Electronic Supplementary Material (ESI) for Chemical Science.
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Computational chemistry experiments performed directly on a blockchain virtual computer

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Supplementary Details

Overview. The outputs from the two molecular dynamics simulations are reported in the Supplementary Information. The details of the interactions with the Ethereum blockchain where these simulations were performed and recorded have been reported using the block explorer tools on the website https://etherchain.org and are also given in the Supplementary Information. These data include the records of these simulations on the Ethereum blockchain, which should remain available for review and replication independent of this publication for as long as the blockchain persists. The results of these simulations are also reported as decimals in Tables S1 and S2 of the Supplementary Information, together with equivalent simulations performed using software written in the C# programming language and executed on a conventional local computer. The source codes for the C# and Solidity implementations of these simulations are also given and the compiled Solidity code is available on the Ethereum blockchain. The blockchain data can be found both in the Supplementary Information and on the blockchain in block number 9360156 with the address 0x9680e167f6221ea0a9dce066a4f9c769621bc577. Working knowledge of how blockchains operate, and how to execute software on the Ethereum network, as well as a downloadable copy of the Ethereum blockchain can be found at the time of writing on the websites https://ethereum.org/ and https://geth.ethereum.org/, and are necessary for review and replication of these data.

External Libraries. The mathematics used in these calculations makes use of decimal numbers. This is normally done in most programming languages through the use of doubles or floating point numbers, however, these are only precise up to a certain value. Two different computers generating slightly different results for the same double value can lead to slightly different simulation histories being recorded by different parts of the blockchain network. This can lead to the calculation being rejected as part of a consensus mechanism such as proof-of-work. Ethereum and similar blockchains that are capable of performing general computation have at the time of writing not yet implemented a method for calculating decimals with a fixed degree of precision, which would allow multiple machines to produce the same exact results from the same calculation. In this case, a third party library has been used in order to imitate floating point numbers using features that are currently available. In order to calculate these molecular dynamics trajectories, the ABDKMathQuad implements IEEE 754 standard fixed precision floating point numbers on the Ethereum blockchain. This library has been included in the code uploaded onto the blockchain as part of this work and can also be found at https://github.com/abdk-consulting/abdk-libraries-solidity/blob/master/ABDKMathQuad.md. Using this library, the results have been scaled by 10^p in order to provide accuracy up to p decimal places, where p is a variable supplied by the user when the code is called on the blockchain and chosen to be $p = 10$ for all of the calculations reported here. The output is then returned a set of integers by ABDKMathQuad and written as part of the simulation onto the blockchain as array of 256 bit integers in bytes displayed as a string of hexadecimal, and these have been divided by 10^p before being reported as decimals in Tables S1 and S2.

Computational Limit. The Ethereum network also has a limit to the maximum amount of computation that can be performed as part of generating a single block. This is measured in units known as gas, with the current limit being set at 10,000,000 gas at the time of writing. A more detailed description of the relationship between gas and computational operations can be found in the Ethereum paper “Ethereum: A Secure Decentralized Generalized Transaction Ledger EIP-150 Revision” by Dr. Gavin Wood on the website https://gavwood.com/paper.pdf at the time of writing.

Application Binary Interface. The procedure for calling a piece of software on the Ethereum blockchain varies depending on the type of software. If the code follows a standard format (such as the ERC20 token standard detailed in the Ethereum documentation) then most software for interacting with the code will already understand how to call it without the need for additional information. In the case of a new and therefore non-standard piece of software such as this, an Application Binary Interface (ABI) is needed to provide a description of the functions in the code.

Developers will usually provide this separately or it can be generated from the source code. The ABI for this contract is:


```
[
{
"constant": true,
"inputs": [
{
"internalType": "uint256",
"name": "steps",
"type": "uint256"
},
{
"internalType": "uint256",
"name": "precision",
"type": "uint256"
}
],
"name": "runMD",
"outputs": [
{
"internalType": "int256[]",
"name": "",
"type": "int256[]"
}
],
"payable": false,
"stateMutability": "pure",
"type": "function"
}
]
```

Preliminary Molecular Dynamics Trajectory Transaction Details
The details of the transaction and the corresponding blockchain output from the 1 fs molecular dynamics preliminary simulation on the Ethereum blockchain are presented here:

Block Number: 9360161
Hash: 0x13eb9c343f380334262706975c676aa5006ac2103b2132dfba0e1667c7dfddc6
Time Stamp: 01/26/2020 10:26:38 PM Greenwich Mean Time (GMT)
From: 0xC120A82d25325c9700652D6f2288EBD2C4224567
To: 0x9680E167F6221ea0A9dcE066A4f9c769621bC577
Fee: 0.00026 ETH (ca. $0.04)
Gas Price: 0.0000000011 ETH
Gas Used: 238,619

Trace [
{
  "action": {
    "callType": "call",
    "from": "0xc120a82d25325c9700652d6f2288ebd2c4224567",
    "gas": "0x350bb",
    "input":
"0x9deac18d0000000000000000000000000000000000000000000000000000000000000a000
0000000000000000000000000000000000000000000000000000000000000a",
    "to": "0x9680e167f6221ea0a9dce066a4f9c769621bc577",
    "value": "0x0"
  },
  "blockHash":
"0x1415b4c454989b7bafdf786ca6adf3d3f50dc8097550b3a9033022ea25c2a29a",
  "blockNumber": 9360161,
  "result": {
    "gasUsed": "0x350bb",
    "output":
"0x0000000000000000000000000000000000000000000000000000000000000020000000000000
0000000000000000000000000000000000000000000000000a0000000000000000000000000000
0000000000000000000000000000000547924e8600000000000000000000000000000000000000
0000000000000000005475fb0cd0000000000000000000000000000000000000000000000000000
00005470b6c020000000000000000000000000000000000000000000000000000000054695a339
0000000000000000000000000000000000000000000000000000545fe877c00000000000000
0000000000000000000000000000000000005454657b0000000000000000000000000000000
0000000000000000000000005446d6082000000000000000000000000000000000000000000000
0000000000000054373fc4400000000000000000000000000000000000000000000000000000000
05425a92c7000000000000000000000000000000000000000000000000000000541219930"
  },
  "subtraces": 0,
  "traceAddress": [],
  "transactionHash":
"0x13eb9c343f380334262706975c676aa5006ac2103b2132dfba0e1667c7dfddc6",
  "transactionPosition": 43,
  "type": "call"
 }
]

