

**Theoretical Investigation of the Mechanism of the Selective Catalytic
Reduction of Nitric Oxide with Ammonia on H-form Zeolites**

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Figure Captions

Figure 1S: Part 1 of the overview of the reaction network involving N_2O_3 . Stated energies are only electronic energies without zero-point correction and are with respect to the gas-phase and the empty zeolite framework. Dotted arrows correspond to two structures that are only slightly different and thus, no transition state was considered between them.

Figure 2S: Structures corresponding to the overview given in Figure 1S. Structures that were presented in the main article are not shown again.

Figure 3S: Part 2 of the overview of the reaction network involving N_2O_3 . Stated energies are only electronic energies without zero-point correction and are with respect to the gas-phase and the empty zeolite framework. Dotted arrows correspond to two structures that are only slightly different and thus, no transition state was considered between them.

Figure 4S: Structures corresponding to the overview given in Figure 3S. Structures that were presented in the main article are not shown again. Starting configurations that are identical with those in part 1 (“a”) are also not shown again.

Figure 5S: Overview of the reaction network involving N_2O_4 . Stated energies are only electronic energies without zero-point correction and are with respect to the gas-phase and the the empty zeolite framework. Dotted arrows correspond to two structures that are only slightly different and thus, no transition state was considered between them.

Figure 6S: Structures corresponding to the overview given in Figure 5S. Structures that were presented in the main article are not shown again.

