

Supplementary Information for

Irreproducibility in the triboelectric charging of insulators: evidence of a non-monotonic charge versus contact time relationship

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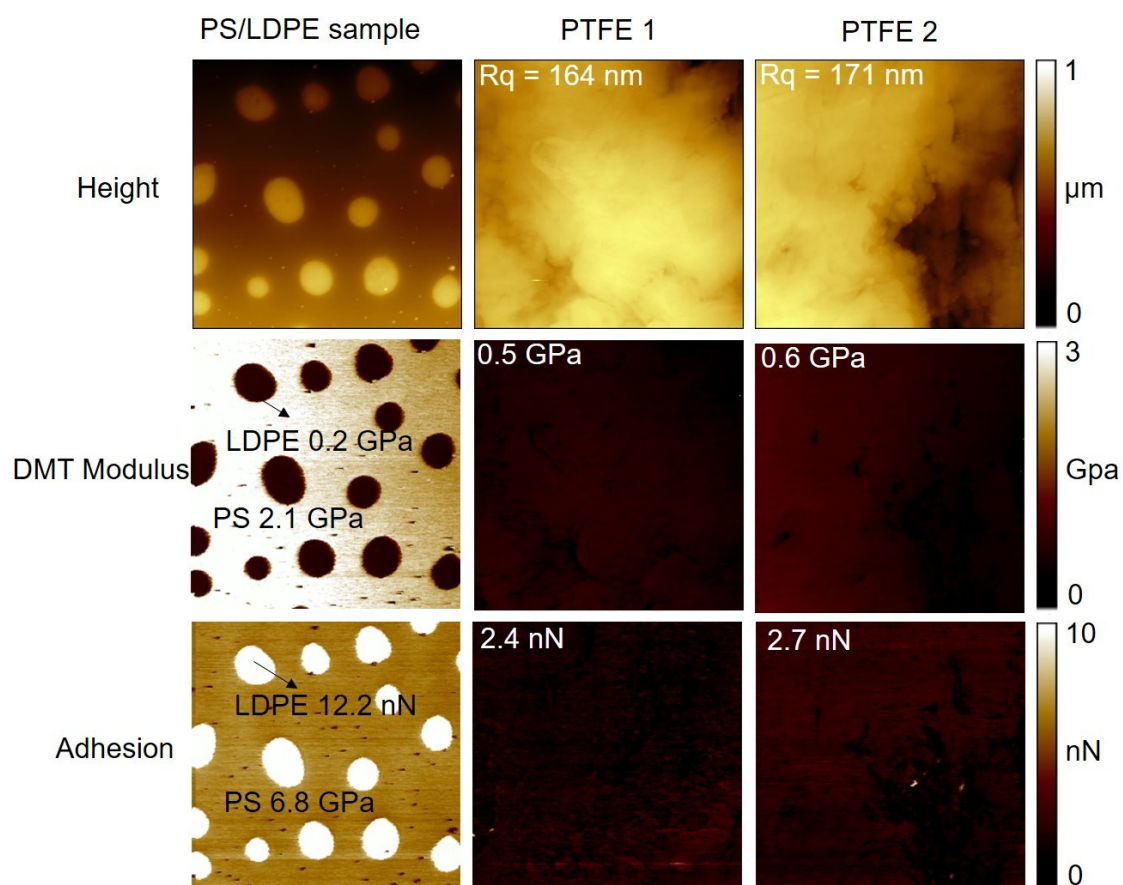


Fig. S1. AFM height images, DMT moduli and surface adhesion data for a standard PS/LDPE reference and PTFE samples. Data are obtained by the AFM Peakforce™ QNM™ mode. Hardness and adhesion are determined with respect to the standard PS and LDPE sample. Imaged areas are $10 \times 10 \mu\text{m}$ for all samples.

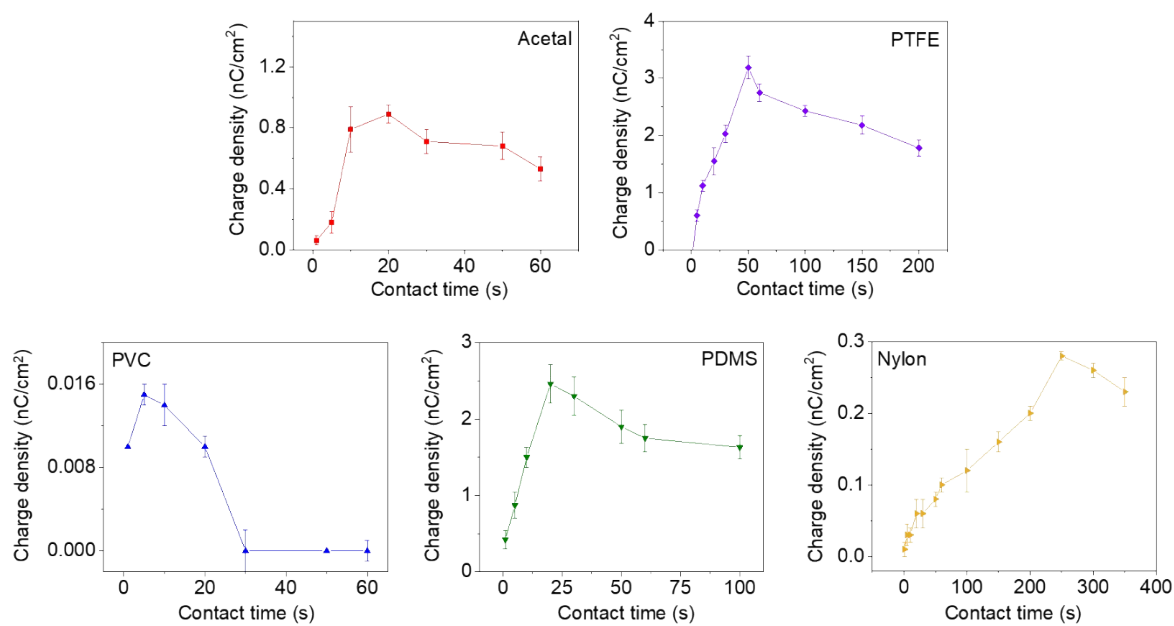


Fig. S2. Evolution with time of the charge density developed on the positive sample of Acetal–Acetal, PTFE–PTFE, PVC–PVC, PDMS–PDMS and Nylon–Nylon dynamic contacts. Error bars shows uncertainty as one standard deviation from the mean of three independently prepared and analyzed samples.

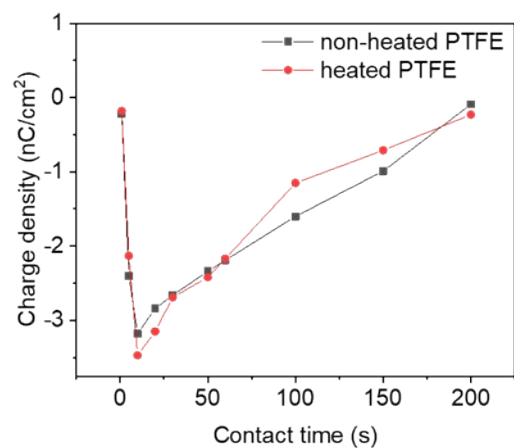


Fig. S3. Faraday pail data showing charge density versus contact time for PTFE–PTFE dynamic contacts, where the samples are either heated (110 °C for 5 min, red trace) or non-heated (black trace) before the tribocharging procedure. Experiments were performed inside a glove box with water and oxygen levels below 1 ppm. The contact time was varied between 0 and 200 s. The glove box temperature is 25 °C.

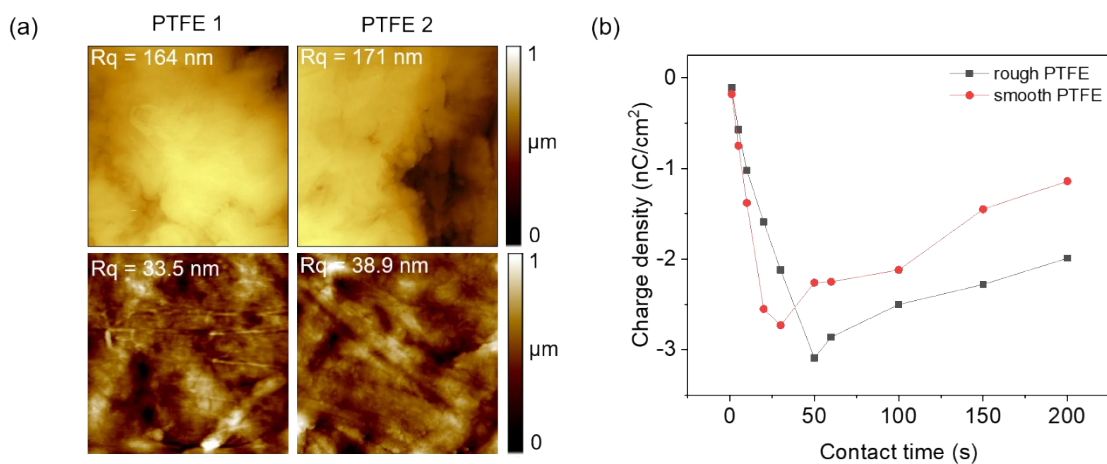


Fig. S4. (a) AFM topography images obtained for PTFE samples of different roughness, which are used as sliding PTFE–PTFE contacts in tribocharging experiments. Roughness values indicated in figure are extracted from unflatten images, and reported as the average root means square surface roughness (R_q , determined using Bruker’s Nanoscope Software). Imaged areas are $10 \times 10 \mu\text{m}$ for all samples. (b) Faraday pail data showing charge density versus contact time for rough (black trace) and smooth PTFE (red trace) samples.

