Supporting Information for:

Insights into the solvent-assisted degradation of organophosphorus compounds by a Zr-based metal-organic framework

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Section S1: Materials and methods

All materials were purchased from commercially available sources and used without further purification.

Section S2: ZrTCPB Synthesis

Zr TCPB Synthesis:

The reaction mixture containing $Cl_2OZr \cdot 8\ H_2O$ (0.0217 g, 0.067 mmol), 1,2,4,5-Tetrakis(4-carboxyphenyl)benzene (TCPB, 0.0067 g, 0.012 mmol), Benzoic acid (BA,0.604 g, 4.95 mmol), N,N'-dimethylformamide (DMF, 2.15 mL), was placed in a 20 mL scintillation vial and was heated to 115 °C for 72 hrs, at a rate of 1.5 °C/minute and cooled to room temperature at a cooling rate of 1 °C/minute. Solid was then washed in 50 mL of DMF 3 times and then 3 times in 50 mL of MeOH.

Zr TCPB HCl Washing Method:

50 mg of the white solid precipitate was re-suspended in 20 mL of DMF with 1.5 mL of 8M HCl and was put in the oven for 12 hours at 115 °C. Then the solution was exchanged with 50 mL of acetone. This acetone was replenished several times over the course of 72 hours before sample was re-activated.

Section S3: Gas Sorption Measurements

Prior to measuring the gas adsorption isotherms, the sample was immersed in 15 mL of methanol for 3 days, with the solvent replenished every 24 hrs. Following this treatment, the sample was activated under vacuum on a Micromeritics ASAP 2020 surface area and porosity analyzer, at 30 °C for 6 hrs and then heated to 150 °C at 1 °C/min for 12 hrs. Nitrogen gas adsorption isotherms were measured at 77 K using nitrogen of ultra-high purity (99.999%, obtained from Matheson Tri-Gas).
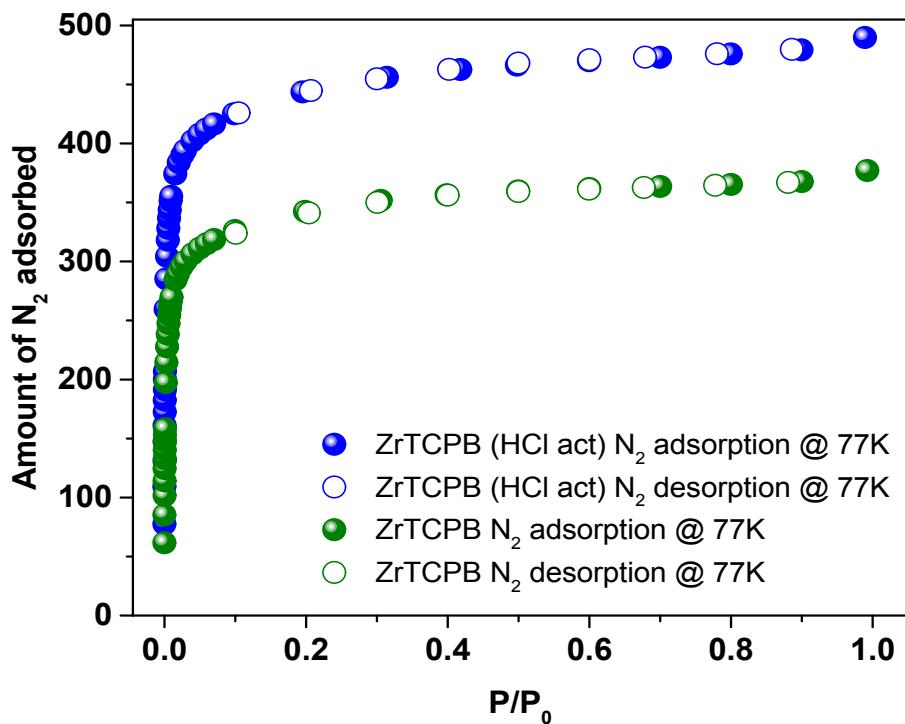
Figure S1. Nitrogen sorption isotherm measured at 77K on pristine (green) and HCl washed (blue) ZrTCPB sample.

Section S4: Powder X-ray Diffraction Studies

Measurements were performed on a Siemens Kristalloflex D500 diffractometer, CuKα radiation (λ = 1.54178 Å).
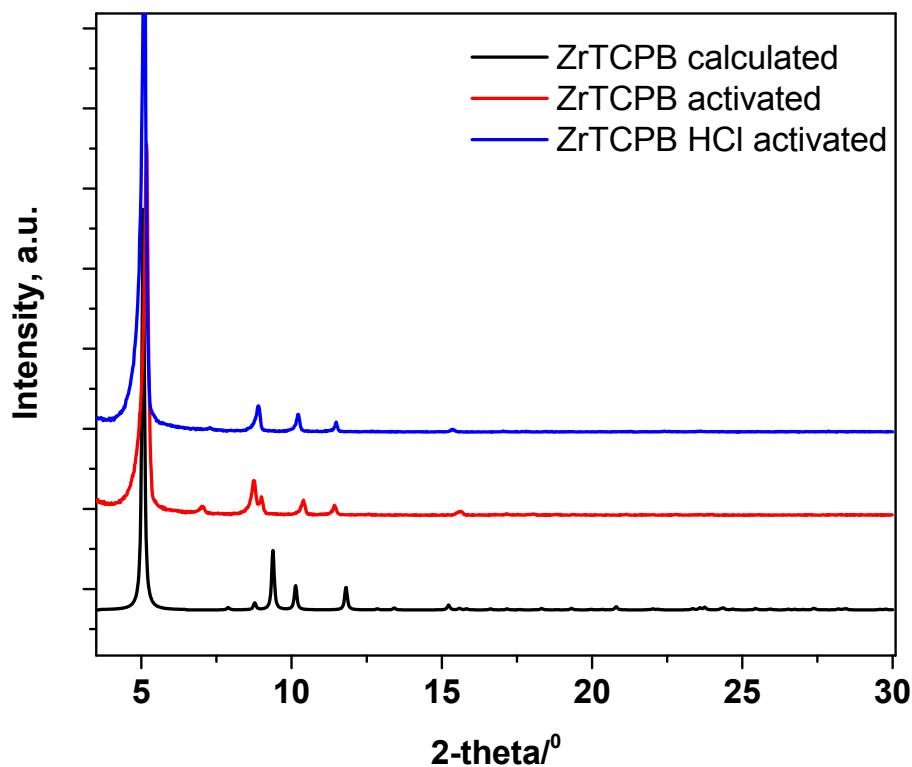
Figure S2. X-ray powder diffraction of pristine (red trace) and HCl washed (blue trace) ZrTCPB sample.

Unit cell	a (Å)	b (Å)	c (Å)	Volume (Å^3)
ZrTCPB (this work)	20.04(3)	34.80(3)	11.86(2)	8271.9
cif file*	20.14	34.89	11.19	7866.8

* M. Lammert, H. Reinsch, C. A. Murray, M. T. Wharmby, H. Terraschke and N. Stock, *Dalton Trans.*, 2016, **45**, 18822-18826.

Section S5: ^{31}P Nuclear Magnetic Resonance (NMR) Experiments

DMNP simulant

Dimethyl 4-nitrophenyl phosphate (DMNP) was used as received from Sigma-Aldrich with no further purification steps performed.

In a representative in situ NMR experiment, the ZrTCPB sample was added to 1 mL of solvent in an NMR tube. To improve the MOF dispersion into the solvent, the sample was vortexed for 30 s, followed by sonication for 1 min, and then vortexed again for 30 s. 4 μL of simulant was added to the mixture, the tube was capped and shaken vigorously twice and then was immediately placed in the instrument, tuned, and the run started.

^{31}P NMR experiments were performed on a Bruker Avance III 500 instrument using a 5 mm broadband probe, with a ^{31}P observed frequency of 202.47 MHz. Experiments were performed in an unlock mode on all reaction mixtures at a stabilized temperature of 50 °C. The ^{31}P NMR experiments were obtained with standard single pulse Bloch decay with inverse gated 1H decoupling pulse sequence (Bruker program zgig) using a spectral width of 100 ppm, recycle delay of 30s, and 16 scan averages. Integration was performed in the Bruker Biospin TOPSPIN software suite and used a normalized total ^{31}P signal for analysis. The ^{31}P NMR chemical shifts were referenced to the external 85% H_3PO_4 standard δ = 0.0 ppm.

Sarin (GB) and GD. *Caution should be taken on any tests involving GB. The experiments should be run by trained personnel using appropriate safety procedures.*
The GB and GD ^{31}P NMR experiments were performed on a Varian 400 instrument using a 5 mm broadband probe, with a ^{31}P observed frequency of 161.85 MHz. Experiments were performed in a lock mode on all reaction mixtures at a stabilized temperature of 50°C. The ^{31}P NMR experiments were obtained with standard single pulse decay with ^{1}H decoupling pulse sequence using a spectral width of 100 ppm, recycle delay of 3.75s, and 128 scan averages. The ZrTCPB sample (9.6 mg) was dispersed into a 5 mm NMR tube containing MeOH (1 mL), followed by the addition of GB and GD, respectively (4.5 μL). The NMR tube was capped and shaken vigorously before being placed into the NMR magnet for monitoring by ^{31}P NMR spectroscopy on a Varian INOVA 400 MHz NMR spectrometer. The temperature was maintained by a temperature controlled probe, and the ^{31}P NMR chemical shifts were referenced to the external standard phosphoric acid δ = 0.0 ppm. Integration was performed utilizing Varian vnmrj 2.3C software. The ^{31}P NMR chemical shifts were referenced to the external 85% H3PO4 standard δ = 0.0 ppm.

Section S6: Computational Details

The previously published crystal structure of ZrTCPB was used for DFT calculations.[1] An initial optimization of the crystal structure was performed in a three step process. First, the ion positions were optimized with fixed cell dimensions, followed by an optimization of ions and cell parameters, and then ended with an additional ion-only optimization. Initial positions for GB and GD were created by manually placing, with Materials Studio,[2] the molecules near the active site. A single solvent molecule was incorporated, which is initially placed between the OH chelated to a Zr and the μ_3-OH. All calculations were performed using the projector augmented wave approach[3] as implemented in the Vienna Ab Initio Simulation Package.[4] The Perdew-Burker-Ernzerhof revised for solids (PBEsol) exchange correlation functional[5] was used on a single Γ point in the Brillouin-zone. Van der Waals corrections were applied using the DFT-D3 method with Becke-Jonson damping.[6] A 400 eV plane wave cutoff energy was used. Optimizations were continued until the force on all atoms was smaller than 0.03 eV $\cdot$ Å^{-1}. Vibrational calculations were performed on all optimized intermediates and transitions to confirm the existence of 0 (intermediates) or 1 (transition state) imaginary frequency. Transition states were located using the climbing image nudge elastic band method[7]. Initial structures were located along the relevant path via a linear interpolation between initial and final states.

Section S7: Additional Tables and Figures

ZrTCPB Ratio Study			
Ratio of MOF to DMNP	MOF (mg)	DMNP (mg)	MeOH (mg)
6.89%	2.9	5.6	779.2
7.79%	3.1	5.3	777.3
14.79%	5	4.5	781
16.82%	7.2	5.7	777.1
28.40%	9.6	4.5	773.1

Table S1. ZrTCPB to DMNP variable mol ratio study.