Figure S1

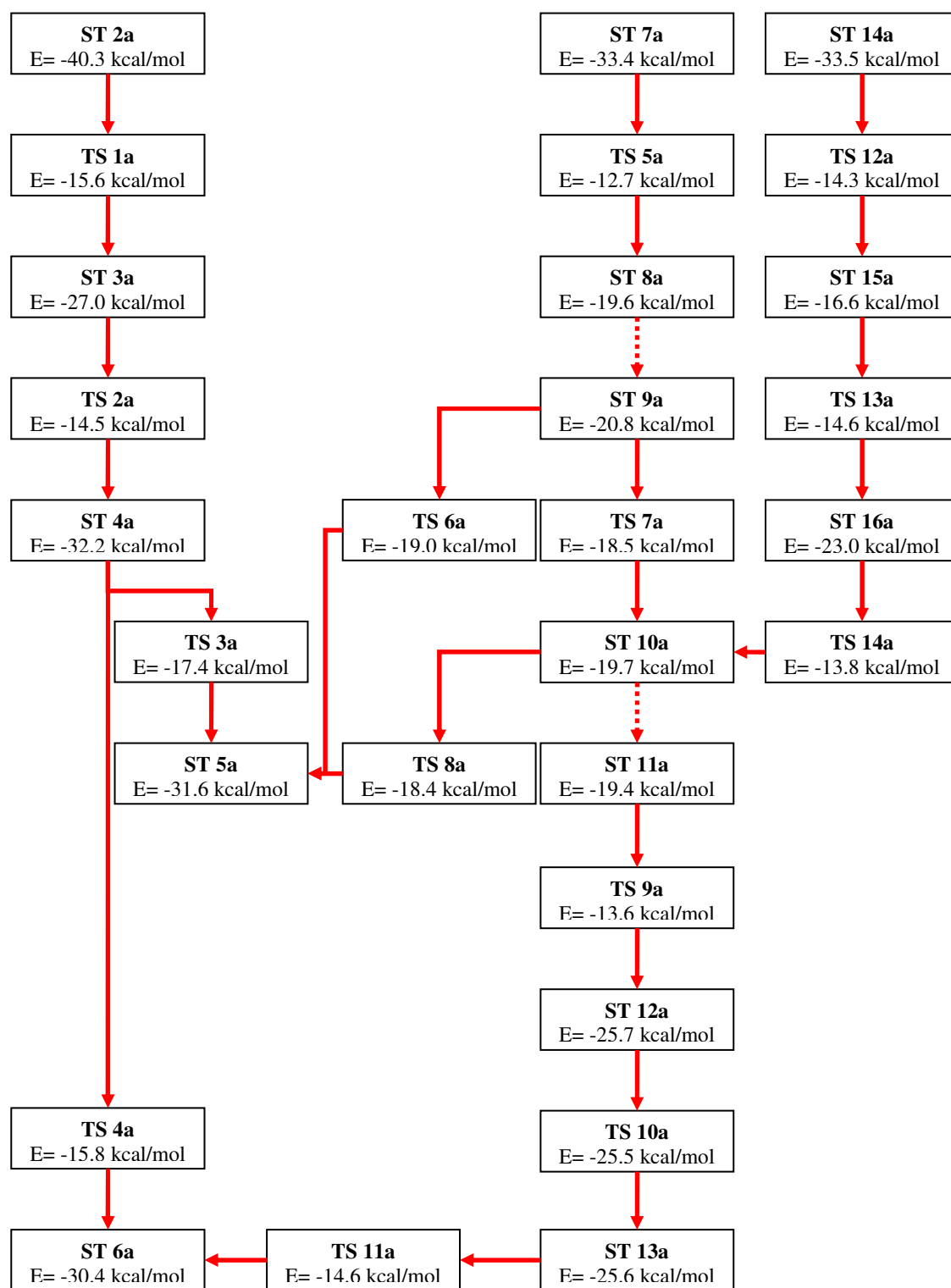
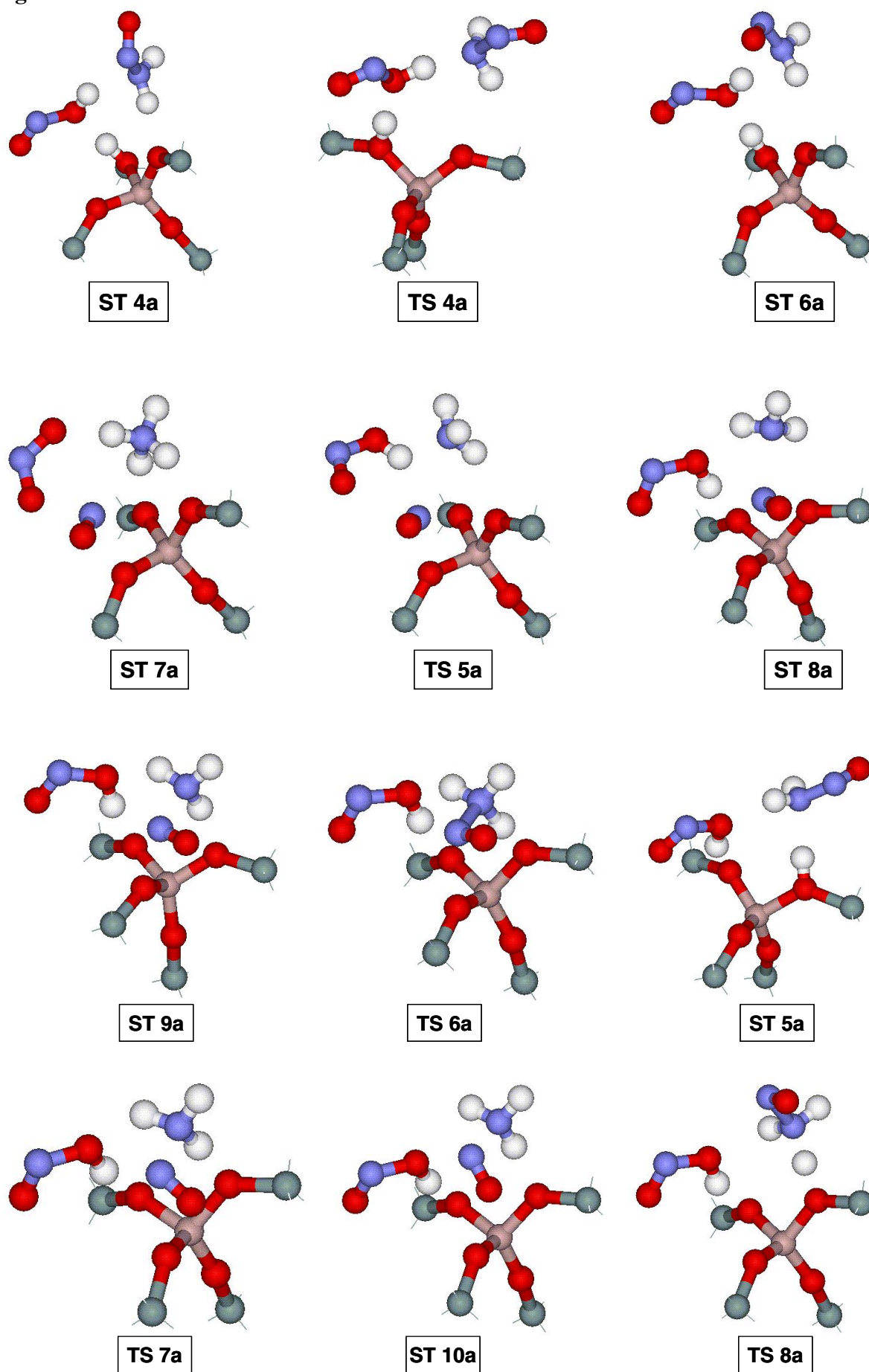
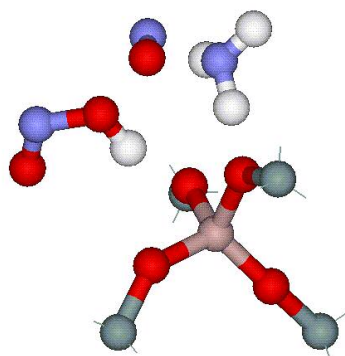
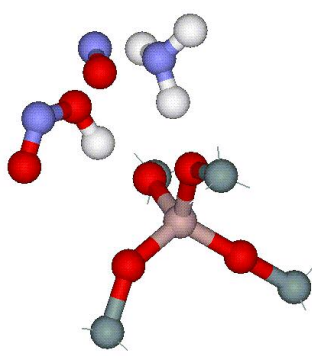


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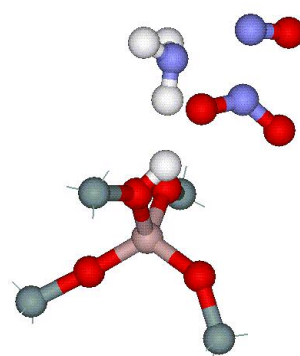




