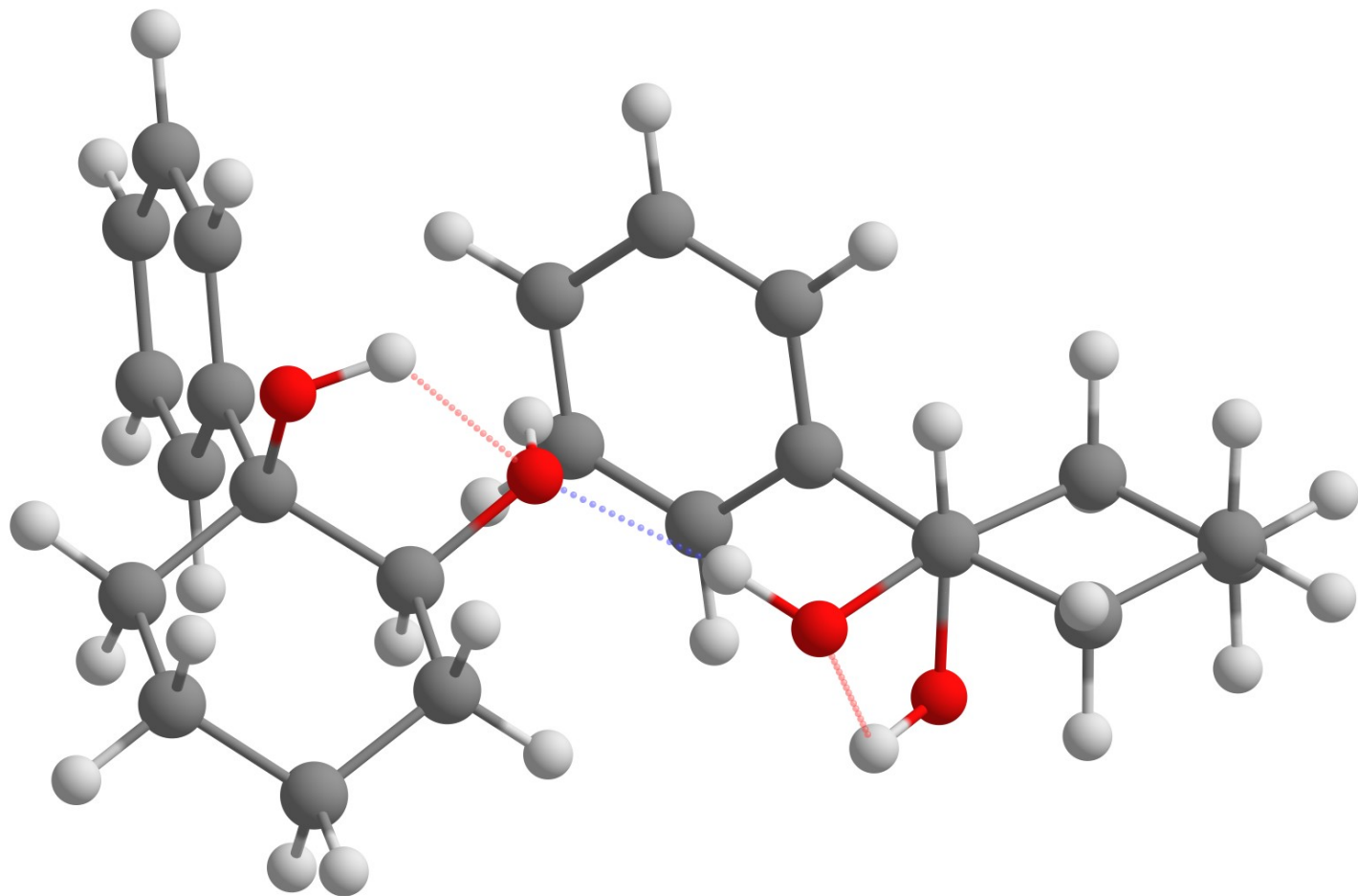


Fig. S3: Interactive 3d representation of the Addition $\text{O}_2\text{H}_2 \rightarrow \text{O}_2(\text{M}_1+\text{M}_1)$ homo-dimer.

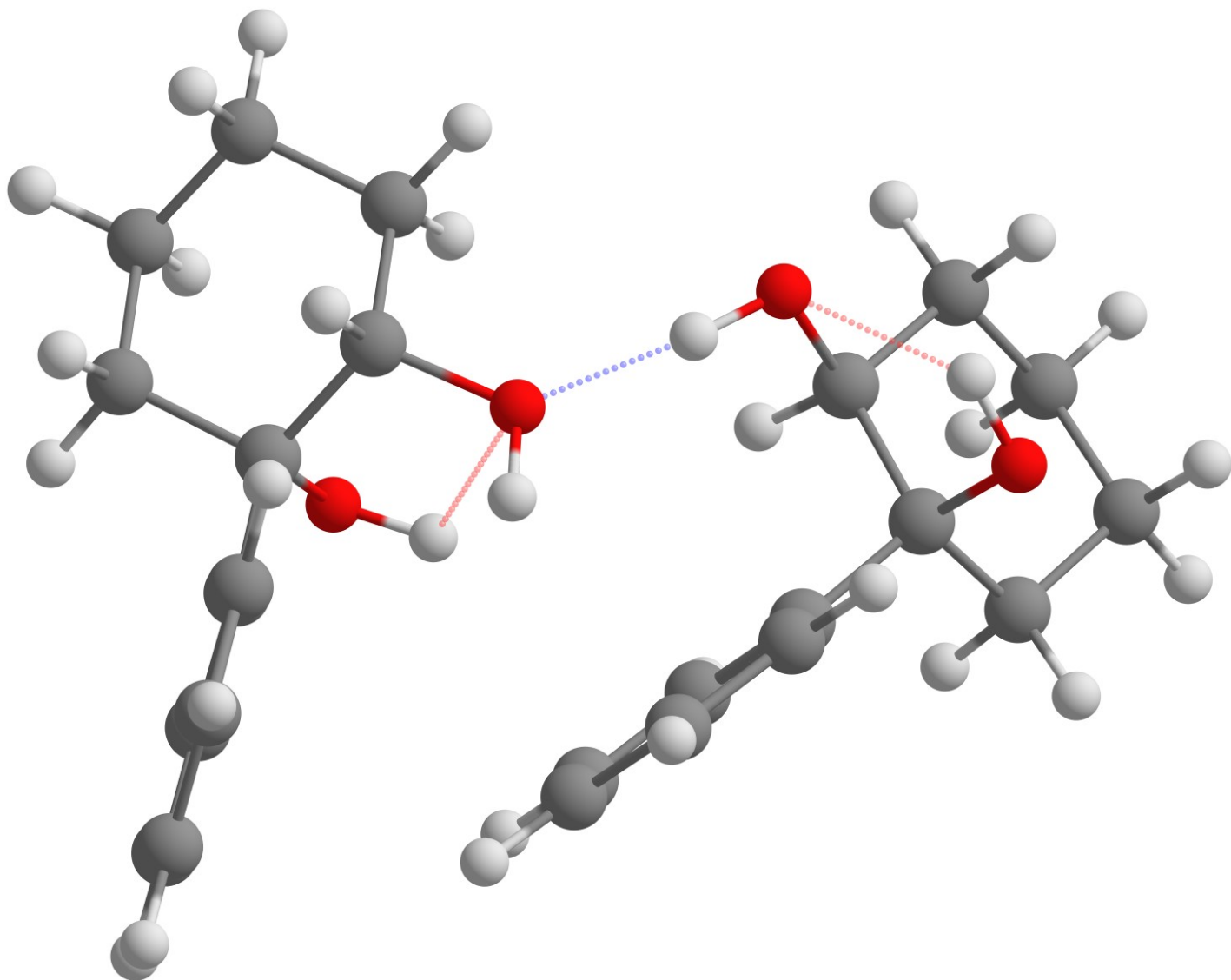


Fig. S4: Interactive 3d representation of the Addition $O_2H_2 \rightarrow O_2(M_1+M_1)$ a homo-dimer.