Solvent	pH	
	Initial	Final
H_2O	7.0	5.0
MeOH	6.5	6.0
IPA	6.5	6.5
HFE	6.5	6.5

Table S2. Initial and final pH of the solutions before and after MOF-based degradation of DMNP.
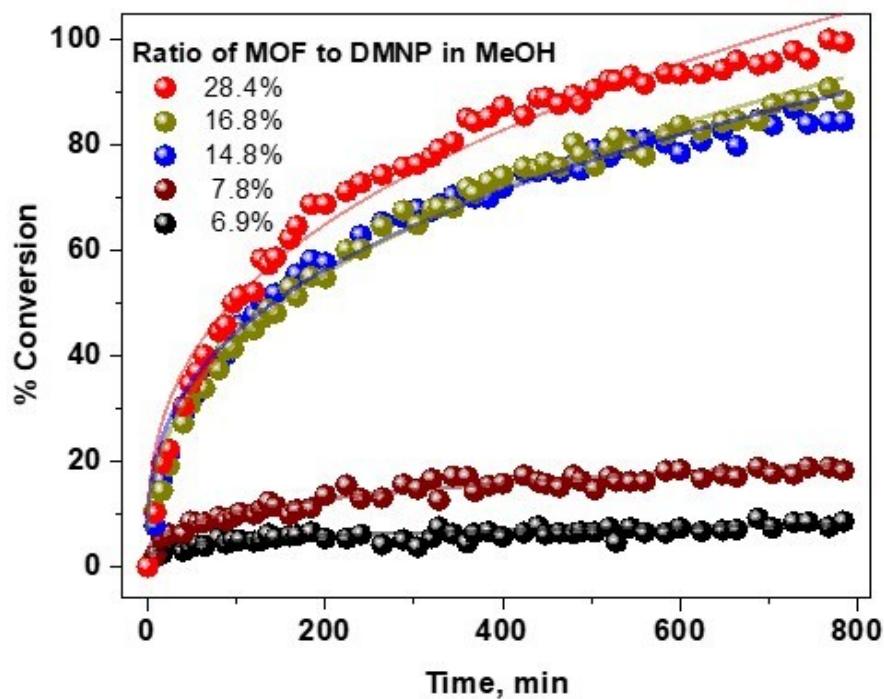
Figure S3. ZrTCPB-based degradation of DMNP in methanol as function of variable MOF:DMNP ratios.
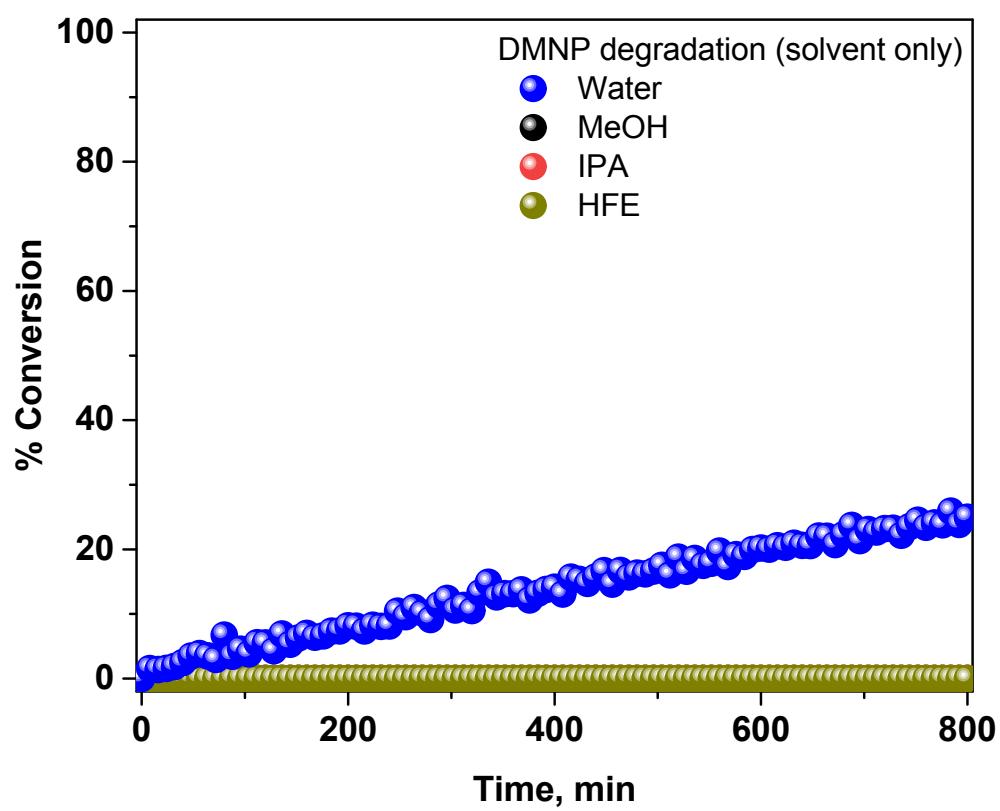
Figure S4. DMNP degradation in water, methanol, isopropyl alcohol and HFE.
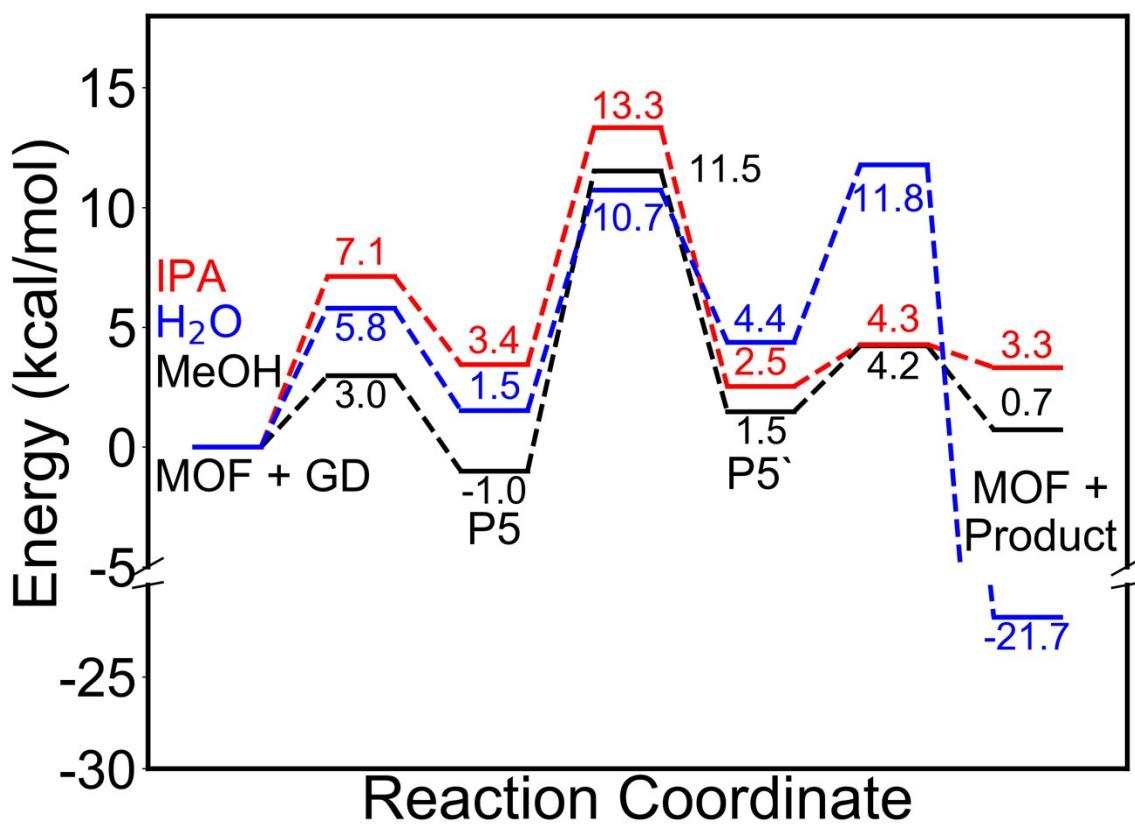
Figure S5. Reaction pathway energies for the degradation of GD on ZrTCPB in H2O (blue), MeOH (black), and IPA (red). The energies shown for each transition state and intermediate are in kcal·mol^{-1} units.
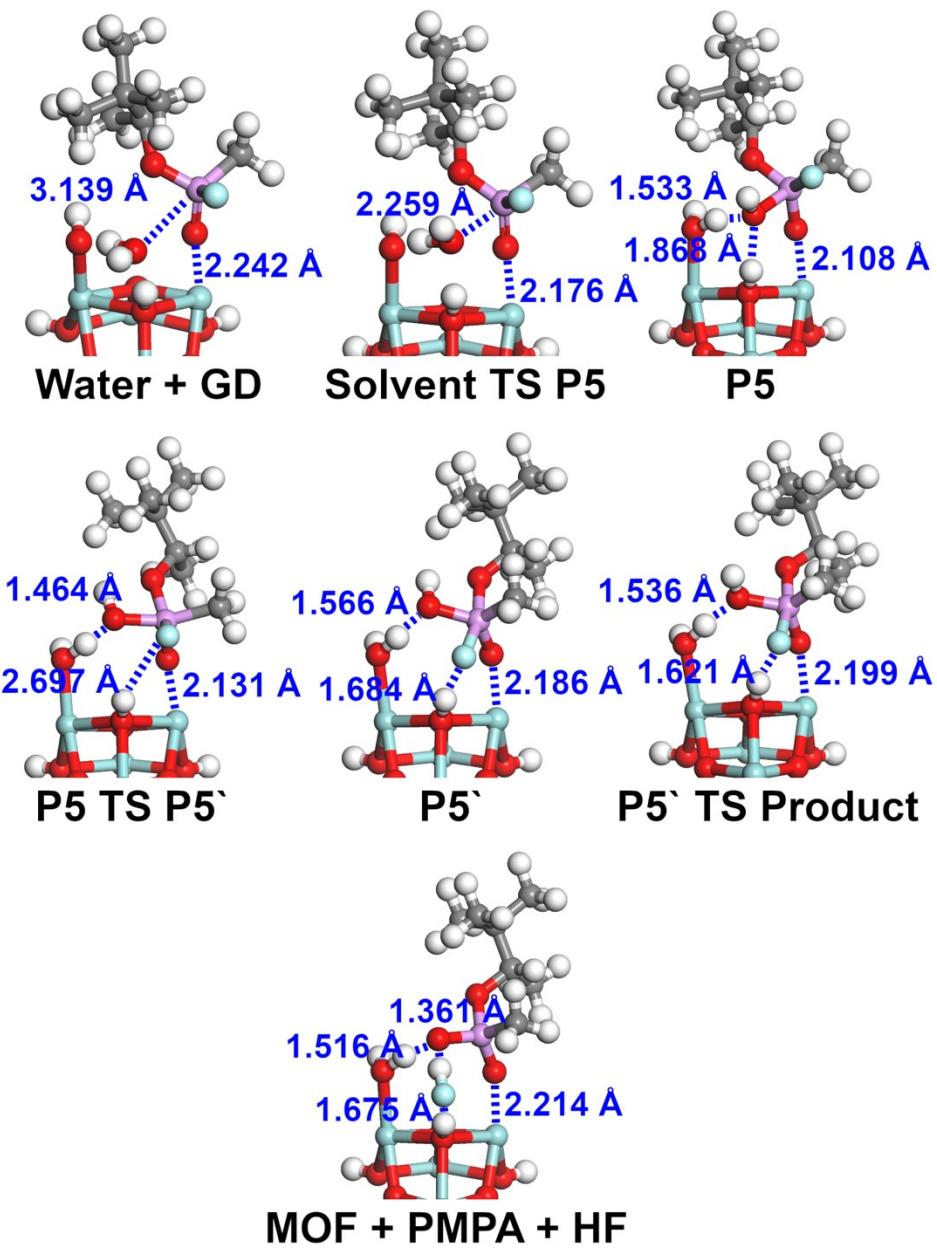
Figure S6. Structures of intermediates and transition states in the degradation pathway of GD with H_2O on ZrTCPB (H = white, O = red, Zr = teal, F = light blue, C = gray). Only the active site is depicted for visual clarity. Relevant distances are shown.
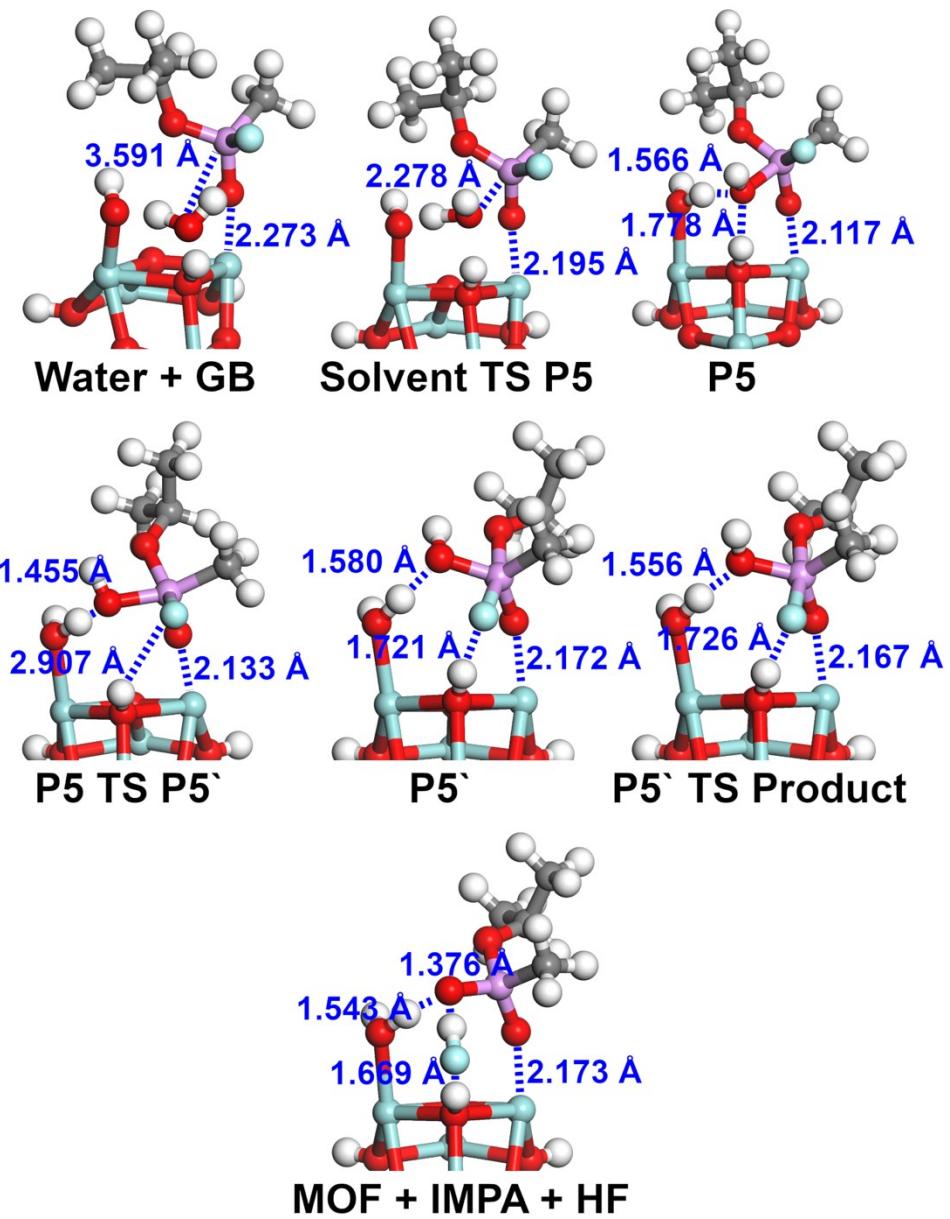
Figure S7. Structures of intermediates and transition states in the degradation pathway of GB with H_2O on ZrTCPB (H = white, O = red, Zr = teal, F = light blue, C = gray). Only the active site is depicted for visual clarity. Relevant distances are shown.
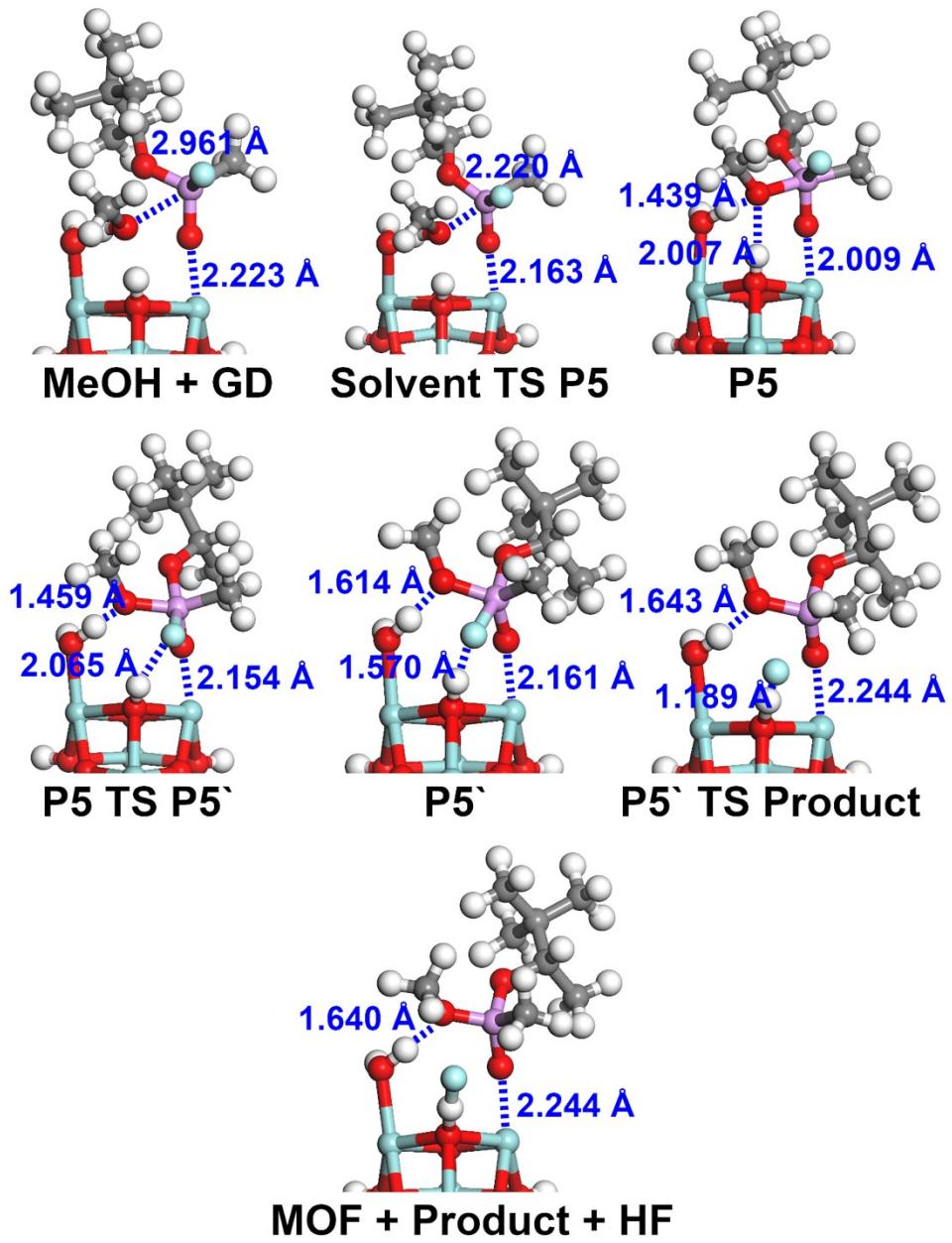
Figure S8. Structures of intermediates and transition states in the degradation pathway of GD with MeOH on ZrTCPB (H = white, O = red, Zr = teal, F = light blue, C = gray). Only the active site is depicted for visual clarity. Relevant distances are shown.
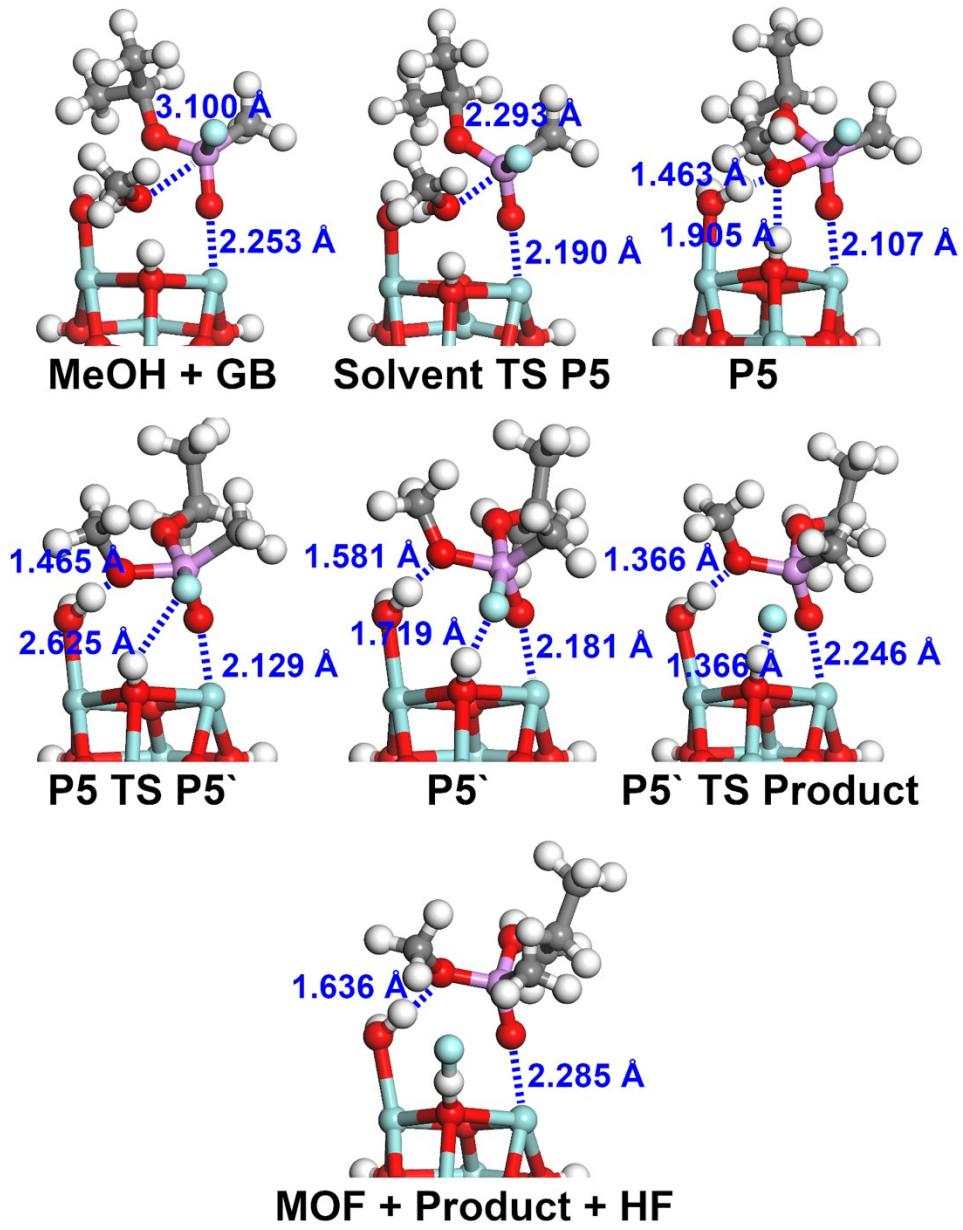
Figure S9. Structures of intermediates and transition states in the degradation pathway of GB with MeOH on ZrTCPB (H = white, O = red, Zr = teal, F = light blue, C = gray). Only the active site is depicted for visual clarity. Relevant distances are shown.
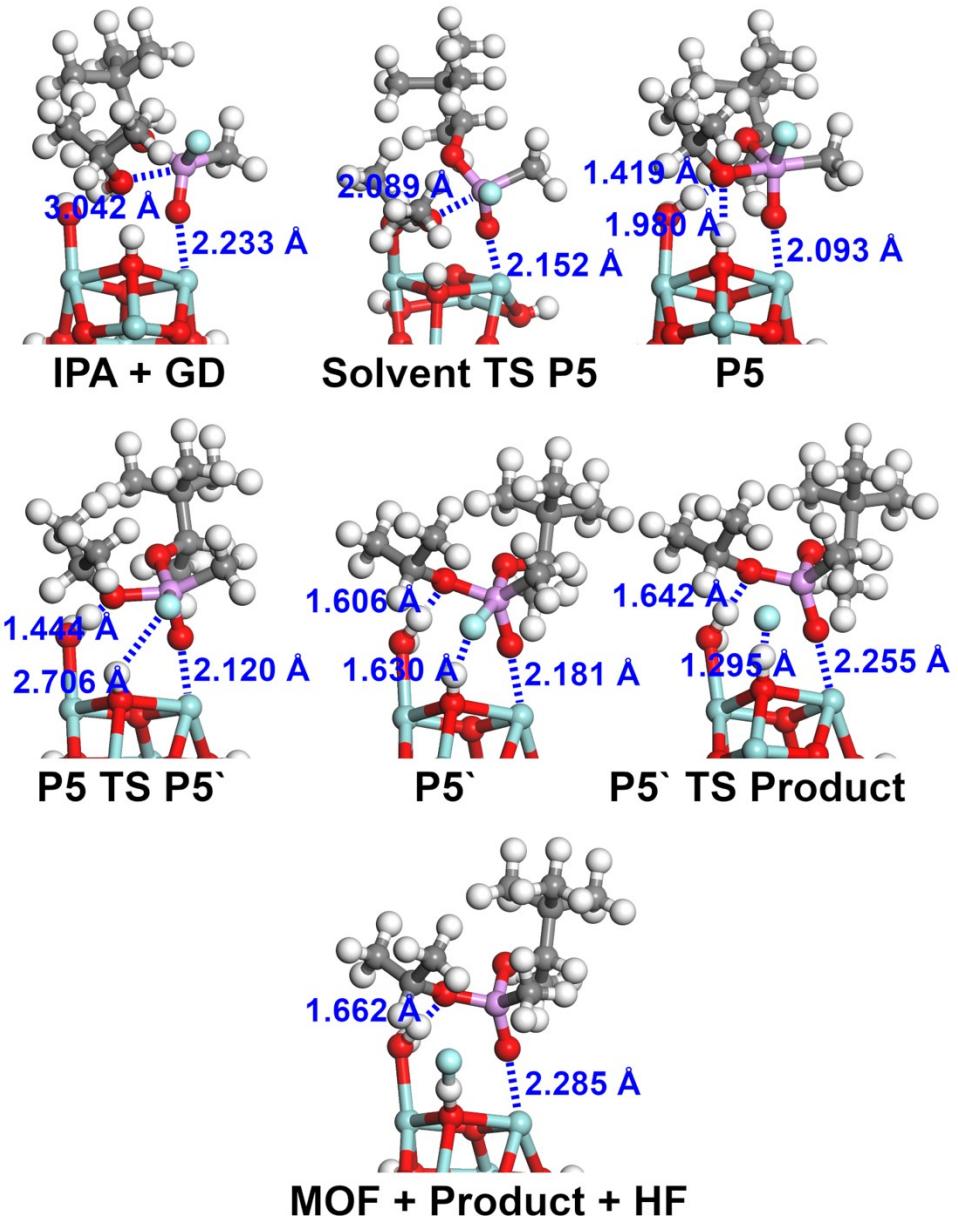
Figure S10. Structures of intermediates and transition states in the degradation pathway of GD with IPA on ZrTCPB (H = white, O = red, Zr = teal, F = light blue, C = gray). Only the active site is depicted for visual clarity. Relevant distances are shown.
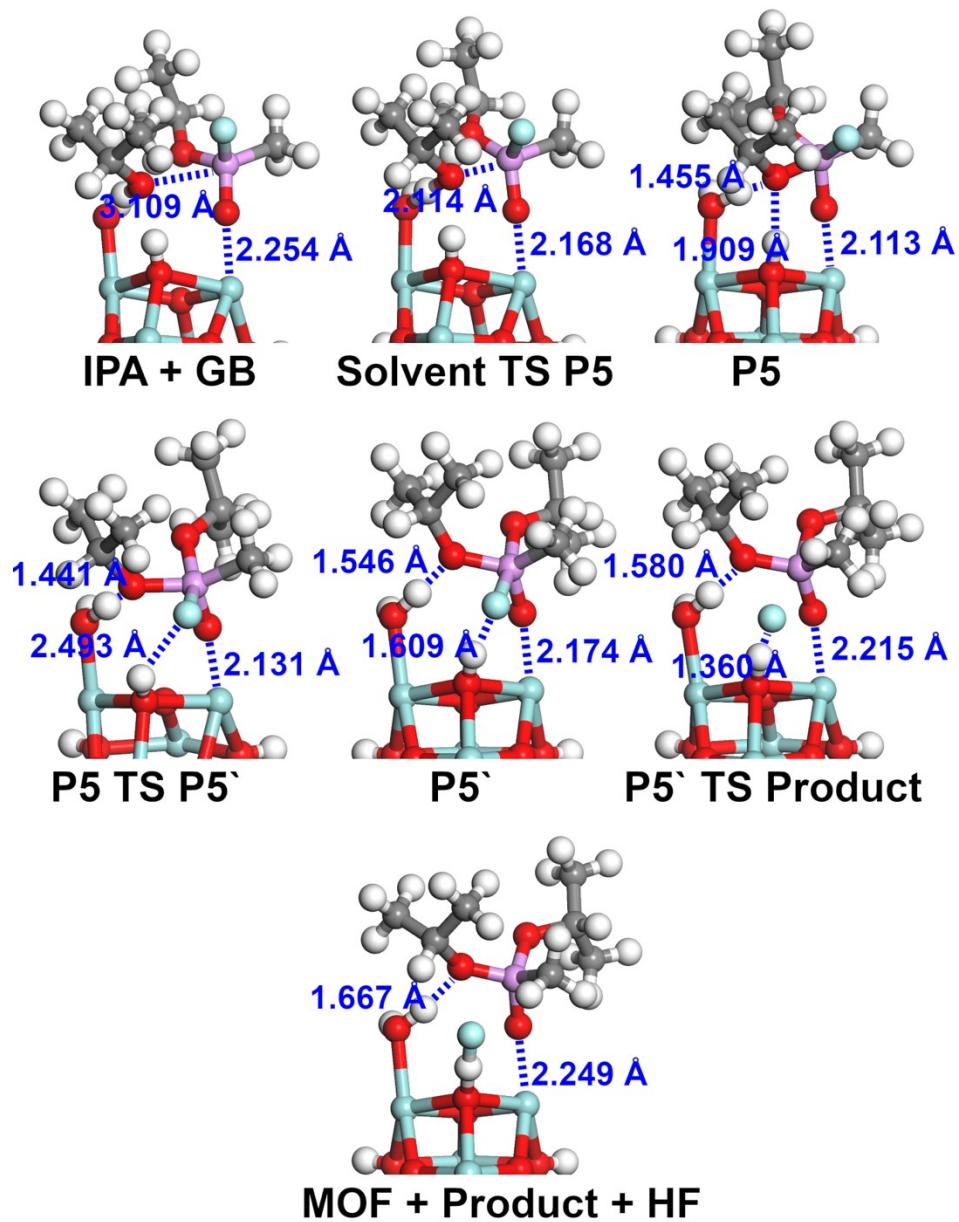
Figure S11. Structures of intermediates and transition states in the degradation pathway of GB with IPA on ZrTCPB (H = white, O = red, Zr = teal, F = light blue, C = gray). Only the active site is depicted for visual clarity. Relevant distances are shown.
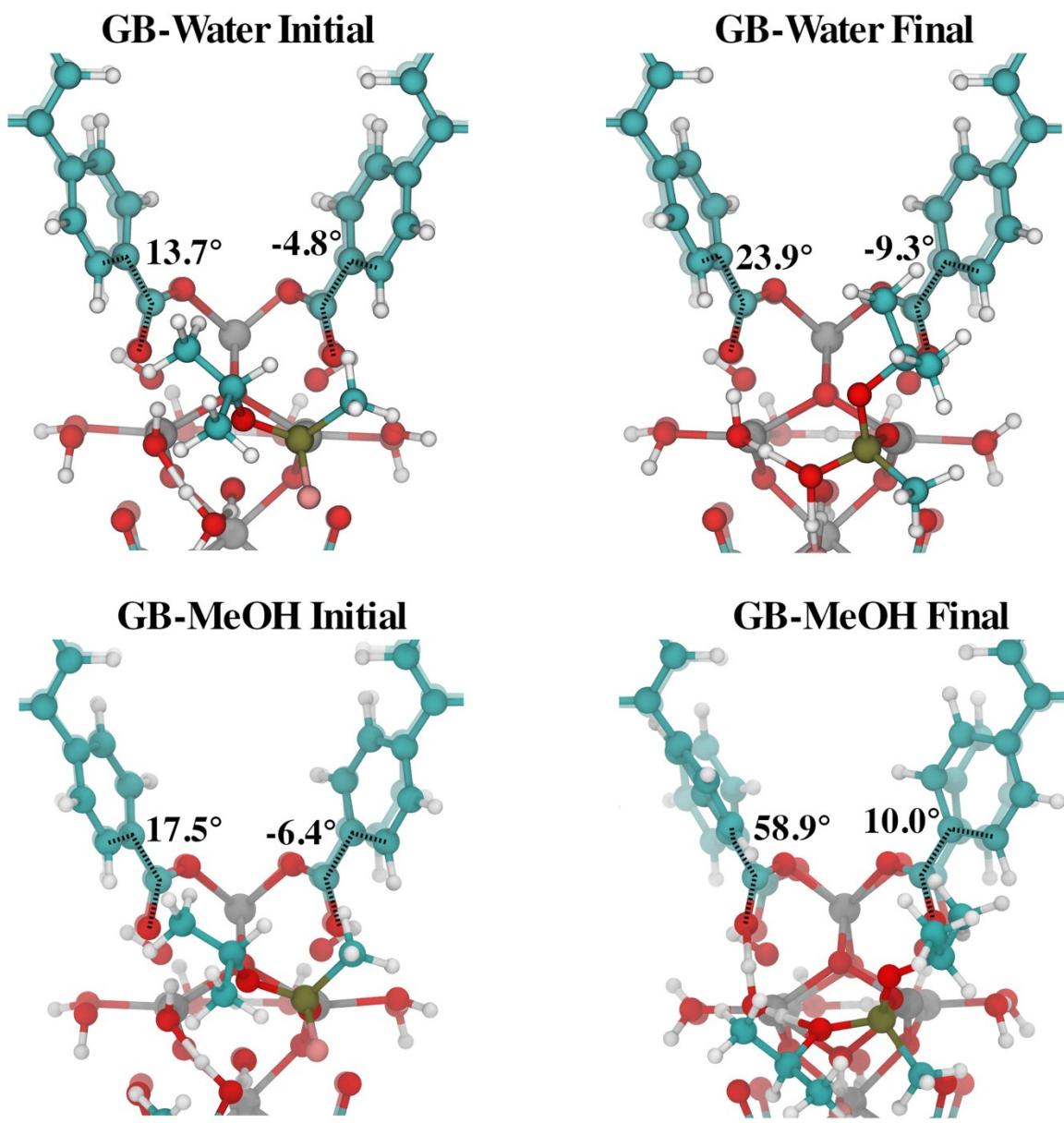
Figure S12. Structures of the initial (left) and final (right) states of GB degradation in H$_2$O (top) and MeOH (bottom). The dihedral angle of two relevant linkers near the active site is indicated. The angle changes more drastically from initial to final for the larger MeOH solvent.

