

```
/*
```

```
This is a program to find out the inter-molecular distance of NaCl.
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```
This program is created by Mohammad Sazzad Hossain.
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```
*/
```

```
# include <iostream>
```

```
# include <math.h>
```

```
using namespace std;
```

```
double funct (double x);
```

```
double f (double x);
```

```
int initial ();
```

```
int main ()
```

```
{
```

```
    double x, dl = 1E-6;
```

```
    int tag = 0;
```

```
    x = initial ();
```

```
    do {
```

```
        if (x + dl < funct (x))
```

```
            tag = 1;
```

```
        x += dl;
```

```
    }while (tag != 1);
```

```
cout << "The inter-molecular distance of NaCl is: " << x << " A." << endl;
```

```
cout << "The error in this value is in the order of: " << dl << endl;
```

```
return 0;
```

```
}
```

```
double funct (double x){
```

```
    double dl = 1E-6;
```

```
    return (x + dl * f(x) / (f(x) - f(x - dl)));
```

```
}
```

```
int initial (){
```

```
    int a = 0, x = 0, tag = 0;
```

```
do {
    if (f(x)<0){
        a = x;
        x++;
    }
    else
        tag = 1;
}while (tag != 1);

return (x);
}

double f (double x){
    double alpha = 1090, ro = 0.33, e2 = 14.4;

    return ((-e2 / (x * x)) + (alpha / ro) * exp (-x / ro));
}
```