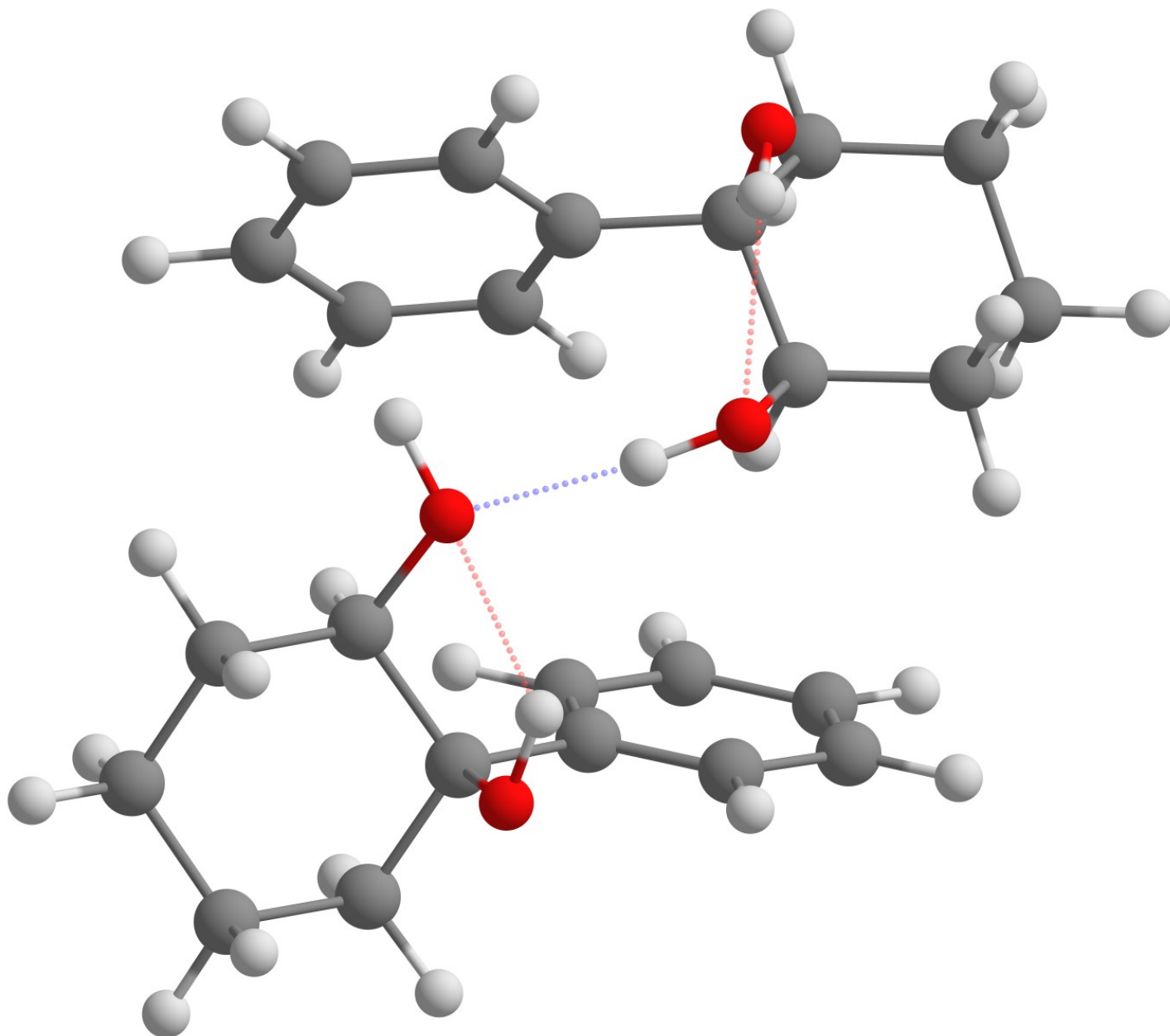


Fig. S5: Interactive 3d representation of the Addition $\text{O}_2\text{H}_2 \rightarrow \text{O}_2(\text{M}_1+\text{M}'_1)$ homo-dimer.