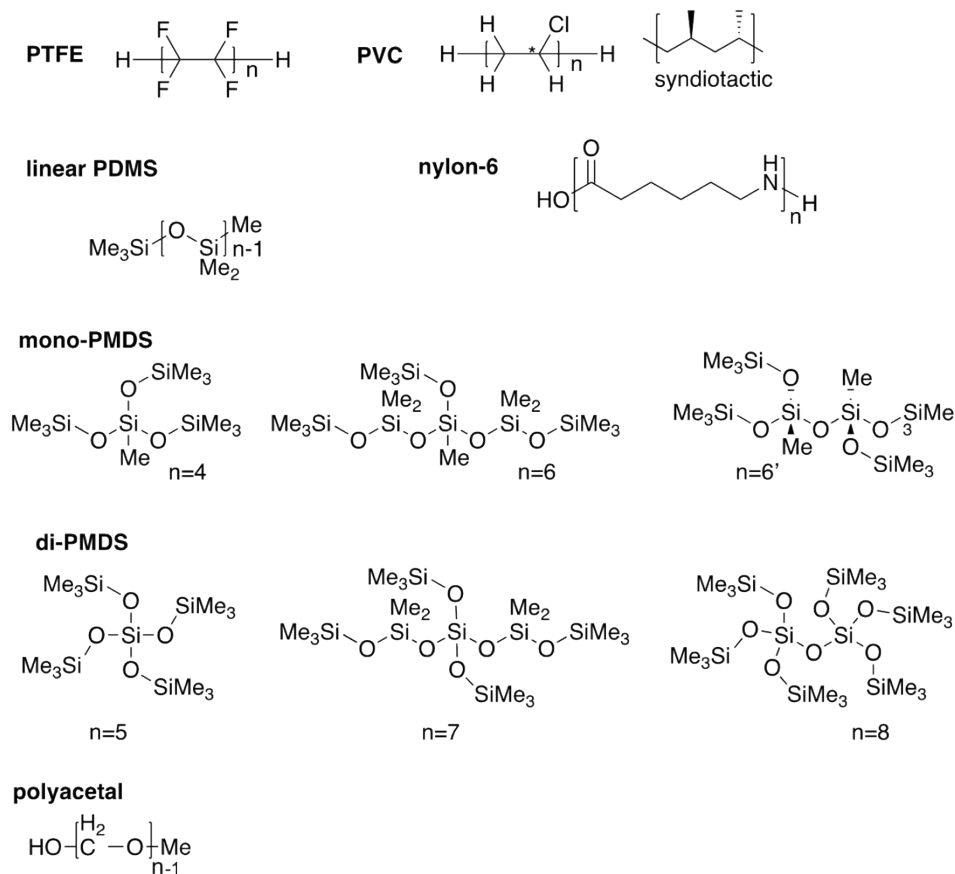


Fig. S5. Chemical structures for the PTFE, PVC, nylon-6, PDMS and polyacetal (Acetal) oligomeric models used in the theoretical calculation of ionization energies and electron affinities.

Table S1. Ionization Energies (IEs) and Electron Affinities (EAs) for polymers

Polymer	n	x	EA (eV)	IE (eV)
PTFE	1	2	-1.57	11.85
	2	4	-1.38	11.70
	3	6	-0.63	11.59
	4	8	-0.32	11.55
	5	10	-0.14	11.54
PVC	1	2	-1.44	11.02
	2	4	-1.20	10.45
	3	6	-0.98	10.41
	4	8	-0.84	10.33
	5	10	-0.74	10.27
nylon-6	1	8	-0.79	8.76
	2	15	-0.91	8.57
	3	22	-0.97	8.52
linear PDMS	1	3	-0.85	9.46
	2	5	-0.79	9.21
	3	7	-0.65	9.08
	4	9	-0.58	8.91
	5	11	-0.53	8.70
polyacetal	1	4	-1.51	10.74
	2	6	-1.36	9.85
	3	8	-1.31	9.68
	4	10	-1.15	9.01
	5	12	-1.05	8.71

x = number of non-hydrogen backbone atoms including end groups¹.

Supporting section. Computational Methodology

Table S2: Calculated H_0 (kJ mol⁻¹), electron affinity (*left*) and Ionisation potential (*right*) (eV).

OLIGOMER	NEUTRAL	CATION	ANION	IP	EA
MONOMER	-303530.2	-302496.9	-303381.3	10.74	-1.51
DIMER	-604027.4	-603079.9	-603893.1	9.85	-1.36
TRIMER	-904521.7	-903590.8	-904392.2	9.68	-1.31
TETRAMER	-1205010.4	-1204144.1	-1204896.4	9.01	-1.15
PENTAMER	-1505500.6	-1504663.1	-1505395.9	8.71	-1.05

We have used the direct as opposed to the thermocycle approach in the calculation of solvent effects in water. Indeed, as shown by Ho and co-workers, the direct solvation method is in fact equivalent to the thermocycle if the level of theory in gas and solvent is unchanged, as is the case here.² Thus, conformer searching was also performed in solvent field, whilst standard state corrections for the change in phase were not added, as these terms cancel in the calculation of reaction Gibbs free energies (ΔG°_{soln}).

Standard reduction potentials E° (volts) for the redox couples (anion/neutral) and (neutral/cation) have been calculated via the Nernst equation³

$$E^\circ = \frac{-\Delta G^\circ_{soln}}{F} - 4.28,$$

where F is faradays constant (96485 C mol⁻¹) and 4.28 V is the absolute potential of the standard hydrogen electrode (SHE).⁴ ΔG°_{soln} is given by the following expression,

$$\Delta G^\circ_{soln} = G^\circ_{soln}(Red) - G^\circ_{soln}(Ox) - G^\circ_{gas}(e),$$

where $G^\circ_{gas}(e)$ is -3.632 kJ mol⁻¹ at 298.15 K assuming EC-FD, *Red* is the reduced species within the redox couple, and *Ox* is the oxidised species.

Table S3: Calculated G°_{soln} (kJ mol⁻¹) and standard reduction potential for electron attachment (*left*) and detachment (*right*) (eV) relative to the SHE.

OLIGOMER	NEUTRAL	CATION	ANION	E°_{-e}	E°_{+e}
MONOMER	-303620.2	-302903.9	-303661.8	3.11	-3.89
DIMER	-604134.8	-603447.6	-604179.5	2.81	-3.85

TRIMER	-904644.3	-903959.8	-904695.4	2.78	-3.79
TETRAMER	-1205154.3	-1204491.6	-1205211.4	2.55	-3.73
PENTAMER	-1505662.2	-1505006.1	-1505722.8	2.48	-3.69

References

- (1) would need to be studied to identify its relevant low energy conformers. One could instead to use MD to search conformational space, but in our experience there is < 0.01 correlation between an MD conformational space and an accurate ab initio space for the same species. So, in essence, any number we could calculate would almost certainly have no real merit. As it is, the calculation on a smaller fragment does capture the local chemistry, so far as it relates to the energetics of ionization or reduction.
- (2) Ho, J. *Phys. Chem. Chem. Phys.* **2015**, *17*, 2859-2868.
- (3) Marenich, A. V.; Ho, J.; Coote, M. L.; Cramer, C. J.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2014**, *16*, 15068-15106.
- (4) Isse, A. A.; Gennaro, A. *J. Phys. Chem. B* **2010**, *114*, 7894-7899.

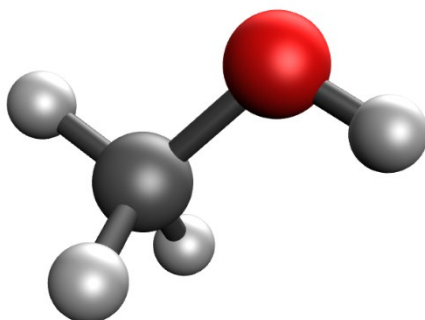
Appendix S1. Optimized Geometries as Gaussian Archive Entries

Gas Phase

Monomer

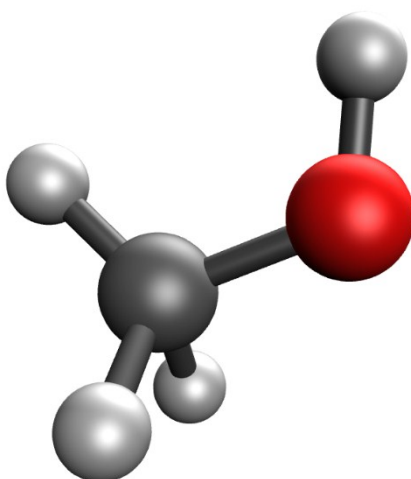
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0568501,-0.1146771063,0.8340513864\H,-3.5366145437,0.0843451969,-0.930
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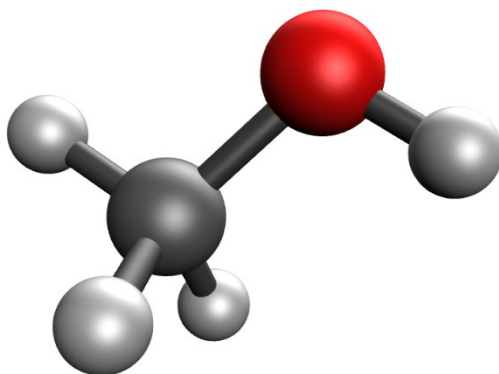
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Anion

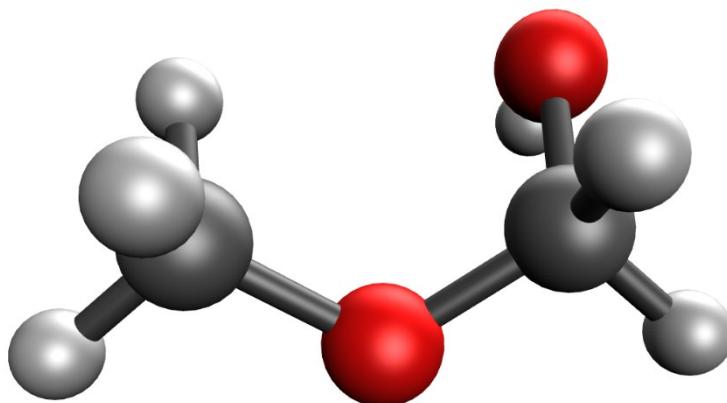
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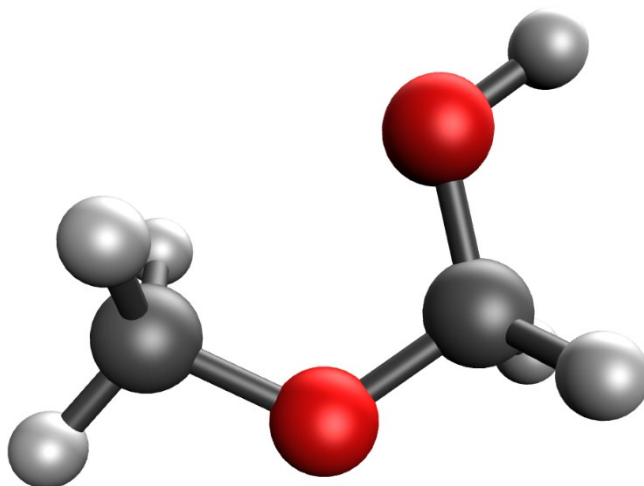
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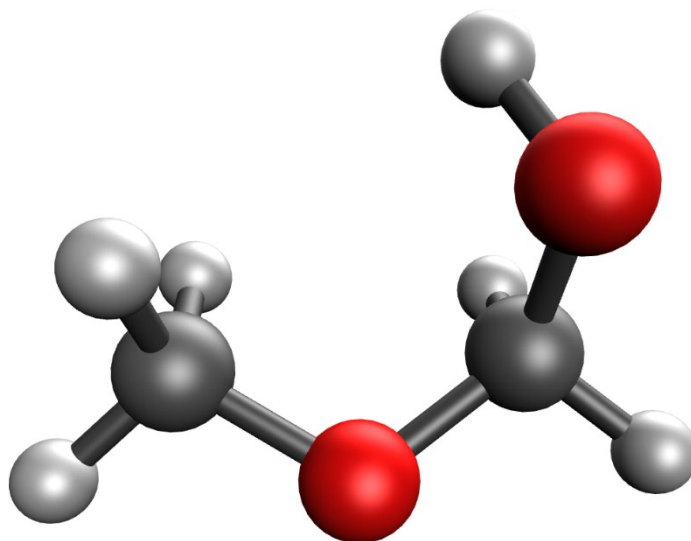
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Anion

