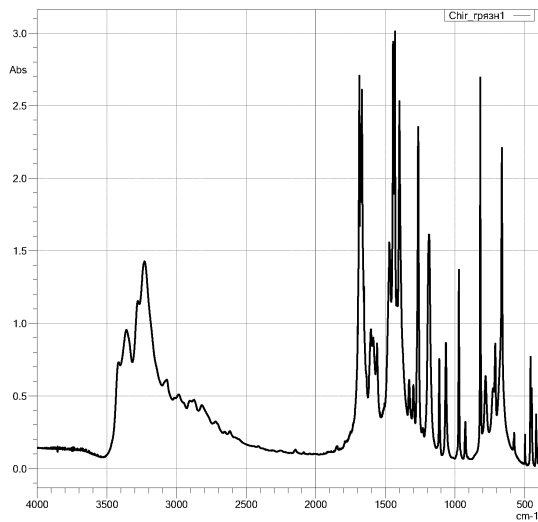
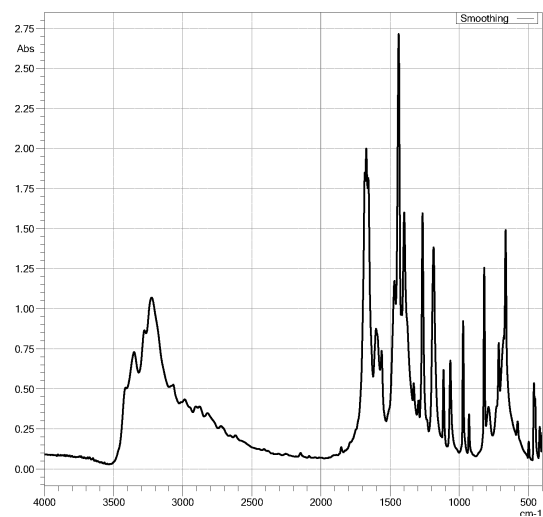


Supplementary Materials: Novel Polymorph of Favipiravir—an Antiviral Medication

Alexander Goloveshkin, Alexander A. Korlyukov and Anna V. Vologzhanina

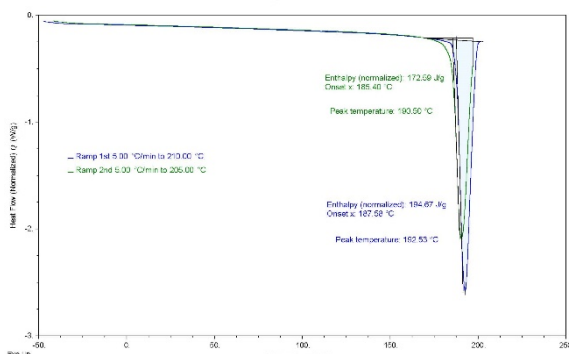


(a)

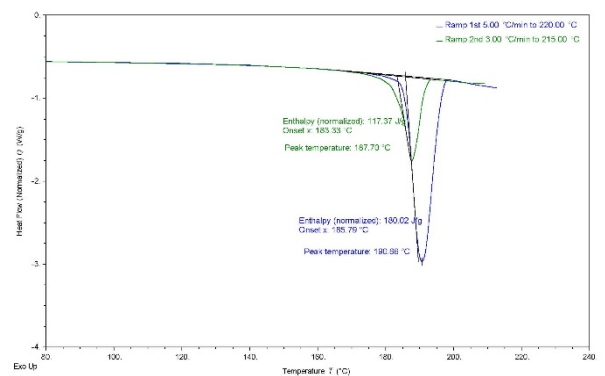


(b)

Figure S1. FT-IR spectra of the (a) tetragonal and (b) orthorhombic polymorphs of favipiravir.



(a)



(b)

Figure S2. DSC curves of the (a) tetragonal and (b) orthorhombic polymorphs of favipiravir.