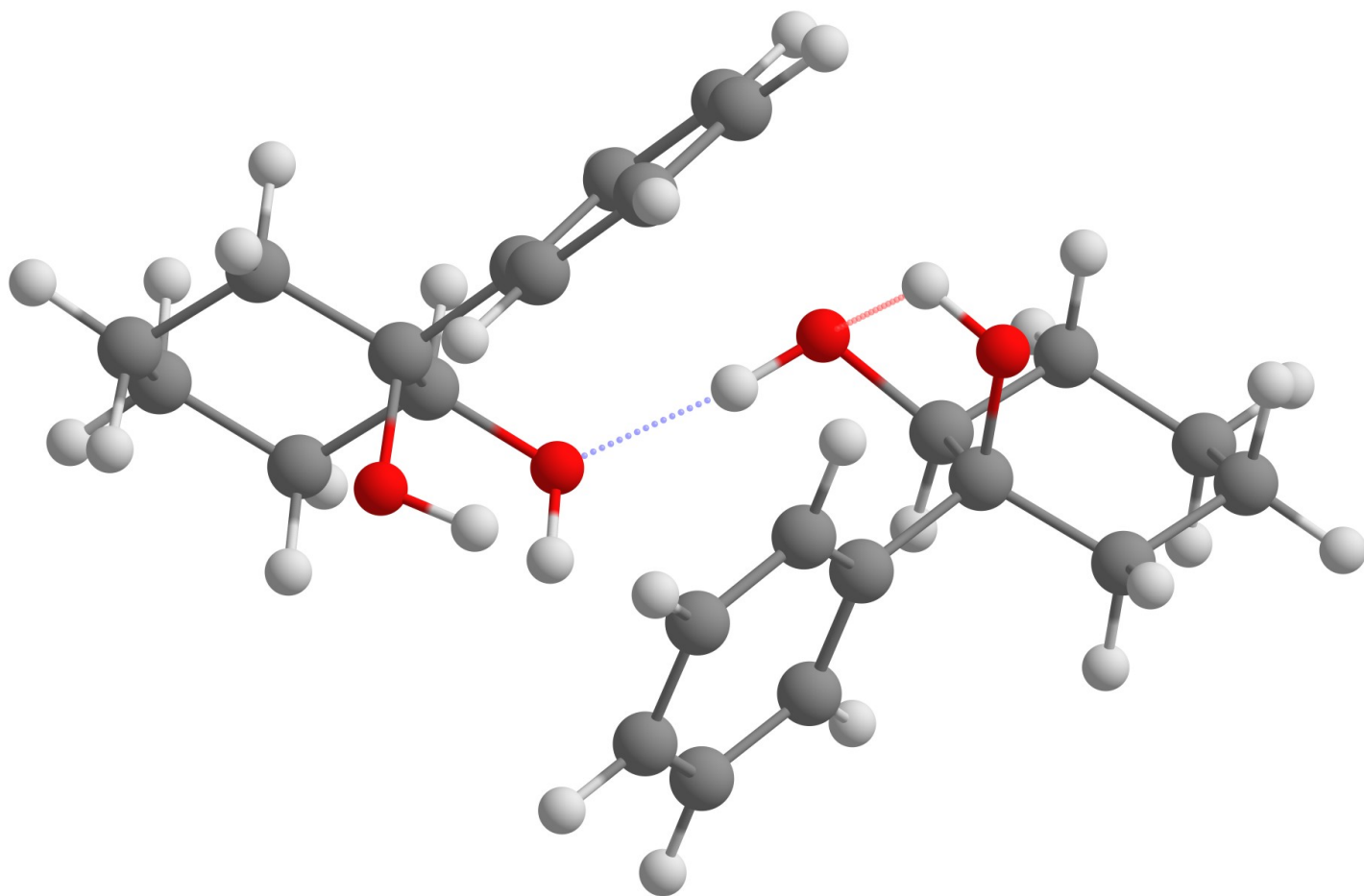


Fig. S6: Interactive 3d representation of the Addition $\text{O}_2\text{H}_2 \rightarrow \text{O}_2(\text{M}_1+\text{M}_2)$ homo-dimer.

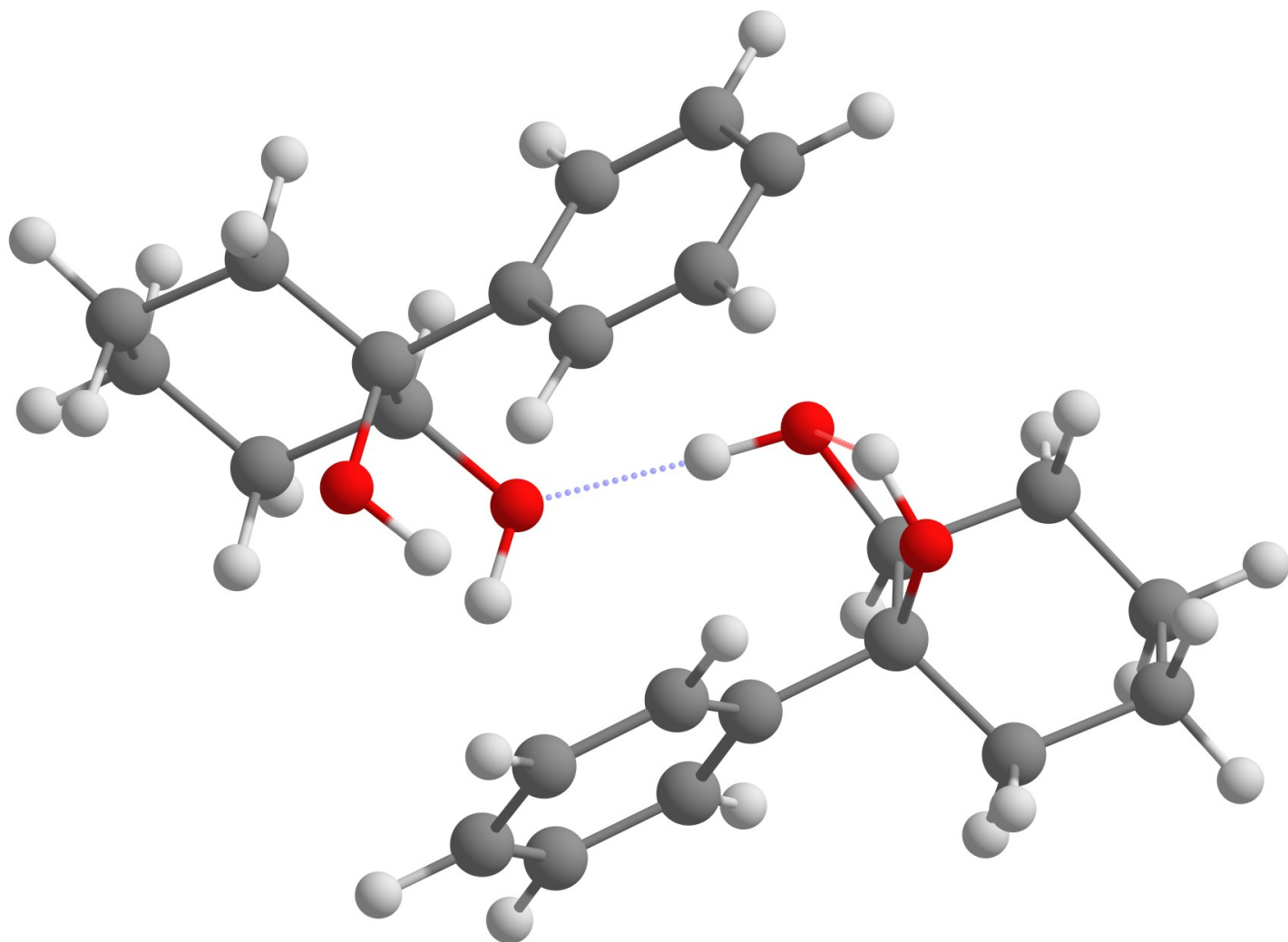


Fig. S7: Interactive 3d representation of the Addition $\text{O}_2\text{H}_2 \rightarrow \text{O}_2(\text{M}_1+\text{M}_2)$ a homo-dimer.

