S P Q R

AB INITIO COMPUTATIONS OF ONE AND TWO HYDROGEN OR DEUTERIUM ATOMS IN THE PALLADIUM TETRAHEDRAL SITE

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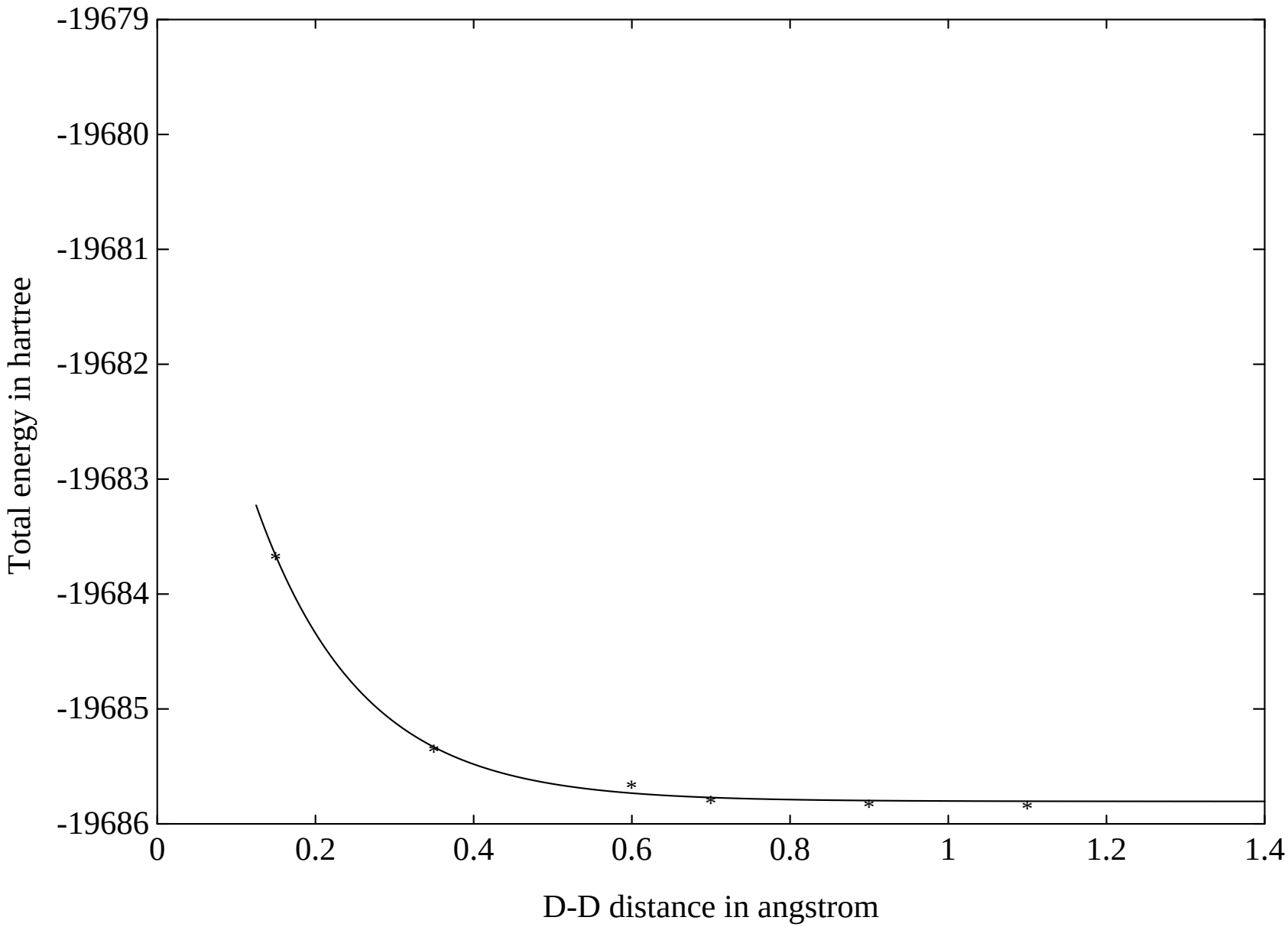