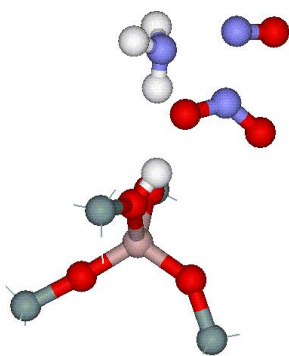
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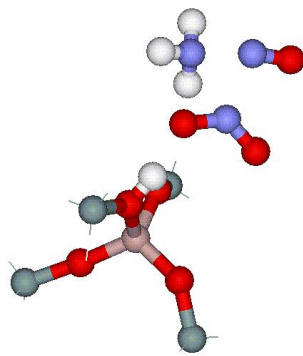
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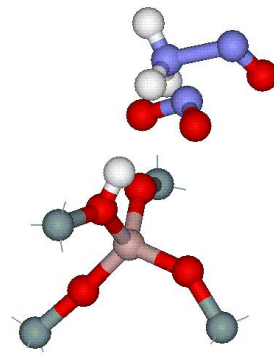
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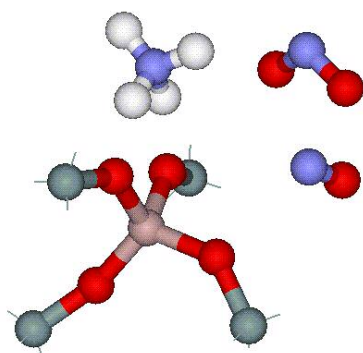
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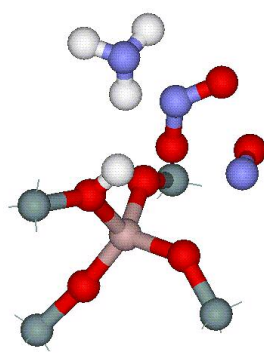
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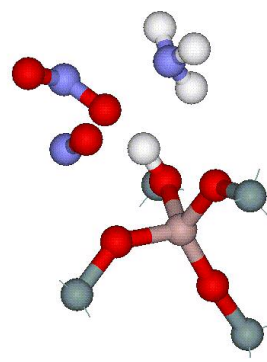
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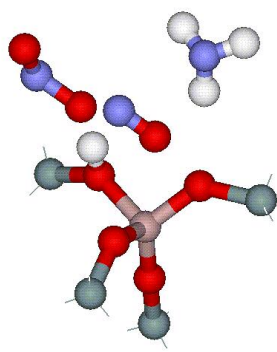
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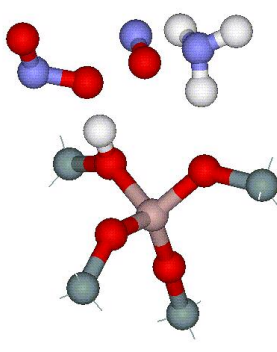
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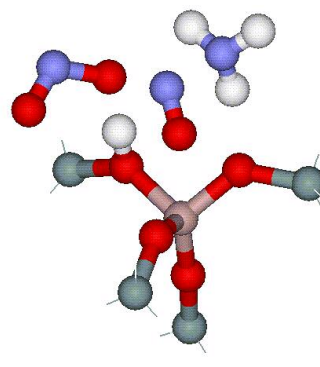
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TS_13a