3 Hetero dimers

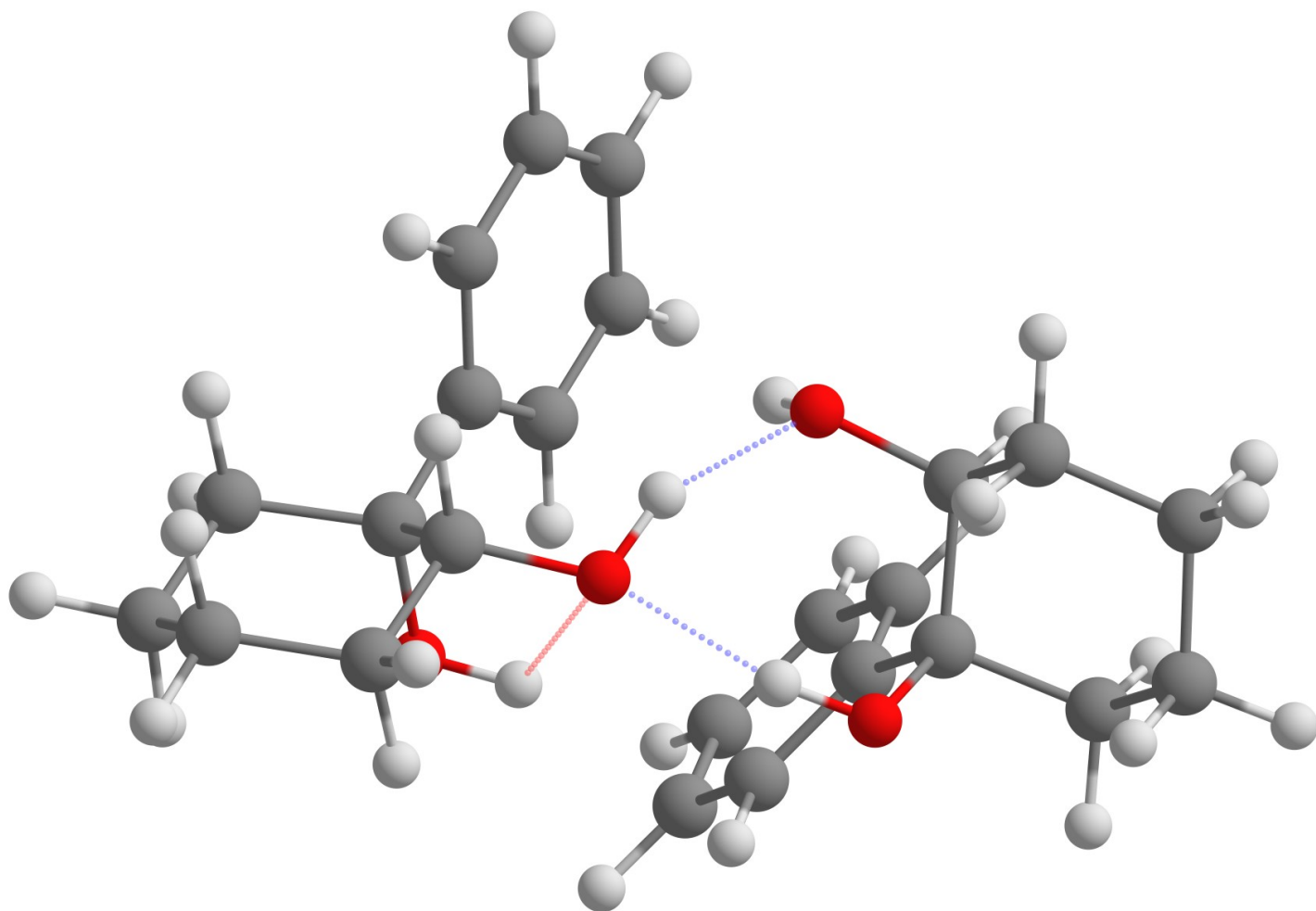


Fig. S8: Interactive 3d representation of the Insertion M_1+M_1 hetero-dimer.

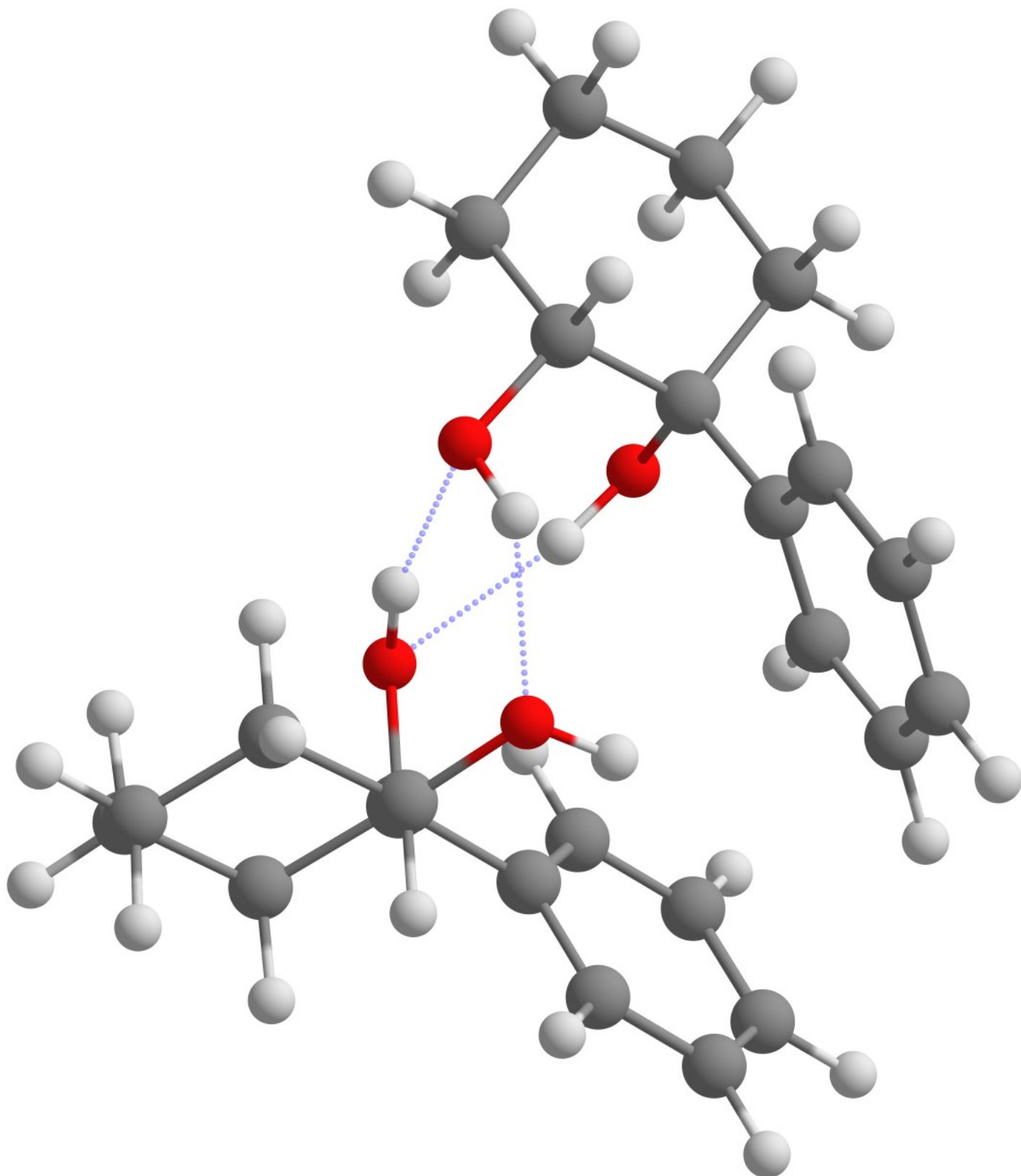


Fig. S9: Interactive 3d representation of the Double insertion hetero-dimer.