Solvent	GB	GD
H_2O	10	14
MeOH	24	25
IPA	33	20

Table S3. Change in the dihedral angle (°) of the linker depicted in Fig. S12 from initial to final state for GB and GD in H_2O, MeOH, and IPA.
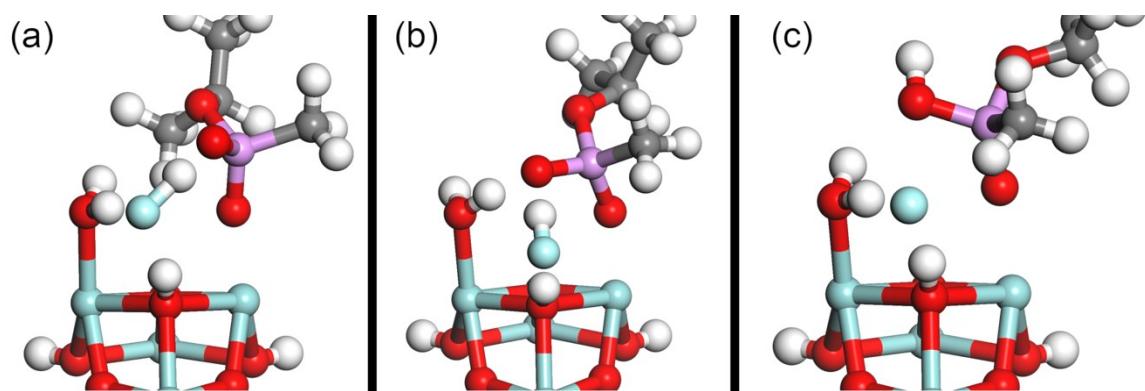
Figure S13. Stable structures of GB degraded on ZrTCPB by H_2O. The relative energies of each are (a) 0.0, (b) 4.9, and (c) 28.4 kcal $\cdot$ mol^{-1}. Only the degraded structure depicted in (c) remains protonated.

Section S8: References

1. M. Lammert, H. Reinsch, C. A. Murray, M. T. Wharmby, H. Terraschke and N. Stock, *Dalton Trans.*, 2016, **45**, 18822-18826.
2. Dassault Systèmes BIOVIA, Materials Studio, 2017 R2 (17.2.0.1626), San Diego: Dassault Systèmes, 2017
3. (a) P. E. Blöchl, *Phys. Rev. B*, 1994, **50**, 17953-17979; (b) G. Kresse and D. Joubert, *Phys. Rev. B*, 1999, **59**, 1758-1775.
4. (a) G. Kresse and J. Furthmuller, *Comp. Mater. Sci.*, 1996, **6**, 15-50; (b) G. Kresse and J. Furthmuller, *Phys. Rev. B*, 1996, **54**, 11169-11186; (c) G. Kresse and J. Hafner, *Phys. Rev. B*, 1994, **49**, 14251-14269; (d) G. Kresse and J. Hafner, *Phys. Rev. B*, 1993, **47**, 558-561.
5. J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou and K. Burke, *Phys. Rev. Lett.*, 2008, **100**, 136406.
6. (a) S. Grimme, S. Ehrlich and L. Goerigk, *J. Comput. Chem.*, 2011, **32**, 1456-1465; (b) S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
7. (a) G. Henkelman and H. Jónsson, *J. Chem. Phys.*, 2000, **113**, 9978-9985; (b) G. Henkelman, B. P. Uberuaga and H. Jónsson, *J. Chem. Phys.*, 2000, **113**, 9901-9904.

Section S9: Input Files for Calculations

Representative INCAR files

Optimization of reactants, products, and intermediates

SYSTEM = gb_solvent_zrtcpb

ISTART = 0   ! 0 = new; 1 = restart
ICHARG = 0   ! 0 = charge density from wave functions; 1 = read from CHGCAR file

ISIF = 2   ! 2 = relax ions; 3 = relax ions and cell boundaries; set ENCUT = 1.3*ENMAX for ISIF=3
ISYM = 0

ENCUT = 400   ! must set ENCUT = 1.3*ENMAX for ISIF = 2

IVDW = 12 ! DFT-D3 method with BJ damping
GGA=PS   ! Perdew-Burke-Ernzerhof revised for solids

ISMEAR = 1 ! confirm 'entropy T*S' in OUTCAR is less than 1 meV/atom; if not, adjust SIGMA or ISMEAR
SIGMA = 0.2 ! change sigma if 'entropy T*S' in OUTCAR is less than 1 meV/atom

MAXMIX = 40 ! should be approx 3*(number of electronic steps in first iteration)

EDIFFG = -0.03   ! remove if change in totoal energy between two ionic steps is greater than 0.001

LREAL = AUTO ! use LREAL=FALSE for final accurate energies

ISPIN = 1   ! 1 for non-spin-polarized; 2 for spin-polarized

NELM = 80   ! number of electronic self-consistent loops in each step
NSW = 1000   ! number of steps; default is 0

IBRION = 2 ! 2 good for systems that are hard to converge
POTIM = 0.2 ! optimal POTIM = original POTIM * trialstep number from OUTCAR

NCORE = 16   ! recommended for linux clusters
LPLANE = .TRUE.   ! recommended for linux clusters
LSCALU = .FALSE.   ! recommended for linux clusters
NSIM = 4   ! recommended for linux clusters

Optimization of transition states (CI-NEB)

SYSTEM = gb_solvent_ts_p5_zrtcpb

ISTART = 0   ! 0 = new; 1 = restart
ICHARG = 0   ! 0 = charge density from wave functions; 1 = read from CHGCAR file

IMAGES = 8   ! number of NEB images
SPRING = -5.0 ! spring < 0 for NEB, -5 = recommended
ICHAIN = 0
LCLIMB = .TRUE.

ISYM = 0
ISIF = 2   ! 2 = relax ions; 3 = relax ions and cell boundaries; set ENCUT = 1.3*ENMAX for ISIF=3

ENCUT = 400   ! must set ENCUT = 1.3*ENMAX for ISIF = 2

IVDW = 12   ! DFT-D3 method with BJ damping
GGA=PS   ! Perdew-Burke-Ernzerhof revised for solids

ISMEAR = 1 ! confirm 'entropy T*S' in OUTCAR is less than 1 meV/atom; if not, adjust SIGMA or ISMEAR
SIGMA = 0.2 ! change sigma if 'entropy T*S' in OUTCAR is less than 1 meV/atom

MAXMIX = 40 ! should be approx 3*(number of electronic steps in first iteration)

EDIFFG = -0.03   ! remove if change in totoal energy between two ionic steps is greater than 0.001

LREAL = AUTO ! use LREAL=FALSE for final accurate energies

ISPIN = 1   ! 1 for non-spin-polarized; 2 for spin-polarized

NELM = 80   ! number of electronic self-consistent loops in each step
NSW = 1000   ! number of steps; default is 0

IBRION = 1   ! 1 recommended for NEB
POTIM = 0.1 ! optimal POTIM = original POTIM * trialstep number from OUTCAR

NCORE = 16   ! recommended for linux clusters
LPLANE = .TRUE.   ! recommended for linux clusters
LSCALU = .FALSE.   ! recommended for linux clusters

NSIM = 4   ! recommended for linux clusters

POSCAR files for h₂o solvent

POSCAR file for gb_solvent

POSCAR file from zrtcpb-gb-h2o-c.res: C: 140 F: 1 H: 114 O: 66 P: 1 ZR: 12
  34.8920000000000
    0.5792995890490465   -0.0000450140396845   0.0007649282407427
   -0.0000781726227076   1.0082675674799713   0.0000166934211398
    0.0004256087542374   0.0000053656439079   0.3214078049098053
140 1 114 66 1 12
Direct
   0.79023   0.88207   0.30393
   0.23310   0.21668   0.56282
   0.73274   0.71652   0.43658
   0.70744   0.68401   0.36688
   0.64843   0.68909   0.30333
   0.61972   0.65899   0.24289
   0.85218   0.81132   0.30654
   0.73821   0.64833   0.36384
   0.61426   0.59095   0.18651
   0.64889   0.62299   0.24586
   0.70878   0.61791   0.30542
   0.88141   0.84152   0.24703
   0.20723   0.18404   0.63189
   0.23333   0.78352   0.56310
   0.20768   0.81611   0.63258
   0.14734   0.81133   0.69266
   0.11810   0.84151   0.75223
   0.23920   0.85152   0.63824
   0.11299   0.90939   0.80970
   0.14801   0.87731   0.75118
   0.20926   0.88210   0.69541
   0.76032   0.85148   0.36115
   0.73406   0.28376   0.56356
   0.14644   0.18870   0.69039
   0.70706   0.31636   0.63162
   0.64542   0.31144   0.68693
   0.61409   0.34168   0.74261
   0.88657   0.90941   0.18987
   0.73765   0.35199   0.63765
   0.60723   0.40976   0.79857
   0.64306   0.37773   0.74138
   0.70544   0.38269   0.69015
   0.85151   0.87731   0.24822
   0.77032   0.21742   0.56295
   0.11678   0.15842   0.74883
   0.79758   0.18507   0.63030
   0.85805   0.19018   0.68918
   0.88899   0.15982   0.74442
   0.76743   0.14920   0.63316
   0.89552   0.09146   0.79720
   0.86040   0.12367   0.74037
   0.79895   0.11854   0.68626
   0.23871   0.14865   0.63728
   0.11203   0.09045   0.80654
   0.14659   0.12261   0.74747
   0.20811   0.11795   0.69265
   0.73325   0.71640   0.56275
   0.70803   0.68386   0.63287
   0.26725   0.71658   0.56322
   0.64846   0.68875   0.69534
   0.61971   0.65861   0.75586
   0.73945   0.64842   0.63740
   0.61423   0.59063   0.81187
   0.64936   0.62273   0.75363
   0.70995   0.61791   0.69561
   0.76700   0.78333   0.56257
   0.79259   0.81569   0.63248
   0.85114   0.81022   0.69713
   0.88032   0.84017   0.75765
   0.29257   0.68415   0.63323
   0.76254   0.85157   0.63485
   0.88700   0.90840   0.81225
   0.82264   0.53180   0.69660
   0.85191   0.87636   0.75388
   0.89930   0.51162   1.09541
   0.85735   0.54778   1.07897
   0.81141   0.55166   1.18796
   0.79228   0.88178   0.69372
   0.26917   0.28300   0.56212
   0.29653   0.31519   0.62980
   0.35632   0.30969   0.69058

S23

0.38707	0.33983	0.74723
0.26684	0.35119	0.63174
0.39366	0.40810	0.80099
0.35135	0.68938	0.69738
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0.26581	0.28375	0.43617
0.29811	0.38161	0.68649
0.76685	0.21667	0.43701
0.79265	0.18401	0.36792
0.85326	0.18868	0.30882
0.29271	0.31635	0.36795
0.88285	0.15838	0.25040
0.76125	0.14858	0.36304
0.88766	0.09037	0.19317
0.38010	0.65938	0.75820
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0.79176	0.11787	0.30764
0.35432	0.31143	0.31255
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0.29196	0.68387	0.36703
0.35159	0.68871	0.30472
0.38032	0.65855	0.24435
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0.35061	0.62269	0.24657
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0.79190	0.81610	0.36682
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0.78723	0.35578	0.60004
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0.23290	0.91011	0.69788
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0.78596	0.64449	0.40780
0.27615	0.41006	0.68694
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0.43397	0.33623	0.79443
0.57338	0.66237	0.19380
0.37930	0.28147	0.68941
0.74491	0.24918	0.27971
0.62435	0.71700	0.30477
0.76994	0.91013	0.69279
0.71515	0.85574	0.58990

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0.92638   0.83644   0.80733
0.87462   0.78214   0.69626
0.24942   0.74974   0.27960
0.73341   0.58986   0.69578
0.78766   0.64477   0.59442
0.57297   0.66189   0.80420
0.62397   0.71652   0.69302
0.23149   0.08987   0.69368
0.28769   0.14517   0.59696
0.06939   0.16160   0.79511
0.12196   0.21648   0.68721
0.72372   0.40999   0.31232
0.78144   0.35508   0.40945
0.56590   0.33608   0.20525
0.62065   0.28136   0.31041
0.22971   0.91012   0.30681
0.28461   0.85573   0.40952
0.07322   0.83642   0.19249
0.12509   0.78212   0.30339
0.26641   0.58986   0.30406
0.21217   0.64481   0.40519
0.42710   0.66178   0.19610
0.37612   0.71648   0.30694
0.75050   0.74979   0.72004
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0.71239   0.14507   0.40375
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0.87762   0.21650   0.31148
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0.06361   0.16331   0.20948
0.11876   0.21833   0.31199
0.71198   0.52243   0.14130
0.57695   0.50072   0.57183
0.28785   0.52246   0.85821
0.42273   0.50092   0.42801
0.49912   0.49963   0.35815
0.57988   0.47200   0.36875
0.50083   0.49998   0.64177
0.41950   0.47251   0.63077
0.36036   0.44491   0.00088
0.49917   0.55409   0.25331
0.50082   0.55432   0.74713
0.63943   0.44482   0.99861
0.30399   0.50070   0.00502
0.29152   0.52506   0.13751
0.07884   0.02413   0.38184
0.21744   0.02136   0.86541
0.19628   0.99895   0.00977
0.99307   0.00188   0.35629
0.78220   0.02124   0.13407
0.80341   0.99892   0.98954
0.92117   0.02421   0.61778
0.00677   0.00191   0.64336
0.13745   0.05516   0.00783
0.86230   0.05512   0.99173
0.99909   0.94455   0.25013
0.00059   0.94455   0.74942
0.20825   0.97508   0.14262
0.91977   0.98882   0.41612
0.79170   0.97495   0.85686
0.08011   0.98879   0.58363
0.27144   0.41090   0.30691
0.21253   0.35573   0.39962
0.43353   0.33820   0.21252
0.37811   0.28346   0.31630
0.75604   0.25124   0.72085
0.76654   0.91005   0.30136
0.71151   0.85499   0.40208
0.92857   0.83828   0.20002
0.87676   0.78358   0.30971
0.25068   0.75022   0.72051
0.26871   0.58984   0.69443
0.21445   0.64443   0.59169
0.42622   0.66292   0.80782
0.37526   0.71734   0.69611
0.74899   0.75014   0.27911
0.77648   0.09021   0.68689
0.71854   0.14558   0.59325
0.93637   0.16324   0.79019
0.88138   0.21830   0.68759
0.24395   0.25120   0.27893
0.72820   0.41094   0.69250
0.80989   0.51106   0.62194
0.79618   0.55995   0.68027
0.87835   0.53676   0.69783
0.93367   0.50793   1.01567
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0.86509	0.48599	1.10254
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0.77750	0.52585	1.19244
0.78047	0.57858	1.17972
0.71508	0.46859	1.06524
0.73730	0.41773	1.01342
0.43564	0.40003	0.12380
0.93784	0.10069	0.87574
0.36825	0.55739	0.79042
0.56731	0.59990	0.88155
0.13011	0.05659	0.78233
0.06650	0.09976	0.87938
0.63163	0.55663	0.78722
0.43527	0.39882	0.88057
0.86949	0.94233	0.78778
0.93123	0.89993	0.11534
0.37785	0.44367	0.23008
0.93392	0.89910	0.88162
0.37964	0.44190	0.76927
0.43290	0.59987	0.11917
0.86956	0.05651	0.21741
0.93316	0.09968	0.12025
0.36835	0.55659	0.21301
0.87149	0.94329	0.21906
0.56448	0.39869	0.11900
0.13032	0.94229	0.21157
0.06575	0.89906	0.11808
0.62030	0.44176	0.23008
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0.93897	0.00229	0.34824
0.69226	0.49929	0.10882
0.44430	0.50264	0.35014
0.80604	0.99913	0.10385
0.06181	0.00026	0.34923
0.30759	0.50048	0.10872
0.56583	0.49787	0.34844
0.80792	0.99945	0.88606
0.06090	0.00236	0.65132
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0.55549	0.50290	0.64970
0.19370	0.99920	0.89554
0.93811	0.00033	0.65046
0.43376	0.49830	0.65162
0.99984	0.96083	0.17994
0.50002	0.47036	0.13265
0.99728	0.02918	0.13391
0.50121	0.53879	0.18095
0.99992	0.96081	0.81966
0.49981	0.47046	0.86722
0.00249	0.02921	0.86585
0.49879	0.53894	0.81931
0.07351	0.97067	0.00022
0.60001	0.46076	0.99974
0.90131	0.03893	0.99313
0.42757	0.52877	0.00149
0.92630	0.97069	0.99921
0.39980	0.46084	0.99995
0.09844	0.03895	0.00659
0.57233	0.52871	0.99872
0.56769	0.60033	0.11636
0.11877	0.05767	0.23400
0.06198	0.10069	0.12402
0.63190	0.55705	0.21050
0.56411	0.40007	0.87572
0.12810	0.94327	0.78066
0.06835	0.89988	0.88424
0.62179	0.44371	0.76923
0.43262	0.60063	0.88438
0.88098	0.05768	0.76580
0.70557	0.50321	0.84017
0.81659	0.54331	0.96699
0.70299	0.44176	1.03054
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0.91423	0.00011	0.83768
0.90980	0.99962	0.15469
0.08555	0.00010	0.16194
0.41135	0.49982	0.84178
0.41349	0.49959	0.15904
0.49988	0.43046	0.99978
0.99988	0.06900	0.99985
0.58852	0.49963	0.15818
0.58639	0.49964	0.84093
0.50003	0.56898	0.00024
0.08995	0.99965	0.84490
0.99989	0.93065	0.99977