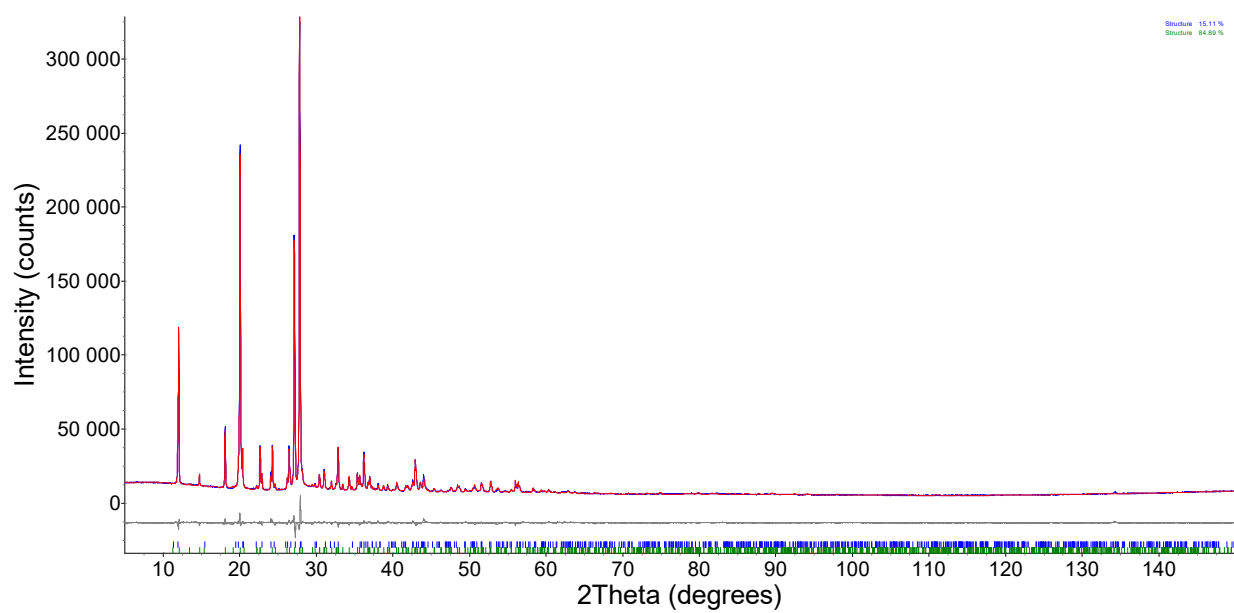


Figure S3. Powder XRD patterns of favipiravir recrystallized from ethyl acetate after 10 months of staying. The Rietveld refinement gives ratio of the tetragonal and orthorhombic forms as 0.85 : 0.15. Experimental (blue), calculated (red) and their difference (grey) curves are depicted.

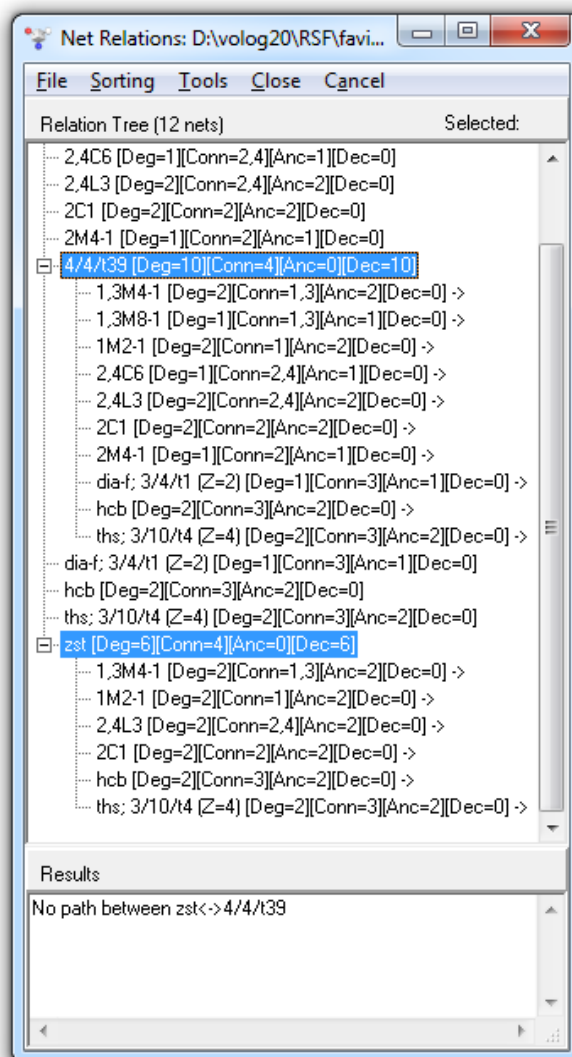


Figure S4. Net relations between zst and 4/4/t39 nets.