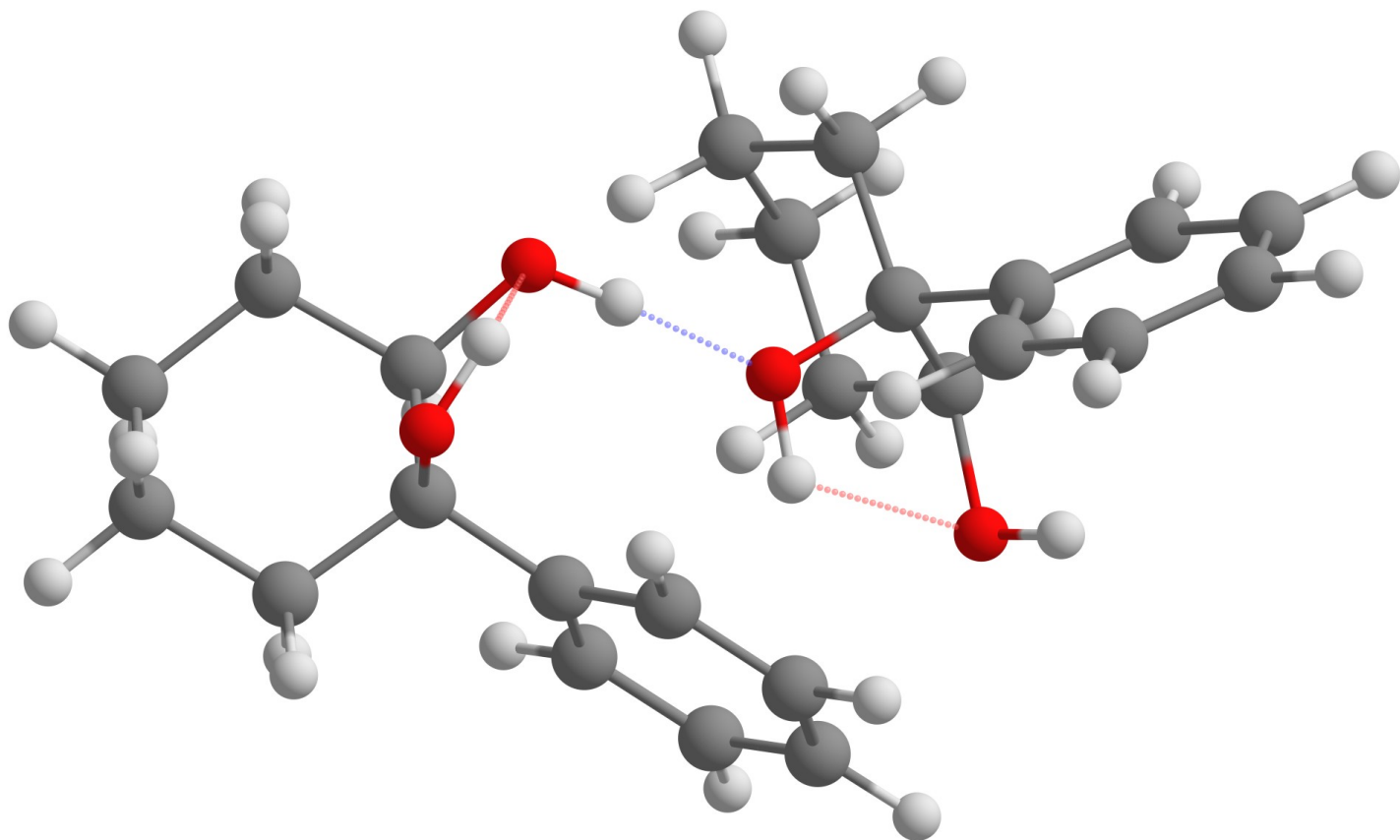


Fig. S10: Interactive 3d representation of the Addition $\text{O}_2\text{H}_2 \rightarrow \text{O}_1(\text{M}_1+\text{M}_1)$ hetero-dimer.

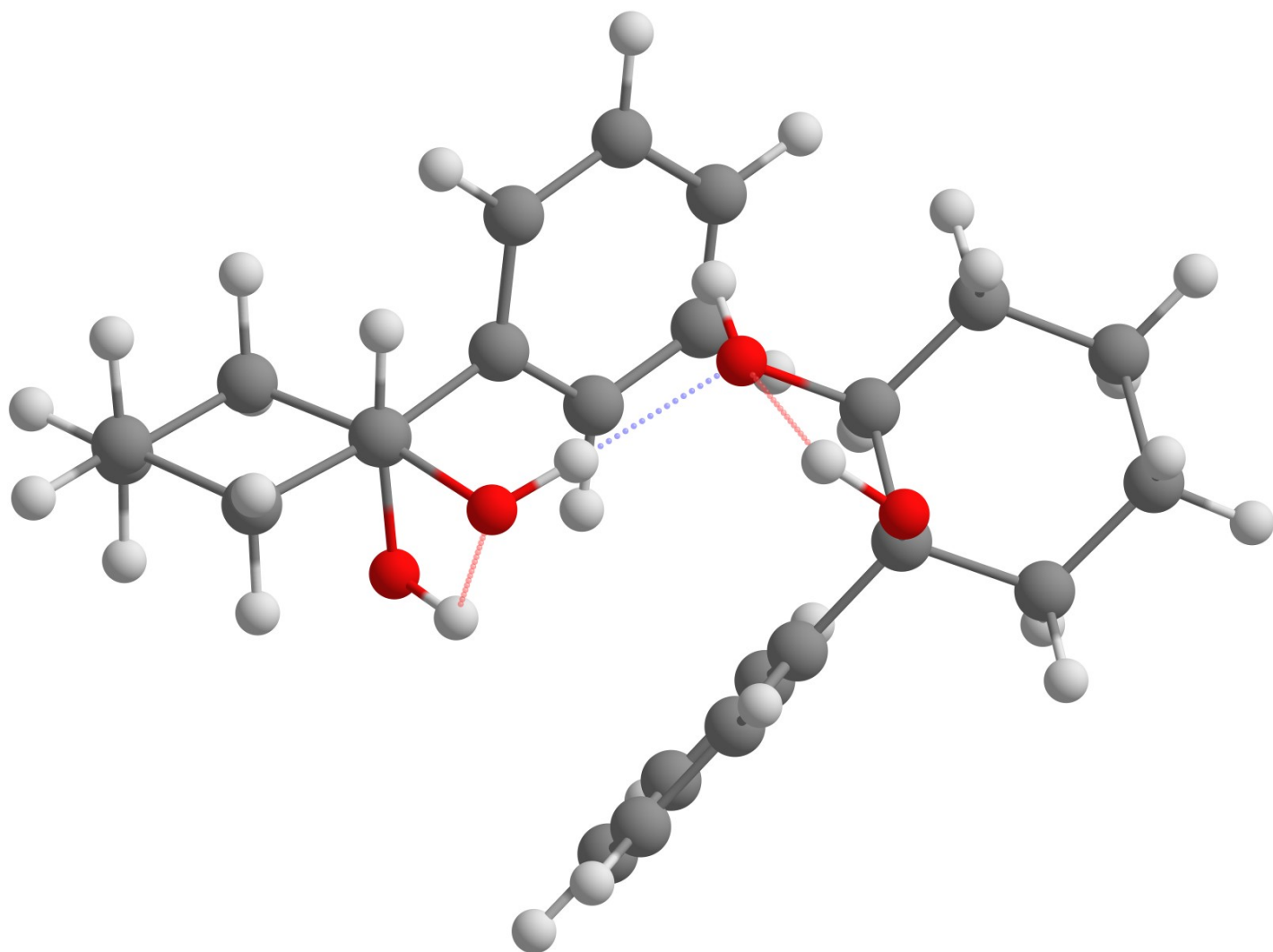


Fig. S11: Interactive 3d representation of the Addition $\text{O}_2\text{H}_2 \rightarrow \text{O}_2(\text{M}_1+\text{M}'_1)$ hetero-dimer.