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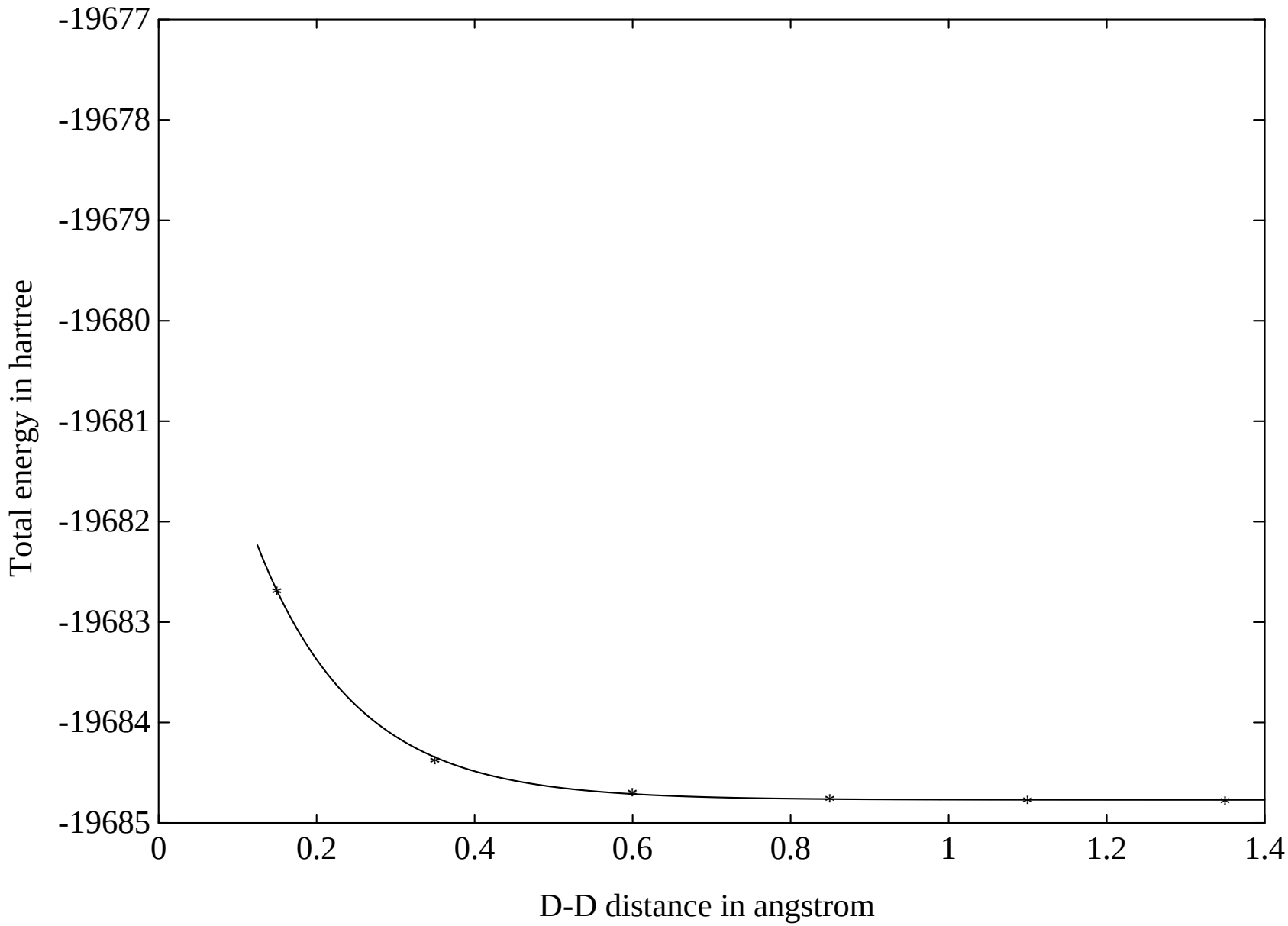
-19680
-19681
-19682
-19683
-19684
-19685
-19686
Total energy in hartree
0
0.2
0.4
0.6
0.8
1
1.2
1.4
D-D distance in angstrom