ST_16a



TS_14a



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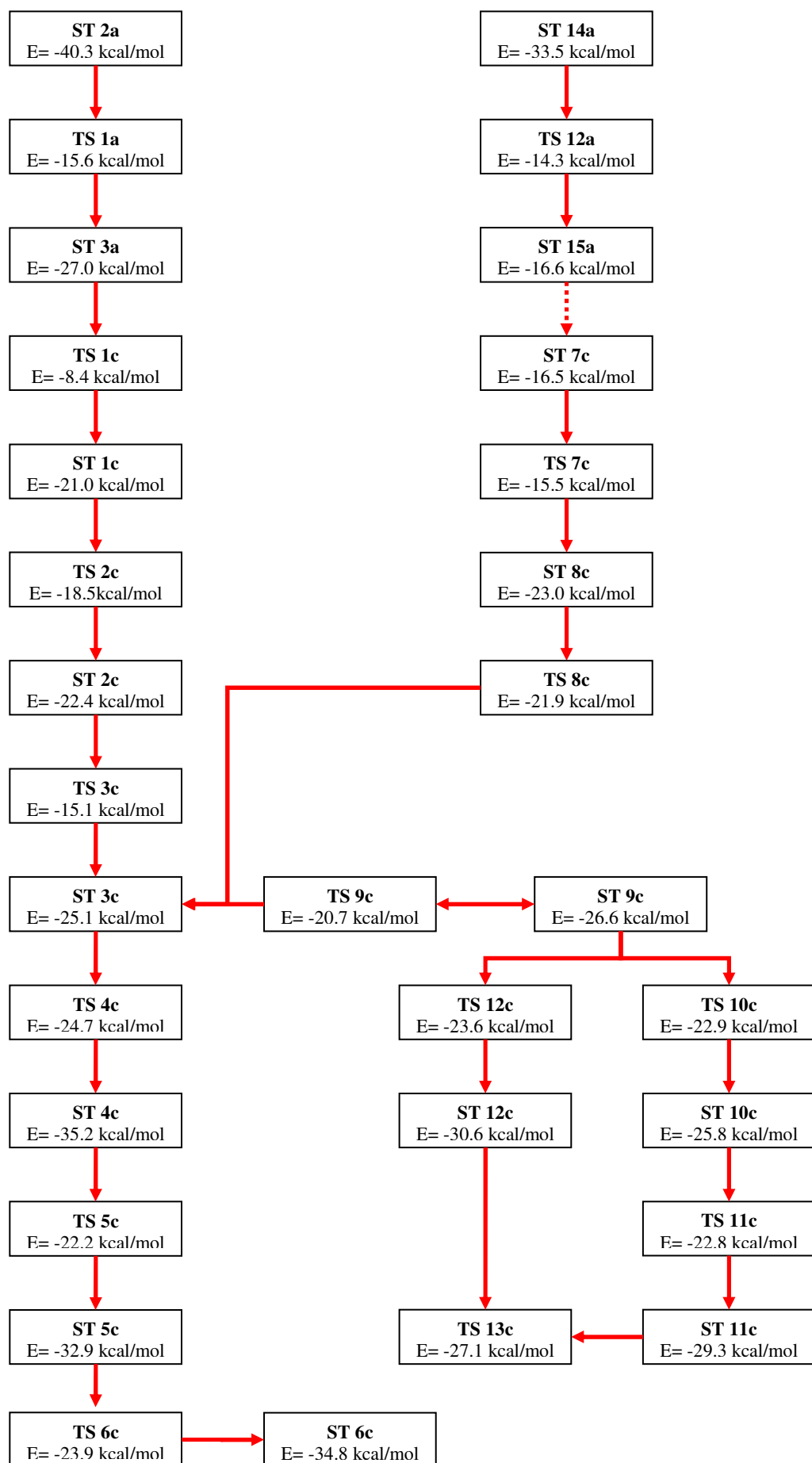
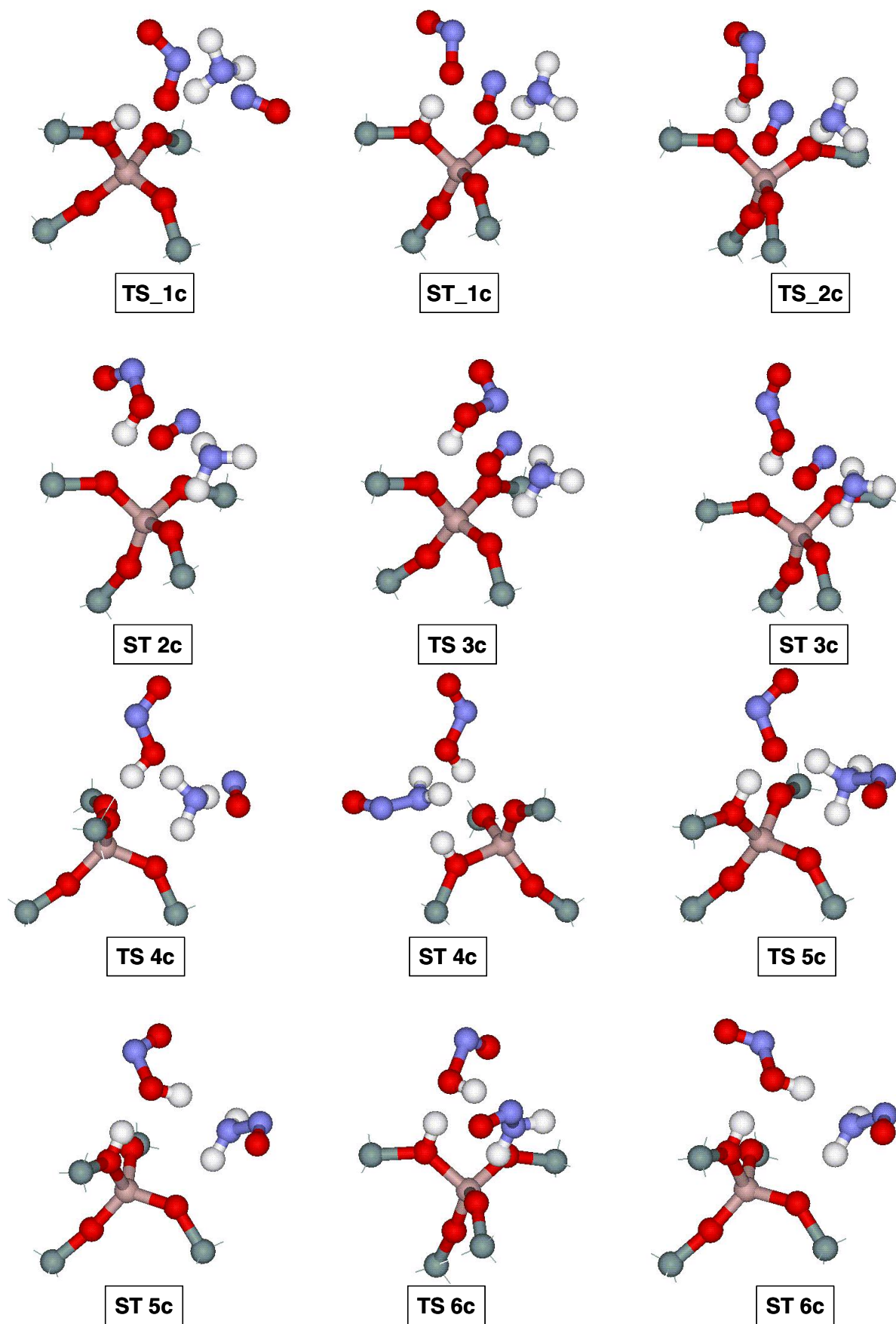
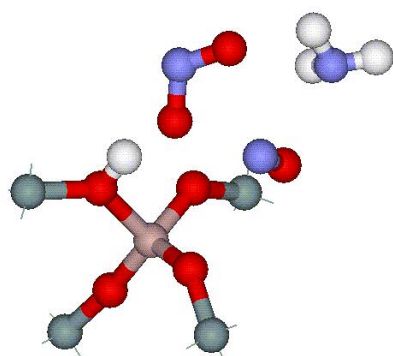
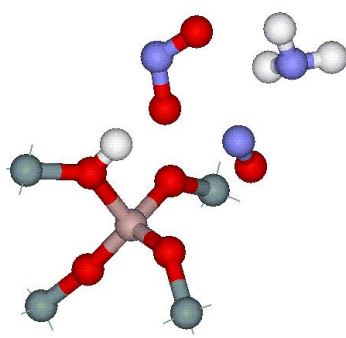


