Asymmetric Transfer Hydrogenation of Ketimines with Trichlorosilane: Structural Studies

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Computational data for all stationary points found on the hypersurfaces

a) Computed absolute energies and ZPVE as well as Gibbs free energies for C1-C10, C1-C4a-b, C1-C5a-b, C1-C8a-d, and TS1-TS6 at B3PW91/cc-pVDZ

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b) Optimized geometries for the structures C1-C5a and C1-C5b at B3PW91/cc-pVDZ

- C1-C5a

-c) Cartesian (xyz) coordinates for all computed species optimized at B3PW91/cc-pVDZ in Å.
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17 -1.683052000 -0.971710000 -0.179798000

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1 -1.187018000 -2.092158000 -0.882627000
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1 -2.072508000 -0.799909000 0.000000000
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1 1.219408000 2.111829000 0.884588000
1 1.219408000 2.111829000 -0.884588000

3- Structure C3

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6- Structure C1-C4b

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