Table S1. Energies (kJ mol⁻¹) of intermolecular interactions in favipiravir polymorphs calculated by the UNI force field and the dimer interaction energies calculated using *Crystal Explorer* based on the PIXEL method [CE-B3LYP/6-31 G(d,p)].

Symmetry Operation; Multiplicity	UNI Empirical Force Field	CE-B3LYP/6-31G(d,p)				
		<i>E</i> _{el}	<i>E</i> _{pol}	<i>E</i> _{dis}	<i>E</i> _{rep}	<i>E</i> _{tot}
Orthorhombic polymorph						
-x+1/2, y+1/2, z+1/2; 2	-5.9	-5.6	-1.5	-5.6	7.2	-7.5
x+1/2, -y+1/2, z; 2	-14.4	-2.5	-1.5	-23	11	-17.1
x+1/2, -y+1/2, z; 2	-28.2	-18.8	-6.7	-11.5	25.1	-19.3
-x, -y, z+1/2; 2	-2.6	-0.8	-0.1	-4.7	1.3	-4.3
-x+1/2, y+1/2, z+1/2; 2	-5.1	-1.2	-0.2	-3.8	0.2	-4.6
x, y, z; 2	-18.1	-3.1	-1.6	-21.5	8.6	-17.8
-x, -y, z+1/2; 2	-28.6	-35.9	-7.8	-7.7	41.2	-25
Tetragonal polymorph						
x+1/2, y+1/2, -z; 2	-18	-17	-6.1	-11.2	21	-19.2
y+1/2, -x, z+1/2; 2	-5.7	-1.2	-0.2	-4	0.3	-4.8
y+1/2, -x, z+1/2; 2	-6.2	-4.8	-1.5	-5.9	7	-7
-x, -y, -z; 1	-31	-11	-2.1	-24	11.8	-26.8
-x, -y, -z; 1	-23.4	1.4	-1.1	-21.3	8.7	-12.5
-x+1/2, -y+1/2, z; 1	-31	-8.7	-2.3	-25.2	12.7	-25
y, -x+1/2, -z+1/2; 2	-2.5	-1	-0.2	-5.4	2	-4.7
-x+1/2, -y+1/2, z; 1	-24.4	-4.4	-1	-18.5	5.8	-17.9
y, -x+1/2, -z+1/2; 2	-14.3	-35.7	-7.7	-7.6	40.6	-25

Supplementary material S1. The results of DFT calculations

The geometry of orthorhombic phase of favipiravir optimized in experimental parameters (VASP POSCAR format)

