

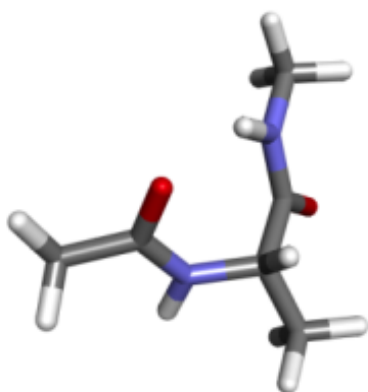
String method (STRING)

1. Calculation setup

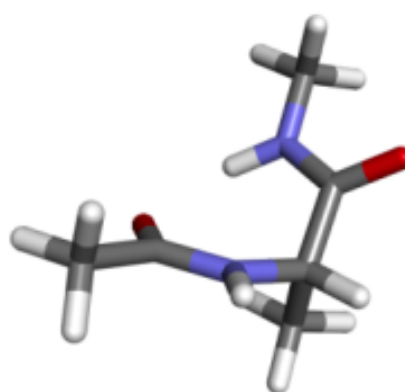
The following setup is used.

- Method: STRING
- Potential: MM (classical force field)
- System: alanine dipeptide
- Number of beads: 256
- Ends of string : fixed

The molecular geometries of reactant and product are shown below.



(a) Reactant



(b) Product

2. Results

The potential profile is printed in "string_pot.out".

1	-0.0262868179181149
2	-0.0262865959492212
3	-0.0262866305346267
4	-0.0262866278134240
5	-0.0262856225311330
6	-0.0262832258810466
7	-0.0262815015946685
8	-0.0262803458522526
9	-0.0262793188292377
10	-0.0262781945587644
...omitted...	

The molecular geometry of each bead is printed in "string.xyz".

22			
4000			
CT3	-3.1543580505402034	0.2388196071695783	0.9999715273529123
C	-1.7151941911535755	0.4674290032928858	0.7421954584734501
O	-1.3015346856074417	1.5551351957417245	0.3620232548691908
HA	-3.7164353289323135	1.1780206360590111	0.8040471621228031
HA	-3.5429468967637572	-0.5567359362541600	0.3296859158782453
HA	-3.3130194503209389	-0.0585991026588972	2.0579437500632354
NH1	-0.8980257755742521	-0.5750459416042859	0.9356463243984348
CT1	0.5378728474257596	-0.5039784879950321	0.7540595603307152
C	0.9525988852139871	-0.6370102110142484	-0.7111008068971502
O	1.5286393646691236	-1.6365964471484895	-1.1342455915902316
H	-1.2614685602318358	-1.4514705300618651	1.2267181509058964
HB	0.8847941530046403	0.4636879407201618	1.0940525922160254
CT3	1.2192796462890960	-1.5922275215727797	1.6092511919652781
HA	2.3249738336041648	-1.5272073921003329	1.5178332686146330
HA	0.9022052766473799	-2.6049558928025647	1.2800229576956974
HA	0.9478796238799629	-1.4650709819323124	2.6781947580123413
NH1	0.6613815016121124	0.3983225226439188	-1.5203454739140030
CT3	1.0201049580200001	0.4123410275791347	-2.9182206230470000
H	0.1397058453563073	1.1666738163315440	-1.1444201714348827
HA	2.1242796900264107	0.3336430231534349	-3.0402275502223683
HA	0.5497020233513568	-0.4443897267070209	-3.4521481307337250
HA	0.6794038122104289	1.3557760331014459	-3.3987133910718312
22			
4000			
CT3	-3.1527188200794050	0.2391387880302395	1.0015301614332632
C	-1.7141812776685337	0.4715640081822566	0.7438227983839130
O	-1.3036711030506112	1.5597768794900790	0.3617063801734307
...omitted...			

The potential profile is shown below. The potential barrier is estimated to be about 0.016 hartree.