Production Molecular Dynamics Trajectory Transaction Details
The details of the transaction and the corresponding blockchain output from the 40 fs molecular dynamics production simulation on the Ethereum blockchain are presented here:

Block Number: 9360178
Hash: 0x36b510f3bdb2fa67a0d4f749899ab8630b54000ee5a211172d699d750f94f94f
Time Stamp: 01/26/2020 10:30:26 PM Greenwich Mean Time (GMT)
From: 0xC120A82d25325c9700652D6f2288EBD2C4224567
To: 0x9680E167F6221ea0A9dcE066A4f9c769621bC577
Fee: 0.00986 ETH (ca. $1.66)
Gas Price: 0.0000000011 ETH
Gas Used: 8,960,757

Trace [
{
"action": {
"callType": "call",
"from": "0xc120a82d25325c9700652d6f2288ebd2c4224567",
"gas": "0x886789",
"input":
"0x9deac18d0000000000000000000000000000000000000000000000000000000000000190000
0000000000000000000000000000000000000000000000000000000000000000a",
"to": "0x9680e167f6221ea0a9dce066a4f9c769621bc577",
"value": "0x0"
},
"blockHash":
"0x6cb36c1011265387c7933e199c1de8a9f3a5ca59fa45ec9e5dd6f388884f958a",
"blockNumber": 9360178,
"result": {
"gasUsed": "0x886789",
"output":
"0x0000000000000000000000000000000000000000000000000000000000000020000000000000
0000000000000000000000000000000000000000000000000190000000000000000000000000000
0000000000000000000000000000000547924e8600000000000000000000000000000000000000
0000000000000000005475fb0cd0000000000000000000000000000000000000000000000000000
00005470b6c0200000000000000000000000000000000000000000000000000000000054695a339
0000000000000000000000000000000000000000000000000545fe877c00000000000000
0000000000000000000000000000000000005454657b0000000000000000000000000000
0000000000000000000000005446d6082000000000000000000000000000000000000000
0000000000000054373fc4400000000000000000000000000000000000000000000000000000
05425a92c7000000000000000000000000000000000000000000000000000541219930000
0000000000000000000000000000000000000000000000053fc991c900000000000000000
0000000000000000000000000000000000053e530bc8000000000000000000000000000000
0000000000000000000000053cbea31500000000000000000000000000000000000000000000
00000000000053b0d0008000000000000000000000000000000000000000000000000000000005
393ed72700000000000000000000000000000000000000000000000000053754e8d300000
0000000000000000000000000000000000000000000005355001010000000000000000000
0000000000000000000000000000000053330f6dd0000000000000000000000000000000
0000000000000000000530f8ac760000000000000000000000000000000000000000000000
00000000052ea80e5e0000000000000000000000000000000000000000000000000052c4
013460000000000000000000000000000000000000000000000529c1bb9a00000000
0000000000000000000000000000000000000000005272e11160000000000000000000000
0000000000000000000000000000000524862653000000000000000000000000000000000000
0000000000000000000521cb165c0000000000000000000000000000000000000000000000000
0000000051efe043200000000000000000000000000000000000000000000000051c201
a560000000000000000000000000000000000000000000519328a4b00000000000