POSCAR file for gb_p5

POSCAR file from zrtcpb-gb-h2o-c.res: C: 140 F: 1 H: 114 O: 66 P: 1 ZR: 12
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   -0.0000781726227076   1.0082675674799713   0.0000166934211398
    0.0004256087542374   0.0000053656439079   0.3214078049098053
140 1 114 66 1 12
Direct
    0.79165   0.88255   0.30407
    0.23212   0.21731   0.56283
    0.73080   0.71780   0.43684
    0.70512   0.68545   0.36721
    0.64765   0.69077   0.29962
    0.61904   0.66061   0.23918
    0.85367   0.81185   0.30989
    0.73439   0.64937   0.36898
    0.61330   0.59196   0.18671
    0.64654   0.62424   0.24753
    0.70448   0.61882   0.31243
    0.88325   0.84185   0.25005
    0.20575   0.18468   0.63158
    0.23331   0.78368   0.56295
    0.20720   0.81625   0.63206
    0.14633   0.81149   0.69026
    0.11676   0.84159   0.74970
    0.23879   0.85160   0.63874
    0.11207   0.90941   0.80856
    0.14682   0.87733   0.74963
    0.20840   0.88216   0.69517
    0.76121   0.85207   0.36077
    0.73483   0.28385   0.56253
    0.14437   0.18896   0.68828
    0.70823   0.31670   0.63016
    0.64552   0.31257   0.68188
    0.61493   0.34307   0.73755
    0.88810   0.90957   0.19097
    0.74039   0.35181   0.63912
    0.60907   0.41077   0.79557
    0.64537   0.37870   0.73899
    0.70860   0.38287   0.69061
    0.85322   0.87758   0.24980
    0.77245   0.21784   0.56287
    0.11483   0.15851   0.74614
    0.79974   0.18551   0.63001
    0.85974   0.19045   0.69051
    0.89009   0.15989   0.74569
    0.76939   0.14966   0.63114
    0.89557   0.09153   0.79806
    0.86125   0.12380   0.74020
    0.80027   0.11883   0.68438
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    0.11132   0.09060   0.80513
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    0.20730   0.11858   0.69231
    0.73212   0.71748   0.56290
    0.70610   0.68507   0.63256
    0.26859   0.71698   0.56378
    0.64630   0.69003   0.69417
    0.61696   0.65987   0.75381
    0.73690   0.64949   0.63608
    0.61167   0.59154   0.80917
    0.64590   0.62385   0.75012
    0.70615   0.61893   0.69140
    0.76797   0.78392   0.56315
    0.79385   0.81615   0.63289
    0.85199   0.81073   0.69851
    0.88069   0.84075   0.75918
    0.29433   0.68471   0.63384
    0.76378   0.85198   0.63372
    0.88684   0.90893   0.81293
    0.81339   0.52473   0.74639
    0.85225   0.87690   0.75400
    0.89030   0.50682   0.05818
    0.84385   0.54004   0.04521
    0.82301   0.55583   0.16464
    0.79317   0.88231   0.69226
    0.27101   0.28308   0.56211
    0.29880   0.31518   0.62993
    0.35792   0.30949   0.69258
    0.38886   0.33963   0.74915
    0.26973   0.35135   0.63051
    0.39596   0.40813   0.80111
    0.35271   0.68998   0.69903
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    0.30113   0.38172   0.68534
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0.88465   0.15819   0.25381
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0.88874   0.09037   0.19443
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0.85433   0.12250   0.25377
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0.26704   0.71648   0.43770
0.29276   0.68398   0.36789
0.35262   0.68901   0.30652
0.38173   0.65903   0.24576
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0.38701   0.59109   0.18797
0.35214   0.62315   0.24694
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0.72904   0.28240   0.43700
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0.61176   0.33892   0.24942
0.73017   0.35063   0.37031
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0.69909   0.38108   0.31568
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0.75062   0.75051   0.62282
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0.75654   0.25155   0.62264
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0.76654   0.78433   0.43722
0.22868   0.21802   0.43700
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0.19990   0.11897   0.31578
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0.28786   0.85516   0.59896
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0.12178   0.78374   0.68617
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0.38026   0.28111   0.69298
0.74187   0.24805   0.27973
0.62469   0.71900   0.29763
0.77107   0.91072   0.69002
0.71675   0.85596   0.58755
0.92642   0.83719   0.81004
0.87538   0.78262   0.69851
0.24805   0.74929   0.27983
0.72733   0.59033   0.68820
0.78535   0.64580   0.59410
0.57026   0.66325   0.80232
0.62236   0.71797   0.69248
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0.56575	0.33524	0.19957
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0.21337	0.64459	0.40536
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0.37689	0.71685	0.30955
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0.87957	0.21615	0.31628
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0.27979	0.14623	0.40935
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0.57595	0.46985	0.36302
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0.42069	0.47282	0.63148
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0.50234	0.55414	0.74667
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0.30518	0.50076	0.01017
0.29631	0.52671	0.13622
0.07858	0.02484	0.38072
0.21691	0.02161	0.86377
0.19632	0.99906	0.00653
0.99424	0.00208	0.35619
0.78308	0.02160	0.13641
0.80360	0.99913	0.99374
0.92131	0.02477	0.61942
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0.13763	0.05539	0.00701
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0.86702	0.56659	0.21166
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0.78756	0.57932	0.15406
0.70772	0.46779	0.11662

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0.12984   0.05675   0.78107
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0.93349   0.89961   0.88285
0.38103   0.44186   0.76993
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0.87037   0.05653   0.21859
0.93421   0.09971   0.12178
0.36863   0.55719   0.21042
0.87264   0.94345   0.21928
0.56666   0.39815   0.11283
0.13089   0.94261   0.21233
0.06672   0.89944   0.11751
0.61490   0.44086   0.23563
0.19215   0.99963   0.11125
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0.69299   0.49359   0.15944
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0.80636   0.99928   0.10631
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0.56369   0.49674   0.35270
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0.06014   0.00254   0.65152
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0.19362   0.99927   0.89373
0.93774   0.00064   0.65109
0.43439   0.49861   0.65327
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0.99796   0.02930   0.13413
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0.50091   0.47113   0.86496
0.00224   0.02931   0.86593
0.49922   0.53924   0.81980
0.07370   0.97089  -0.00005
0.60184   0.46228   0.99660
0.90147   0.03903   0.99438
0.42936   0.52877   0.00207
0.92658   0.97084   0.00013
0.40160   0.46082   0.99966
0.09873   0.03909   0.00570
0.57738   0.53023   0.99751
0.56759   0.60129   0.11479
0.11924   0.05787   0.23368
0.06270   0.10084   0.12289
0.63178   0.55825   0.21047
0.56573   0.40099   0.87164
0.12753   0.94330   0.78021
0.06749   0.89990   0.88326
0.62303   0.44471   0.76497
0.43315   0.60086   0.88600
0.88077   0.05776   0.76667
0.69872   0.49875   0.85028
0.78210   0.52891   0.98579
0.74322   0.47080  -0.04481
0.76958   0.50545   0.86985
0.91373   0.00017   0.83882
0.91064   0.99972   0.15584
0.08637   0.00022   0.16144
0.41131   0.50015   0.84284
0.41538   0.49925   0.16168
0.50250   0.43115  -0.00164
0.00018   0.06901   0.00003
0.59042   0.50002   0.15637
0.58621   0.50010   0.84000
0.50093   0.56922   0.00054
0.08953   0.99976   0.84403
0.00023   0.93082   0.00002
```

POSCAR file for gb_p5_prime

POSCAR file from zrtcpb-gb-h2o-c.res: C: 140 F: 1 H: 114 O: 66 P: 1 ZR: 12
  34.8920000000000
    0.5792995890490465   -0.0000450140396845   0.0007649282407427
   -0.0000781726227076   1.0082675674799713   0.0000166934211398

```
    0.0004256087542374    0.0000053656439079    0.3214078049098053
140 1 114 66 1 12
Direct
  0.79042    0.88197    0.29985
  0.23344    0.21712    0.56421
  0.73231    0.71733    0.43645
  0.70708    0.68498    0.36613
  0.64944    0.69053    0.29905
  0.62016    0.66046    0.23943
  0.85549    0.81233    0.31513
  0.73644    0.64890    0.36642
  0.61170    0.59195    0.19007
  0.64749    0.62403    0.24679
  0.70645    0.61852    0.30888
  0.88494    0.84236    0.25513
  0.20700    0.18452    0.63325
  0.23420    0.78456    0.56320
  0.20783    0.81715    0.63217
  0.14449    0.81303    0.68143
  0.11460    0.84298    0.74101
  0.24137    0.85160    0.64735
  0.11177    0.90989    0.80815
  0.14684    0.87799    0.74913
  0.21058    0.88219    0.70309
  0.76014    0.85138    0.35646
  0.73237    0.28384    0.56448
  0.14292    0.18782    0.67985
  0.70430    0.31626    0.63247
  0.63695    0.31491    0.66181
  0.60687    0.34525    0.71933
  0.88797    0.90961    0.19082
  0.74094    0.34855    0.66314
  0.60897    0.41041    0.80391
  0.64293    0.37827    0.74314
  0.71010    0.37988    0.71471
  0.85328    0.87760    0.25007
  0.77533    0.21903    0.56274
  0.11318    0.15738    0.73728
  0.80337    0.18669    0.62852
  0.86121    0.19171    0.69538
  0.89075    0.16095    0.75105
  0.77455    0.15048    0.62275
  0.89633    0.09219    0.79883
  0.86331    0.12464    0.73956
  0.80464    0.11950    0.67638
  0.24129    0.15031    0.64857
  0.11179    0.09039    0.80474
  0.14622    0.12262    0.74575
  0.21059    0.11925    0.70181
  0.73216    0.71706    0.56250
  0.70585    0.68464    0.63201
  0.26906    0.71787    0.56491
  0.64553    0.68973    0.69183
  0.61634    0.65994    0.75347
  0.73717    0.64922    0.63883
  0.61193    0.59220    0.81466
  0.64620    0.62414    0.75398
  0.70703    0.61896    0.69722
  0.76690    0.78382    0.56363
  0.79183    0.81618    0.63404
  0.84759    0.81036    0.70595
  0.87643    0.84040    0.76640
  0.29437    0.68549    0.63462
  0.76383    0.85259    0.62953
  0.88579    0.90908    0.81323
  0.84298    0.47957    0.81348
  0.85045    0.87706    0.75537
  0.90206    0.54459   -0.18587
  0.82921    0.55316   -0.20168
  0.81308    0.59516   -0.19617
  0.79328    0.88289    0.68831
  0.27346    0.28261    0.56192
  0.30133    0.31501    0.62779
  0.35776    0.30943    0.69807
  0.38786    0.33993    0.75411
  0.27428    0.35162    0.61928
  0.39632    0.40885    0.79853
  0.35079    0.69098    0.70507
  0.36240    0.37662    0.73971
  0.26750    0.28356    0.43650
  0.30496    0.38234    0.67339
  0.76840    0.21762    0.43748
  0.79495    0.18493    0.36890
  0.85958    0.18777    0.32459
  0.29438    0.31612    0.36765
  0.88892    0.15728    0.26674
  0.75987    0.15109    0.35151
  0.88882    0.09055    0.19624
```

0.37938   0.66076   0.76508
0.85496   0.12287   0.25594
0.79018   0.11992   0.29816
0.35964   0.31328   0.32647
0.26606   0.71705   0.43912
0.29121   0.68432   0.36954
0.35335   0.68822   0.31538
0.38170   0.65808   0.25434
0.25722   0.64987   0.35762
0.38319   0.59108   0.18832
0.34907   0.62311   0.24868
0.26566   0.64923   0.63083
0.28644   0.61918   0.29982
0.38965   0.34366   0.26909
0.23137   0.78373   0.43738
0.20617   0.81601   0.36727
0.15127   0.81009   0.29331
0.12273   0.84016   0.23254
0.23361   0.85255   0.37380
0.25934   0.34979   0.34752
0.11343   0.90891   0.18638
0.14827   0.87689   0.24509
0.38723   0.59208   0.81354
0.20454   0.88284   0.31450
0.38992   0.41020   0.19670
0.72594   0.28253   0.43913
0.69773   0.31473   0.37328
0.64460   0.30850   0.29549
0.61386   0.33884   0.23991
0.72131   0.35193   0.38921
0.60078   0.40807   0.20399
0.63552   0.37596   0.26181
0.68997   0.38241   0.33528
0.35254   0.62425   0.75503
0.35566   0.37796   0.25605
0.29024   0.38093   0.29484
0.74404   0.24940   0.37820
0.24742   0.74991   0.37853
0.25638   0.24936   0.62311
0.74947   0.75028   0.62270
0.25317   0.75173   0.62377
0.75780   0.25229   0.62359
0.74958   0.75089   0.37734
0.24429   0.25136   0.37768
0.29490   0.61875   0.68901
0.76685   0.78410   0.43756
0.22738   0.21807   0.43883
0.19933   0.18568   0.37305
0.14133   0.19101   0.30693
0.11122   0.16051   0.25092
0.22769   0.14935   0.37782
0.10439   0.09182   0.20224
0.13813   0.12405   0.26149
0.19694   0.11859   0.32402
0.79318   0.81664   0.36844
0.75138   0.44630   0.92707
0.79401   0.34955   0.64294
0.55468   0.34414   0.74547
0.60824   0.28958   0.63845
0.72783   0.58996   0.31273
0.23547   0.90969   0.71220
0.29213   0.85451   0.61425
0.06533   0.84012   0.78069
0.11849   0.78593   0.67057
0.78331   0.64469   0.41292
0.28494   0.41115   0.66587
0.22844   0.35579   0.56955
0.43205   0.33623   0.80910
0.57474   0.66425   0.18796
0.37875   0.28081   0.70533
0.74039   0.24883   0.28070
0.62677   0.71882   0.29740
0.77286   0.91163   0.68173
0.71844   0.85712   0.57879
0.92052   0.83642   0.82140
0.86926   0.78185   0.71068
0.24619   0.74941   0.28080
0.72992   0.59075   0.69932
0.78584   0.64540   0.59773
0.56929   0.66353   0.80064
0.62111   0.71750   0.68726
0.23618   0.09193   0.70957
0.29231   0.14790   0.61642
0.06336   0.15959   0.77502
0.11618   0.21466   0.66864
0.70681   0.41166   0.34900
0.76466   0.35674   0.44520
0.57196   0.33472   0.17967

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0.62637   0.27947   0.28248
0.22451   0.91165   0.32231
0.27830   0.85713   0.42642
0.07922   0.83616   0.17608
0.12993   0.78153   0.28725
0.26109   0.59173   0.29414
0.20733   0.64710   0.39478
0.43022   0.66068   0.21163
0.37973   0.71529   0.32374
0.74890   0.75016   0.72047
0.76393   0.09286   0.28884
0.70855   0.14900   0.38233
0.93909   0.15921   0.23030
0.88698   0.21432   0.33745
0.25985   0.24898   0.72065
0.21799   0.08995   0.32875
0.27467   0.14543   0.42421
0.06590   0.16403   0.19892
0.11927   0.21943   0.30275
0.71084   0.52269   0.16535
0.58190   0.50554   0.57831
0.29218   0.52536   0.85294
0.41488   0.50230   0.42708
0.49075   0.50013   0.36087
0.57409   0.47414   0.37849
0.50722   0.49990   0.64456
0.42358   0.47347   0.62961
0.36058   0.44546   0.99476
0.49522   0.55507   0.25565
0.50398   0.55531   0.75085
0.64472   0.44984   0.00422
0.30339   0.50177   -0.01257
0.28704   0.52489   0.13141
0.07890   0.02542   0.37835
0.21644   0.02183   0.86384
0.19626   0.99926   0.00350
0.99496   0.00216   0.35615
0.78339   0.02197   0.13677
0.80348   0.99947   0.99560
0.92038   0.02576   0.62169
0.00477   0.00255   0.64366
0.13758   0.05544   0.00701
0.86251   0.05562   0.99379
-0.00005  0.94479   0.25023
-0.00064  0.94503   0.74905
0.21020   0.97619   0.14081
0.92072   0.99112   0.41937
0.78999   0.97617   0.85971
0.07853   0.99116   0.58039
0.26409   0.40790   0.28254
0.20751   0.35181   0.37561
0.44027   0.34166   0.23476
0.38697   0.28681   0.34137
0.76187   0.25293   0.72102
0.76583   0.90961   0.29294
0.71004   0.85447   0.39240
0.93349   0.83938   0.21273
0.88118   0.78504   0.32338
0.25449   0.75229   0.72149
0.27384   0.59014   0.68306
0.21977   0.64501   0.58132
0.42391   0.66449   0.81910
0.37316   0.71932   0.70907
0.75007   0.75102   0.27958
0.78321   0.09097   0.67106
0.72770   0.14688   0.57566
0.93596   0.16414   0.80355
0.88364   0.22002   0.70039
0.24068   0.25175   0.28016
0.73807   0.40569   0.73506
0.84587   0.44833   0.81114
0.83319   0.48941   0.72190
0.89073   0.49072   0.84547
0.91146   0.51374   0.80985
0.91934   0.55510   -0.09857
0.93154   0.55849   -0.25629
0.81204   0.54142   0.71252
0.81647   0.60817   -0.28540
0.84832   0.60988   -0.13681
0.76243   0.59970   -0.16234
0.71486   0.47956   0.11045
0.82545   0.49364   0.09510
0.43416   0.40069   0.12155
0.93746   0.10119   0.87965
0.37026   0.55818   0.78747
0.56668   0.60172   0.88809
0.13039   0.05655   0.78120
0.06591   0.09969   0.87664
```

```
0.62862   0.55840   0.78852
0.43718   0.39976   0.87955
0.86863   0.94305   0.78832
0.93280   0.90004   0.11673
0.37288   0.44399   0.22320
0.93265   0.89975   0.88270
0.38242   0.44264   0.76611
0.43015   0.60040   0.11888
0.86982   0.05677   0.21931
0.93467   0.09982   0.12420
0.36469   0.55714   0.21119
0.87230   0.94351   0.21862
0.56165   0.39896   0.12042
0.13065   0.94283   0.21165
0.06698   0.89962   0.11600
0.61246   0.44169   0.24016
0.19182   0.00003   0.11072
0.94043   0.00258   0.34841
0.69291   0.49698   0.17259
0.43696   0.50201   0.34958
0.80622   0.99950   0.10668
0.06279   0.00089   0.34908
0.30571   0.50112   0.10134
0.55925   0.49949   0.35403
0.80780   0.00020   0.88952
0.05911   0.00292   0.65115
0.30805   0.50100   0.88373
0.56047   0.50115   0.65515
0.19368   0.99930   0.89370
0.93655   0.00126   0.65105
0.43734   0.49928   0.65130
0.00063   0.96109   0.18008
0.49655   0.47113   0.13460
0.99801   0.02940   0.13421
0.49716   0.53950   0.18386
0.99894   0.96129   0.81928
0.50276   0.47165   0.86876
0.00189   0.02954   0.86606
0.50081   0.53978   0.82255
0.07328   0.97100   0.99929
0.60104   0.46260   0.00901
0.90138   0.03931   0.99522
0.42715   0.52951   0.00028
0.92639   0.97106   0.00026
0.39957   0.46174   -0.00436
0.09866   0.03917   0.00521
0.57418   0.53046   0.00577
0.56391   0.60134   0.12282
0.11884   0.05803   0.23355
0.06325   0.10103   0.12160
0.62947   0.55801   0.21362
0.56506   0.40055   0.87941
0.12734   0.94382   0.78045
0.06685   0.90019   0.88185
0.62553   0.44422   0.77827
0.43312   0.60133   0.88511
0.88129   0.05849   0.76736
0.70327   0.50019   0.86261
0.79382   0.53531   -0.10481
0.77925   0.49485   0.07005
0.77247   0.49101   0.91078
0.91315   0.00048   0.83917
0.91075   0.99986   0.15631
0.08666   0.00021   0.16089
0.41461   0.50048   0.83922
0.40848   0.50036   0.15617
0.50031   0.43147   0.00037
0.00018   0.06924   0.00050
0.58259   0.50021   0.16630
0.59076   0.50108   0.84908
0.49946   0.56986   0.00267
0.08891   0.99994   0.84358
-0.00025   0.93088   -0.00045
```

POSCAR file for gb_product

```
POSCAR file from zrtcpb-gb-h2o-c.res: C:
   34.8920000000000
     0.5792995890490465   -0.0000450140396845    0.0007649282407427
    -0.0000781726227076    1.0082675674799713    0.0000166934211398
     0.0004256087542374    0.0000053656439079    0.3214078049098053
   140    1  114   66    1   12
Direct
  0.79138   0.88310   0.30035
  0.23285   0.21776   0.56402
  0.73149   0.71921   0.43215
  0.70675   0.68725   0.35916
```

S34

```
0.64508   0.69162   0.30430
0.61623   0.66159   0.24386
0.85725   0.81372   0.31955
0.74061   0.65281   0.34573
0.61179   0.59393   0.18630
0.64785   0.62629   0.23997
0.71079   0.62221   0.28902
0.88678   0.84360   0.25921
0.20605   0.18520   0.63296
0.23379   0.78391   0.56314
0.20743   0.81649   0.63239
0.14315   0.81312   0.67808
0.11373   0.84323   0.73774
0.24218   0.85038   0.65078
0.11269   0.90979   0.80843
0.14731   0.87774   0.74914
0.21187   0.88121   0.70621
0.76110   0.85266   0.35746
0.72946   0.28277   0.56416
0.14089   0.18774   0.67484
0.70163   0.31539   0.63112
0.63324   0.31636   0.65144
0.60424   0.34726   0.70784
0.88881   0.91033   0.19114
0.74044   0.34605   0.66841
0.61138   0.41121   0.80169
0.64286   0.37866   0.73894
0.71080   0.37794   0.71830
0.85452   0.87861   0.25192
0.77447   0.21855   0.56197
0.11153   0.15719   0.73246
0.80318   0.18632   0.62724
0.85953   0.19188   0.69770
0.88960   0.16129   0.75331
0.77630   0.14968   0.61771
0.89761   0.09234   0.79784
0.86415   0.12463   0.73845
0.80688   0.11893   0.67158
0.24161   0.15166   0.65254
0.11234   0.09069   0.80501
0.14606   0.12305   0.74535
0.21135   0.12042   0.70556
0.72767   0.71871   0.55786
0.70093   0.68593   0.62427
0.26965   0.71739   0.56346
0.64566   0.69150   0.69813
0.61733   0.66125   0.75876
0.72780   0.64934   0.61519
0.61148   0.59251   0.80900
0.64310   0.62462   0.74516
0.69852   0.61883   0.67316
0.76409   0.78511   0.56380
0.78929   0.81716   0.63577
0.84498   0.81085   0.70732
0.87474   0.84064   0.76777
0.29520   0.68488   0.63251
0.76227   0.85376   0.63135
0.88626   0.90934   0.81335
0.81846   0.46242   0.81462
0.84986   0.87752   0.75659
0.89906   0.54671   0.78595
0.82733   0.55133   0.82440
0.81348   0.59168   0.86462
0.79274   0.88382   0.68977
0.27497   0.28278   0.56132
0.30337   0.31509   0.62701
0.35840   0.30913   0.70047
0.38893   0.33951   0.75644
0.27803   0.35200   0.61524
0.39989   0.40856   0.79661
0.35103   0.69044   0.70435
0.36537   0.37645   0.73862
0.26937   0.28364   0.43592
0.30919   0.38258   0.66919
0.76728   0.21715   0.43678
0.79472   0.18467   0.36839
0.86083   0.18683   0.33150
0.29704   0.31604   0.36721
0.89043   0.15643   0.27361
0.75859   0.15164   0.34442
0.88905   0.09056   0.19573
0.37980   0.66019   0.76394
0.85514   0.12276   0.25594
0.78907   0.12046   0.29148
0.36335   0.31381   0.33142
0.26692   0.71684   0.43772
0.29227   0.68420   0.36778
0.35517   0.68773   0.31627
```