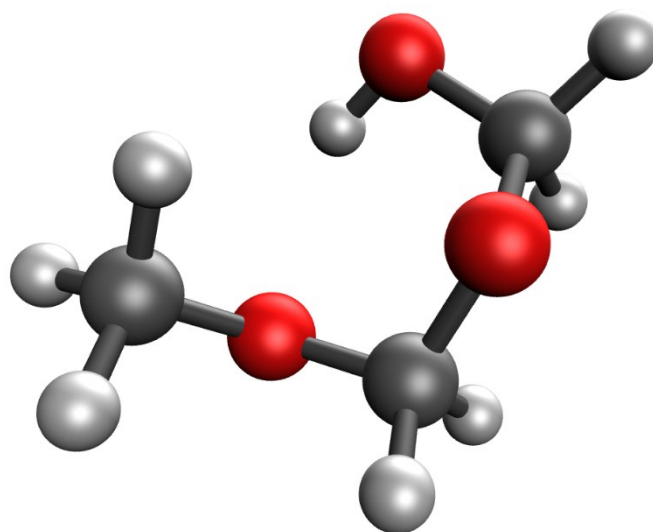
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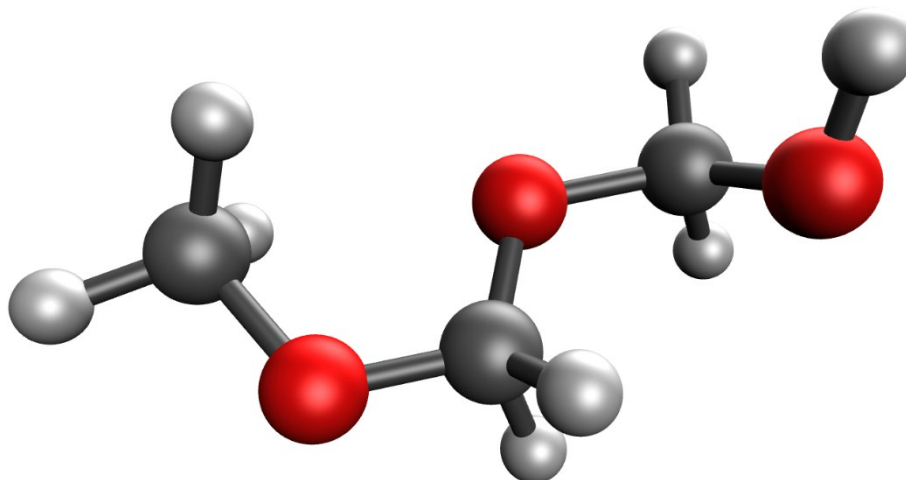
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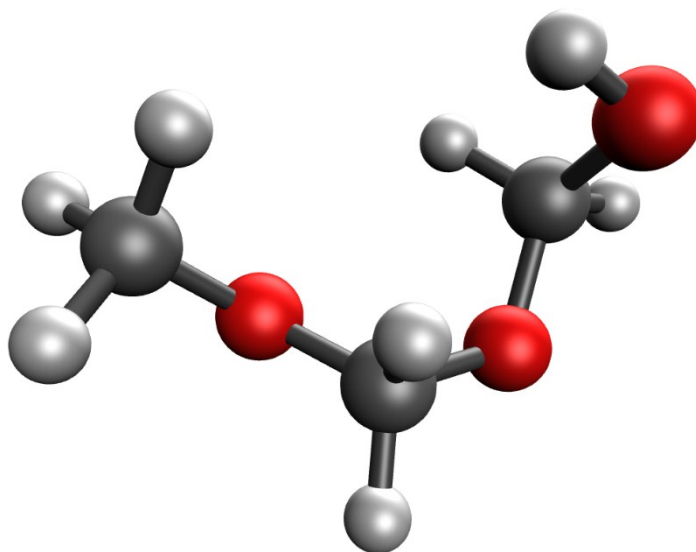
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Anion

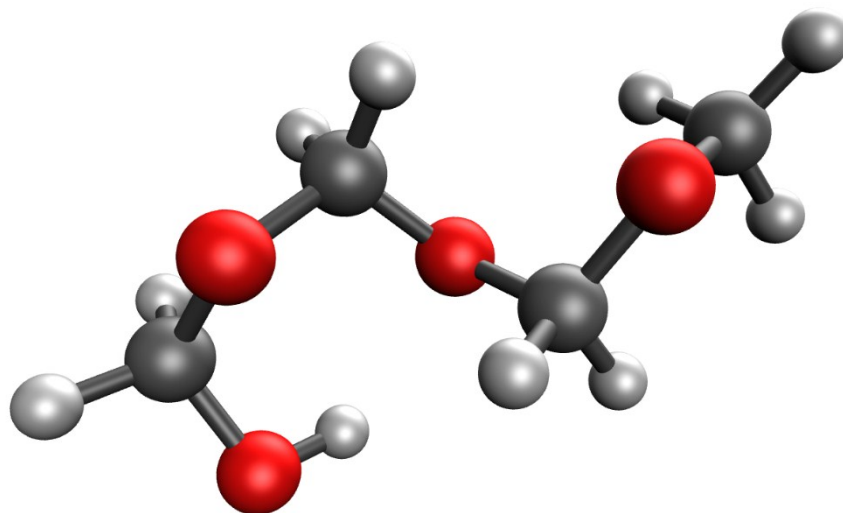
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Tetramer

Neutral

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1\1\GINC-R2113\FOpt\RM062X\6-31+G(d)\C4H10O4\ROOT\15-Dec-2019\0\#\M062
X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=8GB\ \a
3 b3 c3 d3 e2\ \0,1\C,-4.398727516,0.5423253597,-0.1325721787\O,-3.1571
246593,1.2173721138,-0.0457319455\C,-2.0654702985,0.3601521222,0.01356
96676\O,-2.047911519,-0.4036002611,1.207100105\C,-1.7602603244,0.37213
65349,2.3536347201\O,-0.4256581589,0.7766975822,2.3984746714\C,0.48894
5074,-0.2896654054,2.5237805917\O,0.7348185619,-0.9555813035,1.3223644
81\H,-5.1665957879,1.3082636847,-0.2450372708\H,-4.594618407,-0.047738
3272,0.7693531879\H,-4.4157071111,-0.122482804,-1.0072254122\H,-1.1698
332805,0.9835728897,-0.0522414361\H,-2.0945075454,-0.3792747284,-0.797
0518046\H,-2.0047040742,-0.2739796737,3.2058810026\H,-2.3632483989,1.2
837887227,2.3639400608\H,0.1154575163,-0.9854686103,3.2926639568\H,1.4
340471453,0.1514495953,2.8371220574\H,-0.0907282165,-1.3844774918,1.04
71865455\ \Version=ES64L-G16RevC.01\State=1-A\HF=-459.1247296\RMSD=5.59
8e-09\RMSF=1.245e-05\Dipole=-0.8795579,-0.4476807,0.2450427\Quadrupole
=-0.465962,-2.7542427,3.2202047,0.997648,2.1795643,0.2129414\PG=C01 [X
(C4H10O4)]\ \@
```

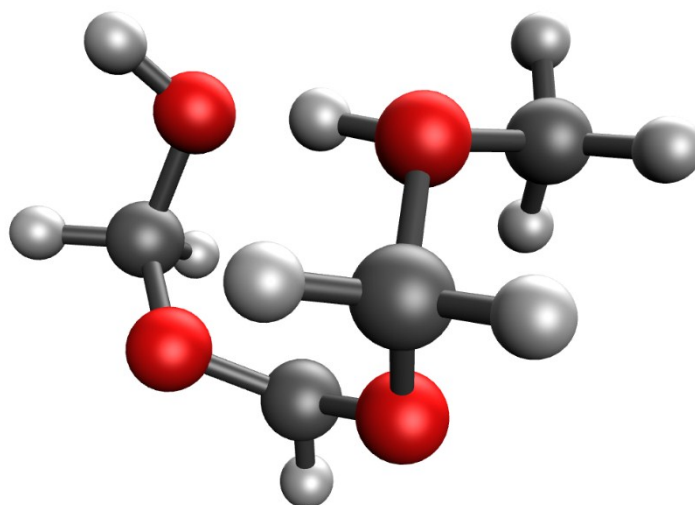


Cation