0000000000000000000000000000000000000000000516368c190000000000000000000000
0000000000000000000000000000005132d5dc8000000000000000000000000000000000000
00000000000000000005101842e0000000000000000000000000000000000000000000000000
00000050cf883dc000000000000000000000000000000000000000000000000000509cf6da
a0000000000000000000000000000000000000000000000000005069e5116000000000000
0000000000000000000000000000000000000000503668248000000000000000000000000
0000000000000000000000000000050029582e000000000000000000000000000000000000
000000000000000004fce82bf2000000000000000000000000000000000000000000000000
0004f9a4586b000000000000000000000000000000000000000000000004f65f3987000
0000000000000000000000000000000000000000000000004f31a2bc200000000000000000
0000000000000000000000000000000000004efd68b8f000000000000000000000000000000
00000000000000000000004ec95b4c8000000000000000000000000000000000000000000
000000000004e959021f000000000000000000000000000000000000000000000004e6
21cc8c000000000000000000000000000000000000000000000004e2f16ac000000000
0000000000000000000000000000000000000000000004dfc9309200000000000000000000
0000000000000000000000000004dcaa6e75000000000000000000000000000000000000
000000000000000004d99670eb000000000000000000000000000000000000000000000000
00000004d68e7ffb000000000000000000000000000000000000000000000004d393de
a70000000000000000000000000000000000000000000000004d0a7ca6700000000000
0000000000000000000000000000000000004cdcb7aa400000000000000000000000000
0000000000000000000000000004cb00203700000000000000000000000000000000000000
000000000000000004c846e4ea000000000000000000000000000000000000000000000000
000004c5a0eafa000000000000000000000000000000000000000000000004c30f4ca3
0000000000000000000000000000000000000000000000004c0931ba50000000000000
0000000000000000000000000000000000000004be2d60d600000000000000000000000000
0000000000000000000000000004bbdf1bb2000000000000000000000000000000000000000
000000000000004b9a941f1000000000000000000000000000000000000000000000000000
04b78cbf2000000000000000000000000000000000000000000000004b58a743f0000
0000000000000000000000000000000000000000000004b3a337680000000000000000
0000000000000000000000000000000004b1d7d36c000000000000000000000000000000
0000000000000000000000004b0290788000000000000000000000000000000000000000
0000000000004ae97871200000000000000000000000000000000000000000000000000004
ad23f92c000000000000000000000000000000000000000000004abcef883000000
0000000000000000000000000000000000000000000004aa991309000000000000000000
0000000000000000000000000000000004a982c9c1000000000000000000000000000000
0000000000000000000004a88c908300000000000000000000000000000000000000000000
00000000004a7b6cdcd000000000000000000000000000000000000000000000000004a7
01da9c000000000000000000000000000000000000000000000004a66e02440000000
0000000000000000000000000000000000000000004a5fb82500000000000000000000000
0000000000000000000000000004a5aa8a6a000000000000000000000000000000000000
0000000000000000000004a57b3c47000000000000000000000000000000000000000000
000000004a56dab970000000000000000000000000000000000000000000000004a581
de010000000000000000000000000000000000000000000004a5b7cb1c000000000
0000000000000000000000000000000000000004a60f5c75000000000000000000000000
0000000000000000000000000004a6886d990000000000000000000000000000000000
0000000000000000004a722cc210000000000000000000000000000000000000000000000
0000004a7de37cb000000000000000000000000000000000000000000000004a8ba62
9200000000000000000000000000000000000000000000000004a9b6f0ce000000000000
0000000000000000000000000000000000000004aad3795f000000000000000000000000
0000000000000000000000000004ac0f85d1000000000000000000000000000000000000
000000000000004ad6a92940000000000000000000000000000000000000000000000000
004aee40f300000000000000000000000000000000000000000000004b07b5e80000
0000000000000000000000000000000000000000000004b22fd6f700000000000000000
0000000000000000000000000000000004b400c2e300000000000000000000000000000
0000000000000000000000004b5ed60ba000000000000000000000000000000000000000
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a1672b4000000000000000000000000000000000000000000000000004bc512b78000000
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0000000000000000000000000000000000004c10e590b000000000000000000000000000000
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e61b900000000000000000000000000000000000000000000000004cb8b438b00000000
0000000000000000000000000000000000000000000004ce5a0a900000000000000000000
0000000000000000000000000000000004d1398b9300000000000000000000000000000000
0000000000000000004d428946600000000000000000000000000000000000000000000000
000000004d725ec650000000000000000000000000000000000000000000000004da30
54f70000000000000000000000000000000000000000000000004dd468a130000000000
0000000000000000000000000000000000000000004e06742c700000000000000000000
0000000000000000000000000000004e39131be000000000000000000000000000000000
0000000000000000004e6c305d000000000000000000000000000000000000000000000000
0000004e9fb6a8c000000000000000000000000000000000000000000000004ed3908c
2000000000000000000000000000000000000000000000004f07a87190000000000000
0000000000000000000000000000000000000004f3be8a990000000000000000000000000
0000000000000000000000004f703b73e000000000000000000000000000000000000000
00000000000004fa48b0870000000000000000000000000000000000000000000000000000
4fd8c1a0c000000000000000000000000000000000000000000000500cc980600000
0000000000000000000000000000000000000000000050408cfea0000000000000000000
0000000000000000000000000000000005073f68f2000000000000000000000000000000
0000000000000000000050a6f0cb000000000000000000000000000000000000000000000000
0000000050d96679a000000000000000000000000000000000000000000000000510b4
299b000000000000000000000000000000000000000000000513c7069c000000000
0000000000000000000000000000000000000516cdb70d0000000000000000000000
0000000000000000000000000000000519c6f87200000000000000000000000000000000
0000000000000000051cb18de60000000000000000000000000000000000000000000000
00000051f8c409f000000000000000000000000000000000000000000000052255e06f
0000000000000000000000000000000000000000000005250d44470000000000000
0000000000000000000000000000000000000527b14aaa000000000000000000000000
0000000000000000000000000052a40da3000000000000000000000000000000000000
0000000000000052cbae1f10000000000000000000000000000000000000000000000000
0052f1e5a000000000000000000000000000000000000000000005316a43d1000
0000000000000000000000000000000000000000000005339daaa70000000000000000
0000000000000000000000000000000000000535b7a3f900000000000000000000000000
0000000000000000000000537b74fd60000000000000000000000000000000000000000000
00000000005399bd93e000000000000000000000000000000000000000000000000053
b64767c000000000000000000000000000000000000000000053d10697b000000
0000000000000000000000000000000000000000000053e9f00180000000000000000000
0000000000000000000000000005400f946400000000000000000000000000000000000000
0000000000000000000541618cf10000000000000000000000000000000000000000000000
0000000542945d0e000000000000000000000000000000000000000000000543a78
503000000000000000000000000000000000000000000005449a92450000000000
0000000000000000000000000000000000000005456d1fa700000000000000000000000000
0000000000000000000000000005461ed582000000000000000000000000000000000000
0000000000000000546af69dc000000000000000000000000000000000000000000000000000
00005471ea086000000000000000000000000000000000000000000000005476c4b34
0000000000000000000000000000000000000000000000005479849910000000000000
0000000000000000000000000000000000000547a2894d000000000000000000000000
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21f909f0000000000000000000000000000000000000000000000000000540e072970000000
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00000000000000000053c6bbbe0000000000000000000000000000000000000000000000000
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43d3000000000000000000000000000000000000000000005092f7f580000000000
0000000000000000000000000000000000000505fcf710000000000000000000000000
0000000000000000000000000000502c3ffb70000000000000000000000000000000000
0000000000000004ff85f0ba0000000000000000000000000000000000000000000000000
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0000000000000000000000000000000000000004f5babc7a000000000000000000
0000000000000000000000000000004f275db0800000000000000000000000000000000
0000000000000000004ef32ab8e0000000000000000000000000000000000000000000000
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fee0000000000000000000000000000000000000000004e580d6be000000000000
0000000000000000000000000000000004e251f456000000000000000000000000000000
0000000000000000000000004df2b7bed0000000000000000000000000000000000000000
0000000000000004dc0ebd3c0000000000000000000000000000000000000000000000000
0004d8fd03ef0000000000000000000000000000000000000000000004d5f79719000
0000000000000000000000000000000000000004d2ffb8b100000000000000000
0000000000000000000000000000000004d016a5090000000000000000000000000000
0000000000000000000004cd3d924a0000000000000000000000000000000000000000000
0000000004ca75aff3000000000000000000000000000000000000000000004c
7c0265d0000000000000000000000000000000000000000004c51e163d000000
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0000000000000000000000000004c018bc32000000000000000000000000000000000
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00000000004bb6dfd380000000000000000000000000000000000000000004b93
d0b900000000000000000000000000000000000000000004b7259de500000000
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0000000000000000000000000004b346bf150000000000000000000000000000000000
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de0000000000000000000000000000000000000000000004acde8da700000000000
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575e7f0000000000000000000000000000000000000000000000000004a56ef9330000000
0000000000000000000000000000000000000000000004a589cd0400000000000000000000
0000000000000000000000000000000004a5c6583800000000000000000000000000000000
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0000000000000004b45f60070000000000000000000000000000000000000000000000000000
004b65156f3000000000000000000000000000000000000000000004b85e091c000
0000000000000000000000000000000000000004ba849c170000000000000000
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ff3000000000000000000000000000000000000000000004ea9e069800000000000
0000000000000000000000000000000000000004eddc8308000000000000000000000000
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0000000000000004f462f4e8000000000000000000000000000000000000000000000000000
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0000000000000000000000000000000000000000000004fe2feb4b000000000000000
0000000000000000000000000000000005016fada400000000000000000000000000000000
0000000000000000000000504aae6030000000000000000000000000000000000000000000
0000000000507e03c0d0000000000000000000000000000000000000000000000000000050
b0e59da0000000000000000000000000000000000000000000000050e33ec83000000
0000000000000000000000000000000000000005114fa4b000000000000000000000
0000000000000000000000000000000051460372400000000000000000000000000000000
0000000000000000000000517645d43000000000000000000000000000000000000000000
00000000051a5ad5a0000000000000000000000000000000000000000000000051d4
2647e0000000000000000000000000000000000000000000000052019d45600000000
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0000000000000000000000000054592a31b000000000000000000000000000000000000000000
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0000000000000000000000000000000000000000000051afb65aa00000000000000000
0000000000000000000000000000000000000051808049f000000000000000000000000000000
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df3c7c000000000000000000000000000000000000000000000050bbbaa0900000000
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00000004fee2644b000000000000000000000000000000000000000000000004fba003
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0000000000000000000000000000000000000004f51642bb000000000000000000000000000
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0000000000000000000000000000000000000000000004e4e026fc00000000000000000
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0000000000000000000000000000000000000004a6c3cd6d00000000000000000000
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0000000000000000000000000000000000000004a593092e000000000000000000000
0000000000000000000000000004a5d631830000000000000000000000000000000000
000000000000000004a63af16f000000000000000000000000000000000000000000000
000004a6c11f0100000000000000000000000000000000000000000004a768825e
0000000000000000000000000000000000000000000000004a830d5d70000000000000
0000000000000000000000000000000000000004a919c609000000000000000000000000
0000000000000000000000004aa22f1fb000000000000000000000000000000000000000
000000000000004ab4beb4c000000000000000000000000000000000000000000000000
004ac94365a"
    },
    "subtraces": 0,
    "traceAddress": [],
    "transactionHash":
"0x36b510f3bdb2fa67a0d4f749899ab8630b54000ee5a211172d699d750f94f94f",
    "transactionPosition": 10,
    "type": "call"
  }
]