C5 H4 F N3 O2

1.0000000000000000

9.1106004714999997 0.0000000000000000 0.0000000000000000

0.0000000000000000 14.7618999480999999 0.0000000000000000

0.0000000000000000 0.0000000000000000 4.6909999847000003

F O N C H

4 8 12 20 16

Direct

0.5289410000000032 0.0630150000000000 0.3958650000000006

0.4710589999999968 0.9369850000000000 0.8958650000000006

0.0289410000000032 0.4369850000000000 0.3958650000000006

0.9710589999999968 0.5630150000000000 0.8958650000000006

0.6447379999999967 0.4448539999999994 0.6018830000000008

0.3552620000000033 0.5551460000000006 0.1018830000000008

0.1447379999999967 0.0551460000000006 0.6018830000000008

0.8552620000000033 0.9448539999999994 0.1018830000000008

0.7974740000000011 0.3393769999999989 0.9118479999999991

0.2025259999999989 0.6606230000000011 0.4118479999999991

0.2974740000000011 0.1606230000000011 0.9118479999999991

0.7025259999999989 0.8393769999999989 0.4118479999999991

0.4806639999999973 0.3886419999999973 0.2798719999999975

0.5193360000000027 0.6113580000000027 0.7798719999999975

0.9806639999999973 0.1113580000000027 0.2798719999999975

0.0193360000000027 0.8886419999999973 0.7798719999999975

0.5559719999999970 0.2150940000000006 0.4394909999999967

0.4440280000000030 0.7849059999999994 0.9394920000000013

0.0559719999999970 0.2849059999999994 0.4394909999999967

```

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0.2362990000000025 0.8128269999999986 0.3682700000000025
0.2637009999999975 0.3128269999999986 0.8682700000000025
0.7362990000000025 0.6871730000000014 0.3682700000000025
0.5819759999999974 0.3784029999999987 0.4801459999999977
0.4180240000000026 0.6215970000000013 0.9801459999999977
0.0819759999999974 0.1215970000000013 0.4801459999999977
0.9180240000000026 0.8784029999999987 0.9801459999999977
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0.3776539999999997 0.7147670000000019 0.0671430000000015
0.1223460000000003 0.2147670000000019 0.5671430000000015
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0.2714629999999971 0.7287549999999996 0.2836879999999979
0.2285370000000029 0.2287549999999996 0.7836879999999979
0.7714629999999971 0.7712450000000004 0.2836879999999979
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0.3037509999999983 0.8819269999999975 0.2414020000000008
0.1962490000000017 0.3819269999999975 0.7414020000000008
0.8037509999999983 0.6180730000000025 0.2414020000000008
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0.4066059999999965 0.8658530000000013 0.0256040000000013
0.0933940000000035 0.3658530000000013 0.5256040000000013
0.9066059999999965 0.6341469999999987 0.0256040000000013
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0.2769899999999978 0.9505270000000010 0.3113880000000009
0.2230100000000022 0.4505270000000010 0.8113880000000009
0.7769899999999978 0.5494729999999990 0.3113880000000009
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0.5525850000000005 0.5477339999999984 0.7168920000000014
0.9474149999999995 0.0477339999999984 0.2168920000000014
0.0525850000000005 0.9522660000000016 0.7168920000000014
0.4295770000000019 0.3346779999999967 0.1850310000000022
0.5704229999999981 0.6653220000000033 0.6850310000000022
0.9295770000000019 0.1653220000000033 0.1850310000000022
0.0704229999999981 0.8346779999999967 0.6850310000000022
0.7549679999999981 0.3957169999999977 0.8184770000000015
0.2450320000000019 0.6042819999999978 0.3184770000000015
0.2549679999999981 0.1042830000000023 0.8184770000000015
0.7450320000000019 0.8957180000000022 0.3184770000000015
Total energy = -412.81351961 eV

```

The geometry of orthorhombic phase of favipiravir entirely optimized (VASP POSCAR format)

```

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  0.0000000000000000  15.0155879696109640  0.0000000000000000
  0.0000000000000000  0.0000000000000000  4.8536951841730431
  C   H   F   N   O
  20  16   4  12   8
Direct
  0.5762005835212705  0.3782561461902461  0.4761132017032779

```

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0.6176026155359295	0.2875539120208117	0.5677093878156754
0.3823973844640776	0.7124460579791858	0.0677093878156754
0.1176026155359224	0.2124460879791883	0.5677093878156754
0.8823973844640705	0.7875539420208142	0.0677093878156754
0.7214725804142930	0.2762520825115189	0.7752669286099518
0.2785274195857070	0.7237479174884811	0.2752669286099518
0.2214725804142930	0.2237479174884811	0.7752669286099518
0.7785274195857070	0.7762520825115189	0.2752669286099518
0.6937635117245193	0.1251757090265997	0.7469428281472261
0.3062364882754736	0.8748243059733980	0.2469428281472261
0.1937635117245193	0.3748243059733980	0.7469428281472261
0.8062364882754807	0.6251756940266020	0.2469428281472261
0.5928336796411600	0.1383272654540875	0.5403654732873520
0.4071663203588400	0.8616727345459125	0.0403654732873520
0.0928336796411600	0.3616727345459125	0.5403654732873520
0.9071663203588400	0.6383272654540875	0.0403654732873520
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0.2784186865397871	0.9416395790799967	0.3176050089676679
0.2215813134602129	0.4416395790800038	0.8176050089676679
0.7784186865397871	0.5583604209200033	0.3176050089676679
0.4476261377627893	0.4467877598214898	0.2107216955605011
0.5523738322372083	0.5532122101785077	0.7107217255605036
0.9476261677627917	0.0532122401785102	0.2107216955605011
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0.9686869940092464	0.5668563486817888	0.9230280532564521
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0.2580452265561064	0.3054537370388317	0.8626556784378963
0.7419547734438936	0.6945462629611683	0.3626556784378963
0.6342143627384829	0.4452666925399029	0.5875784174459397
0.3657856372615171	0.5547333074600971	0.0875784174459397
0.1342143627384829	0.0547333074600900	0.5875784174459397