```

1\1\GINC-R3331\FOpt\UM062X\6-31+G(d)\C4H10O4(1+,2)\ROOT\15-Dec-2019\0\
\#M062X/6-31+G* SCF=XQC IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=8G
B\ \a3 b3 c3 d1 e3\ \1,2\C,-4.0614728557,0.7794263803,0.5691271462\O,-2.
6876483806,1.2841389052,0.4758926341\C,-1.6478196357,0.2934194681,0.14
84203869\O,-1.6846415197,-0.7599931569,1.0295941375\C,-1.4669796814,-0
.4792782999,2.3534649636\O,-0.5918323441,0.5484642633,2.5912331821\C,-
1.1025073342,1.6065153256,3.3527438868\O,-1.8524341229,2.4903015241,2.
500553944\H,-4.6848361652,1.6528389525,0.7485955174\H,-4.123944063,0.0
556227844,1.3818319318\H,-4.2932651989,0.326502864,-0.3935747606\H,-0.
7185398798,0.8630231579,0.1840026879\H,-1.8796655509,-0.0839363608,-0.
8449493574\H,-1.3588693338,-1.3822936904,2.945327534\H,-2.3961446762,1
.8421598774,1.3244131699\H,-0.2569589484,2.1397542646,3.7830970464\H,-
1.7955935868,1.2480930994,4.1144439487\H,-1.3507867227,3.2961136411,2.
2919080006\ \Version=ES64L-G16RevC.01\State=2-A\HF=-458.7928645\S2=0.75
2965\S2-1=0.\S2A=0.750007\RMSD=8.813e-09\RMSF=1.357e-05\Dipole=-0.4618
089,1.0411314,-0.2020344\Quadrupole=-1.3813118,-0.927156,2.3084678,2.8
146911,4.7260877,1.9859359\PG=C01 [X(C4H10O4)]\ \@

```

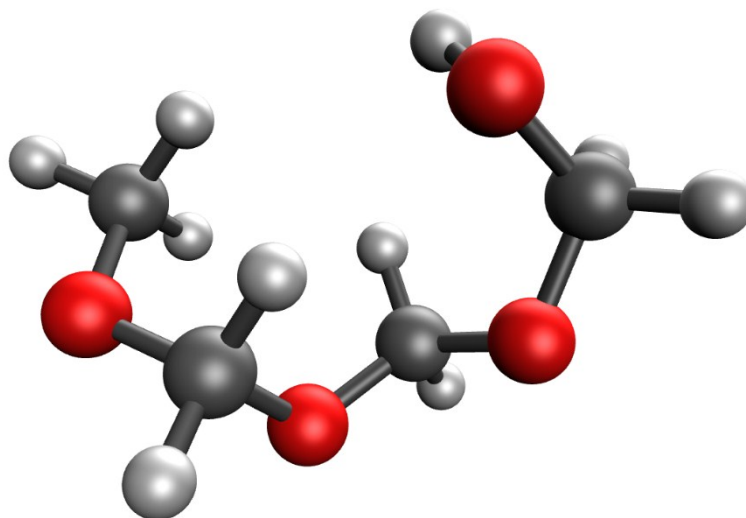


Anion

```

1\1\GINC-R2578\FOpt\UM062X\6-31+G(d)\C4H10O4(1-,2)\ROOT\15-Dec-2019\0\
\#M062X/6-31+G* SCF=XQC IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=8G
B\\a1 b2 c1 d1 e2\\-1,2\C,-3.4949419481,0.6451635373,0.8593565631\O,-2
.7530291756,0.0678135139,-0.2044302434\C,-1.4133139909,0.4648919817,-0
.2189181745\O,-1.2479975458,1.8166566896,-0.581412998\C,-0.9637809075,
2.6920120621,0.4813264295\O,0.3478645441,2.4857420542,0.9504847483\C,0
.4681015886,2.3422147807,2.3578349606\O,-0.1356377487,1.1880051735,2.8
381331149\H,-4.4467519399,0.1099789368,0.9240401386\H,-3.6978462825,1.
7107154667,0.6839010143\H,-2.9659598023,0.549795235,1.819385013\H,-0.9
380567198,-0.1357640062,-0.9984341809\H,-0.944073806,0.287231316,0.759
1701561\H,-1.6803432148,2.5805386709,1.3074156089\H,-1.0485723463,3.69
74648496,0.0571845784\H,0.0569337735,3.2293858074,2.8631155098\H,1.544
5902639,2.2715520408,2.528989078\H,-1.0077737418,1.4222778899,3.249790
6833\\Version=ES64L-G16RevC.01\State=2-A\HF=-459.0788164\S2=0.751313\S
2-1=0.\S2A=0.750002\RMSD=7.774e-09\RMSF=1.624e-05\Dipole=1.0778101,-0.
5859717,-1.8484517\Quadrupole=0.4148086,5.0941523,-5.5089608,-1.082438
1,0.9386795,-2.5540091\PG=C01 [X(C4H10O4)]\\@

```

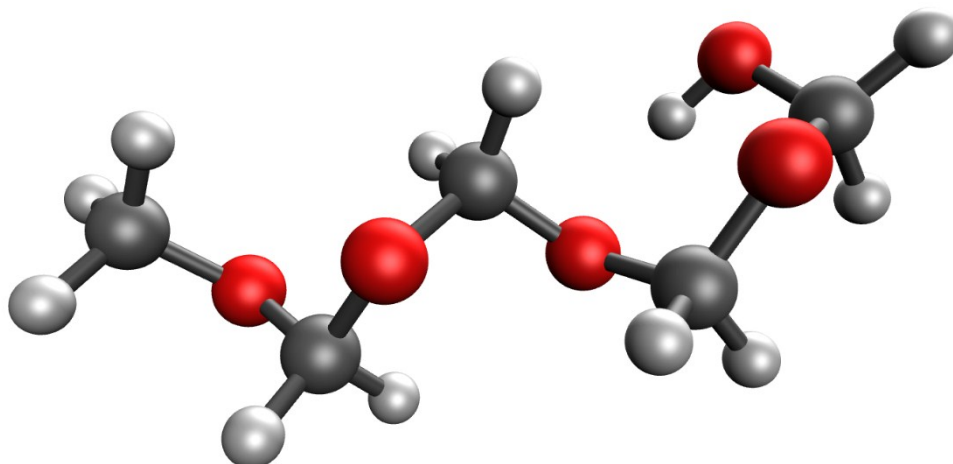


Pentamer

Neutral

```
1\1\GINC-R1812\FOpt\RM062X\6-31+G(d)\C5H12O5\ROOT\15-Dec-2019\0\#\M062
X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=8GB\#a
3 b3 c3 d3 e3 f3 g2\0,1\C,-6.2673651447,1.8750543114,-0.2157098336\O,
-5.003821625,2.5062670866,-0.1129743821\C,-3.9365741404,1.6147540659,-
0.1616155917\O,-3.9100576502,0.7420653305,0.9474214287\C,-3.596708961,
1.3818294022,2.1537121506\O,-2.2312269044,1.7444015241,2.2075574098\C,
-1.3680806108,0.6330308717,2.3480935572\O,-1.4484349796,0.0572473946,3
.6162611026\C,-1.016157475,0.9066152378,4.6565463056\O,-1.9691586204,1
.8531577508,5.0338970112\H,-7.0148045798,2.6686592904,-0.2387442941\H,
-6.4537864595,1.2161114038,0.6391256385\H,-6.3302579509,1.2871809631,-
1.1418676138\H,-3.0291349845,2.2245275564,-0.1957184037\H,-4.006231797
8,0.9589280045,-1.0383283921\H,-3.8376574027,0.67661763,2.9530912068\H
,-4.1567990157,2.3150507943,2.2625474853\H,-0.3620118647,1.0260588353,
2.1567890074\H,-1.6278572179,-0.150764789,1.6321014857\H,-0.0764100351
,1.3920749267,4.3471031072\H,-0.8475235151,0.2687395329,5.5229326895\H
,-2.0984650648,2.459246876,4.2875019249\Version=ES64L-G16RevC.01\Stat
e=1-A\HF=-573.6107556\RMSD=8.575e-09\RMSF=7.259e-06\Dipole=0.1389986,-
0.0361663,-0.7571526\Quadrupole=7.0690701,-4.202833,-2.8662371,0.06053
```

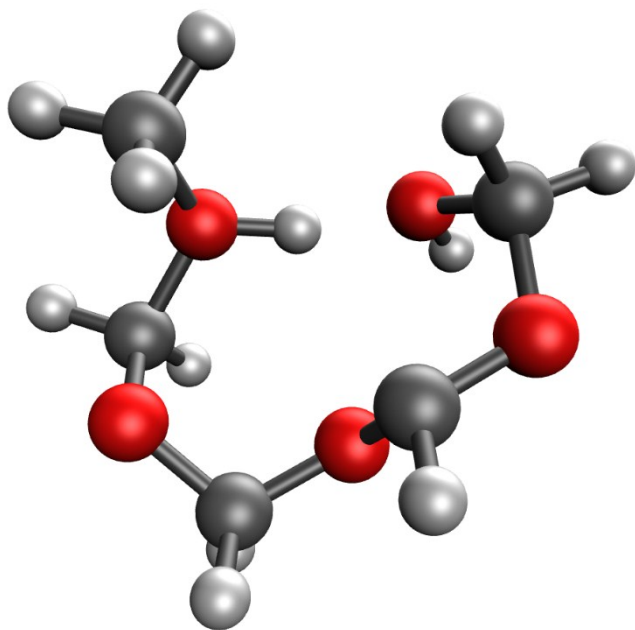
01,1.8961948,1.2975107\PG=C01 [X(C5H12O5)]\@



Cation

```
1\1\GINC-R1851\FOpt\UM062X\6-31+G(d)\C5H12O5(1+,2)\ROOT\15-Dec-2019\0\
\#M062X/6-31+G* SCF=XQC IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=8G
B\ \a1 b1 c1 d3 e1 f1 g1\ \1,2\C,-4.0383034377,3.5680019984,-0.651182800
9\O,-3.2356347661,2.6672423922,-1.4735077161\C,-3.1692238173,1.2684141
071,-1.0045342712\O,-2.6712520959,1.1882474758,0.2619513057\C,-1.26775
44806,0.9976418481,0.3427033748\O,-0.5886024825,2.0147650293,-0.339183
7564\C,-0.4777241567,3.2029504537,0.3456953157\O,0.1570983005,4.148238
985,-0.3884875091\C,-0.6458857691,4.8665816885,-1.2764128899\O,-1.2780
694794,4.013042043,-2.2322233154\H,-4.0288486491,4.5281264537,-1.16520
82591\H,-3.6033397414,3.627000358,0.3472291457\H,-5.0483052482,3.16006
64615,-0.6268598906\H,-2.5631477569,0.7615286749,-1.7603452023\H,-4.20
64484923,0.935147559,-1.0108586517\H,-0.9846626607,0.061010978,-0.1424
593066\H,-1.0334648991,0.9829802441,1.4089645926\H,-0.1459965601,3.131
81829,1.3809871589\H,-2.3262327752,3.125244008,-1.7626143603\H,0.00404
70755,5.5760675401,-1.7858193189\H,-1.4634465068,5.3689281531,-0.75330
23916\H,-0.6098456008,3.5892862586,-2.7996572533\ \Version=ES64L-G16Rev
C.01\State=2-A\HF=-573.2896402\S2=0.753008\S2-1=0.\S2A=0.750008\RMSD=4
.661e-09\RMSF=1.341e-05\Dipole=-0.8986612,-0.0214534,-0.6071846\Quadru
pole=0.0576575,3.085648,-3.1433055,0.9565052,0.110871,-1.8478025\PG=C0
```

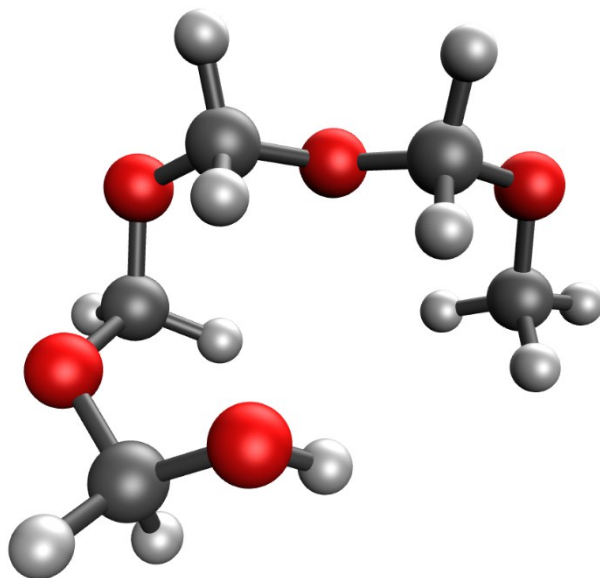
1 [X(C5H12O5)]\ \@



Anion