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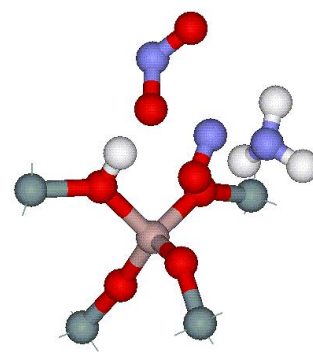




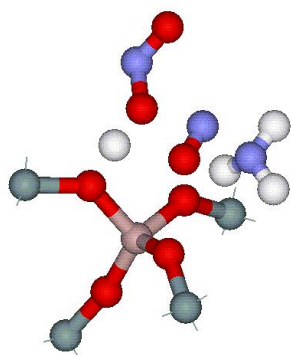
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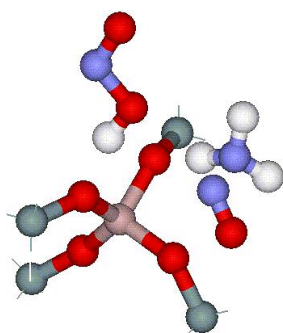
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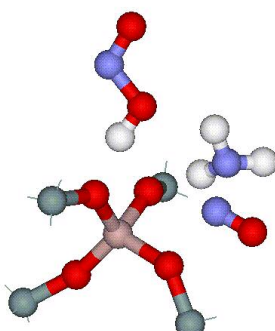
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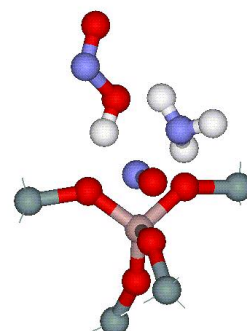
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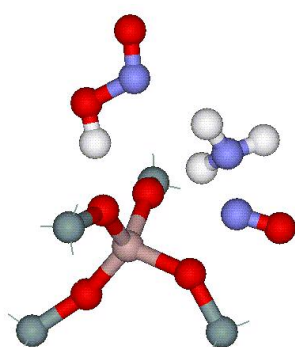
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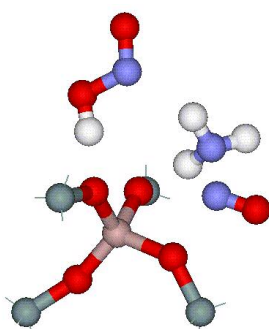
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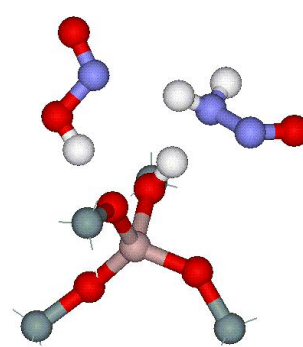
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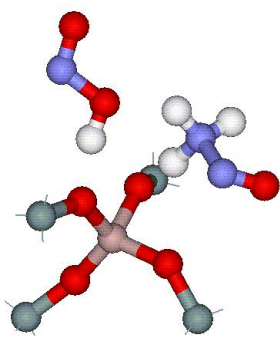
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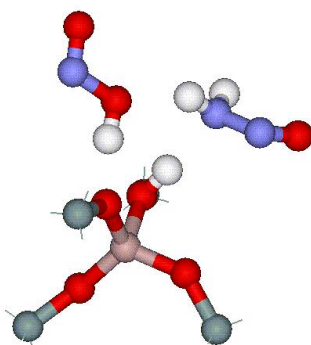
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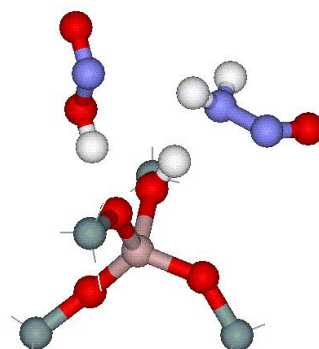
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TS 12c