FIGURE 1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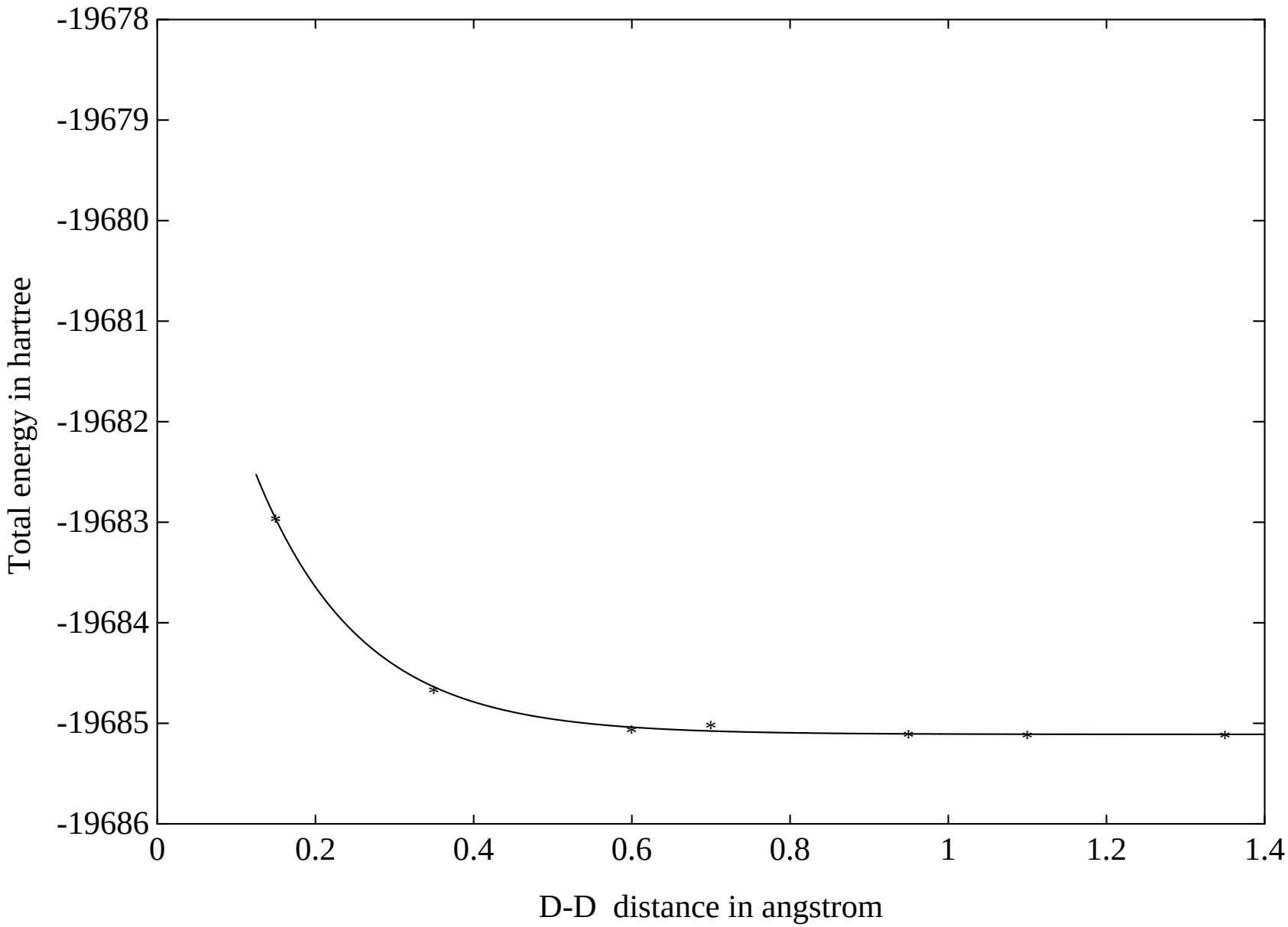
-19679
-19680
-19681
-19682
-19683
-19684
-19685
Total energy in hartree
0
0.2
0.4
0.6
0.8
1
1.2
1.4
D-D distance in angstrom

FIGURE 2


-19678
-19679
-19680
-19681
-19682
-19683
-19684
-19685
-19686
Total energy in hartree
0
0.2
0.4
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0.8
1
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1.4
D-D distance in angstrom