```
1\1\GINC-R1840\FOpt\UM062X\6-31+G(d)\C5H12O5(1-,2)\ROOT\15-Dec-2019\0\
\#M062X/6-31+G* SCF=XQC IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=8G
B\ \a3 b1 c1 d1 e1 f1 g1\ \-1,2\C,-4.4595633825,0.1351664098,-0.98988397
71\O,-4.1135554448,1.3239424254,-0.2840019753\C,-3.3240279619,1.074303
7976,0.822233187\O,-4.0905141645,0.4339805681,1.8192027899\C,-3.327253
9006,0.0380393824,2.9357416806\O,-4.0273113402,-0.9327593757,3.6449393
358\C,-4.0035800783,-2.2034243028,3.0318961514\O,-2.7523505526,-2.8121
04927,3.2168269765\C,-2.0826444968,-3.2270677846,2.0335787916\O,-1.753
4960449,-2.1620628397,1.2078792577\H,-5.0331957048,0.4413656175,-1.870
4485376\H,-5.0579232153,-0.5421662342,-0.3688942018\H,-3.5612867589,-0
.407890487,-1.3086644291\H,-2.9757889921,2.0540496997,1.1842996955\H,-
2.4630630147,0.4322695083,0.5627723941\H,-3.199649827,0.8854475291,3.6
23400302\H,-2.3531590506,-0.3494191192,2.6035557667\H,-4.2471627331,-2
.1224127023,1.9630986794\H,-4.7668729508,-2.7848967945,3.5562586693\H,
-2.6996344867,-3.9571182206,1.4886250116\H,-1.1691951721,-3.701742713,
2.4003135549\H,-2.3203517269,-2.1957314373,0.3889838769\ \Version=ES64L
-G16RevC.01\State=2-A\HF=-573.5656576\S2=0.752113\S2-1=0.\S2A=0.750004
\RMSD=8.029e-09\RMSF=5.783e-06\Dipole=0.2442324,1.5525361,1.9920389\Qu
adrupole=6.0299785,0.8230089,-6.8529874,5.3972461,-0.5710881,-1.594419
```

6\PG=C01 [X(C5H12O5)]\ \@

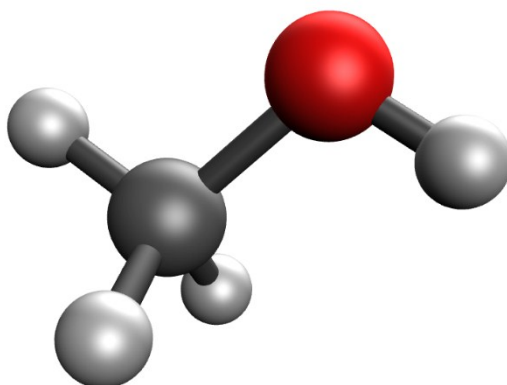


Solution Phase

Monomer

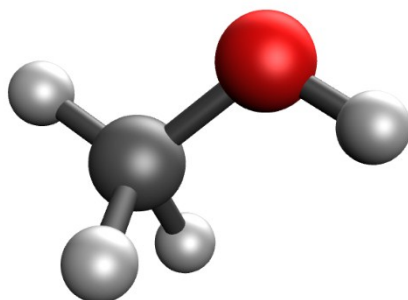
Neutral

```
1\1\GINC-R1810\FOpt\RM062X\6-31+G(d)\C1H4O1\ROOT\29-Nov-2019\0\#M062X
/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD,Solve
nt=Water) maxdisk=5GB\ \a1\ \0,1\C,-3.4579298695,0.6131158402,0.01299050
67\O,-2.208513917,1.2994629728,-0.0084162364\H,-4.294166001,1.31438284
78,0.1041388103\H,-3.4997699082,-0.1089174617,0.8353600217\H,-3.544812
5509,0.078010683,-0.9341867118\H,-2.1133543146,1.7817810529,0.82702049
16\ \Version=ES64L-G16RevC.01\State=1-A'\HF=-115.6718197\RMSD=9.751e-09
\RMSF=1.030e-04\Dipole=-0.6639239,0.0126085,0.7458266\Quadrupole=-1.01
72675,0.2961615,0.721106,0.4769734,1.2625237,1.4397527\PG=CS [SG(C1H2O
1),X(H2)]\ \@
```



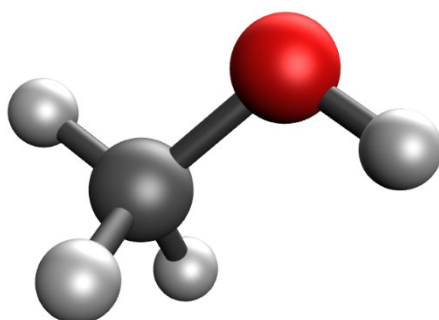
Cation

```
1\1\GINC-R2505\FOpt\UM062X\6-31+G(d)\C1H4O1(1+,2)\ROOT\28-Nov-2019\0\
#M062X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD
,Solvent=Water) maxdisk=5GB\\a1\\1,2\C,-3.4290888885,0.5951829942,-0.0
532479819\O,-2.2515674477,1.2736591991,-0.0118693126\H,-4.2598112153,1
.3124447171,0.1809510745\H,-3.5083350152,-0.0339570562,0.8726656263\H,
-3.5278918429,0.0588357927,-0.989892661\H,-2.1418521492,1.771670289,0.
8383001358\\Version=ES64L-G16RevC.01\State=2-A"\HF=-115.3936996\S2=0.7
55512\S2-1=0.\S2A=0.750017\RMSD=4.581e-09\RMSF=1.829e-04\Dipole=-0.529
0047,0.1939101,0.952149\Quadrupole=-0.0547075,0.0550051,-0.0002976,1.2
165036,1.0585018,1.2379429\PG=CS [SG(C1H2O1),X(H2)]\\@
```



Anion

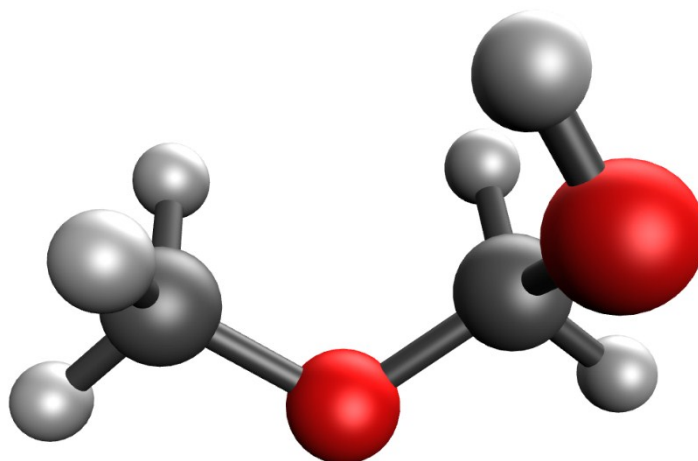
```
1\1\GINC-R2505\FOpt\UM062X\6-31+G(d)\C1H4O1(1-,2)\ROOT\28-Nov-2019\0\
#M062X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD
,Solvent=Water) maxdisk=5GB\\a1\\-1,2\C,-3.4558976729,0.6093972863,0.0
035446814\O,-2.1971120883,1.2938525298,-0.0317237023\H,-4.2890380452,1
.3175641589,0.1087007795\H,-3.4960763933,-0.1031660974,0.8386016248\H,
-3.5580577172,0.067695825,-0.9398747747\H,-2.1223646419,1.7924922333,0
.8576582724\\Version=ES64L-G16RevC.01\State=2-A'\HF=-115.6836099\S2=0.
750753\S2-1=0.\S2A=0.75\RMSD=9.449e-09\RMSF=1.860e-04\Dipole=-1.504357
4,-1.1720645,-0.6470602\Quadrupole=0.1305602,0.1696326,-0.3001928,0.20
82336,0.3226874,-0.0021192\PG=CS [SG(C1H2O1),X(H2)]\\@
```



Dimer

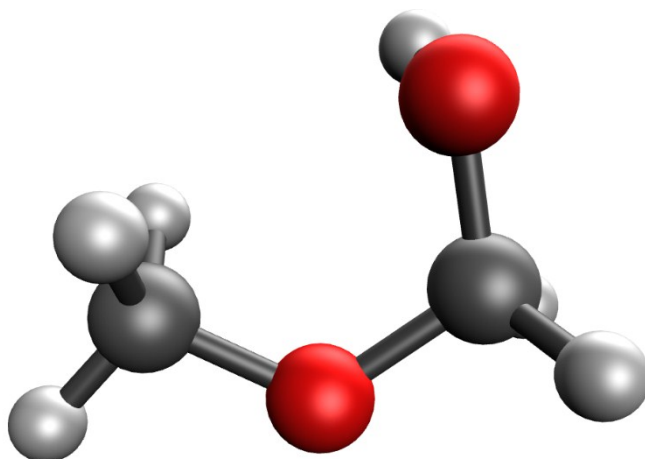
Neutral