Molecular Dynamics C# Source Code

```
using System;
using System.Collections.Generic;

namespace DiatomicMD.CommandLine
{
   class Program
   {
      static void Main(string[] args)
      {
         var proc = new DiatomicMD();
         var res = proc.RunMD();
         foreach (var result in res) Console.WriteLine(result);
         Console.ReadKey();
      }
   }

   /// <summary>
   /// Initializes a diatomic molecular dynamics trajectory for the carbon monoxide molecule run with a variation of the velocity Verlet algorithm used to integrate Newton's equations of motion in atomic units.
   /// </summary>
   public class DiatomicMD
   {
      public DiatomicMD()
      {
         R1 = 2.26767135; // !initial bond length in a0(120.0 pm)
         TMax = 400; // !total number of time steps
         R2 = 0;
         V1 = 0;
         V2 = 0;
      }

      public const double Re = 2.1316; // !equilibrium bond length in a0(112.8 pm)
      public const double K = 1.1915; // !reciprocal force constant in a_0 ^ 2 / Eh(19.02 N / cm)
      public const double M1 = 21875; // !mass of atom one in m_e(Carbon)
      public const double M2 = 29156.9457; // !mass of atom two in m_e(Oxygen)
      public const double DT = 4.13; // !0.1 fs time step in hbar / Eh
      public static double dTbyM1x2 => DT / (M1 * 2);
      public static double dTbyM2x2 => DT / (M2 * 2);
      public static double dTdTbyM1x2 => (DT * DT) / (M1 * 2);
      public static double dTdTbyM2x2 => (DT * DT) / (M2 * 2);

      public double Rmag { get; set; }
      public double R { get; set; }
      public double R1 { get; set; }
      public double R2 { get; set; }
      public double V1 { get; set; }
      public double V2 { get; set; }
      public double F { get; set; }
      public double FNew { get; set; }
      public double T { get; set; }
      public double TMax { get; set; }

      /// <summary>
```

```
        /// Executes a diatomic molecular dynamics trajectory for the carbon monoxide molecule run with a variation of the velocity Verlet algorithm used to integrate Newton's equations of motion in atomic units.
        /// </summary>
        /// <returns></returns> A list of doubles representing the carbon monoxide bond length in atomic units.
        public List<double> RunMD()
        {
            var res = new List<double>();
            T = 0;
            while (T < TMax)
            {
                R = R1 - R2;
                Rmag = Math.Abs(R);
                F = -K * (Rmag - Re) * R / Rmag;
                R1 = R1 + DT * V1 + dTdTbyM1x2 * F;
                R2 = R2 + DT * V2 - dTdTbyM2x2 * F;

                R = R1 - R2;
                Rmag = Math.Abs(R);

                FNew = -K * (Rmag - Re) * R / Rmag;

                V1 = V1 + dTbyM1x2 * (FNew + F);
                V2 = V2 - dTbyM2x2 * (FNew + F);

                res.Add(Rmag);
                T++;
            }
            return res;
        }
    }
}
```