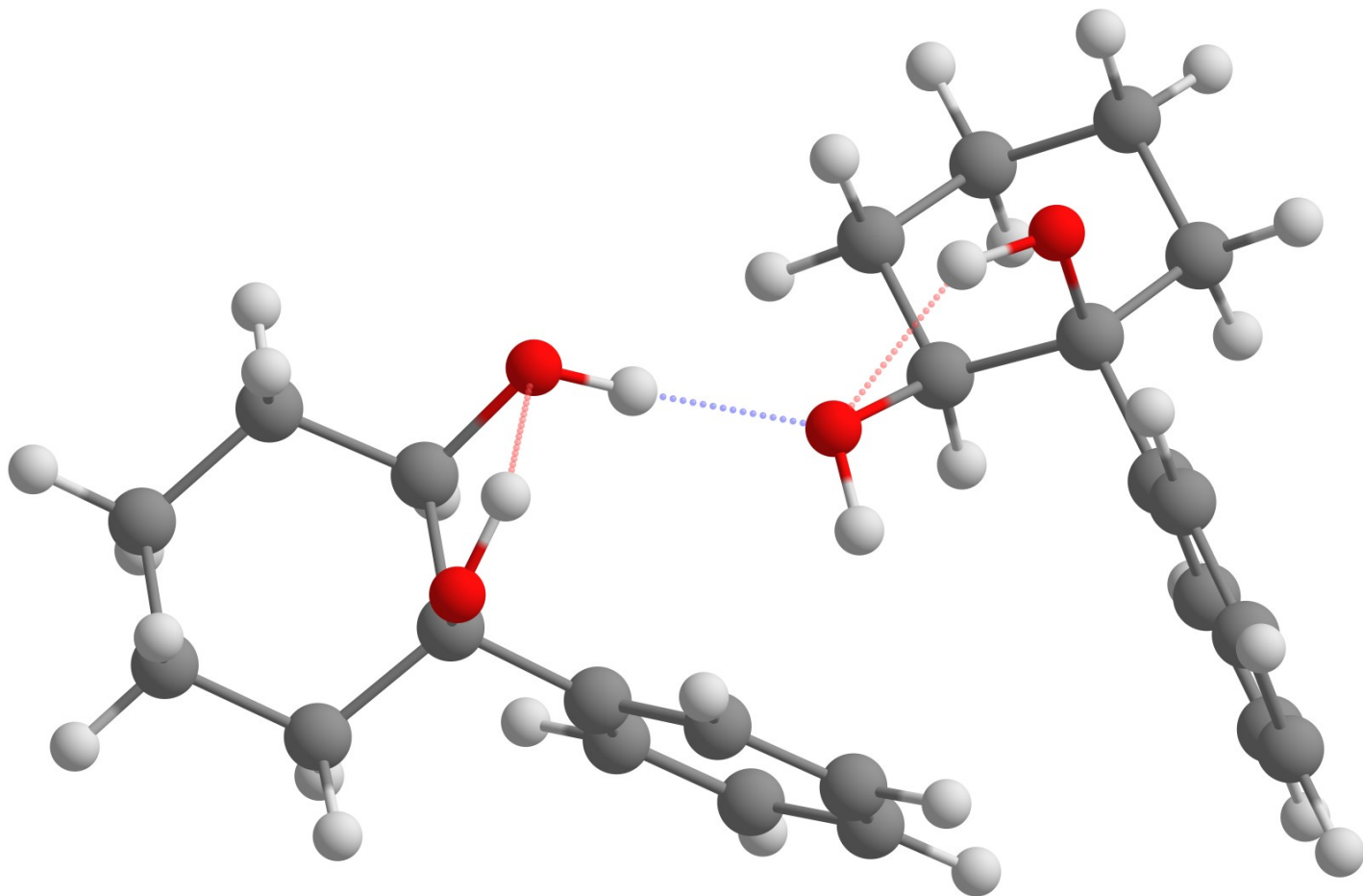


Fig. S12: Interactive 3d representation of the Addition $O_2H_2 \rightarrow O_2(M_1+M_1)$ a hetero-dimer.