```
1\1\GINC-R1930\FOpt\RM062X\6-31+G(d)\C2H6O2\ROOT\29-Nov-2019\0\#\M062X
/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD,Solve
nt=Water) maxdisk=5GB\ \a2\ \0,1\C,-3.1931942122,0.2303891578,0.04006934
51\O,-1.9451095694,0.909363801,-0.0392360366\C,-0.8425594677,0.0365165
27,-0.0496174744\O,-0.7257313774,-0.6757732345,-1.2611371075\H,-3.9658
475864,0.9921538857,0.1519062764\H,-3.2095666045,-0.4391372283,0.90935
93392\H,-3.3889093685,-0.3476749149,-0.8700632827\H,-0.9153472823,-0.6
620690965,0.793767035\H,0.0438516011,0.6642663019,0.0366616596\H,-1.29
83611328,-1.4591671992,-1.2321827541\ \Version=ES64L-G16RevC.01\State=1
-A\HF=-230.162199\RMSD=4.777e-09\RMSF=1.396e-05\Dipole=-0.7133699,-1.1
346126,0.7437513\Quadrupole=1.1137362,0.5230842,-1.6368204,1.2490957,2
.0064857,-0.1113379\PG=C01 [X(C2H6O2)]\ \@
```



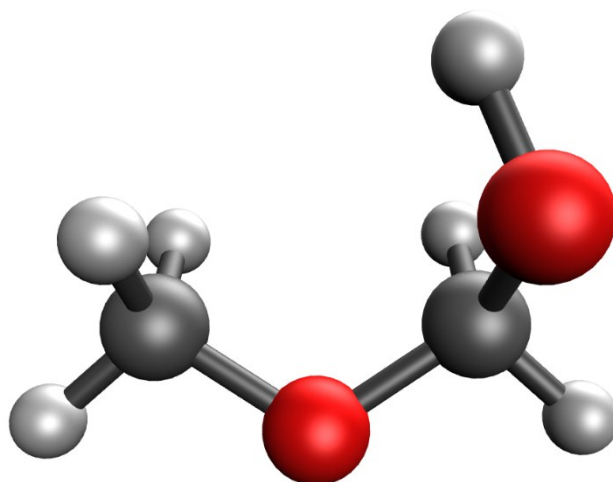
Cation

```
1\1\GINC-R2471\FOpt\UM062X\6-31+G(d)\C2H6O2(1+,2)\ROOT\28-Nov-2019\0\
#M062X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD
,Solvent=Water) maxdisk=5GB\\a2\\1,2\C,-3.2334240337,0.2802714293,-0.0
520541397\O,-1.9725671834,0.6687345329,0.4253599417\C,-0.8100782713,0.
0131073541,-0.0644850484\O,-1.0346745798,-0.8910718203,-1.0495952725\H
,-3.9695418963,0.9226229017,0.4199503562\H,-3.3706040473,-0.7880584043
,0.1930002972\H,-3.2187407427,0.3447348609,-1.1522345415\H,-0.35632864
02,-0.3912572288,0.8605160622\H,-0.1826571581,0.8478970686,-0.41652229
89\H,-1.2921584473,-1.7581126941,-0.6844083564\\Version=ES64L-G16RevC.
01\State=2-A\HF=-229.8958429\S2=0.754758\S2-1=0.\S2A=0.750017\RMSD=1.3
24e-09\RMSF=3.891e-05\Dipole=-0.4495917,-0.3873099,0.7797347\Quadrupol
e=3.3961212,0.859672,-4.2557932,-0.0621055,1.4783093,-1.2919446\PG=C01
[X(C2H6O2)]\\@
```



Anion

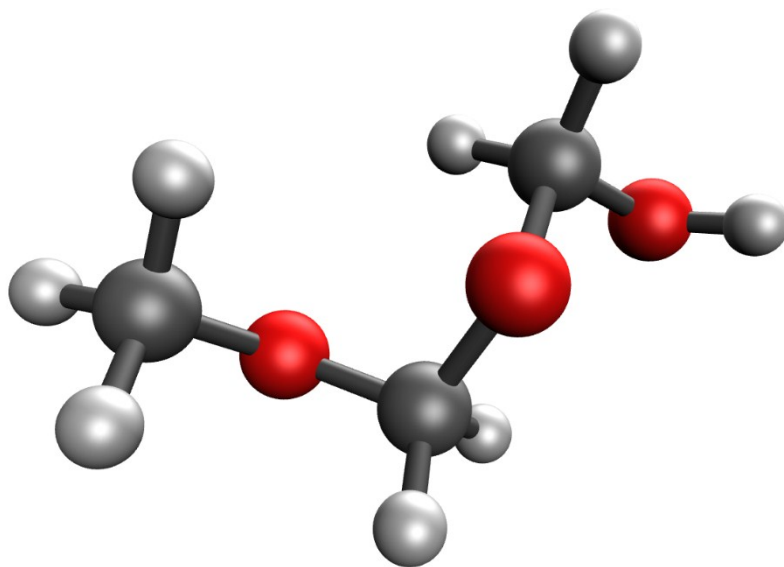
```
1\1\GINC-R1824\FOpt\UM062X\6-31+G(d)\C2H6O2(1-,2)\ROOT\28-Nov-2019\0\
#M062X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD
,Solvent=Water) maxdisk=5GB\\a2\\-1,2\C,-3.2107985099,0.2541000662,0.0
48020472\O,-1.9559450245,0.913861411,-0.0170366469\C,-0.8431468748,0.0
390154151,-0.075278142\O,-0.7345484669,-0.6408624177,-1.2974471206\H,-
3.9699688623,1.0290840087,0.18022856\H,-3.2416392124,-0.4420093951,0.8
962964819\H,-3.4127199534,-0.3093260167,-0.8731905971\H,-0.9108199765,
-0.6892051423,0.750172895\H,0.0308065092,0.6798585791,0.0497676376\H,-
1.1919946284,-1.5856485083,-1.1820065398\\Version=ES64L-G16RevC.01\Sta
te=2-A\HF=-230.1738946\S2=0.750926\S2-1=0.\S2A=0.750001\RMSD=9.360e-09
\RMSF=4.031e-05\Dipole=-1.3229613,1.9555513,1.8137025\Quadrupole=4.555
8964,-4.8251263,0.2692299,2.9634937,2.6554892,-2.8933437\PG=C01 [X(C2H
6O2)]\@
```



Trimer

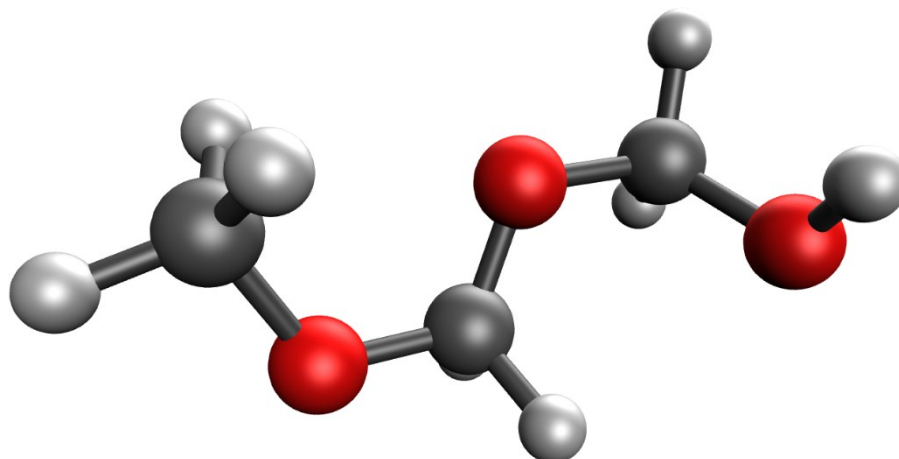
Neutral

```
1\1\GINC-R2636\FOpt\RM062X\6-31+G(d)\C3H8O3\ROOT\29-Nov-2019\0\#\M062X
/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD,Solve
nt=Water) maxdisk=5GB\ \a3 b3 c3\ \0,1\C,-4.3418276492,-0.1858807847,-0.
1041315784\O,-3.1867974568,0.6429107471,-0.0273376968\C,-1.9886105511,
-0.0855089842,0.0053368703\O,-1.8946035193,-0.917208178,1.143528607\C,
-1.7682578372,-0.211479735,2.3608986323\O,-0.4929594814,0.3661846168,2
.5045392008\H,-5.1918792309,0.4712941507,-0.2921438627\H,-4.5012454598
,-0.726983483,0.8342170008\H,-4.2429838492,-0.9043293944,-0.9273626735
\H,-1.1818772297,0.651948842,-0.0075205803\H,-1.9210042788,-0.7596071,
-0.8548296976\H,-1.9623557541,-0.9436955411,3.146941156\H,-2.487315186
6,0.6098724131,2.4059965107\H,0.1526794841,-0.3446955694,2.6530631114\
\Version=ES64L-G16RevC.01\State=1-A\HF=-344.6511564\RMSD=6.237e-09\RMS
F=1.209e-05\Dipole=-0.1854343,-0.9308955,0.0884849\Quadrupole=3.001979
5,-4.7897344,1.7877549,-1.6246256,0.7722459,-1.1742212\PG=C01 [X(C3H8O
3)]\ \@
```



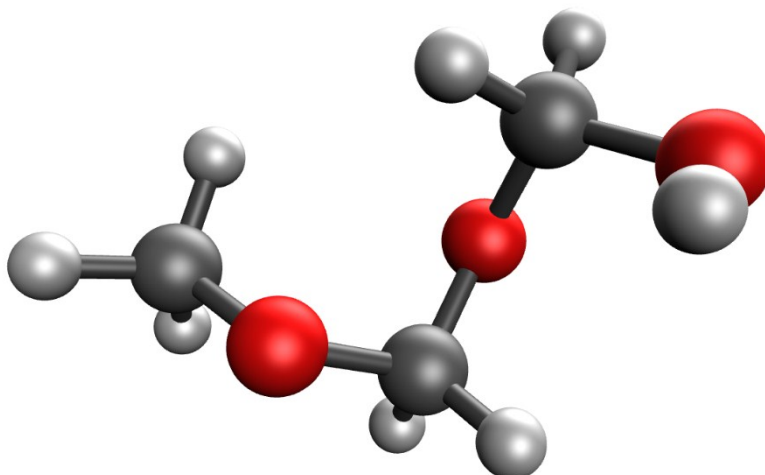
Cation