Molecular Dynamics Solidity Source Code
The Solidity source code for the molecular dynamics simulation that was used to run these simulations on the Ethereum blockchain is given here:

```
pragma solidity ^0.5.16;
import "github.com/abdk-consulting/abdk-libraries-solidity/ABDKMathQuad.sol";
/**
* Copyright (c) 2019, ABDK Consulting

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**/

/// @title Diatomic Molecular Dynamics
/// @notice A diatomic molecular dynamics trajectory for the carbon monoxide molecule run with a variation of the velocity Verlet algorithm used to integrate Newton's equations of motion in atomic units.
/// @author Alex Ashmore <kezyma@yahoo.co.uk>, Magnus Hanson-Heine <magnus.hansonheine@gmail.com>
contract DiatomicMD {

    bytes16 constant Re = 0x400010d844d013a92a305532617c1bda;
// 2.1316      - equilibrium bond length in a_0 (112.8 pm)
    bytes16 constant K = 0x3fff310624dd2f1a9fbe76c8b4395810;
// 1.1915      - force constant in Eh/a_0^2 (18.55 N/cm)
    bytes16 constant M1 = 0x400d55cc000000000000000000000000;
// 21875       - mass of atom one in m_e (Carbon)
    bytes16 constant M2 = 0x400dc793c86594af4f0d844d013a92a3;
// 29156.9457  - mass of atom two in m_e (Oxygen)
    bytes16 constant dT = 0x40010851eb851eb851eb851eb851eb85;
// 4.13        - 0.1 fs time step in hbar/E_h
    bytes16 constant dTdTbyM1x2 = 0x3ff398cf77d58230a4ec10bd70161b26;
// ((dT*dT)/(M1*2))
    bytes16 constant dTdTbyM2x2 = 0x3ff332b5c5317be96318c8a728b2194e;
```

```
// ((dT*dT)/(M2*2))
    bytes16 constant dTbyM1x2 = 0x3ff18bf13a6a5f196b0b10d53a599821;
// (dT/(M1*2))
    bytes16 constant dTbyM2x2 = 0x3ff1290e444148485119dcfda2c40c1e;
// (dT/(M2*2))

    /// @notice Initializes a molecular dynamics trajectory
    /// @param steps Number of steps in time in units of 0.1 femtosecond
    /// @param precision Number of decimal places to include in output
    function runMD(uint256 steps, uint precision) public returns (int256[] memory) {

        bytes16 r1 = 0x400022430e0729bfecea7985fddb6291; // 2.26767135  - initial bond length in
a_0 (120.0 pm)
        bytes16 r2 = 0x00000000000000000000000000000000; // 0
        bytes16 v1 = 0x00000000000000000000000000000000; // 0
        bytes16 v2 = 0x00000000000000000000000000000000; // 0

        bytes16 r;
        bytes16 rMag;
        bytes16 f;
        bytes16 fNew;

        uint256 t = 0;

        uint ten = 10;
        uint multiplier = ten**precision;
        bytes16 convertedMultiplier = ABDKMathQuad.fromUInt(multiplier);
        int256[] memory results = new int256[](steps);

        while (t < steps) {
            r = ABDKMathQuad.sub(r1,r2);
            rMag = ABDKMathQuad.abs(r);

            f                                                                                   =
ABDKMathQuad.div(ABDKMathQuad.mul(ABDKMathQuad.mul(ABDKMathQuad.neg(K),ABDKM
athQuad.sub(rMag,Re)),r),rMag);

            r1                                                                                  =
ABDKMathQuad.add(ABDKMathQuad.add(r1,ABDKMathQuad.mul(dT,v1)),ABDKMathQuad.mul(
dTdTbyM1x2,f));
            r2        =        ABDKMathQuad.sub(ABDKMathQuad.add(r2,ABDKMathQuad.mul(dT,v2)),
ABDKMathQuad.mul(dTdTbyM2x2,f));

            r = ABDKMathQuad.sub(r1,r2);
            rMag = ABDKMathQuad.abs(r);

            fNew                                                                                =
ABDKMathQuad.div(ABDKMathQuad.mul(ABDKMathQuad.mul(ABDKMathQuad.neg(K),ABDKM
athQuad.sub(rMag,Re)),r),rMag);

            v1                                                                                  =
ABDKMathQuad.add(v1,ABDKMathQuad.mul(dTbyM1x2,ABDKMathQuad.add(fNew,f)));
            v2                                                                                  =
ABDKMathQuad.sub(v2,ABDKMathQuad.mul(dTbyM2x2,ABDKMathQuad.add(fNew,f)));

            results[t] = ABDKMathQuad.toInt(ABDKMathQuad.mul(rMag, convertedMultiplier));
```

```
            t = t + 1;
        }
        return results;
    }
}
```

Molecular Dynamics Solidity Source Code Upload Transaction Details
The details of the transaction in which the Solidity source code for the molecular dynamics simulation was uploaded onto the Ethereum blockchain are presented here:

Block Number: 9360156
Hash: 0x1c98dbb671dbe76b7cb4188d7585296e5adbe0f64fe8144546b4a82081089152
Time Stamp: 01/26/2020 10:25:44 PM Greenwich Mean Time (GMT)
From: 0xC120A82d25325c9700652D6f2288EBD2C4224567
To: 0x9680E167F6221ea0A9dcE066A4f9c769621bC577
Fee: 0.00091 ETH (ca. $0.15)
Gas Price: 0.0000000011 ETH
Gas Used: 825,151

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    },
    "subtraces": 0,
    "traceAddress": [],
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    "transactionPosition": 56,
    "type": "create"
  }
]

Table S1. Calculated bond lengths (a_0) and simulation times (fs) for the preliminary run molecular dynamics trajectory of 10 steps when run on Ethereum network using the Solidity language and on a local computer using the C# language.

Time	Bond Length (Solidity)	Bond Length (C#)
0.1	2.2675607174	2.2675607175
0.2	2.2672289997	2.2672289997
0.3	2.2666767362	2.2666767362
0.4	2.2659048249	2.2659048250
0.5	2.2649145212	2.2649145212
0.6	2.2637074352	2.2637074352
0.7	2.2622855298	2.2622855298
0.8	2.2606511172	2.2606511173
0.9	2.2588068551	2.2588068552
1.0	2.2567557424	2.2567557425

Column 1 shows the elapsed simulation time in fs. Columns 2-3 show the calculated carbon-oxygen bond lengths (in a_0) predicted by the Solidity and C# implementations of the trajectory, respectively.