0.38337	0.65758	0.25499
0.25751	0.65010	0.35304
0.38378	0.59088	0.18588
0.34989	0.62292	0.24664
0.26730	0.64844	0.62666
0.28658	0.61936	0.29526
0.39345	0.34414	0.27386
0.23125	0.78337	0.43737
0.20604	0.81580	0.36778
0.15203	0.80989	0.29177
0.12365	0.84002	0.23104
0.23272	0.85248	0.37670
0.26124	0.34911	0.34215
0.11375	0.90891	0.18694
0.14843	0.87684	0.24571
0.38859	0.59150	0.81057
0.20381	0.88282	0.31741
0.39239	0.41001	0.19533
0.72299	0.28153	0.43885
0.69546	0.31405	0.37365
0.64290	0.30842	0.29431
0.61333	0.33918	0.23896
0.71963	0.35103	0.39166
0.60222	0.40846	0.20394
0.63561	0.37607	0.26265
0.68949	0.38191	0.33792
0.35370	0.62355	0.75214
0.35841	0.37784	0.25551
0.29210	0.38026	0.28951
0.74169	0.24860	0.37756
0.24798	0.74979	0.37776
0.25662	0.24982	0.62280
0.74420	0.75169	0.62053
0.25315	0.75103	0.62306
0.75597	0.25154	0.62327
0.75091	0.75263	0.37530
0.24520	0.25164	0.37719
0.29668	0.61793	0.68447
0.76710	0.78557	0.43806
0.22714	0.21862	0.43865
0.19903	0.18614	0.37321
0.14211	0.19149	0.30413
0.11220	0.16086	0.24837
0.22652	0.14965	0.38133
0.10472	0.09198	0.20283
0.13820	0.12429	0.26212
0.19594	0.11880	0.32777
0.79446	0.81809	0.37086
0.64985	0.41650	0.99154
0.79409	0.34531	0.65404
0.55117	0.34773	0.72762
0.60286	0.29232	0.62229
0.73587	0.59468	0.28339
0.23778	0.90831	0.71751
0.29349	0.85271	0.62003
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0.11605	0.78650	0.66461
0.79058	0.64992	0.38192
0.29050	0.41160	0.65906
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0.37798	0.28026	0.71047
0.73821	0.24808	0.28003
0.61927	0.71888	0.31249
0.77326	0.91277	0.68286
0.71712	0.85878	0.58032
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0.86598	0.78216	0.71184
0.24705	0.74954	0.27999
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0.11310	0.21406	0.66024
0.70714	0.41096	0.35257
0.76265	0.35530	0.44893
0.57200	0.33554	0.17716
0.62429	0.27954	0.27954
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0.26052	0.59219	0.28745
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0.76189	0.09393	0.27714
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0.21632	0.09006	0.33500
0.27266	0.14565	0.43034
0.06774	0.16437	0.19399
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0.58445	0.51238	0.58515
0.29448	0.52442	0.84940
0.41519	0.50202	0.42383
0.49189	0.50087	0.35886
0.57598	0.47686	0.38343
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0.42715	0.47359	0.62623
0.36365	0.44486	0.99169
0.49633	0.55499	0.25381
0.50506	0.55565	0.75031
0.64824	0.44955	0.00171
0.30552	0.50081	0.98199
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0.26520	0.40679	0.27348
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0.39136	0.28785	0.35040
0.76004	0.25215	0.72072
0.76667	0.91065	0.29157
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0.93571	0.84074	0.21815
0.88303	0.78651	0.32949
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0.22189	0.64410	0.57578
0.42394	0.66403	0.81888
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0.75342	0.75316	0.27763
0.78693	0.09011	0.66369
0.73062	0.14558	0.56738
0.93376	0.16487	0.80843
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0.24195	0.25192	0.27962
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0.79855	0.43467	0.78910
0.82401	0.48062	0.73539
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0.91028	0.51736	0.75825
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0.91121	0.56591	0.71126
0.79346	0.54388	0.75005
0.82491	0.61232	0.79342
0.84467	0.59845	0.94248
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0.37222	0.55748	0.78459
0.56798	0.60160	0.88615
0.13149	0.05692	0.78216
0.06639	0.09995	0.87693
0.62879	0.55873	0.78253
0.44059	0.39957	0.87804
0.86972	0.94338	0.78787
0.93321	0.90053	0.11659
0.37512	0.44380	0.22132
0.93329	0.89987	0.88242
0.38679	0.44239	0.76329

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0.86973   0.05677   0.21780
0.93516   0.09997   0.12441
0.36530   0.55692   0.20824
0.87306   0.94429   0.21834
0.56437   0.39954   0.11801
0.13098   0.94284   0.21237
0.06735   0.89967   0.11626
0.61320   0.44199   0.24098
0.19260  -0.00007   0.11183
0.94060   0.00306   0.34809
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0.43771   0.50242   0.34681
0.80675   0.99957   0.10437
0.06311   0.00092   0.34918
0.30765   0.50022   0.09847
0.55939   0.50103   0.35211
0.80898   0.00073   0.88730
0.06088   0.00300   0.65166
0.31061   0.50011   0.88027
0.56489   0.49962   0.65397
0.19462   0.99938   0.89462
0.93846   0.00115   0.65044
0.44131   0.49915   0.64978
0.00118   0.96132   0.17994
0.49845   0.47111   0.13310
0.99864   0.02965   0.13428
0.49830   0.53964   0.18155
0.00019   0.96137   0.81929
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0.00312   0.02969   0.86613
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0.60593   0.46363   0.00946
0.90223   0.03954   0.99422
0.42887   0.52924  -0.00195
0.92724   0.97129  -0.00038
0.40230   0.46141   0.99315
0.09952   0.03931   0.00585
0.57619   0.53089   0.00510
0.56338   0.60261   0.11994
0.11923   0.05820   0.23431
0.06370   0.10113   0.12185
0.62927   0.56012   0.21247
0.56801   0.40143   0.87826
0.12866   0.94370   0.78114
0.06763   0.90016   0.88203
0.62911   0.44489   0.77766
0.43433   0.60086   0.88243
0.88342   0.05861   0.76554
0.70112   0.50399   0.87897
0.81422   0.52666   0.92256
0.75767   0.46056   0.04415
0.76634   0.48642   0.92135
0.91445   0.00062   0.83835
0.91139   0.00014   0.15525
0.08710   0.00036   0.16132
0.41774   0.50008   0.83678
0.40957   0.50024   0.15405
0.50307   0.43151  -0.00105
0.00095   0.06937   0.00036
0.58359   0.50031   0.16564
0.59504   0.50169   0.84915
0.50047   0.56994   0.00068
0.09019   0.00001   0.84422
0.00055   0.93106   0.99919
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POSCAR file for gd_solvent

POSCAR file from zrtcpb-gd-h2o-c.res: C: 143 F: 1 H: 120 O: 66 P: 1 ZR: 12
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    -0.0000781726227076    1.0082675674799713    0.0000166934211398
     0.0004256087542374    0.0000053656439079    0.3214078049098053
143 1 120 66 1 12
Direct
  0.79102   0.88175   0.29982
  0.64919   0.62376   0.24267
  0.23247   0.78362   0.43772
  0.20691   0.81587   0.36790
  0.15159   0.80993   0.29502
  0.12298   0.83994   0.23410
  0.23456   0.85236   0.37353
  0.26009   0.34983   0.35104
  0.11398   0.90854   0.18664
  0.14883   0.87662   0.24559
  0.38684   0.59189   0.81619
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0.69530	0.31311	0.37313
0.64057	0.30676	0.29911
0.61008	0.33697	0.24231
0.72054	0.35013	0.38432
0.60003	0.40601	0.19967
0.63371	0.37392	0.25930
0.68961	0.38044	0.32902
0.35335	0.62416	0.75594
0.88589	0.84219	0.25672
0.35669	0.37770	0.25969
0.29146	0.38095	0.29921
0.74154	0.24788	0.37876
0.24893	0.74996	0.37842
0.25571	0.24886	0.62380
0.74814	0.75023	0.62180
0.25459	0.75149	0.62367
0.75866	0.25177	0.62345
0.74955	0.75092	0.37653
0.24449	0.25106	0.37824
0.20698	0.18394	0.63304
0.29560	0.61881	0.69018
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0.22759	0.21770	0.43894
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0.10510	0.09137	0.20242
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0.11577	0.84251	0.74238
0.24212	0.85138	0.64708
0.11250	0.90949	0.80831
0.23325	0.21663	0.56431
0.14771	0.87763	0.74956
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0.76062	0.85119	0.35626
0.73249	0.28309	0.56427
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0.63790	0.31357	0.66519
0.60714	0.34404	0.72070
0.88864	0.90926	0.19118
0.74008	0.34888	0.65720
0.73183	0.71735	0.43499
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0.64175	0.37792	0.73896
0.70840	0.38020	0.70726
0.85404	0.87736	0.25081
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0.61118	0.59097	0.80894
0.64510	0.62325	0.74882
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0.87653	0.83998	0.76619

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0.06652   0.09914   0.87746
0.62851   0.55715   0.78344
0.43460   0.39923   0.88327
0.86942   0.94262   0.78815
0.93339   0.89966   0.11700
0.37479   0.44370   0.22833
```

```
0.93320   0.89927   0.88269
0.37964   0.44207   0.76986
0.43452   0.60047   0.12141
0.87021   0.05595   0.22003
0.93518   0.09917   0.12574
0.36737   0.55752   0.21078
0.87291   0.94319   0.21869
0.56346   0.39711   0.11202
0.13117   0.94248   0.21178
0.06758   0.89921   0.11620
0.60956   0.43938   0.23895
0.19256   0.99951   0.11119
0.94133   0.00208   0.34894
0.69058   0.49180   0.16895
0.44023   0.50312   0.34557
0.80670   0.99888   0.10580
0.06382   0.00043   0.34937
0.30627   0.50200   0.10972
0.56113   0.49640   0.35378
0.80870  -0.00001   0.88881
0.05981   0.00262   0.65151
0.30691   0.49979   0.88967
0.55401   0.50253   0.65230
0.19428   0.99876   0.89421
0.93726   0.00096   0.65116
0.43330   0.49864   0.65439
0.00124   0.96060   0.18045
0.49937   0.47034   0.13342
0.99868   0.02884   0.13476
0.50208   0.53892   0.18161
0.99958   0.96084   0.81944
0.49942   0.47092   0.86708
0.00252   0.02906   0.86673
0.49846   0.53905   0.82096
0.07384   0.97052  -0.00036
0.60094   0.46142   0.00015
0.90203   0.03882   0.99579
0.42805   0.52908   0.00289
0.92702   0.97059   0.00046
0.39929   0.46128   0.00051
0.09932   0.03866   0.00582
0.57586   0.52957   0.99892
0.56756   0.60083   0.11545
0.11969   0.05760   0.23371
0.06369   0.10052   0.12211
0.63292   0.55767   0.20804
0.56208   0.40045   0.87091
0.12792   0.94343   0.78047
0.06758   0.89979   0.88201
0.62233   0.44400   0.76871
0.43289   0.60098   0.88767
0.88271   0.05819   0.76772
0.69701   0.49870   0.85843
0.78679   0.52490   0.98887
0.71363   0.42983   0.06012
0.76840   0.50530   0.86837
0.58497   0.49957   0.84211
0.58887   0.49945   0.15795
0.00080   0.06873   0.00124
0.49994   0.43092   0.00033
0.41338   0.49959   0.16217
0.40998   0.50041   0.84415
0.08740  -0.00029   0.16136
0.91149   0.99932   0.15666
0.91373   0.00001   0.83933
0.50045   0.56905   0.00163
0.00034   0.93037  -0.00040
0.08953   0.99948   0.84397
```

POSCAR file for gd_p5

POSCAR file from zrtcpb-gd-h2o-c.res: C: 143 F: 1 H: 120 O: 66 P: 1 ZR: 12
```
  34.8920000000000
    0.5792995890490465   -0.0000450140396845    0.0007649282407427
   -0.0000781726227076    1.0082675674799713    0.0000166934211398
    0.0004256087542374    0.0000053656439079    0.3214078049098053
143 1 120 66 1 12
Direct
   0.79062   0.88169   0.29923
   0.64897   0.62385   0.24266
   0.23252   0.78370   0.43769
   0.20695   0.81595   0.36794
   0.15198   0.80990   0.29435
   0.12329   0.83987   0.23340
   0.23427   0.85251   0.37427
   0.25997   0.34947   0.34909
   0.11381   0.90853   0.18678
```

```
0.14875   0.87662   0.24558
0.38541   0.59181   0.81672
0.20503   0.88271   0.31483
0.70917   0.61906   0.30120
0.39152   0.41003   0.20173
0.72370   0.28123   0.43927
0.69476   0.31312   0.37315
0.64029   0.30676   0.29853
0.60986   0.33698   0.24164
0.71978   0.35017   0.38499
0.59978   0.40605   0.19904
0.63332   0.37395   0.25902
0.68893   0.38047   0.32947
0.35224   0.62406   0.75602
0.88596   0.84230   0.25777
0.35687   0.37775   0.26015
0.29126   0.38070   0.29776
0.74136   0.24795   0.37869
0.24911   0.75011   0.37827
0.25581   0.24885   0.62351
0.74807   0.75031   0.62220
0.25427   0.75146   0.62361
0.75839   0.25186   0.62347
0.74950   0.75087   0.37691
0.24462   0.25095   0.37786
0.20667   0.18402   0.63290
0.29462   0.61879   0.68984
0.76683   0.78400   0.43768
0.22755   0.21766   0.43875
0.19967   0.18527   0.37275
0.14158   0.19055   0.30689
0.11149   0.16000   0.25106
0.22820   0.14900   0.37740
0.10477   0.09133   0.20282
0.13853   0.12358   0.26165
0.19747   0.11819   0.32385
0.23508   0.78432   0.56345
0.79356   0.81652   0.36908
0.20849   0.81679   0.63262
0.14508   0.81265   0.68159
0.11515   0.84258   0.74117
0.24208   0.85122   0.64815
0.11240   0.90946   0.80864
0.23312   0.21664   0.56413
0.14747   0.87758   0.74963
0.21128   0.88180   0.70388
0.76022   0.85111   0.35561
0.73202   0.28313   0.56423
0.14263   0.18729   0.67973
0.70415   0.31580   0.63153
0.63700   0.31420   0.66226
0.60647   0.34476   0.71767
0.88848   0.90931   0.19142
0.74020   0.34857   0.65937
0.73173   0.71736   0.43556
0.60641   0.41055   0.79610
0.64174   0.37827   0.73836
0.70881   0.38005   0.70918
0.85388   0.87740   0.25105
0.93317   0.49132   0.94388
0.98110   0.55337   0.00251
0.90889   0.51739   0.14615
0.77560   0.21848   0.56292
0.11309   0.15686   0.73751
0.80413   0.18623   0.62842
0.86141   0.19147   0.69662
0.89119   0.16078   0.75228
0.77612   0.14983   0.62107
0.70693   0.68501   0.36423
0.89752   0.09193   0.79914
0.86453   0.12432   0.73957
0.80643   0.11895   0.67481
0.24111   0.14987   0.64828
0.11219   0.08993   0.80558
0.14631   0.12214   0.74613
0.21063   0.11881   0.70190
0.73072   0.71714   0.56149
0.70431   0.68467   0.63028
0.27063   0.71780   0.56416
0.64772   0.68985   0.30134
0.64635   0.69013   0.69700
0.61678   0.66008   0.75684
0.73296   0.64845   0.62842
0.60921   0.59137   0.80766
0.64364   0.62358   0.74837
0.70196   0.61804   0.68422
0.76636   0.78373   0.56352
0.79164   0.81605   0.63401
```

0.84740	0.81010	0.70568
0.87647	0.84006	0.76634
0.61942	0.65976	0.24013
0.29577	0.68533	0.63368
0.76399	0.85253	0.62945
0.88633	0.90872	0.81323
0.75913	0.54009	0.75755
0.85079	0.87679	0.75542
0.92061	0.52761	0.01536
0.86057	0.54855	-0.03676
0.83836	0.58365	0.02988
0.79373	0.88276	0.68816
0.27307	0.28207	0.56258
0.85637	0.81232	0.31771
0.30054	0.31444	0.62899
0.35694	0.30893	0.69931
0.38638	0.33944	0.75645
0.27289	0.35089	0.62106
0.39334	0.40827	0.80285
0.35251	0.69055	0.70342
0.36021	0.37597	0.74297
0.26760	0.28310	0.43718
0.30288	0.38160	0.67633
0.76731	0.21662	0.43799
0.73851	0.64962	0.35909
0.79426	0.18395	0.36970
0.85972	0.18647	0.32930
0.29482	0.31574	0.36921
0.88931	0.15604	0.27153
0.75871	0.15048	0.34881
0.88875	0.08977	0.19707
0.38029	0.66029	0.76445
0.85473	0.12196	0.25708
0.78923	0.11932	0.29576
0.36033	0.31293	0.32939
0.61445	0.59157	0.18401
0.26798	0.71721	0.43841
0.29335	0.68466	0.36846
0.35518	0.68884	0.31337
0.38380	0.65877	0.25242
0.25982	0.65005	0.35727
0.38615	0.59144	0.18906
0.35176	0.62362	0.24800
0.26621	0.64932	0.63066
0.28935	0.61945	0.29966
0.39071	0.34340	0.27317
0.80535	0.46800	0.79981
0.79311	0.34978	0.63803
0.55442	0.34352	0.74459
0.60873	0.28849	0.64133
0.73192	0.59082	0.30184
0.23617	0.90930	0.71323
0.29288	0.85409	0.61524
0.06577	0.83975	0.78052
0.11905	0.78557	0.67039
0.78667	0.64606	0.40184
0.28252	0.41035	0.66954
0.22717	0.35491	0.57086
0.43051	0.33589	0.81167
0.57304	0.66309	0.19112
0.37834	0.28040	0.70584
0.73643	0.24707	0.28143
0.62328	0.71764	0.30354
0.77361	0.91157	0.68137
0.71875	0.85722	0.57843
0.92051	0.83592	0.82137
0.86889	0.78154	0.71034
0.24800	0.74977	0.28057
0.72146	0.58913	0.67686
0.77983	0.64415	0.58162
0.57150	0.66396	0.80911
0.62382	0.71845	0.69894
0.23633	0.09153	0.70982
0.29211	0.14753	0.61601
0.06329	0.15903	0.77546
0.11582	0.21411	0.66849
0.70738	0.40961	0.33780
0.76429	0.35483	0.43811
0.56713	0.33283	0.18330
0.62101	0.27781	0.28879
0.22489	0.91156	0.32232
0.27899	0.85716	0.42677
0.07976	0.83577	0.17706
0.13082	0.78128	0.28858
0.26463	0.59179	0.29486
0.21013	0.64707	0.39508
0.43210	0.66152	0.20897
0.38114	0.71607	0.32105

```
0.74722    0.75014    0.71994
0.76252    0.09250    0.28389
0.70689    0.14863    0.37704
0.94011    0.15778    0.23792
0.88750    0.21274    0.34491
0.25903    0.24843    0.72105
0.21862    0.08958    0.32854
0.27526    0.14516    0.42360
0.06610    0.16347    0.19921
0.11949    0.21896    0.30273
0.71326    0.51600    0.15939
0.57353    0.49846    0.57482
0.28578    0.52264    0.85758
0.41515    0.49866    0.41891
0.50565    0.49871    0.35817
0.57269    0.46963    0.36372
0.49563    0.49970    0.64464
0.41726    0.47274    0.63432
0.35965    0.44504    0.00124
0.49907    0.55408    0.25455
0.49986    0.55414    0.74810
0.64212    0.44595    0.00517
0.30217    0.50159    0.01221
0.29391    0.52778    0.13710
0.07970    0.02490    0.37887
0.21727    0.02128    0.86484
0.19689    0.99872    0.00456
0.99540    0.00177    0.35657
0.78362    0.02121    0.13547
0.80416    0.99902    0.99618
0.92150    0.02542    0.62204
0.00563    0.00209    0.64401
0.13824    0.05491    0.00790
0.86301    0.05514    0.99374
0.00035    0.94431    0.25062
0.00011    0.94456    0.74948
0.21077    0.97567    0.14181
0.92131    0.99088    0.41994
0.79034    0.97638    0.85744
0.07954    0.99073    0.58112
0.26530    0.40776    0.28576
0.20801    0.35145    0.37642
0.44153    0.34145    0.23977
0.38753    0.28643    0.34443
0.76340    0.25276    0.72072
0.76584    0.90926    0.29116
0.70982    0.85406    0.39028
0.93489    0.83942    0.21671
0.88226    0.78513    0.32733
0.25553    0.75182    0.72131
0.27303    0.59030    0.68482
0.22028    0.64536    0.58105
0.42496    0.66376    0.81828
0.37558    0.71872    0.70645
0.75022    0.75112    0.27918
0.78558    0.09029    0.66849
0.72973    0.14601    0.57269
0.93601    0.16417    0.80576
0.88321    0.21992    0.70274
0.24136    0.25137    0.28033
0.73610    0.40637    0.72635
0.72829    0.52990    0.68323
0.73393    0.56409    0.80138
0.80775    0.54907    0.72326
0.87175    0.55578    0.86901
0.87757    0.60538    0.02997
0.82631    0.57660    0.12329
0.79406    0.59619    -0.01140
0.70466    0.47027    0.12954
0.80400    0.43999    -0.03252
0.93298    0.49684    0.84671
0.89600    0.46931    0.96327
0.98211    0.47951    -0.03373
0.02492    0.53866    0.03843
0.99142    0.56004    -0.09204
0.97554    0.58034    0.05160
0.90906    0.54279    0.20387
0.94855    0.49834    0.17754
0.86120    0.50262    0.15886
0.43567    0.40048    0.12649
0.93806    0.10097    0.88096
0.36690    0.55808    0.79255
0.56455    0.60084    0.88195
0.13092    0.05610    0.78221
0.06638    0.09924    0.87768
0.62556    0.55758    0.78026
0.43426    0.39919    0.88387
0.86944    0.94272    0.78815
```