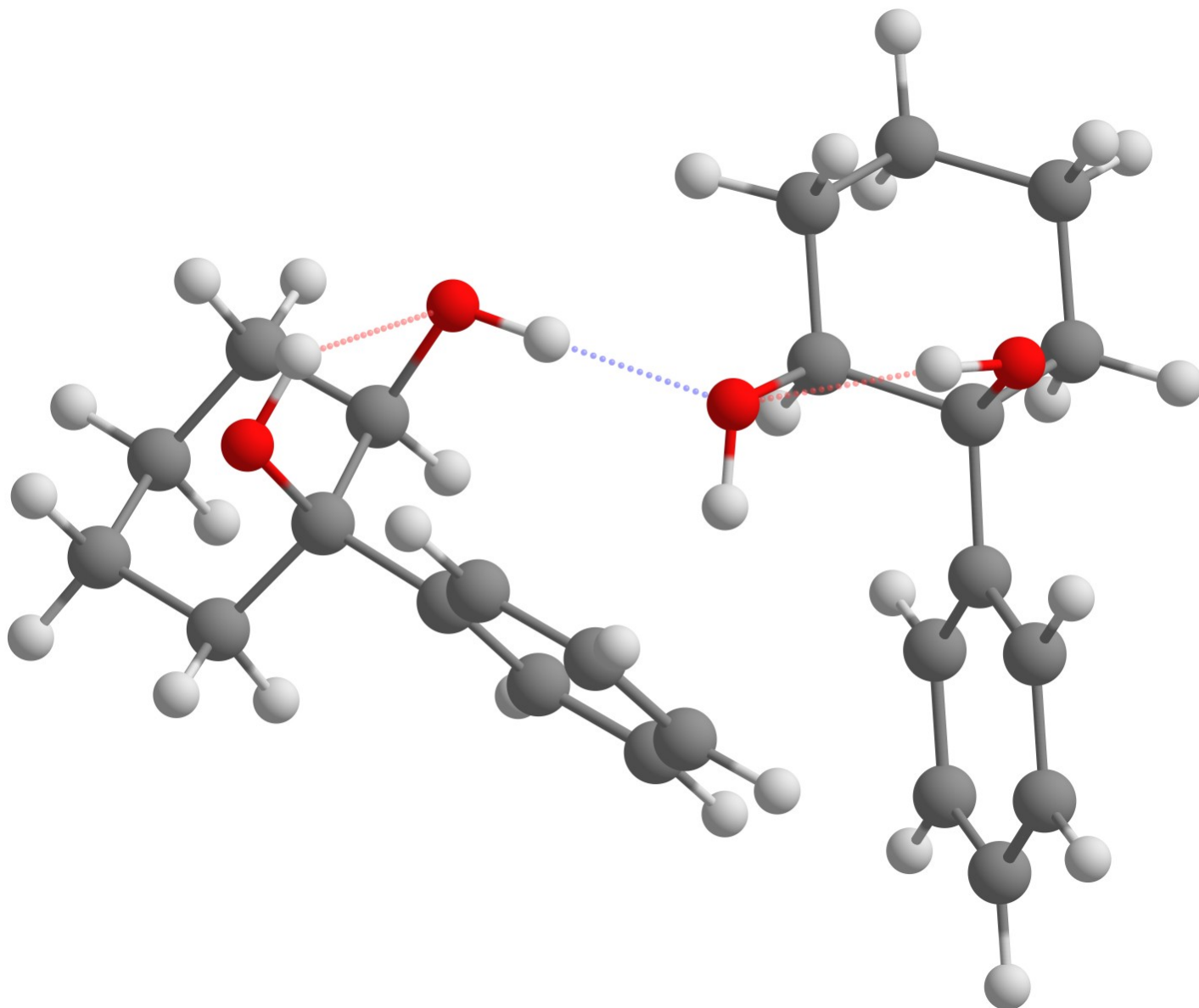


Fig. S13: Interactive 3d representation of the Addition $O_2H_2 \rightarrow O_2(M_1+M_1)b$ hetero-dimer.

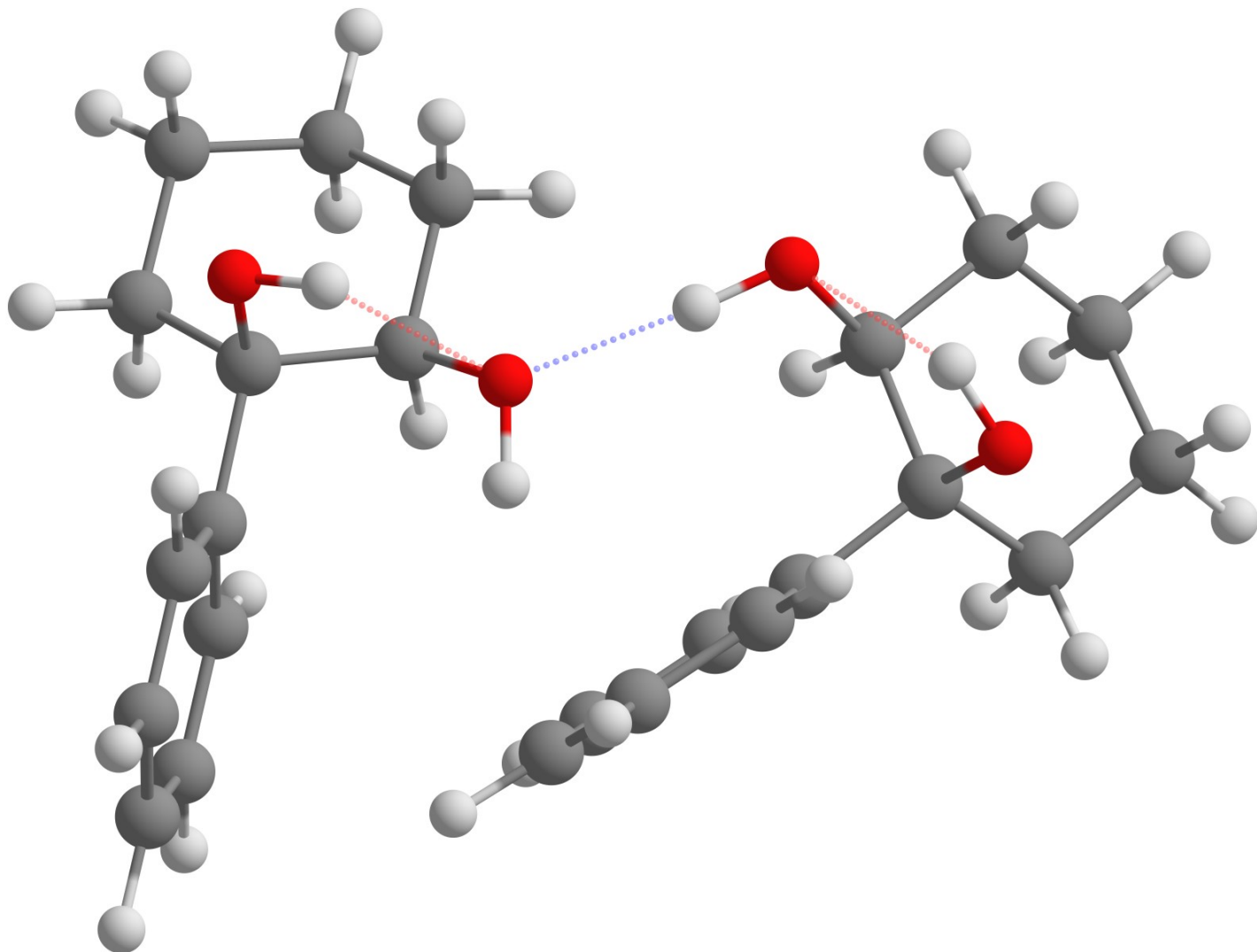


Fig. S14: Interactive 3d representation of the Addition $O_2H_2 \rightarrow O_2(M_1+M_1)c$ hetero-dimer.