Table S2. Ccalculated bond lengths (a_0) and simulation times (fs) for the production run molecular dynamics trajectory of 400 steps when run on Ethereum network using the Solidity language and on a local computer using the C# language.

Time	Bond Length (Solidity)	Bond Length (C#)
0.1	2.2675607174	2.2675607175
0.2	2.2672289997	2.2672289997
0.3	2.2666767362	2.2666767362
0.4	2.2659048249	2.2659048250
0.5	2.2649145212	2.2649145212
0.6	2.2637074352	2.2637074352
0.7	2.2622855298	2.2622855298
0.8	2.2606511172	2.2606511173
0.9	2.2588068551	2.2588068552
1.0	2.2567557424	2.2567557425
1.1	2.2545011145	2.2545011146
1.2	2.2520466376	2.2520466376
1.3	2.2493963029	2.2493963029
1.4	2.2465544200	2.2465544201
1.5	2.2435256103	2.2435256103
1.6	2.2403147987	2.2403147988
1.7	2.2369272065	2.2369272066
1.8	2.2333683421	2.2333683422
1.9	2.2296439926	2.2296439927
2.0	2.2257602142	2.2257602142
2.1	2.2217233222	2.2217233222
2.2	2.2175398810	2.2175398811
2.3	2.2132166934	2.2132166934
2.4	2.2087607891	2.2087607892
2.5	2.2041794140	2.2041794141
2.6	2.1994800178	2.1994800179
2.7	2.1946702422	2.1946702423
2.8	2.1897579083	2.1897579084
2.9	2.1847510041	2.1847510041
3.0	2.1796576712	2.1796576713
3.1	2.1744861920	2.1744861920
3.2	2.1692449756	2.1692449757
3.3	2.1639425450	2.1639425450
3.4	2.1585875222	2.1585875223
3.5	2.1531886152	2.1531886152
3.6	2.1477546030	2.1477546030
3.7	2.1422943218	2.1422943218
3.8	2.1368166507	2.1368166507
3.9	2.1313304967	2.1313304968
4.0	2.1258447810	2.1258447811
4.1	2.1203684239	2.1203684240
4.2	2.1149103304	2.1149103304
4.3	2.1094793759	2.1094793759
4.4	2.1040843916	2.1040843917
4.5	2.0987341504	2.0987341504
4.6	2.0934373522	2.0934373522
4.7	2.0882026101	2.0882026101
4.8	2.0830384363	2.0830384364
4.9	2.0779532283	2.0779532284

5.0	2.0729552551	2.0729552552
5.1	2.0680526439	2.0680526440
5.2	2.0632533668	2.0632533669
5.3	2.0585652279	2.0585652280
5.4	2.0539958506	2.0539958506
5.5	2.0495526650	2.0495526650
5.6	2.0452428963	2.0452428963
5.7	2.0410735525	2.0410735526
5.8	2.0370514134	2.0370514135
5.9	2.0331830194	2.0331830195
6.0	2.0294746609	2.0294746609
6.1	2.0259323680	2.0259323680
6.2	2.0225619007	2.0225619008
6.3	2.0193687400	2.0193687400
6.4	2.0163580780	2.0163580780
6.5	2.0135348104	2.0135348105
6.6	2.0109035282	2.0109035282
6.7	2.0084685100	2.0084685101
6.8	2.0062337155	2.0062337155
6.9	2.0042027785	2.0042027786
7.0	2.0023790017	2.0023790018
7.1	2.0007653507	2.0007653507
7.2	1.9993644493	1.9993644494
7.3	1.9981785756	1.9981785757
7.4	1.9972096580	1.9972096581
7.5	1.9964592720	1.9964592721
7.6	1.9959286378	1.9959286379
7.7	1.9956186183	1.9956186183
7.8	1.9955297175	1.9955297176
7.9	1.9956620801	1.9956620801
8.0	1.9960154908	1.9960154908
8.1	1.9965893749	1.9965893750
8.2	1.9973827993	1.9973827993
8.3	1.9983944737	1.9983944737
8.4	1.9996227531	1.9996227531
8.5	2.0010656402	2.0010656402
8.6	2.0027207886	2.0027207887
8.7	2.0045855071	2.0045855071
8.8	2.0066567633	2.0066567633
8.9	2.0089311892	2.0089311892
9.0	2.0114050864	2.0114050864
9.1	2.0140744320	2.0140744321
9.2	2.0169348855	2.0169348856
9.3	2.0199817955	2.0199817956
9.4	2.0232102074	2.0232102075
9.5	2.0266148715	2.0266148716
9.6	2.0301902516	2.0301902516
9.7	2.0339305336	2.0339305336
9.8	2.0378296355	2.0378296356
9.9	2.0418812171	2.0418812171
10.0	2.0460786900	2.0460786900
10.1	2.0504152287	2.0504152288
10.2	2.0548837817	2.0548837818

10.3	2.0594770827	2.0594770827
10.4	2.0641876624	2.0641876625
10.5	2.0690078611	2.0690078611
10.6	2.0739298406	2.0739298406
10.7	2.0789455973	2.0789455973
10.8	2.0840469751	2.0840469752
10.9	2.0892256787	2.0892256788
11.0	2.0944732871	2.0944732871
11.1	2.0997812670	2.0997812670
11.2	2.1051409872	2.1051409873
11.3	2.1105437324	2.1105437324
11.4	2.1159807170	2.1159807171
11.5	2.1214431001	2.1214431002
11.6	2.1269219993	2.1269219994
11.7	2.1324085054	2.1324085054
11.8	2.1378936967	2.1378936968
11.9	2.1433686540	2.1433686540
12.0	2.1488244742	2.1488244743
12.1	2.1542522858	2.1542522859
12.2	2.1596432626	2.1596432627
12.3	2.1649886384	2.1649886384
12.4	2.1702797210	2.1702797211
12.5	2.1755079067	2.1755079068
12.6	2.1806646940	2.1806646940
12.7	2.1857416973	2.1857416973
12.8	2.1907306610	2.1907306611
12.9	2.1956234726	2.1956234726
13.0	2.2004121759	2.2004121759
13.1	2.2050889839	2.2050889840
13.2	2.2096462919	2.2096462919
13.3	2.2140766890	2.2140766891
13.4	2.2183729712	2.2183729712
13.5	2.2225281521	2.2225281522
13.6	2.2265354752	2.2265354752
13.7	2.2303884241	2.2303884241
13.8	2.2340807335	2.2340807335
13.9	2.2376063993	2.2376063994
14.0	2.2409596886	2.2409596887
14.1	2.2441351486	2.2441351486
14.2	2.2471276156	2.2471276156
14.3	2.2499322235	2.2499322236
14.4	2.2525444120	2.2525444120
14.5	2.2549599332	2.2549599332
14.6	2.2571748593	2.2571748593
14.7	2.2591855886	2.2591855887
14.8	2.2609888515	2.2609888516
14.9	2.2625817157	2.2625817158
15.0	2.2639615911	2.2639615912
15.1	2.2651262338	2.2651262339
15.2	2.2660737500	2.2660737501
15.3	2.2668025990	2.2668025991
15.4	2.2673115956	2.2673115957
15.5	2.2675999121	2.2675999122