```
0.93323    0.89968    0.11723
0.37477    0.44379    0.22914
0.93314    0.89934    0.88287
0.37871    0.44195    0.77109
0.43424    0.60056    0.12179
0.86963    0.05593    0.21936
0.93479    0.09918    0.12562
0.36695    0.55765    0.21095
0.87278    0.94326    0.21895
0.56343    0.39714    0.11101
0.13094    0.94248    0.21204
0.06739    0.89919    0.11635
0.60922    0.43942    0.23828
0.19246    0.99951    0.11159
0.94100    0.00226    0.34879
0.69005    0.49190    0.16821
0.44010    0.50333    0.34597
0.80658    0.99879    0.10529
0.06348    0.00040    0.34958
0.30553    0.50201    0.11128
0.56099    0.49660    0.35333
0.80876    0.00012    0.88833
0.06001    0.00252    0.65173
0.30586    0.49979    0.89115
0.55206    0.50221    0.65199
0.19427    0.99881    0.89458
0.93748    0.00083    0.65105
0.43143    0.49857    0.65481
0.00107    0.96065    0.18052
0.49893    0.47047    0.13328
0.99848    0.02890    0.13473
0.50171    0.53906    0.18168
0.99966    0.96087    0.81965
0.49843    0.47104    0.86701
0.00257    0.02913    0.86679
0.49683    0.53921    0.82113
0.07378    0.97053    0.99987
0.60029    0.46168   -0.00042
0.90194    0.03886    0.99543
0.42718    0.52918    0.00354
0.92696    0.97062    0.00043
0.39861    0.46133    0.00118
0.09921    0.03870    0.00607
0.57503    0.52981    0.99834
0.56717    0.60096    0.11558
0.11933    0.05754    0.23406
0.06339    0.10051    0.12248
0.63298    0.55779    0.20691
0.56184    0.40082    0.86977
0.12803    0.94341    0.78108
0.06741    0.89973    0.88222
0.62255    0.44443    0.76867
0.43144    0.60090    0.88823
0.88300    0.05823    0.76703
0.69456    0.50093    0.85876
0.80362    0.52284    0.96391
0.77089    0.45968   -0.02022
0.76710    0.50207    0.86068
0.58370    0.49991    0.84118
0.58836    0.49962    0.15729
0.00064    0.06881    0.00127
0.49957    0.43104    0.00010
0.41295    0.49969    0.16263
0.40877    0.50045    0.84494
0.08722    0.99973    0.16151
0.91132    0.99936    0.15646
0.91380    0.00005    0.83915
0.49962    0.56920    0.00171
0.00024    0.93038    0.99980
0.08957    0.99951    0.84427
```

POSCAR file for gd_p5_prime

```
POSCAR file from zrtcpb-gd-h2o-c.res: C: 143 F: 1 H: 120 O: 66 P: 1 ZR: 12
    34.8920000000000
     0.5792995890490465   -0.0000450140396845    0.0007649282407427
    -0.0000781726227076    1.0082675674799713    0.0000166934211398
     0.0004256087542374    0.0000053656439079    0.3214078049098053
143 1 120 66 1 12
Direct
  0.79061    0.88165    0.29793
  0.64889    0.62438    0.24088
  0.23196    0.78363    0.43753
  0.20660    0.81595    0.36763
  0.15262    0.80982    0.29175
  0.12397    0.83983    0.23082
  0.23304    0.85267    0.37621
```

```
0.26118   0.34899   0.34486
0.11338   0.90865   0.18693
0.14843   0.87672   0.24538
0.38265   0.59134   0.81783
0.20382   0.88291   0.31687
0.71121   0.62017   0.29239
0.39368   0.40981   0.20121
0.72351   0.28184   0.43963
0.69569   0.31422   0.37389
0.64228   0.30860   0.29636
0.61328   0.33925   0.23926
0.72086   0.35111   0.38908
0.60441   0.40842   0.19843
0.63699   0.37608   0.25923
0.69135   0.38189   0.33346
0.34948   0.62357   0.75710
0.88670   0.84268   0.25746
0.35901   0.37763   0.26018
0.29264   0.38021   0.29376
0.74154   0.24870   0.37865
0.24847   0.74996   0.37833
0.25580   0.24910   0.62327
0.74521   0.75116   0.62085
0.25336   0.75142   0.62375
0.75764   0.25217   0.62376
0.75151   0.75084   0.37562
0.24514   0.25104   0.37752
0.20614   0.18434   0.63275
0.29227   0.61844   0.68969
0.76771   0.78414   0.43666
0.22739   0.21789   0.43858
0.19933   0.18547   0.37284
0.14224   0.19091   0.30436
0.11208   0.16035   0.24868
0.22682   0.14897   0.38036
0.10416   0.09153   0.20337
0.13800   0.12375   0.26211
0.19597   0.11816   0.32703
0.23446   0.78430   0.56328
0.79456   0.81660   0.36838
0.20798   0.81684   0.63234
0.14389   0.81317   0.67863
0.11418   0.84314   0.73835
0.24240   0.85085   0.65057
0.11254   0.90969   0.80866
0.23282   0.21694   0.56397
0.14742   0.87777   0.74949
0.21187   0.88153   0.70630
0.76066   0.85100   0.35449
0.73112   0.28345   0.56472
0.14122   0.18709   0.67565
0.70309   0.31610   0.63178
0.63497   0.31576   0.65498
0.60483   0.34641   0.71061
0.88820   0.90955   0.19047
0.74036   0.34776   0.66625
0.73203   0.71767   0.43411
0.60733   0.41107   0.79760
0.64174   0.37881   0.73829
0.70966   0.37951   0.71577
0.85402   0.87759   0.25026
0.94774   0.51817   0.91230
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0.77706   0.15003   0.61753
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0.24146   0.15069   0.65181
0.11215   0.09018   0.80579
0.14604   0.12240   0.74599
0.21114   0.11956   0.70533
0.72830   0.71792   0.55988
0.70086   0.68573   0.62802
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0.60491   0.59337   0.80667
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0.69580   0.61882   0.67809
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0.27427	0.35123	0.61853
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0.39045	0.28713	0.35188
0.76218	0.25293	0.72113
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0.93779	0.10117	0.88063
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0.93306   0.89950   0.88199
0.37917   0.44215   0.77134
0.43193   0.59999   0.12347
0.86874   0.05630   0.21815
0.93448   0.09947   0.12562
0.36715   0.55655   0.21647
0.87229   0.94346   0.21787
0.56495   0.39938   0.11522
0.13022   0.94262   0.21266
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0.61790   0.44211   0.23196
0.19187   0.99969   0.11293
0.93989   0.00247   0.34807
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0.80621   0.99900   0.10398
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0.99786   0.02913   0.13447
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0.49562   0.53975   0.82102
0.07356   0.97077   0.00007
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0.42632   0.52903   0.00354
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0.39964   0.46118   0.00056
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0.56491   0.60141   0.11835
0.11831   0.05771   0.23503
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0.56387   0.40104   0.87385
0.12830   0.94363   0.78152
0.06744   0.89999   0.88200
0.62294   0.44487   0.77049
0.42822   0.60056   0.89009
0.88316   0.05849   0.76606
0.70678   0.50715   0.87157
0.81039   0.52818   0.88744
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0.77224   0.48781   0.90392
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0.58599   0.50052   0.15919
0.00033   0.06911   0.00114
0.50085   0.43136  -0.00129
0.41151   0.49985   0.16005
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0.91064   0.99963   0.15557
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0.08972   0.99977   0.84476
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POSCAR file for gd_product

POSCAR file from zrtcpb-gd-h2o-c.res: C: 143 F: 1 H: 120 O: 66 P: 1 ZR: 12
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     0.0004256087542374   0.0000053656439079   0.3214078049098053
143 1 120 66 1 12
Direct
  0.79112   0.88254   0.29865
  0.64826   0.62573   0.24078
  0.23155   0.78334   0.43758
  0.20637   0.81573   0.36763
  0.15295   0.80970   0.29037
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0.38613	0.59145	0.81511
0.20332	0.88285	0.31844
0.71291	0.62294	0.28303
0.39408	0.40966	0.19819
0.72143	0.28086	0.43755
0.69441	0.31330	0.37122
0.64161	0.30784	0.29234
0.61296	0.33866	0.23567
0.71974	0.35009	0.38757
0.60379	0.40788	0.19819
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0.07838	0.02503	0.38029
0.21801	0.02166	0.86663
0.19697	0.99914	0.00743
0.99420	0.00217	0.35598
0.78296	0.02137	0.13295
0.80424	0.99952	0.99294
0.92309	0.02559	0.61983
0.00698	0.00245	0.64384
0.13830	0.05544	0.00882
0.86312	0.05563	0.99192
0.00015	0.94478	0.25001
0.00087	0.94500	0.74914
0.21009	0.97583	0.14349
0.92004	0.99043	0.41708
0.79093	0.97694	0.85443
0.08098	0.99026	0.58301
0.26626	0.40605	0.27230
0.20946	0.34978	0.36384
0.44723	0.34257	0.25100
0.39314	0.28790	0.35682
0.75696	0.25190	0.72048
0.76597	0.90992	0.28900
0.71050	0.85472	0.38979
0.93643	0.84071	0.21916
0.88416	0.78644	0.33082
0.25341	0.75158	0.72176
0.27371	0.58947	0.68108
0.22032	0.64444	0.57888
0.42249	0.66376	0.82209
0.37250	0.71868	0.71158
0.75466	0.75233	0.27827
0.78958	0.08963	0.65734
0.73300	0.14492	0.56087
0.93089	0.16536	0.81474
0.87721	0.22087	0.71227
0.24352	0.25146	0.27969
0.73340	0.40395	0.73151
0.80648	0.42379	0.81212
0.79677	0.46182	0.70667
0.86593	0.46159	0.80594
0.86722	0.51478	0.74401
0.84098	0.58039	0.67622
0.80077	0.59002	0.81579
0.76810	0.55477	0.71973
0.72895	0.48882	0.13559
0.79358	0.44064	0.02842
0.96422	0.49256	0.85296
0.92572	0.50207	0.99330
0.00388	0.52282	0.95821
0.01514	0.57172	0.80392
0.97215	0.54433	0.69508
0.94560	0.59162	0.72929
0.89086	0.60617	0.92492
0.95799	0.58628	0.00659
0.87561	0.56946	0.03127
0.43754	0.40015	0.12165
0.93794	0.10145	0.88026
0.36942	0.55746	0.78918
0.56501	0.60223	0.88791
0.13161	0.05671	0.78327

```
0.06627   0.09978   0.87726
0.62747   0.55973   0.78625
0.43766   0.39980   0.87969
0.87024   0.94335   0.78690
0.93309   0.90034   0.11596
0.37727   0.44342   0.22531
0.93345   0.89978   0.88185
0.38264   0.44266   0.76693
0.43179   0.59999   0.12090
0.86878   0.05634   0.21693
0.93485   0.09960   0.12534
0.36726   0.55656   0.21438
0.87255   0.94398   0.21732
0.56523   0.39916   0.11333
0.13044   0.94272   0.21300
0.06722   0.89956   0.11624
0.61611   0.44140   0.23430
0.19226   0.99982   0.11339
0.93980   0.00280   0.34769
0.69435   0.50025   0.19044
0.44093   0.50158   0.34997
0.80637   0.99915   0.10248
0.06219   0.00069   0.34965
0.30819   0.50007   0.10675
0.56290   0.49868   0.35037
0.80922   0.00068   0.88559
0.06141   0.00294   0.65202
0.30837   0.50035   0.88834
0.55954   0.50510   0.65263
0.19463   0.99931   0.89627
0.93899   0.00116   0.65016
0.43690   0.49931   0.65144
0.00071   0.96111   0.17991
0.49943   0.47070   0.13310
0.99816   0.02938   0.13423
0.49996   0.53909   0.18280
0.00045   0.96132   0.81927
0.50411   0.47231   0.86810
0.00326   0.02960   0.86647
0.50080   0.53995   0.82192
0.07403   0.97101   0.00019
0.60499   0.46334   0.00331
0.90206   0.03938   0.99384
0.42812   0.52911   0.00137
0.92720   0.97113   0.99909
0.40135   0.46139   0.99673
0.09933   0.03919   0.00675
0.57573   0.53060   0.00291
0.56407   0.60198   0.12085
0.11843   0.05794   0.23538
0.06336   0.10088   0.12242
0.63161   0.55942   0.20938
0.56494   0.40145   0.87320
0.12899   0.94376   0.78171
0.06783   0.90019   0.88199
0.62142   0.44508   0.76474
0.43174   0.60073   0.88713
0.88409   0.05861   0.76495
0.70021   0.50093   0.86439
0.81611   0.51989   0.90464
0.75871   0.46029   0.03559
0.76428   0.48127   0.90344
0.59264   0.50182   0.84497
0.58500   0.49985   0.16201
0.00072   0.06934   0.00074
0.50208   0.43156   0.99767
0.41085   0.49990   0.15773
0.41514   0.50032   0.84001
0.08672   0.00021   0.16214
0.91089   0.99991   0.15477
0.91457   0.00060   0.83771
0.49984   0.56970   0.00225
0.00054   0.93090   0.99911
0.09042  -0.00000   0.84484
```

POSCAR files for ipa solvent

POSCAR file for gb_solvent

```
POSCAR file from zrtcpb-gb-ipa-c.res: C: 143 F: 1 H: 120 O: 66 P: 1 ZR: 12
   34.8920000000000
     0.5792995890490465  -0.0000450140396845   0.0007649282407427
    -0.0000781726227076   1.0082675674799713   0.0000166934211398
     0.0004256087542374   0.0000053656439079   0.3214078049098053
143 1 120 66 1 12
```

Direct
0.79023 0.88207 0.30393
0.23310 0.21668 0.56282
0.73274 0.71652 0.43658
0.70744 0.68401 0.36688
0.64843 0.68909 0.30333
0.61972 0.65899 0.24289
0.85218 0.81132 0.30654
0.73821 0.64833 0.36384
0.61426 0.59095 0.18651
0.64889 0.62299 0.24586
0.70878 0.61791 0.30542
0.88141 0.84152 0.24703
0.20723 0.18404 0.63189
0.23333 0.78352 0.56310
0.20768 0.81611 0.63258
0.14734 0.81133 0.69266
0.11810 0.84151 0.75223
0.23920 0.85152 0.63824
0.11299 0.90939 0.80970
0.14801 0.87731 0.75118
0.20926 0.88210 0.69541
0.76032 0.85148 0.36115
0.73406 0.28376 0.56356
0.14644 0.18870 0.69039
0.70706 0.31636 0.63162
0.64542 0.31144 0.68693
0.61409 0.34168 0.74261
0.88657 0.90941 0.18987
0.73765 0.35199 0.63765
0.60723 0.40976 0.79857
0.64306 0.37773 0.74138
0.70544 0.38269 0.69015
0.85151 0.87731 0.24822
0.77032 0.21742 0.56295
0.11678 0.15842 0.74883
0.79758 0.18507 0.63030
0.85805 0.19018 0.68918
0.88899 0.15982 0.74442
0.76743 0.14920 0.63316
0.89552 0.09146 0.79720
0.86040 0.12367 0.74037
0.79895 0.11854 0.68626
0.23871 0.14865 0.63728
0.11203 0.09045 0.80654
0.14659 0.12261 0.74747
0.20811 0.11795 0.69265
0.73325 0.71640 0.56275
0.70803 0.68386 0.63287
0.26725 0.71658 0.56322
0.64846 0.68875 0.69534
0.61971 0.65861 0.75586
0.73945 0.64842 0.63740
0.61423 0.59063 0.81187
0.64936 0.62273 0.75363
0.70995 0.61791 0.69561
0.76700 0.78333 0.56257
0.79259 0.81569 0.63248
0.85114 0.81022 0.69713
0.88032 0.84017 0.75765
0.29257 0.68415 0.63323
0.76254 0.85157 0.63485
0.88700 0.90840 0.81225
0.82264 0.53180 0.69660
0.85191 0.87636 0.75388
0.89930 0.51162 1.09541
0.85735 0.54778 1.07897
0.81141 0.55166 1.18796
0.79228 0.88178 0.69372
0.75606 0.41591 1.02650
0.80466 0.42594 0.92541
0.26917 0.28300 0.56212
0.79518 0.41524 1.14423
0.29653 0.31519 0.62980
0.35632 0.30969 0.69058
0.38707 0.33983 0.74723
0.26684 0.35119 0.63174
0.39366 0.40810 0.80099
0.35135 0.68938 0.69738
0.35886 0.37608 0.74273
0.26581 0.28375 0.43617
0.29811 0.38161 0.68649
0.76685 0.21667 0.43701
0.79265 0.18401 0.36792
0.85326 0.18868 0.30882
0.29271 0.31635 0.36795
0.88285 0.15838 0.25040
0.76125 0.14858 0.36304

```
0.88766    0.09037    0.19317
0.38010    0.65938    0.75820
0.85314    0.12254    0.25229
0.79176    0.11787    0.30764
0.35432    0.31143    0.31255
0.26672    0.71642    0.43704
0.29196    0.68387    0.36703
0.35159    0.68871    0.30472
0.38032    0.65855    0.24435
0.26045    0.64844    0.36242
0.38583    0.59059    0.18854
0.35061    0.62269    0.24657
0.26202    0.64840    0.63622
0.28994    0.61790    0.30437
0.38558    0.34167    0.25667
0.23276    0.78331    0.43693
0.20716    0.81567    0.36700
0.14856    0.81020    0.30246
0.11932    0.84014    0.24206
0.23719    0.85156    0.36465
0.26209    0.35197    0.36189
0.11275    0.90837    0.18732
0.14776    0.87634    0.24579
0.38594    0.59128    0.81437
0.20739    0.88176    0.30588
0.39244    0.40973    0.20079
0.73078    0.28298    0.43761
0.70338    0.31514    0.36988
0.64358    0.30960    0.30913
0.61282    0.33972    0.25238
0.73308    0.35114    0.36775
0.60619    0.40795    0.19841
0.64102    0.37597    0.25673
0.70180    0.38153    0.31287
0.35122    0.62330    0.75506
0.35660    0.37770    0.25792
0.29425    0.38266    0.30925
0.74703    0.24946    0.37739
0.24952    0.74978    0.37737
0.25291    0.24949    0.62240
0.75035    0.74980    0.62226
0.25060    0.75016    0.62274
0.75402    0.25097    0.62317
0.74918    0.75009    0.37689
0.24591    0.25093    0.37661
0.29148    0.61809    0.69506
0.76635    0.78350    0.43640
0.22965    0.21739    0.43689
0.20237    0.18501    0.36965
0.14198    0.19018    0.31054
0.11095    0.15984    0.25531
0.23236    0.14910    0.36700
0.10427    0.09146    0.20260
0.13940    0.12365    0.25951
0.20075    0.11846    0.31392
0.79190    0.81610    0.36682
0.83520    0.46561    0.86657
0.78723    0.35578    0.60004
0.56611    0.33818    0.78664
0.62169    0.28345    0.68325
0.73172    0.58972    0.30603
0.23290    0.91011    0.69788
0.28799    0.85505    0.59726
0.07090    0.83826    0.79914
0.12274    0.78358    0.68948
0.78596    0.64449    0.40780
0.27615    0.41006    0.68694
0.21851    0.35509    0.58995
0.43397    0.33623    0.79443
0.57338    0.66237    0.19380
0.37930    0.28147    0.68941
0.74491    0.24918    0.27971
0.62435    0.71700    0.30477
0.76994    0.91013    0.69279
0.71515    0.85574    0.58990
0.92638    0.83644    0.80733
0.87462    0.78214    0.69626
0.24942    0.74974    0.27960
0.73341    0.58986    0.69578
0.78766    0.64477    0.59442
0.57297    0.66189    0.80420
0.62397    0.71652    0.69302
0.23149    0.08987    0.69368
0.28769    0.14517    0.59696
0.06939    0.16160    0.79511
0.12196    0.21648    0.68721
0.72372    0.40999    0.31232
0.78144    0.35508    0.40945
```

```
0.56590   0.33608   0.20525
0.62065   0.28136   0.31041
0.22971   0.91012   0.30681
0.28461   0.85573   0.40952
0.07322   0.83642   0.19249
0.12509   0.78212   0.30339
0.26641   0.58986   0.30406
0.21217   0.64481   0.40519
0.42710   0.66178   0.19610
0.37612   0.71648   0.30694
0.75050   0.74979   0.72004
0.76843   0.08977   0.30699
0.71239   0.14507   0.40375
0.93009   0.16159   0.20365
0.87762   0.21650   0.31148
0.25505   0.24921   0.72007
0.22309   0.09011   0.31330
0.28119   0.14539   0.40713
0.06361   0.16331   0.20948
0.11876   0.21833   0.31199
0.71198   0.52243   0.14130
0.57695   0.50072   0.57183
0.28785   0.52246   0.85821
0.42273   0.50092   0.42801
0.49912   0.49963   0.35815
0.57988   0.47200   0.36875
0.50083   0.49998   0.64177
0.41950   0.47251   0.63077
0.36036   0.44491   0.00088
0.49917   0.55409   0.25331
0.50082   0.55432   0.74713
0.63943   0.44482   0.99861
0.30399   0.50070   0.00502
0.29152   0.52506   0.13751
0.07884   0.02413   0.38184
0.21744   0.02136   0.86541
0.19628   0.99895   0.00977
0.99307   0.00188   0.35629
0.78220   0.02124   0.13407
0.80341   0.99892   0.98954
0.92117   0.02421   0.61778
0.00677   0.00191   0.64336
0.13745   0.05516   0.00783
0.86230   0.05512   0.99173
0.99909   0.94455   0.25013
0.00059   0.94455   0.74942
0.20825   0.97508   0.14262
0.91977   0.98882   0.41612
0.79170   0.97495   0.85686
0.08011   0.98879   0.58363
0.27144   0.41090   0.30691
0.21253   0.35573   0.39962
0.43353   0.33820   0.21252
0.37811   0.28346   0.31630
0.75604   0.25124   0.72085
0.76654   0.91005   0.30136
0.71151   0.85499   0.40208
0.92857   0.83828   0.20002
0.87676   0.78358   0.30971
0.25068   0.75022   0.72051
0.26871   0.58984   0.69443
0.21445   0.64443   0.59169
0.42622   0.66292   0.80782
0.37526   0.71734   0.69611
0.74899   0.75014   0.27911
0.77648   0.09021   0.68689
0.71854   0.14558   0.59325
0.93637   0.16324   0.79019
0.88138   0.21830   0.68759
0.24395   0.25120   0.27893
0.72820   0.41094   0.69250
0.80989   0.51106   0.62194
0.79618   0.55995   0.68027
0.87835   0.53676   0.69783
0.93367   0.50793   1.01567
0.86509   0.48599   1.10254
0.92983   0.51420   1.18045
0.89093   0.57367   1.07149
0.84249   0.55318   1.27244
0.77750   0.52585   1.19244
0.78047   0.57858   1.17972
0.73644   0.38721   1.00923
0.71508   0.46859   1.06524
0.78163   0.42653   0.85164
0.82369   0.45016   0.94038
0.83863   0.40732   0.92184
0.83047   0.39752   1.13800
0.81257   0.43983   1.15972
```

```
0.76663   0.40796   1.20760
0.43564   0.40003   0.12380
0.93784   0.10069   0.87574
0.36825   0.55739   0.79042
0.56731   0.59990   0.88155
0.13011   0.05659   0.78233
0.06650   0.09976   0.87938
0.63163   0.55663   0.78722
0.43527   0.39882   0.88057
0.86949   0.94233   0.78778
0.93123   0.89993   0.11534
0.37785   0.44367   0.23008
0.93392   0.89910   0.88162
0.37964   0.44190   0.76927
0.43290   0.59987   0.11917
0.86956   0.05651   0.21741
0.93316   0.09968   0.12025
0.36835   0.55659   0.21301
0.87149   0.94329   0.21906
0.56448   0.39869   0.11900
0.13032   0.94229   0.21157
0.06575   0.89906   0.11808
0.62030   0.44176   0.23008
0.19179   0.99950   0.11330
0.93897   0.00229   0.34824
0.69226   0.49929   0.10882
0.44430   0.50264   0.35014
0.80604   0.99913   0.10385
0.06181   0.00026   0.34923
0.30759   0.50048   0.10872
0.56583   0.49787   0.34844
0.80792   0.99945   0.88606
0.06090   0.00236   0.65132
0.30769   0.49940   0.89092
0.55549   0.50290   0.64970
0.19370   0.99920   0.89554
0.93811   0.00033   0.65046
0.43376   0.49830   0.65162
0.99984   0.96083   0.17994
0.50002   0.47036   0.13265
0.99728   0.02918   0.13391
0.50121   0.53879   0.18095
0.99992   0.96081   0.81966
0.49981   0.47046   0.86722
0.00249   0.02921   0.86585
0.49879   0.53894   0.81931
0.07351   0.97067   0.00022
0.60001   0.46076   0.99974
0.90131   0.03893   0.99313
0.42757   0.52877   0.00149
0.92630   0.97069   0.99921
0.39980   0.46084   0.99995
0.09844   0.03895   0.00659
0.57233   0.52871   0.99872
0.56769   0.60033   0.11636
0.11877   0.05767   0.23400
0.06198   0.10069   0.12402
0.63190   0.55705   0.21050
0.56411   0.40007   0.87572
0.12810   0.94327   0.78066
0.06835   0.89988   0.88424
0.62179   0.44371   0.76923
0.43262   0.60063   0.88438
0.88098   0.05768   0.76580
0.70557   0.50321   0.84017
0.81659   0.54331   0.96699
0.70299   0.44176   1.03054
0.79540   0.51137   0.84272
0.90980   0.99962   0.15469
0.91423   0.00011   0.83768
0.41135   0.49982   0.84178
0.41349   0.49959   0.15904
0.49988   0.43046   0.99978
0.99988   0.06900   0.99985
0.58852   0.49963   0.15818
0.08555   0.00010   0.16194
0.50003   0.56898   0.00024
0.08995   0.99965   0.84490
0.58639   0.49964   0.84093
0.99989   0.93065   0.99977
```