FIGURE 3

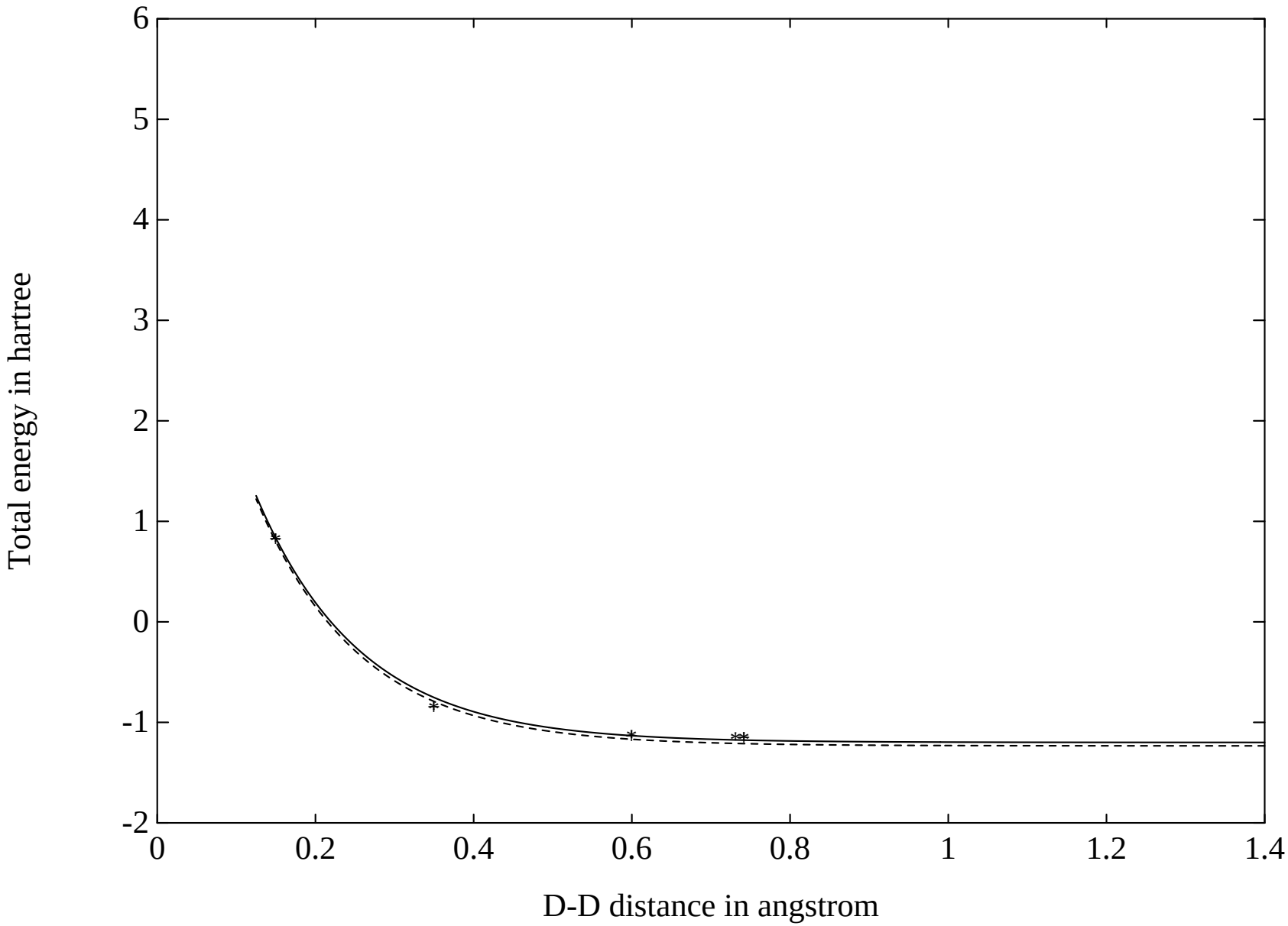
Total energy in hartree
D-D distance in angstrom
6
5
4
3
2
1
0
-1
-2
0
0.2
0.4
0.6
0.8
1
1.2
1.4