15.6	2.2676670797	2.2676670798
15.7	2.2675129892	2.2675129892
15.8	2.2671378911	2.2671378911
15.9	2.2665423953	2.2665423954
16.0	2.2657274703	2.2657274703
16.1	2.2646944411	2.2646944412
16.2	2.2634449876	2.2634449876
16.3	2.2619811415	2.2619811415
16.4	2.2603052831	2.2603052831
16.5	2.2584201375	2.2584201376
16.6	2.2563287703	2.2563287703
16.7	2.2540345821	2.2540345821
16.8	2.2515413035	2.2515413035
16.9	2.2488529888	2.2488529888
17.0	2.2459740095	2.2459740095
17.1	2.2429090471	2.2429090471
17.2	2.2396630854	2.2396630855
17.3	2.2362414029	2.2362414029
17.4	2.2326495633	2.2326495634
17.5	2.2288934075	2.2288934076
17.6	2.2249790432	2.2249790433
17.7	2.2209128357	2.2209128358
17.8	2.2167013969	2.2167013970
17.9	2.2123515751	2.2123515751
18.0	2.2078704434	2.2078704435
18.1	2.2032652887	2.2032652888
18.2	2.1985435993	2.1985435994
18.3	2.1937130533	2.1937130533
18.4	2.1887815054	2.1887815055
18.5	2.1837569749	2.1837569750
18.6	2.1786476322	2.1786476322
18.7	2.1734617855	2.1734617855
18.8	2.1682078675	2.1682078675
18.9	2.1628944216	2.1628944216
19.0	2.1575300880	2.1575300880
19.1	2.1521235895	2.1521235896
19.2	2.1466837178	2.1466837178
19.3	2.1412193184	2.1412193185
19.4	2.1357392771	2.1357392772
19.5	2.1302525050	2.1302525051
19.6	2.1247679240	2.1247679241
19.7	2.1192944526	2.1192944527
19.8	2.1138409913	2.1138409913
19.9	2.1084164078	2.1084164078
20.0	2.1030295230	2.1030295230
20.1	2.0976890966	2.0976890966
20.2	2.0924038125	2.0924038126
20.3	2.0871822652	2.0871822653
20.4	2.0820329455	2.0820329455
20.5	2.0769642265	2.0769642265
20.6	2.0719843505	2.0719843505
20.7	2.0671014153	2.0671014153
20.8	2.0623233610	2.0623233610

20.9	2.0576579571	2.0576579572
21.0	2.0531127901	2.0531127902
21.1	2.0486952509	2.0486952509
21.2	2.0444125227	2.0444125228
21.3	2.0402715698	2.0402715698
21.4	2.0362791256	2.0362791257
21.5	2.0324416824	2.0324416824
21.6	2.0287654800	2.0287654801
21.7	2.0252564965	2.0252564966
21.8	2.0219204378	2.0219204378
21.9	2.0187627285	2.0187627286
22.0	2.0157885035	2.0157885035
22.1	2.0130025991	2.0130025991
22.2	2.0104095454	2.0104095455
22.3	2.0080135591	2.0080135591
22.4	2.0058185362	2.0058185362
22.5	2.0038280460	2.0038280460
22.6	2.0020453253	2.0020453253
22.7	2.0004732729	2.0004732730
22.8	1.9991144452	1.9991144452
22.9	1.9979710517	1.9979710518
23.0	1.9970449517	1.9970449518
23.1	1.9963376512	1.9963376512
23.2	1.9958503002	1.9958503002
23.3	1.9955836912	1.9955836913
23.4	1.9955382579	1.9955382579
23.5	1.9957140740	1.9957140740
23.6	1.9961108536	1.9961108537
23.7	1.9967279516	1.9967279517
23.8	1.9975643646	1.9975643646
23.9	1.9986187323	1.9986187323
24.0	1.9998893403	1.9998893404
24.1	2.0013741226	2.0013741226
24.2	2.0030706646	2.0030706646
24.3	2.0049762076	2.0049762077
24.4	2.0070876531	2.0070876531
24.5	2.0094015676	2.0094015677
24.6	2.0119141885	2.0119141886
24.7	2.0146214300	2.0146214301
24.8	2.0175188900	2.0175188900
24.9	2.0206018567	2.0206018568
25.0	2.0238653171	2.0238653172
25.1	2.0273039644	2.0273039645
25.2	2.0309122071	2.0309122072
25.3	2.0346841779	2.0346841779
25.4	2.0386137430	2.0386137431
25.5	2.0426945128	2.0426945128
25.6	2.0469198513	2.0469198514
25.7	2.0512828880	2.0512828880
25.8	2.0557765280	2.0557765280
25.9	2.0603934642	2.0603934643
26.0	2.0651261891	2.0651261892
26.1	2.0699670068	2.0699670068