POSCAR file for gb_p5

POSCAR file from zrtcpb-gb-ipa-c.res: C: 143 F: 1 H: 120 O: 66 P: 1 ZR: 12
   34.8920000000000
     0.5792995890490465   -0.0000450140396845   0.0007649282407427
    -0.0000781726227076   1.0082675674799713   0.0000166934211398

0.0004256087542374   0.0000053656439079   0.3214078049098053
143 1 120 66 1 12
Direct
0.79232   0.88298   0.30252
0.23260   0.21733   0.56319
0.73117   0.71851   0.43343
0.70696   0.68608   0.36158
0.64600   0.69007   0.30381
0.61807   0.65976   0.24314
0.85501   0.81246   0.31266
0.74048   0.65137   0.35210
0.61579   0.59194   0.18331
0.64954   0.62439   0.24234
0.71118   0.62038   0.29641
0.88497   0.84233   0.25293
0.20599   0.18481   0.63217
0.23450   0.78394   0.56318
0.20830   0.81658   0.63200
0.14595   0.81225   0.68504
0.11631   0.84233   0.74449
0.24116   0.85139   0.64328
0.11282   0.90962   0.80770
0.14778   0.87762   0.74898
0.21064   0.88202   0.69929
0.76169   0.85265   0.35956
0.73106   0.28284   0.56310
0.14324   0.18856   0.68405
0.70300   0.31566   0.62928
0.63525   0.31465   0.65556
0.60445   0.34555   0.70850
0.88923   0.90970   0.19061
0.73928   0.34824   0.65803
0.60558   0.41112   0.78883
0.64014   0.37886   0.72987
0.70764   0.38021   0.70399
0.85438   0.87792   0.25021
0.77437   0.21816   0.56230
0.11378   0.15805   0.74169
0.80317   0.18604   0.62803
0.86216   0.19113   0.69134
0.89220   0.16049   0.74676
0.77380   0.14996   0.62524
0.89734   0.09195   0.79810
0.86408   0.12428   0.73849
0.80436   0.11910   0.67862
0.23926   0.15010   0.64252
0.11175   0.09053   0.80458
0.14571   0.12287   0.74541
0.20884   0.11908   0.69636
0.72782   0.71855   0.55939
0.70121   0.68609   0.62725
0.26950   0.71725   0.56492
0.64650   0.69187   0.70236
0.61748   0.66166   0.76228
0.72679   0.64926   0.61630
0.60884   0.59243   0.80694
0.64148   0.62478   0.74554
0.69599   0.61880   0.67164
0.76405   0.78502   0.56242
0.78989   0.81715   0.63341
0.84756   0.81109   0.69986
0.87738   0.84077   0.76077
0.29466   0.68492   0.63530
0.76133   0.85339   0.63373
0.88656   0.90908   0.81272
0.79937   0.53986   0.74966
0.85062   0.87732   0.75470
0.90395   0.51392   0.03666
0.84789   0.54175   0.01907
0.83007   0.56345   0.13065
0.79193   0.88339   0.69228
0.77967   0.44105   -0.00527
0.81193   0.41858   0.89522
0.27294   0.28277   0.56070
0.82845   0.45270   0.09069
0.30042   0.31519   0.62728
0.35809   0.30987   0.69438
0.38766   0.34031   0.75162
0.27187   0.35148   0.62281
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0.35216   0.69020   0.70303
0.36055   0.37672   0.74145
0.26926   0.28322   0.43496
0.30208   0.38219   0.67789
0.76639   0.21624   0.43734
0.79325   0.18368   0.36874
0.85717   0.18728   0.32167
0.29724   0.31549   0.36642

S59

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0.75929   0.14937   0.35362
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0.85438   0.12215   0.25521
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0.26760   0.71658   0.43896
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0.29137   0.61829   0.30454
0.39230   0.34162   0.26343
0.23252   0.78323   0.43721
0.20710   0.81552   0.36706
0.15034   0.80991   0.29754
0.12169   0.83998   0.23685
0.23598   0.85173   0.36951
0.26468   0.35028   0.35282
0.11433   0.90849   0.18591
0.14893   0.87642   0.24510
0.38558   0.59176   0.81871
0.20681   0.88203   0.31034
0.39637   0.40918   0.20045
0.72308   0.28088   0.43804
0.69456   0.31278   0.37196
0.64253   0.30647   0.29170
0.61271   0.33679   0.23434
0.71732   0.35001   0.39036
0.60254   0.40620   0.19563
0.63376   0.37387   0.25848
0.68619   0.38042   0.33671
0.35189   0.62392   0.75839
0.36110   0.37695   0.25760
0.29690   0.38117   0.30154
0.74076   0.24760   0.37771
0.24919   0.74952   0.37842
0.25468   0.24977   0.62204
0.74450   0.75180   0.62058
0.25304   0.75101   0.62368
0.75714   0.25156   0.62265
0.74999   0.75184   0.37528
0.24689   0.25082   0.37613
0.29331   0.61864   0.69493
0.76638   0.78507   0.43660
0.22864   0.21783   0.43752
0.20069   0.18540   0.37146
0.14107   0.19043   0.30994
0.11080   0.15991   0.25420
0.23044   0.14942   0.37186
0.10526   0.09151   0.20190
0.13918   0.12374   0.26069
0.19953   0.11861   0.31852
0.79354   0.81744   0.36850
0.82173   0.48043   0.80159
0.79260   0.34896   0.64002
0.55198   0.34464   0.73278
0.60681   0.28911   0.63320
0.73516   0.59248   0.29535
0.23508   0.90973   0.70571
0.29124   0.85452   0.60721
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0.12041   0.78489   0.67707
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0.28089   0.41079   0.67310
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0.77123   0.64453   0.56293
0.57493   0.66576   0.82142
0.62600   0.72058   0.71079
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0.06497   0.16057   0.78346
0.11726   0.21579   0.67676
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0.62474   0.27739   0.27765
0.22806   0.91062   0.31499
0.28194   0.85607   0.41879
0.07689   0.83618   0.18367
0.12778   0.78160   0.29488
0.26759   0.59034   0.30198
0.21228   0.64534   0.40174
0.43123   0.66175   0.20611
0.37932   0.71623   0.31669
0.74282   0.75167   0.71834
0.76496   0.09107   0.29208
0.70844   0.14671   0.38643
0.93676   0.15948   0.22532
0.88357   0.21425   0.33266
0.25693   0.24968   0.71972
0.22158   0.09019   0.32015
0.27855   0.14577   0.41471
0.06429   0.16322   0.20561
0.11800   0.21861   0.30910
0.71642   0.51698   0.15677
0.57559   0.49691   0.57760
0.28636   0.52211   0.86371
0.42011   0.49825   0.42013
0.51093   0.49816   0.35733
0.57826   0.46942   0.36005
0.49449   0.50065   0.64446
0.42036   0.47257   0.63541
0.36274   0.44470   0.00239
0.50220   0.55357   0.25503
0.50018   0.55460   0.74754
0.64662   0.44776   0.99442
0.30501   0.50072   0.01647
0.29611   0.52595   0.14384
0.08099   0.02482   0.37785
0.21723   0.02195   0.86286
0.19731   0.99908   0.00288
0.99646   0.00192   0.35554
0.78423   0.02140   0.13532
0.80458   0.99919   0.99586
0.92211   0.02549   0.62067
0.00578   0.00219   0.64315
0.13856   0.05523   0.00625
0.86320   0.05525   0.99305
0.00121   0.94457   0.24961
0.00047   0.94477   0.74874
0.21123   0.97572   0.13918
0.92249   0.99079   0.41892
0.79044   0.97668   0.85730
0.08003   0.99062   0.58068
0.27285   0.40898   0.29455
0.21370   0.35329   0.38465
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0.38642   0.28399   0.32895
0.76209   0.25251   0.71993
0.76882   0.91097   0.29715
0.71224   0.85617   0.39781
0.93303   0.83903   0.20898
0.87968   0.78481   0.31931
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0.75194   0.75206   0.27754
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0.72611   0.14640   0.58088
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0.24469   0.25085   0.27848
0.73507   0.40643   0.72198
0.78257   0.53024   0.66126
0.77856   0.56823   0.76763
0.85379   0.54091   0.75115
0.91498   0.49769   -0.04502
0.89152   0.49360   0.10825
0.94904   0.52946   0.06273
0.85972   0.56205   -0.05344
0.87221   0.58095   0.15999
0.81765   0.54343   0.20318
0.78740   0.58228   0.11521
0.74146   0.42252   0.03704
0.71181   0.47118   0.11478
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0.83648   0.39299   -0.06928
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0.84671   0.42760   0.13960
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0.44008   0.39987   0.12385
0.93798   0.10111   0.87954
0.36781   0.55791   0.79381
0.56421   0.60160   0.88169
0.13045   0.05674   0.78061
0.06612   0.09970   0.87729
0.62683   0.55877   0.78126
0.43554   0.39957   0.88150
0.86957   0.94311   0.78804
0.93365   0.90000   0.11601
0.38059   0.44290   0.22992
0.93351   0.89955   0.88175
0.37959   0.44268   0.77091
0.43580   0.60023   0.12392
0.87034   0.05616   0.21888
0.93487   0.09949   0.12418
0.36981   0.55694   0.21432
0.87379   0.94364   0.21877
0.56761   0.39737   0.10578
0.13205   0.94240   0.21026
0.06765   0.89922   0.11596
0.61401   0.43956   0.23304
0.19314   0.99969   0.10952
0.94204   0.00245   0.34808
0.69359   0.49277   0.16689
0.44477   0.50274   0.34669
0.80714   0.99894   0.10525
0.06454   0.00042   0.34815
0.30912   0.50062   0.11597
0.56583   0.49629   0.35018
0.80893   0.00038   0.88825
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0.93808   0.00098   0.65032
0.43362   0.49870   0.65431
0.00187   0.96087   0.17944
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0.07436   0.97079  -0.00138
0.60389   0.46227   0.99440
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0.92743   0.97087  -0.00027
0.40153   0.46114   0.00195
0.09956   0.03902   0.00475
0.57697   0.53027   0.99628
0.56839   0.60123   0.11495
0.12019   0.05772   0.23256
0.06353   0.10074   0.12224
0.63505   0.55824   0.20525
0.56310   0.40110   0.86626
0.12836   0.94354   0.77976
0.06792   0.89999   0.88162
0.62053   0.44496   0.76010
0.43134   0.60095   0.89069
0.88274   0.05823   0.76619
0.69720   0.49894   0.84769
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0.74804   0.47326  -0.05499
0.76820   0.50742   0.85778
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0.08783  -0.00005   0.15997
0.50097   0.56940   0.00192
0.08984  -0.00019   0.84294
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POSCAR file for gb_p5_prime

POSCAR file from zrtcpb-gb-ipa-c.res: C: 143 F: 1 H: 120 O: 66 P: 1 ZR: 12
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      0.0004256087542374    0.0000053656439079    0.3214078049098053
143 1 120 66 1 12
Direct
   0.79248   0.88304   0.30286
   0.23343   0.21728   0.56203
   0.73130   0.71855   0.43352
   0.70660   0.68606   0.36234
   0.64434   0.68969   0.30907
   0.61621   0.65942   0.24849
   0.85521   0.81245   0.31070
   0.74101   0.65179   0.34911
   0.61448   0.59209   0.18477
   0.64888   0.62445   0.24308
   0.71173   0.62087   0.29286
   0.88490   0.84246   0.25123
   0.20674   0.18474   0.63096
   0.23439   0.78429   0.56228
   0.20811   0.81694   0.63101
   0.14499   0.81289   0.68124
   0.11538   0.84293   0.74085
   0.24171   0.85143   0.64511
   0.11279   0.90994   0.80704
   0.14766   0.87796   0.74804
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0.39429   0.34239   0.26750
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0.37850   0.28093   0.70441
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0.61758   0.71663   0.31785
0.77126   0.91245   0.68766
0.71472   0.85847   0.58565
0.92207   0.83668   0.81260
0.86909   0.78283   0.70103
0.24742   0.74911   0.28001
0.71449   0.59054   0.66787
0.77054   0.64478   0.56507
0.57427   0.66751   0.82298
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0.29109   0.14766   0.60963
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0.22622   0.91119   0.31901
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0.12943   0.78148   0.28893
0.26497   0.59036   0.30322
0.20982   0.64596   0.39987
0.43102   0.66051   0.21127
0.37940   0.71547   0.31987
0.74165   0.75223   0.71794
0.76388   0.09212   0.28612
0.70776   0.14800   0.37996
0.93942   0.15867   0.23363
0.88640   0.21350   0.34089
0.25771   0.24951   0.71888
0.22079   0.09006   0.32320
0.27792   0.14565   0.41743
0.06581   0.16365   0.20183
0.11982   0.21911   0.30440
0.71420   0.52308   0.14891
0.57527   0.50089   0.57164
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0.42419   0.50150   0.42914
0.49953   0.49844   0.35807
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0.50024   0.50174   0.64146
0.41751   0.47386   0.63196
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0.30432   0.50073   0.00117
0.29152   0.52419   0.14223
0.08025   0.02496   0.37822
0.21769   0.02188   0.86294
0.19733   0.99924   0.00370
0.99577   0.00209   0.35512
0.78410   0.02160   0.13441
0.80466   0.99960   0.99409
0.92228   0.02594   0.62025
0.00621   0.00258   0.64279
0.13866   0.05542   0.00623
0.86345   0.05569   0.99235
0.00089   0.94491   0.24921
0.00061   0.94515   0.74814
0.21075   0.97571   0.13934
0.92176   0.99118   0.41847
0.79091   0.97694   0.85616
0.08007   0.99067   0.58065
0.27134   0.40815   0.28548
0.21287   0.35236   0.37636
0.44471   0.33989   0.23251
0.38970   0.28529   0.33761
0.75852   0.25332   0.71832
0.76887   0.91101   0.29823
0.71288   0.85602   0.39890
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0.87986   0.78478   0.31624
0.25410   0.75201   0.72086
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0.21693   0.64550   0.58606
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0.37461   0.71833   0.70487
0.75346   0.75163   0.27733
0.78419   0.09068   0.67027
0.72712   0.14615   0.57561
0.93565   0.16498   0.80147
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0.24511   0.25120   0.27757
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0.89141   0.48493   0.80360
0.92212   0.54661   0.94480
0.88217   0.59170  -0.03916
0.94416   0.58517  -0.15120
0.87074   0.53947   0.74220
0.85739   0.60908  -0.30538
0.79471   0.61213  -0.19326
0.78245   0.58311  -0.32345
0.84143   0.50438   0.19640
0.71695   0.48096   0.08431
0.87763   0.44364   1.09846
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0.43980   0.40002   0.12095
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0.06667   0.09995   0.87685
0.62316   0.56052   0.78054
0.43675   0.39971   0.87889
0.86972   0.94341   0.78704
0.93341   0.90026   0.11528
0.37989   0.44306   0.22624
0.93346   0.89981   0.88093
0.37989   0.44262   0.76904
0.43290   0.59980   0.12462
0.87027   0.05635   0.21786
0.93510   0.09974   0.12399
0.36913   0.55616   0.21878
0.87348   0.94385   0.21805
0.56736   0.39871   0.10654
0.13161   0.94266   0.21037
0.06750   0.89949   0.11528
0.61926   0.44114   0.22591
0.19299   0.99979   0.10989
0.94141   0.00263   0.34743
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0.44520   0.50063   0.35062
0.80717   0.99926   0.10392
0.06390   0.00061   0.34797
0.30891   0.50019   0.11134
0.56716   0.49775   0.34650
0.80910   0.00075   0.88692
0.06063   0.00298   0.65046
0.30682   0.49984   0.89427
0.55378   0.50524   0.64856
0.19460   0.99946   0.89279
0.93814   0.00139   0.64972
0.43139   0.49977   0.65224
0.00156   0.96112   0.17886
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0.99899   0.02945   0.13327
0.50162   0.53888   0.18249
0.00010   0.96144   0.81828
0.50099   0.47238   0.86533
0.00304   0.02973   0.86543
0.49697   0.54061   0.82072
0.07430   0.97101   0.99841
0.60339   0.46330   0.99602
0.90241   0.03946   0.99381
0.42760   0.52918   0.00340
0.92736   0.97115   0.99885
0.40111   0.46126   0.99846
0.09961   0.03925   0.00469
0.57437   0.53110   0.99881
0.56568   0.60129   0.11973
0.12005   0.05787   0.23276
0.06375   0.10093   0.12197
0.63425   0.55829   0.20475
0.56431   0.40214   0.86515
0.12844   0.94386   0.77931
0.06786   0.90028   0.88084
0.62163   0.44640   0.76058
0.42914   0.60114   0.89095
0.88317   0.05881   0.76529
0.70792   0.50630   0.83079
0.79690   0.54123   0.87325
0.79490   0.50113   1.03906
0.77655   0.49649   0.87894
0.91188  -0.00007   0.15477
0.91440   0.00070   0.83773
0.41169   0.50065   0.84225
0.41334   0.49945   0.15936
0.50242   0.43153   0.99431
0.00102   0.06940   0.99974
0.58726   0.50022   0.15676
0.08755   0.00020   0.15994
0.49913   0.57001   0.00247
0.09006   0.00008   0.84295
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0.00073   0.93099   0.99806
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POSCAR file for gb_product