ST 12c



TS 13c



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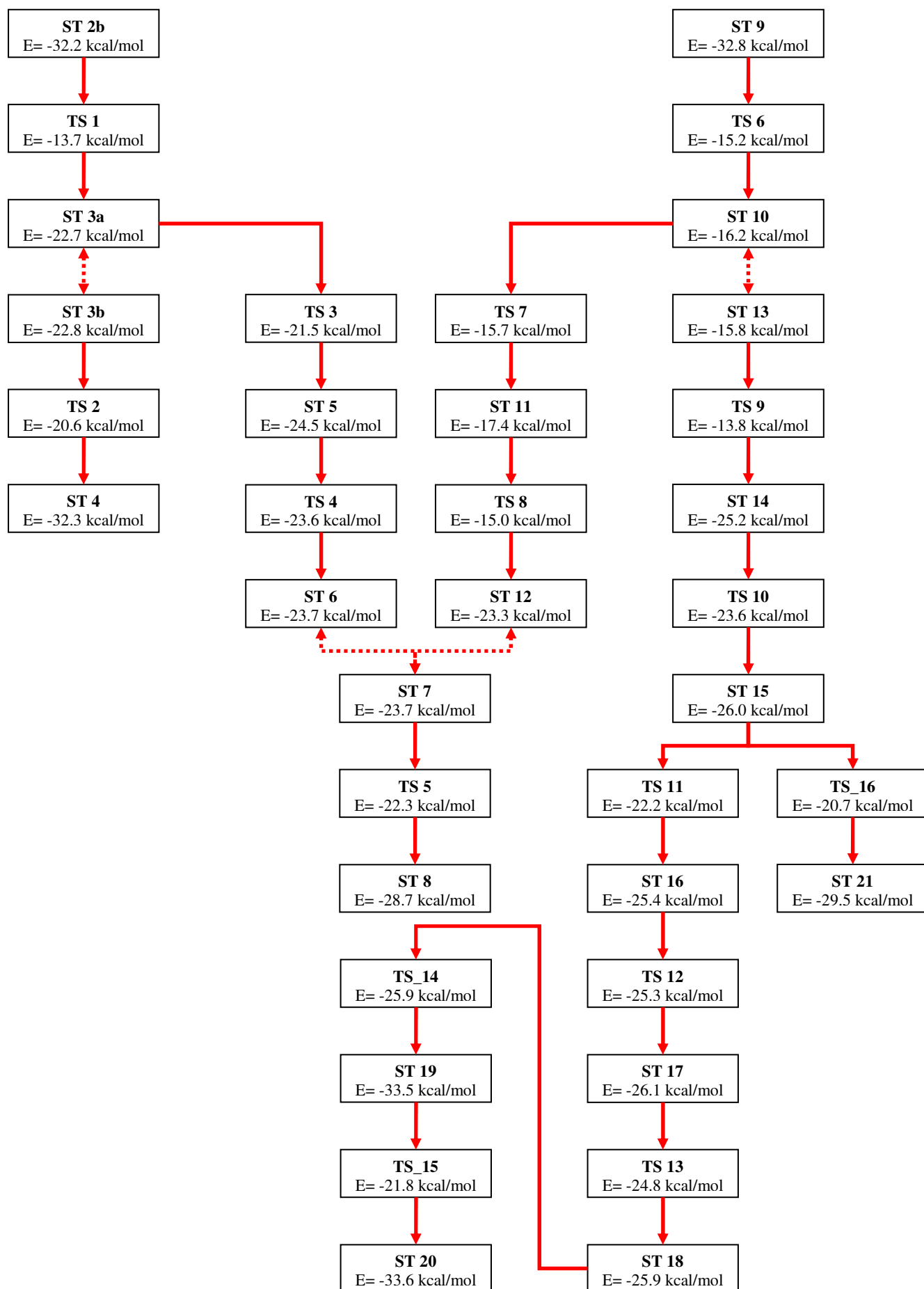
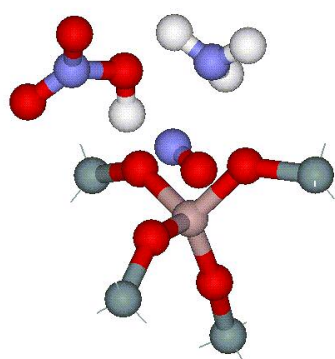
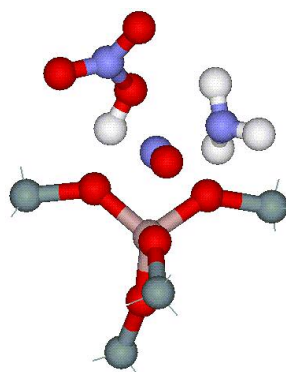