FIGURE 4

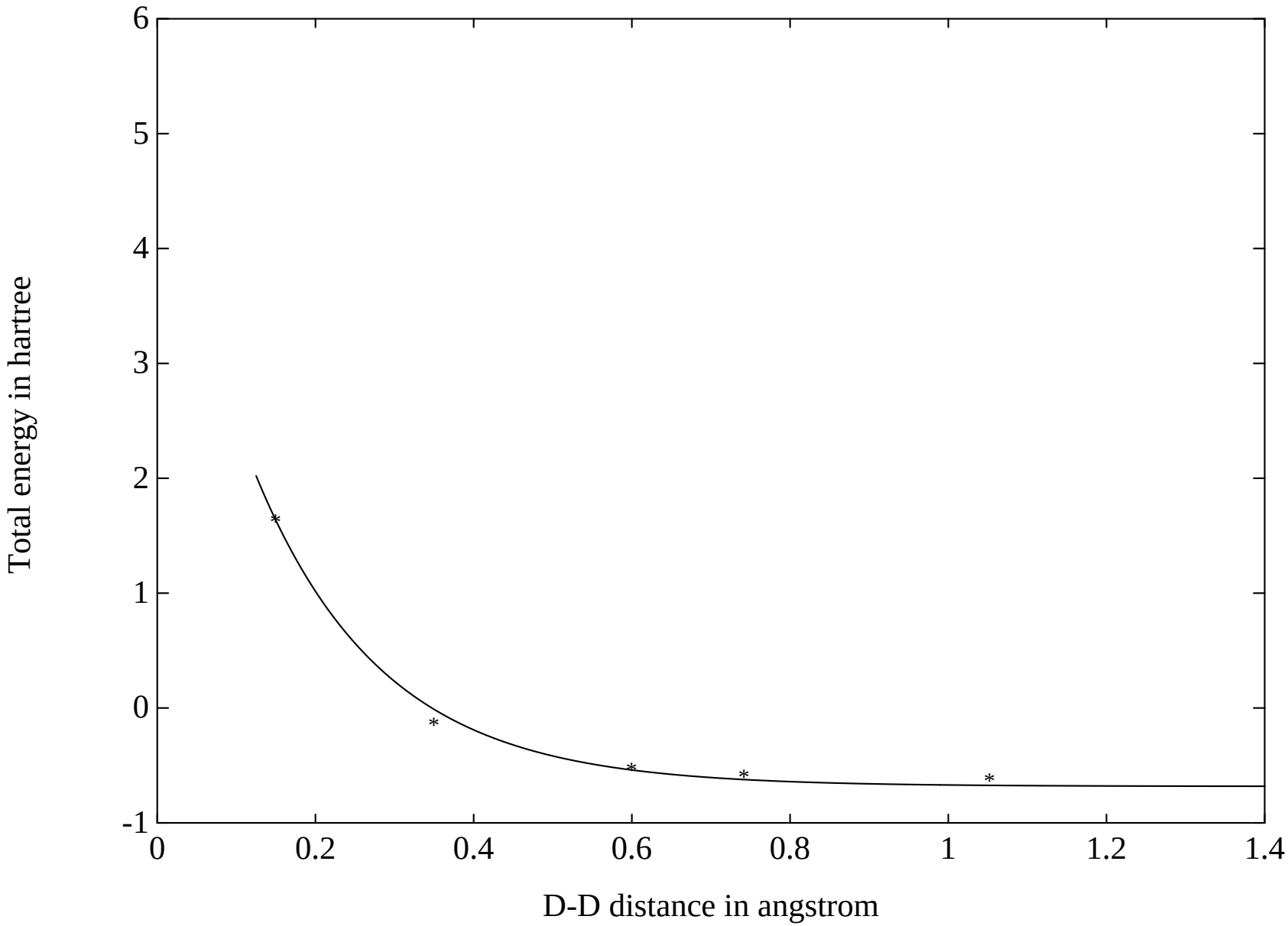
Total energy in hartree
D-D distance in angstrom
6
5
4
3
2
1
0
-1
0
0.2
0.4
0.6
0.8
1
1.2
1.4

FIGURE 5