```
1\1\GINC-R3499\FOpt\UM062X\6-31+G(d)\C3H8O3(1+,2)\ROOT\28-Nov-2019\0\
#M062X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD
,Solvent=Water) maxdisk=5GB\ \a3 b1 c3\ \1,2\C,-4.3094804421,-0.02432725
4,0.1687038685\O,-3.0868076794,0.4174744518,-0.4101407597\C,-1.9454964
745,-0.2492747289,-0.1086438353\O,-2.1062621508,-1.2695918604,0.758257
6994\C,-0.8910469158,-2.0072051351,1.0389808705\O,-0.4177929564,-2.635
0122956,-0.1058430451\H,-5.0819076856,0.6288630504,-0.2256093059\H,-4.
2185949415,0.0421934347,1.2605774889\H,-4.4640496805,-1.0760423031,-0.
1050841877\H,-1.2036062798,0.526534804,0.2278760524\H,-1.5008594573,-0.
5568339034,-1.0975929679\H,-1.1866430832,-2.7045314922,1.8207922647\H
,-0.1289396779,-1.3042405529,1.3785340442\H,-0.9660895753,-3.416028215
3,-0.2926491871\ \Version=ES64L-G16RevC.01\State=2-A\HF=-344.3826558\S2
=0.755756\S2-1=0.\S2A=0.750024\RMSD=4.943e-09\RMSF=2.614e-05\Dipole=-0.
8271937,0.5050473,0.1671348\Quadrupole=1.0625661,2.222835,-3.2854011,
-1.2446207,2.1138044,-0.6957403\PG=C01 [X(C3H8O3)]\ \@
```



Anion

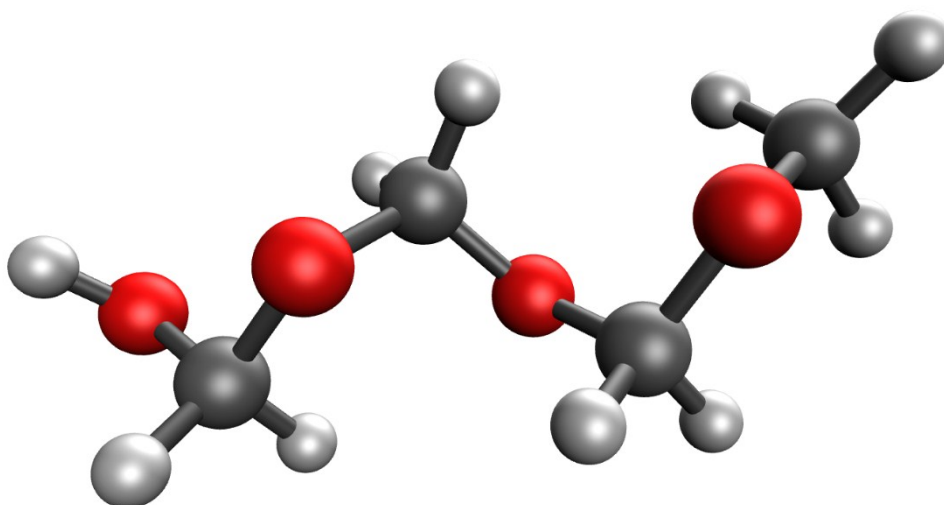
```
1\1\GINC-R2534\FOpt\UM062X\6-31+G(d)\C3H8O3(1-,2)\ROOT\28-Nov-2019\0\
#M062X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD
,Solvent=Water) maxdisk=5GB\ \a2 b2 c2\ \-1,2\C,-4.3122008295,-0.1355976
478,0.0799521641\O,-3.099668913,0.6032714074,0.1711680929\C,-1.9523778
695,-0.1984619276,0.0403963932\O,-1.8878868911,-0.8755079055,-1.191514
0048\C,-1.8218448538,-0.0361760866,-2.3408212506\O,-0.6328402771,0.702
583243,-2.4035142608\H,-5.1195135679,0.5459353017,0.3523673974\H,-4.29
8512008,-0.9856278035,0.7737940823\H,-4.4755116476,-0.5025575229,-0.93
90979401\H,-1.9469764183,-0.983686214,0.8047503523\H,-1.1009667287,0.4
835059304,0.1588590904\H,-2.6854231258,0.6461537792,-2.3520989319\H,-1
.8650609801,-0.722776646,-3.1864227632\H,-0.8210278896,1.6453760921,-1
.9653744212\ \Version=ES64L-G16RevC.01\State=2-A\HF=-344.66536\S2=0.751
021\S2-1=0.\S2A=0.750001\RMSD=4.341e-09\RMSF=2.308e-05\Dipole=-3.04380
74,-2.8349489,1.8486691\Quadrupole=0.2534764,-3.6803828,3.4269064,-4.0
657448,6.4185749,2.6503621\PG=C01 [X(C3H8O3)]\ \@
```



Tetramer

Neutral

```
1\1\GINC-R2545\FOpt\RM062X\6-31+G(d)\C4H10O4\ROOT\03-Dec-2019\0\#\M062
X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD,Solv
ent=Water) maxdisk=8GB\ \a3 b3 c3 d3 e3\ \0,1\C,-4.3112289584,0.68353637
82,-0.0987447759\O,-3.017318755,1.274527033,-0.032056492\C,-1.98049364
72,0.3324326117,-0.0698764291\O,-2.0093344418,-0.5512335252,1.03367189
73\C,-1.8652268609,0.0796527585,2.2871187593\O,-0.6105325238,0.7079948
946,2.4221870209\C,0.4740024607,-0.1913744692,2.5391853777\O,0.5063308
533,-0.8122845643,3.8011537357\H,-5.0259574334,1.4987516687,-0.2183017
433\H,-4.5400926906,0.1307430092,0.8183966864\H,-4.3776216618,0.006242
8942,-0.9590644649\H,-1.0483907164,0.9024068593,-0.0879832809\H,-2.067
6239386,-0.3099251772,-0.9522962106\H,-1.9951618468,-0.7096571022,3.03
13126733\H,-2.6112509302,0.8664663693,2.4188368239\H,1.3712018279,0.40
63272476,2.3681746549\H,0.3919211942,-0.9921210932,1.8006734695\H,0.76
23760688,-0.1492437931,4.4638392978\ \Version=ES64L-G16RevC.01\State=1-
A\HF=-459.1394349\RMSD=4.094e-09\RMSF=8.660e-06\Dipole=0.0063134,0.106
2084,-0.1051502\Quadrupole=6.1983855,-8.6088951,2.4105096,2.6188161,1.
9293663,4.2944244\PG=C01 [X(C4H10O4)]\ \@
```

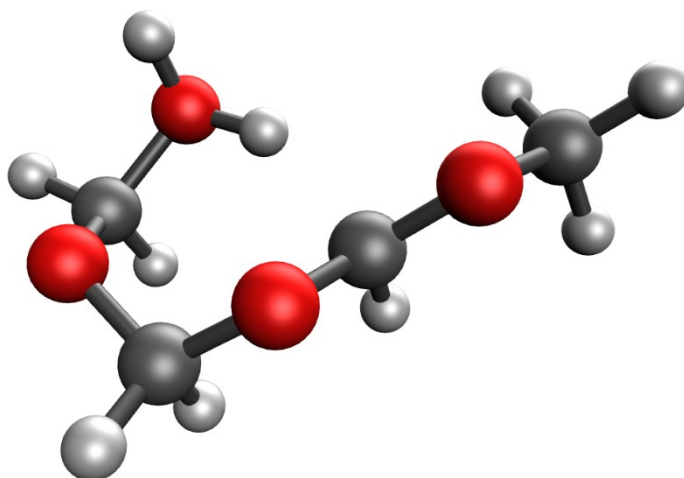


Cation

```

1\1\GINC-R2397\FOpt\UM062X\6-31+G(d)\C4H10O4(1+,2)\ROOT\30-Nov-2019\0\
\#M062X/6-31+G* SCF=XQC IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD,
Solvent=Water) maxdisk=8GB\\a1 b1 c1 d2 e3\\1,2\C,-3.8982883096,0.5683
429977,0.2486553804\O,-2.8026426242,0.8249538481,-0.6396671677\C,-1.61
36388599,0.4281620237,-0.1554666204\O,-0.6450603998,0.5970448249,-1.10
84304176\C,0.6669150806,0.2915912512,-0.6857567932\O,1.2600066031,1.38
12816916,-0.001281613\C,1.0335170483,1.4721623551,1.349813367\O,-0.247
2417557,2.1835928892,1.6345786718\H,-4.7906492284,0.9332943247,-0.2566
270433\H,-3.7485487649,1.1084320027,1.1880204456\H,-3.9813260449,-0.50
58258816,0.4366345507\H,-1.5797064058,-0.507670819,0.417868616\H,-1.01
37110247,1.6925569052,1.1798883994\H,1.2509448909,0.1485171155,-1.5905
01245\H,0.6699877843,-0.6007864206,-0.050375652\H,1.7911815748,2.09882
01338,1.810491013\H,0.9028845173,0.5063237815,1.8398500369\H,-0.235016
0815,3.1041749762,1.2852110714\\Version=ES64L-G16RevC.01\State=2-A\HF=
-458.8860128\S2=0.752619\S2-1=0.\S2A=0.750006\RMSD=9.264e-09\RMSF=3.99
1e-05\Dipole=0.7893862,0.3655196,2.8156357\Quadrupole=4.4632258,1.8251
702,-6.2883961,1.552258,1.0151137,4.450258\PG=C01 [X(C4H10O4)]\\@

```

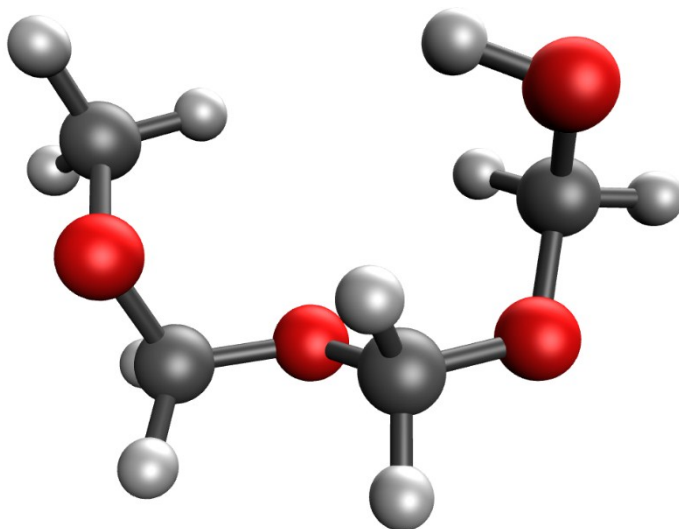


Anion