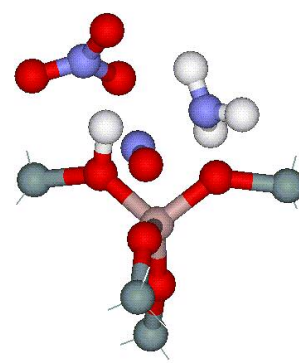
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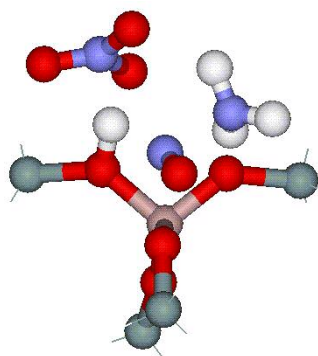
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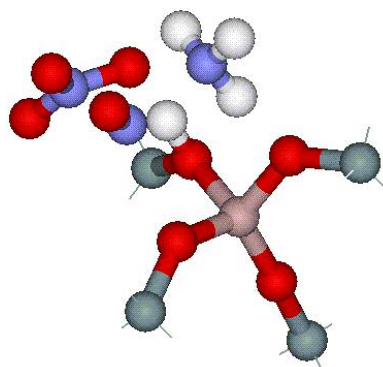
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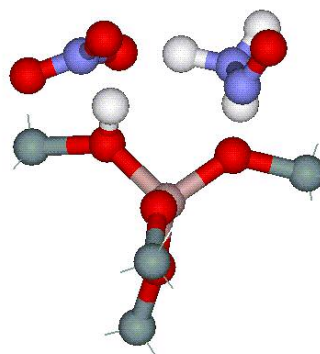
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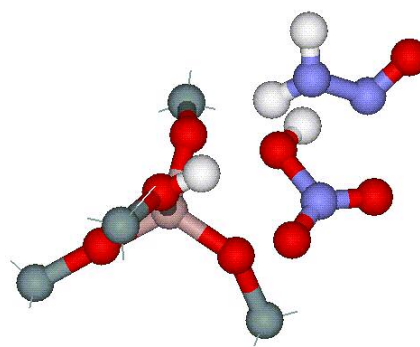
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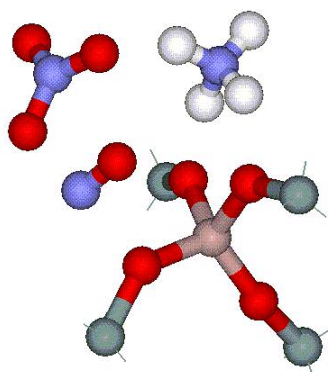
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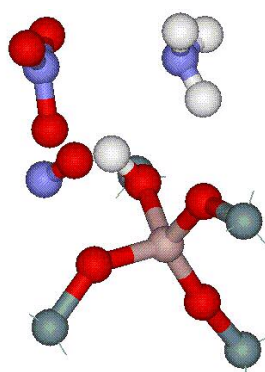
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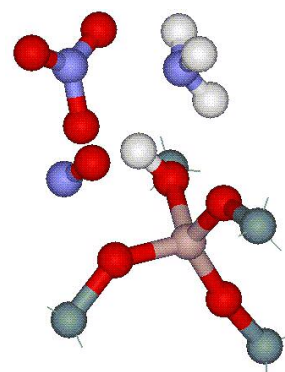
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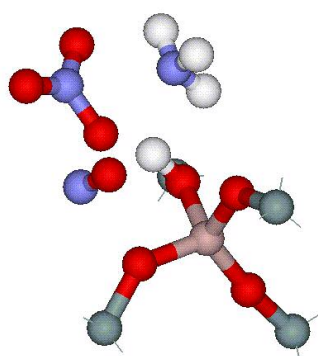
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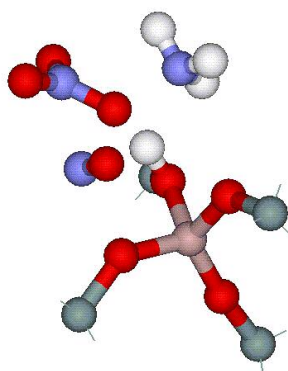
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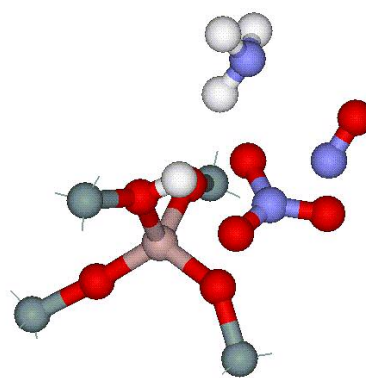
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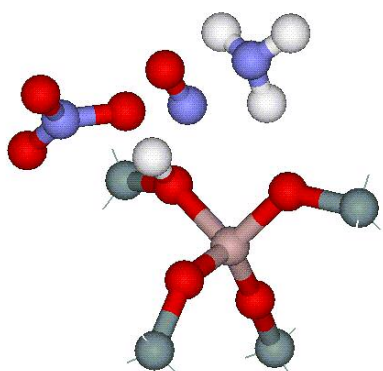
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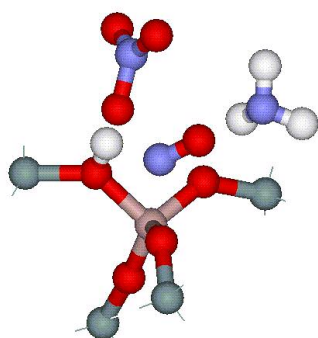
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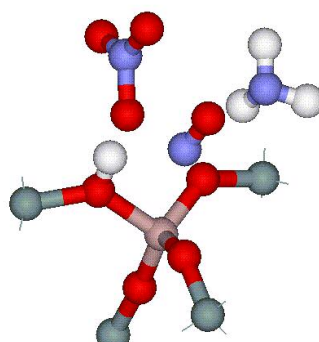
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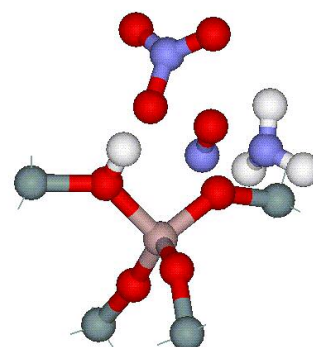