26.2	2.0749080457	2.0749080457
26.3	2.0799412711	2.0799412711
26.4	2.0850584986	2.0850584986
26.5	2.0902514070	2.0902514070
26.6	2.0955115522	2.0955115522
26.7	2.1008303807	2.1008303807
26.8	2.1061992435	2.1061992436
26.9	2.1116094104	2.1116094105
27.0	2.1170520840	2.1170520840
27.1	2.1225184138	2.1225184138
27.2	2.1279995112	2.1279995112
27.3	2.1334864633	2.1334864633
27.4	2.1389703478	2.1389703479
27.5	2.1444422475	2.1444422475
27.6	2.1498932644	2.1498932644
27.7	2.1553145347	2.1553145347
27.8	2.1606972429	2.1606972429
27.9	2.1660326362	2.1660326362
28.0	2.1713120387	2.1713120388
28.1	2.1765268656	2.1765268657
28.2	2.1816686372	2.1816686372
28.3	2.1867289923	2.1867289923
28.4	2.1916997024	2.1916997024
28.5	2.1965726846	2.1965726846
28.6	2.2013400150	2.2013400150
28.7	2.2059939414	2.2059939414
28.8	2.2105268961	2.2105268961
28.9	2.2149315081	2.2149315082
29.0	2.2192006151	2.2192006151
29.1	2.2233272751	2.2233272751
29.2	2.2273047777	2.2273047777
29.3	2.2311266551	2.2311266552
29.4	2.2347866927	2.2347866927
29.5	2.2382789387	2.2382789388
29.6	2.2415977146	2.2415977147
29.7	2.2447376237	2.2447376237
29.8	2.2476935601	2.2476935601
29.9	2.2504607172	2.2504607172
30.0	2.2530345954	2.2530345954
30.1	2.2554110092	2.2554110093
30.2	2.2575860945	2.2575860946
30.3	2.2595563143	2.2595563144
30.4	2.2613184648	2.2613184649
30.5	2.2628696807	2.2628696808
30.6	2.2642074395	2.2642074395
30.7	2.2653295658	2.2653295658
30.8	2.2662342350	2.2662342350
30.9	2.2669199760	2.2669199761
31.0	2.2673856737	2.2673856738
31.1	2.2676305709	2.2676305710
31.2	2.2676542694	2.2676542694
31.3	2.2674567305	2.2674567305
31.4	2.2670382755	2.2670382756

31.5	2.2663995849	2.2663995850
31.6	2.2655416972	2.2655416973
31.7	2.2644660075	2.2644660075
31.8	2.2631742649	2.2631742649
31.9	2.2616685698	2.2616685699
32.0	2.2599513708	2.2599513709
32.1	2.2580254602	2.2580254602
32.2	2.2558939696	2.2558939697
32.3	2.2535603651	2.2535603651
32.4	2.2510284413	2.2510284413
32.5	2.2483023154	2.2483023154
32.6	2.2453864203	2.2453864204
32.7	2.2422854976	2.2422854977
32.8	2.2390045896	2.2390045897
32.9	2.2355490315	2.2355490316
33.0	2.2319244423	2.2319244423
33.1	2.2281367158	2.2281367159
33.2	2.2241920115	2.2241920115
33.3	2.2200967436	2.2200967436
33.4	2.2158575715	2.2158575715
33.5	2.2114813885	2.2114813885
33.6	2.2069753107	2.2069753107
33.7	2.2023466654	2.2023466654
33.8	2.1976029792	2.1976029792
33.9	2.1927519658	2.1927519659
34.0	2.1878015135	2.1878015136
34.1	2.1827596721	2.1827596722
34.2	2.1776346402	2.1776346403
34.3	2.1724347516	2.1724347516
34.4	2.1671684617	2.1671684617
34.5	2.1618443341	2.1618443341
34.6	2.1564710262	2.1564710263
34.7	2.1510572757	2.1510572758
34.8	2.1456118859	2.1456118859
34.9	2.1401437113	2.1401437113
35.0	2.1346616438	2.1346616439
35.1	2.1291745979	2.1291745979
35.2	2.1236914958	2.1236914959
35.3	2.1182212537	2.1182212538
35.4	2.1127727668	2.1127727669
35.5	2.1073548948	2.1073548948
35.6	2.1019764476	2.1019764476
35.7	2.0966461711	2.0966461712
35.8	2.0913727330	2.0913727330
35.9	2.0861647082	2.0861647083
36.0	2.0810305656	2.0810305657
36.1	2.0759786538	2.0759786538
36.2	2.0710171876	2.0710171876
36.3	2.0661542348	2.0661542349
36.4	2.0613977032	2.0613977033
36.5	2.0567553273	2.0567553273
36.6	2.0522346559	2.0522346560
36.7	2.0478430403	2.0478430403

36.8	2.0435876214	2.0435876215
36.9	2.0394753192	2.0394753193
37.0	2.0355128206	2.0355128206
37.1	2.0317065689	2.0317065690
37.2	2.0280627535	2.0280627536
37.3	2.0245872997	2.0245872997
37.4	2.0212858588	2.0212858588
37.5	2.0181637992	2.0181637993
37.6	2.0152261978	2.0152261979
37.7	2.0124778314	2.0124778315
37.8	2.0099231691	2.0099231691
37.9	2.0075663650	2.0075663650
38.0	2.0054112515	2.0054112515
38.1	2.0034613330	2.0034613330
38.2	2.0017197803	2.0017197803
38.3	2.0001894252	2.0001894253
38.4	1.9988727565	1.9988727565
38.5	1.9977719149	1.9977719149
38.6	1.9968886907	1.9968886907
38.7	1.9962245199	1.9962245200
38.8	1.9957804828	1.9957804828
38.9	1.9955573012	1.9955573012
39.0	1.9955553380	1.9955553381
39.1	1.9957745966	1.9957745967
39.2	1.9962147203	1.9962147204
39.3	1.9968749935	1.9968749936
39.4	1.9977543425	1.9977543425
39.5	1.9988513374	1.9988513374
39.6	2.0001641943	2.0001641944
39.7	2.0016907785	2.0016907785
39.8	2.0034286075	2.0034286076
39.9	2.0053748556	2.0053748556
40.0	2.0075263578	2.0075263579

Column 1 shows the elapsed simulation time in fs. Columns 2-3 show the calculated carbon-oxygen bond lengths (in a_0) predicted by the Solidity and C# implementations of the trajectory, respectively.