```

1\1\GINC-R2108\FOpt\UM062X\6-31+G(d)\C4H10O4(1-,2)\ROOT\03-Dec-2019\0\
\#M062X/6-31+G* SCF=XQC IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD,
Solvent=Water) maxdisk=8GB\ \a2 b2 c1 d2 e2\ \-1,2\C,-4.1947223197,0.619
1065844,0.5542698714\O,-2.997000115,1.2579997132,0.1245683714\C,-1.915
1229281,0.3731172515,-0.0151981026\O,-2.0250169747,-0.4576231454,-1.14
8418365\C,-1.801760611,0.2462504397,-2.3647610824\O,-1.9983952527,-0.6
266816333,-3.4361857684\C,-3.3544292724,-1.0278937699,-3.6538082537\O,
-4.196035383,0.0474837704,-3.9554352995\H,-4.9735346031,1.3845765252,0
.5786155686\H,-4.0537760607,0.1972981746,1.5584103625\H,-4.5001401539,
-0.1662615362,-0.1479817136\H,-1.8536018164,-0.3002285407,0.8457852184
\H,-1.0183205093,0.9976193257,-0.087627153\H,-0.758168874,0.5744880582
,-2.4104182324\H,-2.4876419378,1.102749028,-2.4239976136\H,-3.72538782
42,-1.5571481114,-2.7647165443\H,-3.3035326614,-1.7001052429,-4.510052
0121\H,-4.6405817026,0.3725491091,-3.0580492518\ \Version=ES64L-G16RevC
.01\State=2-A\HF=-459.1575495\S2=0.751383\S2-1=0.\S2A=0.750002\RMSD=7.
950e-09\RMSF=1.151e-05\Dipole=2.9206739,-0.6185549,2.7902016\Quadrupol
e=-2.4293178,3.0611238,-0.631806,4.8837836,-5.1061275,-0.0677489\PG=C0
1 [X(C4H10O4)]\ \@

```

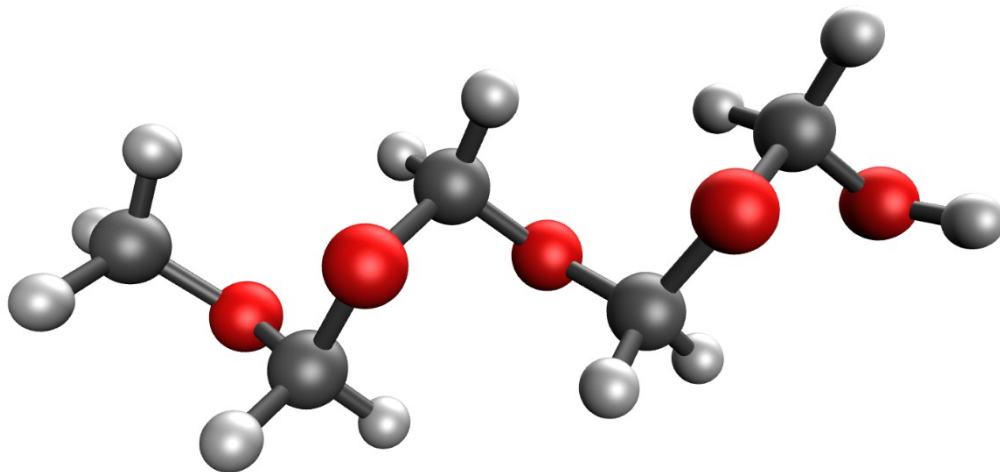


Pentamer

Neutral

```
1\1\GINC-R2390\FOpt\RM062X\6-31+G(d)\C5H12O5\ROOT\05-Dec-2019\0\#\M062
X/6-31+G* SCF=Tight IOP(2/17=4) INT(grid=ultrafine) Opt SCRF=(SMD,Solv
ent=Water) maxdisk=8GB\ \a3 b3 c3 d3 e3 f3 g3\ \0,1\C,-6.1793822316,1.92
25005544,-0.1210721926\O,-4.8452667804,2.4209109189,-0.1329987262\C,-3
.8794622196,1.4063330584,-0.1157464934\O,-3.9336553368,0.6257858928,1.
0629487989\C,-3.7122476107,1.3504091129,2.2513390842\O,-2.4245647267,1
.9248775665,2.2977718014\C,-1.3633555795,0.9948203537,2.2578147835\O,-
1.3807494308,0.1174522647,3.3604259107\C,-1.1177785609,0.7408751207,4.
6024272579\O,0.2154440345,1.1775081062,4.7015142754\H,-6.8376422277,2.
7764810013,-0.2855736456\H,-6.4186459451,1.4589714207,0.8416911273\H,-
6.3196458143,1.1886954563,-0.9241683176\H,-2.9107484637,1.9035467187,-
0.2096688232\H,-4.0405054411,0.6971633435,-0.9343273174\H,-3.855571809
6,0.6348604903,3.0640012003\H,-4.4083523285,2.1874818692,2.3407024886\
H,-0.4505682163,1.5942554914,2.2417103848\H,-1.4292921931,0.3602820083
,1.3712944238\H,-1.3487897057,-0.0112183012,5.3590245264\H,-1.74385198
72,1.6270876722,4.7287028627\H,0.7923185749,0.3981658803,4.7649165901\
\Version=ES64L-G16RevC.01\State=1-A\HF=-573.627685\RMSD=6.516e-09\RMSF
=6.532e-06\Dipole=-0.3315729,-0.8816004,0.0703072\Quadrupole=4.8736047
```

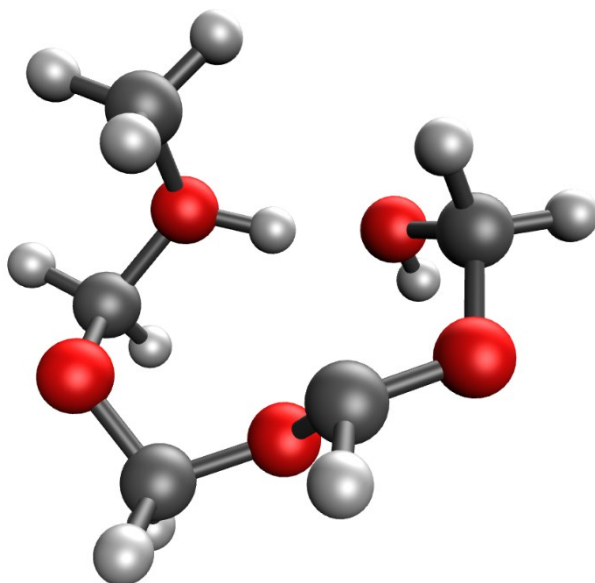
, -8.1560662, 3.2824615, -4.5858681, 1.1464467, -1.899671 \PG=C01 [X(C5H12O5)
)]\@



Cation

```
1\1\GINC-R1804\FOpt\UM062X\6-31+G(d)\C5H12O5(1+,2)\ROOT\17-Dec-2019\0\
\#M062X/6-31+G* SCF=XQC IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=8G
B\ \a1 b1 c1 d3 e1 f1 g2\ \1,2\C, -4.058297552, 3.5706128238, -0.1539582542
\O, -3.5464102672, 2.667238557, -1.1804516744\C, -3.410855827, 1.2541179597
, -0.7736395767\O, -2.5918537698, 1.1212128593, 0.3080227722\C, -1.22760903
61, 0.8822868441, 0.0007344329\O, -0.7194882663, 1.8942686234, -0.822842574
9\C, -0.3764492304, 3.0584129136, -0.1748251849\O, 0.0717046636, 4.00035554
5, -1.0395670985\C, -0.9134034125, 4.771253068, -1.6594568163\O, -1.8172912
605, 3.9677939528, -2.4209587331\H, -4.1505361839, 4.5441283981, -0.6334383
432\H, -3.3660721004, 3.5865071895, 0.6886912228\H, -5.039066243, 3.1963005
927, 0.1377315923\H, -3.0528193957, 0.7494743225, -1.6751012394\H, -4.42325
57885, 0.9554765217, -0.5038160805\H, -1.1236732508, -0.0498039264, -0.5589
256825\H, -0.7138217202, 0.8310277618, 0.9627189984\H, 0.2226928381, 2.9474
00897, 0.7283156837\H, -2.7326305176, 3.1029321737, -1.6988400465\H, -0.399
3196267, 5.4724804735, -2.3146336705\H, -1.5356565476, 5.2857612174, -0.922
9581161\H, -1.3474465056, 3.5385242314, -3.1578706105\ \Version=ES64L-G16R
evC.01\State=2-A\HF=-573.2896399\S2=0.753009\S2-1=0.\S2A=0.750008\RMSD
=7.930e-09\RMSF=2.944e-05\Dipole=-1.0287551, 0.0276429, -0.3385813\Quadr
```

upole=-0.0838055,3.1081481,-3.0243426,0.5643287,-0.8039803,-1.9002129\
PG=C01 [X(C5H12O5)]\ \@



Anion

```
1\1\GINC-R1805\FOpt\UM062X\6-31+G(d)\C5H12O5(1-,2)\ROOT\17-Dec-2019\0\
\#M062X/6-31+G* SCF=XQC IOP(2/17=4) INT(grid=ultrafine) Opt maxdisk=8G
B\ \a3 b1 c1 d3 e3 f1 g1\ \-1,2\C,-4.622777476,2.2169103085,-0.173133988
3\O,-5.6500150328,2.0374993672,0.7902862615\C,-5.2194333682,1.38210204
07,1.9431677686\O,-5.0012656002,0.0037886235,1.7712914817\C,-3.7088430
939,-0.3892338354,1.3501185094\O,-3.1322598592,-1.2746300328,2.2629170
486\C,-2.639492208,-0.6911424877,3.4523201381\O,-1.2826311611,-0.94897
35696,3.6218638442\C,-0.4240687945,-0.2248638155,2.7493298821\O,-0.429
058874,1.1393512887,3.0055516582\H,-4.9894600865,2.9388284658,-0.90725
40805\H,-4.3758933485,1.2763482943,-0.6894696132\H,-3.7040694139,2.608
8992399,0.2849823683\H,-6.0362372229,1.4731875415,2.6625843326\H,-4.30
28086609,1.8633487918,2.3223422122\H,-3.0684374989,0.4938501175,1.2043
151847\H,-3.7948928938,-0.9424837695,0.4092712634\H,-3.1411350167,-1.1
635392263,4.3007963142\H,-2.8302275789,0.3928612161,3.4482472681\H,-0.
6963271592,-0.4315675369,1.703139958\H,0.5689687347,-0.6230603166,2.96
80290617\H,-0.9500183867,1.6086122949,2.3066401263\ \Version=ES64L-G16R
evC.01\State=2-A\HF=-573.5682353\S2=0.751615\S2-1=0.\S2A=0.750002\RMSD
=5.858e-09\RMSF=1.311e-05\Dipole=-1.3852082,-1.2183812,1.0426957\Quadr
```

upole=-3.7797353,0.2968889,3.4828464,-2.1190703,-5.3361293,5.9729073\p
G=C01 [X(C5H12O5)]\@