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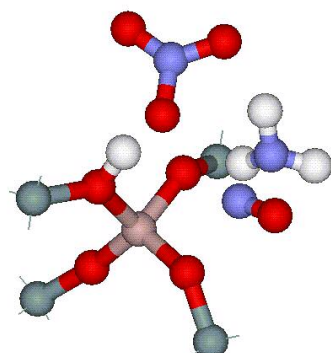
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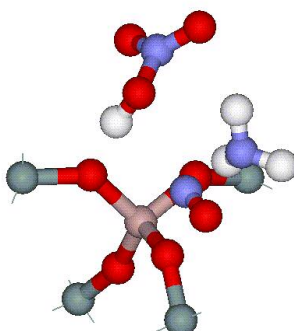
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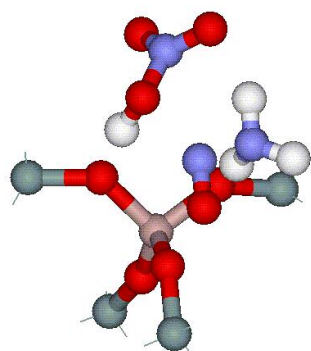
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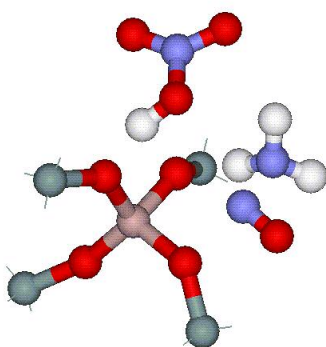
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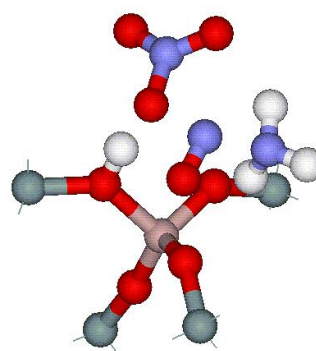
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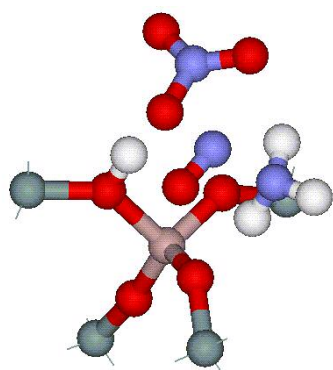
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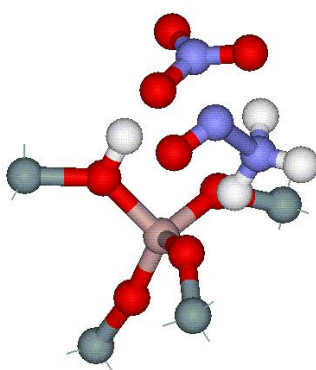
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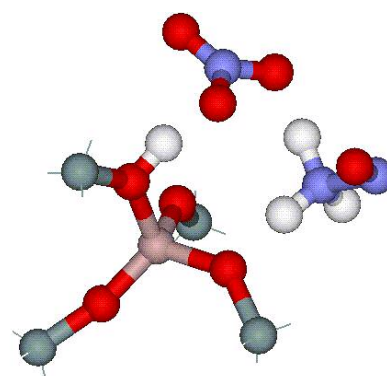
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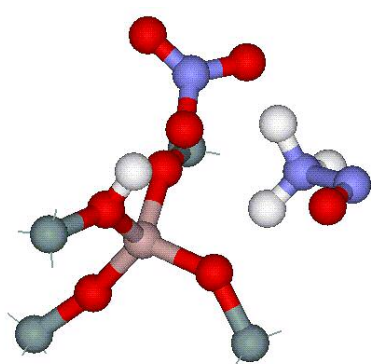
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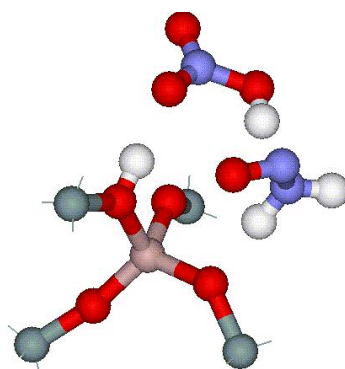
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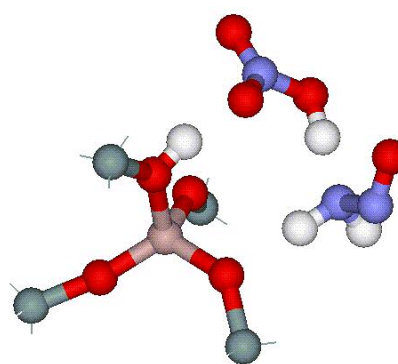
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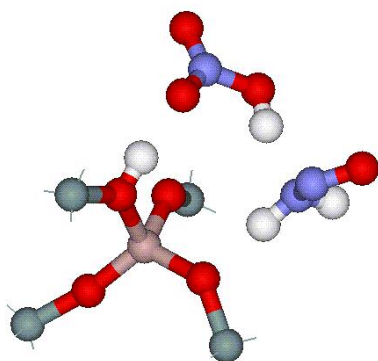
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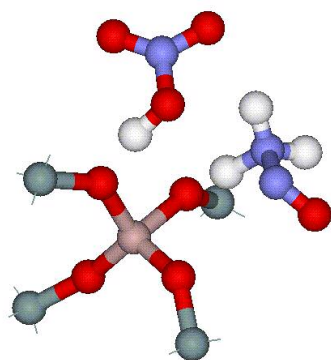
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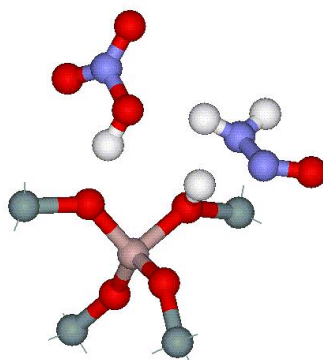
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TS 16



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