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0.8657856372615171 0.9452666925399029 0.0875784174459397
0.7867763704692905 0.3449245192942030 0.8921210214073767
0.2132236295307095 0.6550754807057970 0.3921210214073767
0.2867763704692976 0.1550754807057970 0.8921210214073767
0.7132236295307095 0.8449245192942030 0.3921210214073767

```

Total energy = -412.90789928 eV

The geometry of tetragonal phase of favipiravir optimized in experimental parameters (VASP POSCAR format)

C40 H32 F8 N24 O16

1.0000000000000000

```

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0.0000000052983579 9.6594038995192619 0.0000000000000000
-0.0000000000000000 0.0000000000000000 14.8975776383443037

```

F O H N C

8 16 32 24 40

Direct

```

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0.8427964140371680 0.5872801151780784 0.8129394565297239
0.9127198848219216 0.8427964140371680 0.6870605434702761
0.0872801151780781 0.1572036149628309 0.3129394865297201
0.5872801151780784 0.6572035859628320 0.6870605434702761
0.4127198848219149 0.3427963850371691 0.3129394865297201
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0.2565594887617987 0.5064915437282035 0.8064571446732783
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0.0064915437282030 0.7434405112382014 0.3064571446732786
0.9935084562717965 0.2565594887617987 0.6935428553267217
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0.3421332741541532 0.9052430611709892 0.4089562180372622
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0.3616328490785822 0.6139361233291253 0.8538716416539953
0.6383671509214180 0.3860638766708747 0.1461283283460020
0.1139361083291277 0.6383671509214180 0.3538716716539981
0.8860638766708747 0.3616328490785822 0.6461283583460047
0.3860638766708747 0.8616328490785820 0.3538716716539981
0.6139361233291253 0.1383671439214208 0.6461283583460047
0.4299637024884405 0.1804305636387983 0.8030628718144213
0.5700362975115664 0.8195694363612017 0.1969371431855769
0.0700362975115596 0.3195694363612018 0.8030628718144213
0.9299637024884336 0.6804305636387983 0.1969371431855769
0.8195694363612017 0.9299637024884336 0.3030628718144209
0.1804305636387983 0.0700362975115596 0.6969371281855787

```

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0.6905318400678944	0.5561407955747901	0.4205528473687474
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0.8561500329398354	0.0993088156960856	0.8025927331869835
0.3561500329398355	0.5993088306960831	0.1974072518130192
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0.0993088156960856	0.6438499670601646	0.6974072668130165
0.9006911693039169	0.3561500329398355	0.3025927331869835
0.4006911693039164	0.8561500329398354	0.6974072668130165
0.5993088306960831	0.1438499820601694	0.3025927331869835
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0.1007534779180788	0.3534289622773372	0.8653678728495585
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0.9503538351488073	0.8023037453060333	0.3733412793069997
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0.7393234388143053	0.9930581054199624	0.0346960607723076
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0.6564195734687085	0.4050688944775321	0.0223402777752782
0.0949311055224677	0.6564195734687085	0.4776597322247226
0.9050688944775320	0.3435804565312950	0.5223402977752731
0.4050688944775321	0.8435804265312915	0.4776597322247226
0.5949311055224680	0.1564195434687055	0.5223402977752731
0.1768289195797618	0.9294672256492088	0.1297710514869487
0.8231710654202409	0.0705327893507886	0.8702289335130468
0.3231710654202409	0.5705327743507912	0.1297710514869487
0.6768289345797591	0.4294672256492091	0.8702289335130468
0.0705327893507886	0.6768289345797591	0.6297710664869532
0.9294672256492088	0.3231710654202409	0.3702289335130468
0.4294672256492091	0.8231710654202409	0.6297710664869532
0.5705327743507912	0.1768289195797618	0.3702289335130468