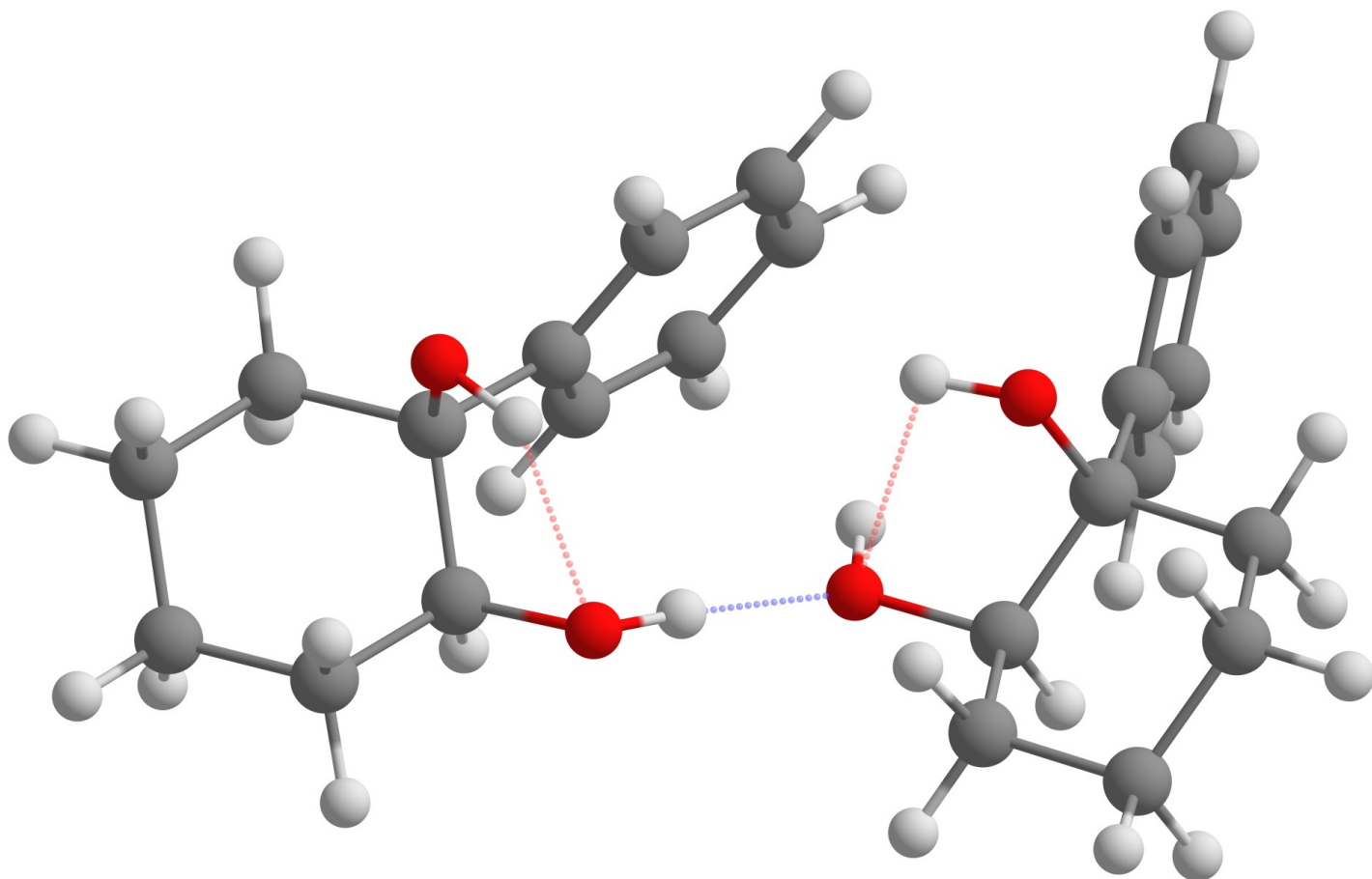


Fig. S15: Interactive 3d representation of the Addition $\text{O}_2\text{H}_2 \rightarrow \text{O}_2(\text{M}_1+\text{M}_1)\text{d}$ hetero-dimer.

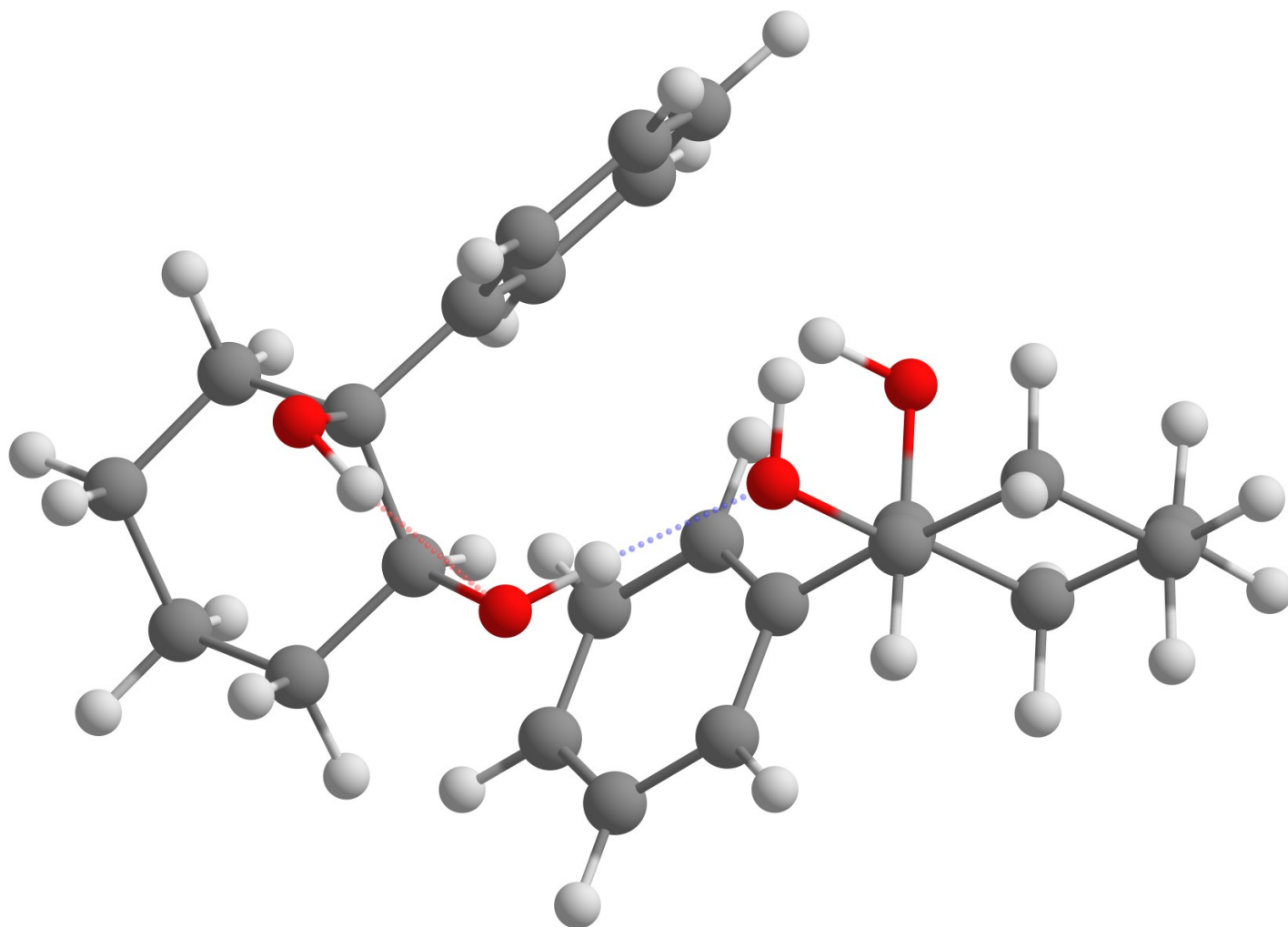


Fig. S16: Interactive 3d representation of the Addition $\text{O}_2\text{H}_2 \rightarrow \text{O}_2(\text{M}_1+\text{M}_2)$ hetero-dimer.

Literature

- [1] B. Hartwig, M. Lange, A. Poblitzki, R. Medel, A. Zehnacker, M. A. Suhm, “The reduced cohesion of homo-configurational 1,2-diols”, *Phys. Chem. Chem. Phys.* **2020**, *22*, 1122–1136.