0.2807070652258103	0.0284220396406243	0.1156352278278773
0.7192929347741823	0.9715779543593747	0.8843647571721249
0.2192929347741895	0.4715779543593754	0.1156352278278773
0.7807070652258177	0.5284220456406253	0.8843647571721249
0.9715779543593747	0.7807070652258177	0.6156352428278751
0.0284220396406243	0.2192929347741895	0.3843647571721245
0.5284220456406253	0.7192929347741823	0.6156352428278751
0.4715779543593754	0.2807070652258103	0.3843647571721245

Total energy = -825.25388750 eV

The geometry of orthorhombic phase of favipiravir entirely optimized (VASP POSCAR format)

C40 H32 F8 N24 O16

1.0000000000000000

9.2751998900999997	0.0000000000000000	0.0000000000000000
0.0000000000000000	9.2751998900999997	0.0000000000000000
0.0000000000000000	0.0000000000000000	14.6443004608000003

F O H N C

8 16 32 24 40

Direct

0.3489697395244922	0.0983232435047875	0.1893327043003330
0.6510302314755096	0.9016767564952123	0.8106672656996718
0.1510302604755080	0.4016767564952127	0.1893327043003330
0.8489697685244904	0.5983232435047877	0.8106672656996718
0.9016767564952123	0.8489697685244904	0.6893327343003282
0.0983232435047875	0.1510302604755080	0.3106672956996669
0.5983232435047877	0.6510302314755096	0.6893327343003282
0.4016767564952127	0.3489697395244922	0.3106672956996669
0.2373337871072032	0.9782326021543593	0.8062376518831177
0.7626662128927976	0.0217673978456406	0.1937623481168824
0.2626662128927969	0.5217673978456407	0.8062376518831177
0.7373337871072024	0.4782326021543594	0.1937623481168824
0.0217673978456406	0.7373337871072024	0.3062376518831177
0.9782326021543593	0.2626662128927969	0.6937623481168823
0.4782326021543594	0.7626662128927976	0.3062376518831177

0.5217673978456407	0.2373337871072032	0.6937623481168823
0.0844814556650385	0.8282963418322064	0.9146456401097620
0.9155185593349587	0.1717036731677983	0.0853543748902430
0.4155185593349592	0.6717036581677936	0.9146456401097620
0.5844814406650413	0.3282963418322064	0.0853543748902430
0.1717036731677983	0.5844814406650413	0.4146456401097617
0.8282963418322064	0.4155185593349592	0.5853543598902380
0.3282963418322064	0.9155185593349587	0.4146456401097617
0.6717036581677936	0.0844814556650385	0.5853543598902380
0.1291960792257675	0.8708355580172188	0.8572566569515423
0.8708039137742356	0.1291644269827831	0.1427433130484549
0.3708039137742351	0.6291644419827812	0.8572566569515423
0.6291960862257644	0.3708355580172193	0.1427433130484549
0.1291644269827831	0.6291960862257644	0.3572566869515452
0.8708355580172188	0.3708039137742351	0.6427433430484577
0.3708355580172193	0.8708039137742356	0.3572566869515452
0.6291644419827812	0.1291960792257675	0.6427433430484577
0.4336736858893239	0.1719464351433451	0.7968199455110498
0.5663263141106837	0.8280535648566546	0.2031800694889475
0.0663263141106762	0.3280535648566549	0.7968199455110498
0.9336736858893163	0.6719464351433454	0.2031800694889475
0.8280535648566546	0.9336736858893163	0.2968199455110502
0.1719464351433451	0.0663263141106762	0.7031800544889502
0.6719464351433454	0.5663263141106837	0.2968199455110502
0.3280535648566549	0.4336736858893239	0.7031800544889502
0.4476717949558430	0.1919132668946719	0.9152858537264861
0.5523282050441563	0.8080867031053256	0.0847141312735233
0.0523282050441568	0.3080867331053281	0.9152858537264861
0.9476717949558437	0.6919132968946744	0.0847141312735233
0.8080867031053256	0.9476717949558437	0.4152858537264789
0.1919132668946719	0.0523282050441568	0.5847141462735139
0.6919132968946744	0.5523282050441563	0.4152858537264789
0.3080867331053281	0.4476717949558430	0.5847141462735139
0.1431637426924825	0.9030691564810096	0.2059563712733100
0.8568362723075226	0.0969308285189926	0.7940436137266924
0.3568362723075226	0.5969308435189904	0.2059563712733100
0.6431637276924774	0.4030691564810099	0.7940436137266924
0.0969308285189926	0.6431637276924774	0.7059563862733076
0.9030691564810096	0.3568362723075226	0.2940436137266924
0.4030691564810099	0.8568362723075226	0.7059563862733076
0.5969308435189904	0.1431637426924825	0.2940436137266924
0.4000493227432765	0.1415595404213349	0.8609836675502277
0.5999506772567232	0.8584404295786628	0.1390163474497702
0.0999506772567234	0.3584404595786580	0.8609836675502277
0.9000493227432768	0.6415595704213372	0.1390163474497702
0.8584404295786628	0.9000493227432768	0.3609836675502274
0.1415595404213349	0.0999506772567234	0.6390163324497723
0.6415595704213372	0.5999506772567232	0.3609836675502274
0.3584404595786580	0.4000493227432765	0.6390163324497723
0.3232250752562813	0.0700357210901750	0.0365374248944633
0.6767748947437231	0.9299642519098190	0.9634625711055358
0.1767749247437185	0.4299642819098219	0.0365374248944633
0.8232251052562769	0.5700357480901810	0.9634625711055358
0.9299642519098190	0.8232251052562769	0.5365374288944642

0.0700357210901750	0.1767749247437185	0.4634625711055360
0.5700357480901810	0.6767748947437231	0.5365374288944642
0.4299642819098219	0.3232250752562813	0.4634625711055360
0.1098771767039883	0.8632144126304283	0.0676681446780291
0.8901227932960161	0.1367855723695670	0.9323318553219708
0.3901228232960116	0.6367855873695717	0.0676681446780291
0.6098772067039839	0.3632144126304280	0.9323318553219708
0.1367855723695670	0.6098772067039839	0.5676681446780292
0.8632144126304283	0.3901228232960116	0.4323318553219709
0.3632144126304279	0.8901227932960161	0.5676681446780292
0.6367855873695717	0.1098771767039883	0.4323318553219709
0.2996691250504578	0.0416076121617825	0.8723188839723161
0.7003308749495415	0.9583923858382242	0.1276811310276817
0.2003308749495420	0.4583923858382173	0.8723188839723161
0.7996691250504585	0.5416076141617758	0.1276811310276817
0.9583923858382242	0.7996691250504585	0.3723188839723158
0.0416076121617825	0.2003308749495420	0.6276811160276839
0.5416076141617758	0.7003308749495415	0.3723188839723158
0.4583923858382173	0.2996691250504578	0.6276811160276839
0.2577998875918425	0.0032566275091291	0.9668399969111509
0.7422000824081616	0.9967433424908611	0.0331599770888541
0.2422001124081573	0.4967433724908710	0.9668399969111509
0.7577999175918384	0.5032566575091389	0.0331599770888541
0.9967433424908682	0.7577999175918384	0.4668400269111463
0.0032566275091291	0.2422001124081573	0.5331600030888491
0.5032566575091389	0.7422000824081616	0.4668400269111463
0.4967433724908710	0.2577998875918425	0.5331600030888491
0.1500205950213397	0.8977267006950447	0.9824670298651057
0.8499793749786574	0.1022732993049549	0.0175329501349000
0.3499794049786600	0.6022732993049553	0.9824670298651057
0.6500206250213426	0.3977267006950451	0.0175329501349000
0.1022732993049549	0.6500206250213426	0.4824670598651007
0.8977267006950447	0.3499794049786600	0.5175329701348943
0.3977267006950451	0.8499793749786574	0.4824670598651007
0.6022732993049553	0.1500205950213397	0.5175329701348943
0.1752723005771718	0.9307301574877053	0.1364171894152803
0.8247276844228306	0.0692698575122923	0.8635827955847147
0.3247276844228306	0.5692698425122947	0.1364171894152803
0.6752723155771694	0.4307301574877055	0.8635827955847147
0.0692698575122923	0.6752723155771694	0.6364172044152853
0.9307301574877053	0.3247276844228306	0.3635827955847149
0.4307301574877055	0.8247276844228306	0.6364172044152853
0.5692698425122947	0.1752723005771718	0.3635827955847149
0.2823508750876392	0.0333818388300495	0.1187544792340569
0.7176491249123538	0.9666181551699498	0.8812455057659455
0.2176491249123610	0.4666181551699499	0.1187544792340569
0.7823508750876462	0.5333818448300502	0.8812455057659455
0.9666181551699498	0.7823508750876462	0.6187544942340545
0.0333818388300495	0.2176491249123610	0.3812455057659452
0.5333818448300502	0.7176491249123538	0.6187544942340545
0.4666181551699499	0.2823508750876392	0.3812455057659452

Total energy = -825.52517965 eV