POSCAR file from zrtcpb-gb-ipa-c.res: C: 143 F: 1 H: 120 O: 66 P: 1 ZR: 12
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     -0.0000781726227076   1.0082675674799713   0.0000166934211398
      0.0004256087542374   0.0000053656439079   0.3214078049098053
143 1 120 66 1 12
Direct
   0.79431   0.88551   0.30413
   0.23451   0.21858   0.56273
   0.72689   0.72270   0.43056
   0.70188   0.69089   0.35701
   0.63473   0.69122   0.32765
   0.60681   0.66074   0.26809
   0.85676   0.81480   0.31451
   0.74129   0.66026   0.32078
   0.61067   0.59568   0.18872
   0.64511   0.62875   0.24180
   0.71268   0.62874   0.26672
   0.88656   0.84448   0.25375
   0.20707   0.18616   0.63150
   0.23254   0.78387   0.56175
   0.20653   0.81673   0.63009
   0.14228   0.81372   0.67612
   0.11333   0.84403   0.73543
   0.24176   0.85050   0.64804
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   0.14742   0.87840   0.74644
   0.21199   0.88152   0.70331
   0.76384   0.85539   0.36221
   0.73051   0.28429   0.56029
   0.14226   0.18892   0.67505
   0.70369   0.31791   0.62376
   0.63493   0.32088   0.63726
   0.60700   0.35265   0.69034
   0.89030   0.91159   0.18959
   0.74378   0.34764   0.66407
   0.61574   0.41570   0.78771
   0.64717   0.38306   0.72481
   0.71555   0.38049   0.71087
   0.85596   0.88007   0.25081
   0.77444   0.21978   0.56279
   0.11277   0.15837   0.73248
   0.80284   0.18777   0.62969
   0.85842   0.19358   0.70185
   0.88898   0.16307   0.75717
   0.77690   0.15095   0.61880
   0.89897   0.09392   0.79839
   0.86475   0.12621   0.74038
   0.80797   0.12028   0.67231
   0.24207   0.15230   0.64913
   0.11326   0.09168   0.80376
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   0.21176   0.12112   0.70228
   0.71943   0.72273   0.55583
   0.69165   0.69026   0.62135
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   0.64636   0.69654   0.71446
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   0.63685   0.62902   0.74668
   0.68087   0.62245   0.65312
   0.76092   0.78805   0.56268
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   0.84987   0.87935   0.75526
   0.90905   0.56489   0.82953
   0.84748   0.54297   0.79375
   0.79632   0.56853   0.73773
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   0.82375   0.49428   0.21180
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   0.36137   0.30996   0.69837
   0.39239   0.34042   0.75332
   0.28126   0.35280   0.61277
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   0.35098   0.69041   0.70224
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   0.27470   0.28356   0.43368
   0.31283   0.38344   0.66575

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0.85634    0.12311    0.25774
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0.25747    0.64876    0.36007
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0.39931    0.34235    0.26560
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0.93950	0.00264	0.64929
0.44355	0.50192	0.64860
0.00288	0.96215	0.17845
0.50303	0.47112	0.12926
0.00045	0.03042	0.13319
0.50048	0.53944	0.18216
0.00124	0.96255	0.81767
0.50991	0.47441	0.86565
0.00452	0.03083	0.86567
0.50409	0.54204	0.82117
0.07546	0.97196	0.99783
0.61071	0.46643	0.00211
0.90375	0.04072	0.99380
0.43045	0.52937	0.99878
0.92878	0.97246	0.99833
0.40648	0.46129	0.98980
0.10106	0.04014	0.00454
0.57788	0.53329	0.00435
0.56072	0.60390	0.12559
0.12148	0.05858	0.23246
0.06511	0.10172	0.12236
0.63062	0.56219	0.21236
0.57469	0.40527	0.86724
0.12947	0.94447	0.77859
0.06830	0.90110	0.87973
0.63050	0.44968	0.76104
0.43232	0.60157	0.88677
0.88534	0.06022	0.76501
0.70522	0.50657	0.86963
0.82247	0.52517	0.89906
0.75988	0.46918	0.03961
0.77083	0.48824	0.90703
0.91321	0.00117	0.15432
0.91563	0.00207	0.83722
0.42000	0.50106	0.83570
0.41327	0.49922	0.15343
0.50853	0.43278	0.99187
0.00247	0.07054	0.00001
0.58718	0.50140	0.16093
0.08898	0.00101	0.15969
0.50015	0.57100	0.00306
0.09146	0.00104	0.84237
0.59753	0.50517	0.84621
0.00185	0.93202	0.99734

POSCAR file for gd_solvent

POSCAR file from zrtcpb-gd-ipa-c.res: C: 146 F: 1 H: 126 O: 66 P: 1 ZR: 12
```
  34.8920000000000
    0.5792995890490465   -0.0000450140396845    0.0007649282407427
   -0.0000781726227076    1.0082675674799713    0.0000166934211398
    0.0004256087542374    0.0000053656439079    0.3214078049098053
146 1 126 66 1 12
Direct
  0.79241   0.88298   0.30290
  0.64952   0.62447   0.24179
  0.26482   0.64901   0.63477
  0.29124   0.61833   0.30453
  0.39247   0.34179   0.26470
  0.23242   0.78321   0.43733
  0.20708   0.81548   0.36708
  0.15063   0.80981   0.29681
  0.12204   0.83987   0.23604
  0.23584   0.85172   0.37002
  0.26436   0.35018   0.35218
  0.11443   0.90843   0.18580
  0.71167   0.62073   0.29409
  0.14906   0.87636   0.24489
  0.38548   0.59173   0.81864
  0.20673   0.88201   0.31073
  0.39607   0.40922   0.20029
  0.72287   0.28067   0.43843
  0.69441   0.31262   0.37241
  0.64249   0.30637   0.29188
  0.61255   0.33674   0.23496
  0.71712   0.34986   0.39112
  0.60234   0.40619   0.19633
  0.88497   0.84232   0.25296
  0.63353   0.37382   0.25932
  0.68605   0.38029   0.33747
  0.35188   0.62387   0.75810
  0.36088   0.37701   0.25771
  0.29646   0.38109   0.30070
  0.74092   0.24747   0.37796
  0.24910   0.74950   0.37849
  0.25484   0.24970   0.62228
  0.74414   0.75177   0.62062
  0.25322   0.75105   0.62382
  0.20628   0.18472   0.63220
  0.75696   0.25138   0.62302
  0.75012   0.75187   0.37543
  0.24684   0.25086   0.37636
  0.29349   0.61859   0.69414
  0.76651   0.78507   0.43693
  0.22872   0.21783   0.43764
  0.20078   0.18540   0.37159
  0.14129   0.19045   0.30966
  0.11104   0.15992   0.25402
  0.23042   0.14940   0.37249
  0.23449   0.78393   0.56323
  0.10539   0.09147   0.20219
  0.13929   0.12372   0.26099
  0.19951   0.11858   0.31925
  0.79369   0.81745   0.36894
  0.20821   0.81656   0.63199
  0.14565   0.81232   0.68428
  0.11602   0.84241   0.74362
  0.24129   0.85127   0.64389
  0.11285   0.90964   0.80754
  0.23283   0.21726   0.56326
  0.14773   0.87763   0.74871
  0.21078   0.88193   0.69970
  0.76184   0.85266   0.36010
  0.73065   0.28259   0.56355
  0.14340   0.18844   0.68354
  0.70250   0.31539   0.62969
  0.63451   0.31479   0.65399
  0.60392   0.34578   0.70685
  0.88923   0.90969   0.19058
  0.73920   0.34764   0.66043
  0.73099   0.71857   0.43334
  0.60562   0.41111   0.78904
  0.64010   0.37877   0.73020
  0.70784   0.37972   0.70631
  0.85440   0.87791   0.25031
  0.77450   0.21805   0.56255
  0.89835   0.48395   1.13566
  0.96479   0.53684   1.07502
  0.92483   0.49814   0.91235
  0.11389   0.15794   0.74114
  0.80337   0.18595   0.62825
  0.86207   0.19116   0.69236
```

```
0.89218   0.16055   0.74785
0.77437   0.14977   0.62459
0.70676   0.68618   0.36127
0.89771   0.09196   0.79834
0.86442   0.12426   0.73881
0.80502   0.11895   0.67804
0.23968   0.15008   0.64305
0.11202   0.09047   0.80462
0.14596   0.12280   0.74533
0.20921   0.11904   0.69677
0.72743   0.71856   0.55926
0.70089   0.68608   0.62709
0.26964   0.71729   0.56499
0.64528   0.68996   0.30521
0.64694   0.69192   0.70391
0.61811   0.66171   0.76407
0.72599   0.64918   0.61484
0.60884   0.59246   0.80755
0.64158   0.62477   0.74616
0.69542   0.61873   0.67071
0.76394   0.78497   0.56273
0.78978   0.81705   0.63391
0.84736   0.81099   0.70061
0.87718   0.84070   0.76132
0.61745   0.65966   0.24429
0.29485   0.68494   0.63519
0.76131   0.85330   0.63392
0.88660   0.90906   0.81265
0.79959   0.54009   0.74860
0.85058   0.87728   0.75484
0.90409   0.51364   0.03526
0.84830   0.54159   0.01735
0.83064   0.56364   0.12834
0.79195   0.88333   0.69224
0.75992   0.40934   0.07813
0.85509   0.81246   0.31282
0.79171   0.38548   0.98139
0.27300   0.28272   0.56101
0.80911   0.42152   0.17280
0.30047   0.31512   0.62769
0.35788   0.30967   0.69541
0.38756   0.34008   0.75266
0.27215   0.35146   0.62275
0.39437   0.40871   0.80148
0.35231   0.69017   0.70304
0.36079   0.37656   0.74172
0.74089   0.65174   0.34983
0.26926   0.28323   0.43533
0.30247   0.38212   0.67783
0.76665   0.21615   0.43755
0.79365   0.18360   0.36903
0.85781   0.18706   0.32298
0.29724   0.31552   0.36683
0.88762   0.15679   0.26481
0.75940   0.14943   0.35290
0.88909   0.08993   0.19573
0.38036   0.66004   0.76434
0.61573   0.59195   0.18317
0.85460   0.12205   0.25531
0.79021   0.11852   0.29900
0.36132   0.31152   0.32076
0.26757   0.71659   0.43910
0.29338   0.68398   0.36982
0.35440   0.68862   0.31216
0.38359   0.65857   0.25197
0.26118   0.64885   0.36171
0.38796   0.59092   0.19187
0.35295   0.62297   0.25049
0.81098   0.47135   0.83027
0.79267   0.34802   0.64391
0.55125   0.34516   0.72979
0.60572   0.28952   0.63031
0.73615   0.59299   0.29167
0.23534   0.90960   0.70654
0.29150   0.85430   0.60835
0.06733   0.83950   0.78554
0.11997   0.78502   0.67593
0.79073   0.64917   0.38692
0.28149   0.41077   0.67301
0.22560   0.35545   0.57502
0.43238   0.33648   0.80605
0.56960   0.66223   0.19963
0.37980   0.28123   0.69992
0.73652   0.24657   0.28058
0.61889   0.71707   0.31214
0.77121   0.91206   0.68874
0.71480   0.85804   0.58671
0.92249   0.83648   0.81287
```

```
0.86956   0.78257   0.70144
0.24839   0.74907   0.28073
0.71167   0.58953   0.65486
0.76981   0.64440   0.55990
0.57599   0.66585   0.82415
0.62682   0.72068   0.71356
0.23406   0.09143   0.70139
0.28993   0.14736   0.60749
0.06498   0.16043   0.78246
0.11734   0.21563   0.67583
0.70250   0.40956   0.35206
0.75992   0.35458   0.44840
0.57229   0.33267   0.17116
0.62493   0.27729   0.27707
0.22784   0.91062   0.31576
0.28160   0.85607   0.41982
0.07743   0.83604   0.18229
0.12824   0.78146   0.29368
0.26742   0.59039   0.30189
0.21203   0.64543   0.40134
0.43129   0.66173   0.20671
0.37939   0.71621   0.31744
0.74232   0.75158   0.71837
0.76471   0.09120   0.29058
0.70839   0.14689   0.38505
0.93745   0.15912   0.22709
0.88451   0.21390   0.33478
0.25706   0.24959   0.71996
0.22148   0.09014   0.32127
0.27840   0.14574   0.41571
0.06463   0.16323   0.20510
0.11831   0.21865   0.30840
0.71579   0.51748   0.15564
0.57568   0.49651   0.57830
0.28717   0.52263   0.86264
0.41964   0.49831   0.41983
0.51027   0.49825   0.35703
0.57779   0.46955   0.36060
0.49466   0.50074   0.64448
0.42023   0.47263   0.63527
0.36229   0.44475   0.00205
0.50181   0.55359   0.25475
0.50013   0.55491   0.74834
0.64688   0.44795   0.99411
0.30474   0.50102   0.01564
0.29641   0.52649   0.14243
0.08078   0.02476   0.37827
0.21747   0.02188   0.86303
0.19742   0.99904   0.00305
0.99632   0.00188   0.35556
0.78424   0.02130   0.13514
0.80471   0.99923   0.99545
0.92201   0.02554   0.62087
0.00589   0.00226   0.64311
0.13868   0.05523   0.00652
0.86350   0.05528   0.99310
0.00135   0.94453   0.24971
0.00062   0.94481   0.74851
0.21120   0.97560   0.13922
0.92230   0.99088   0.41895
0.79083   0.97664   0.85697
0.07990   0.99051   0.58067
0.27213   0.40878   0.29273
0.21323   0.35307   0.38332
0.44223   0.33898   0.22699
0.38691   0.28427   0.33116
0.76180   0.25229   0.72032
0.76887   0.91096   0.29754
0.71241   0.85617   0.39847
0.93296   0.83902   0.20876
0.87973   0.78479   0.31923
0.25414   0.75153   0.72157
0.27143   0.59019   0.69091
0.21821   0.64505   0.58719
0.42562   0.66357   0.81651
0.37575   0.71825   0.70429
0.75226   0.75211   0.27773
0.78349   0.09042   0.67448
0.72696   0.14610   0.57937
0.93808   0.16385   0.79830
0.88469   0.21945   0.69530
0.24456   0.25098   0.27869
0.73569   0.40567   0.72599
0.78236   0.53082   0.66015
0.77956   0.56860   0.76733
0.85406   0.54068   0.74949
0.86028   0.56163  -0.05576
0.87313   0.58090   0.15758
```

```
0.81742    0.54391    0.20121
0.78856    0.58283    0.11199
0.72131    0.39154    0.12230
0.71976    0.46268    0.08940
0.75462    0.37595    0.91613
0.82970    0.40228    0.93389
0.81544    0.36011    0.02011
0.82766    0.39666    0.22247
0.85177    0.43589    0.13059
0.78578    0.44137    0.23645
0.95294    0.51376    0.83902
0.96732    0.47779    0.93208
0.88073    0.47922    0.89029
0.88213    0.49482    1.22688
0.95219    0.47534    1.12179
0.86985    0.45648    1.15220
0.97582    0.56069    1.00910
0.94679    0.53496    1.17122
1.01561    0.52311    1.08416
0.43981    0.39992    0.12393
0.93834    0.10113    0.87978
0.36766    0.55789    0.79374
0.56417    0.60163    0.88217
0.13064    0.05668    0.78062
0.06647    0.09967    0.87747
0.62673    0.55877    0.78180
0.43572    0.39951    0.88158
0.86970    0.94308    0.78790
0.93368    0.89997    0.11607
0.38011    0.44297    0.22953
0.93355    0.89954    0.88172
0.37983    0.44254    0.77056
0.43566    0.60028    0.12399
0.87035    0.05608    0.21866
0.93505    0.09941    0.12426
0.36969    0.55698    0.21422
0.87378    0.94362    0.21856
0.56721    0.39738    0.10680
0.13207    0.94234    0.21041
0.06780    0.89917    0.11575
0.61412    0.43958    0.23331
0.19318    0.99961    0.10968
0.94190    0.00244    0.34802
0.69337    0.49310    0.16470
0.44437    0.50267    0.34642
0.80724    0.99892    0.10482
0.06439    0.00038    0.34828
0.30883    0.50101    0.11496
0.56540    0.49639    0.35001
0.80913    0.00040    0.88783
0.06042    0.00266    0.65071
0.30772    0.49973    0.89501
0.55338    0.50448    0.65136
0.19467    0.99932    0.89257
0.93804    0.00101    0.65026
0.43351    0.49875    0.65417
0.00195    0.96080    0.17948
0.50266    0.47025    0.13115
0.99922    0.02911    0.13404
0.50430    0.53883    0.18132
0.00012    0.96109    0.81871
0.50017    0.47161    0.86631
0.00302    0.02937    0.86583
0.49778    0.53975    0.82100
0.07442    0.97077   -0.00134
0.60384    0.46225    0.99450
0.90247    0.03905    0.99470
0.42892    0.52901    0.00465
0.92755    0.97083   -0.00035
0.40118    0.46111    0.00155
0.09973    0.03898    0.00493
0.57661    0.53025    0.99662
0.56816    0.60116    0.11520
0.12028    0.05768    0.23289
0.06370    0.10070    0.12246
0.63507    0.55827    0.20526
0.56313    0.40112    0.86647
0.12843    0.94355    0.77968
0.06796    0.90000    0.88148
0.62046    0.44495    0.76006
0.43118    0.60091    0.89064
0.88315    0.05826    0.76637
0.69694    0.49942    0.84712
0.78773    0.52151    0.98392
0.72903    0.44133    0.02539
0.76810    0.50765    0.85617
0.91215   -0.00041    0.15554
0.50071    0.56940    0.00212
```

```
0.08790  -0.00011   0.16016
0.59120   0.49999   0.15393
0.00114   0.06894   0.00040
0.50207   0.43111  -0.00305
0.41625   0.49918   0.16359
0.41029   0.50065   0.84613
0.91437   0.00025   0.83853
0.09000  -0.00021   0.84304
0.58559   0.50073   0.83769
0.00094   0.93069  -0.00135
```

POSCAR file for gd_p5

```
POSCAR file from zrtcpb-gd-ipa-c.res: C: 146 F: 1 H: 126 O: 66 P: 1 ZR: 12
  34.8920000000000
    0.5792995890490465  -0.0000450140396845   0.0007649282407427
   -0.0000781726227076   1.0082675674799713   0.0000166934211398
    0.0004256087542374   0.0000053656439079   0.3214078049098053
146 1 126 66 1 12
Direct
  0.79249   0.88300   0.30315
  0.65043   0.62429   0.24148
  0.26508   0.64905   0.63414
  0.29081   0.61849   0.30345
  0.39341   0.34236   0.26881
  0.23223   0.78328   0.43717
  0.20693   0.81560   0.36707
  0.15136   0.80983   0.29472
  0.12288   0.83991   0.23383
  0.23493   0.85201   0.37219
  0.26390   0.34983   0.35008
  0.11434   0.90856   0.18610
  0.71436   0.62155   0.28712
  0.14905   0.87653   0.24491
  0.38561   0.59190   0.81901
  0.20586   0.88233   0.31298
  0.39585   0.40940   0.20034
  0.71984   0.28011   0.44093
  0.69033   0.31203   0.37621
  0.63960   0.30573   0.29330
  0.60953   0.33612   0.23669
  0.71117   0.34944   0.39853
  0.59946   0.40577   0.19916
  0.88520   0.84247   0.25303
  0.62885   0.37329   0.26428
  0.67946   0.37985   0.34614
  0.35186   0.62401   0.75846
  0.36081   0.37718   0.25835
  0.29575   0.38081   0.29847
  0.73848   0.24714   0.37971
  0.24887   0.74959   0.37827
  0.25537   0.24946   0.62272
  0.74419   0.75178   0.62053
  0.25330   0.75112   0.62352
  0.20685   0.18450   0.63218
  0.75671   0.25116   0.62440
  0.75062   0.75183   0.37541
  0.24718   0.25089   0.37685
  0.29370   0.61866   0.69384
  0.76691   0.78503   0.43697
  0.22918   0.21779   0.43782
  0.20123   0.18536   0.37171
  0.14214   0.19048   0.30870
  0.11185   0.15995   0.25310
  0.23045   0.14926   0.37385
  0.23445   0.78398   0.56296
  0.10562   0.09143   0.20278
  0.13962   0.12366   0.26136
  0.19945   0.11843   0.32080
  0.79408   0.81744   0.36906
  0.20810   0.81661   0.63173
  0.14485   0.81264   0.68142
  0.11521   0.84271   0.74082
  0.24178   0.85106   0.64612
  0.11286   0.90966   0.80767
  0.23338   0.21708   0.56335
  0.14763   0.87770   0.74843
  0.21128   0.88175   0.70177
  0.76205   0.85260   0.36016
  0.72888   0.28208   0.56579
  0.14349   0.18804   0.68170
  0.70123   0.31498   0.63204
  0.63280   0.31566   0.65186
  0.60305   0.34710   0.70349
  0.88915   0.90981   0.19068
  0.73917   0.34651   0.66531
  0.73115   0.71859   0.43336
```

```
0.60703   0.41187   0.78919
0.64064   0.37938   0.72953
0.70876   0.37917   0.70917
0.85447   0.87802   0.25047
0.77451   0.21799   0.56327
0.92017   0.55074   0.08144
0.95469   0.59638  -0.07818
0.94270   0.52770   0.87497
0.11400   0.15760   0.73958
0.80384   0.18590   0.62831
0.86148   0.19134   0.69527
0.89164   0.16077   0.75085
0.77590   0.14948   0.62178
0.70688   0.68616   0.36132
0.89827   0.09203   0.79873
0.86498   0.12429   0.73910
0.80660   0.11872   0.67539
0.24074   0.15006   0.64509
0.11256   0.09041   0.80533
0.14661   0.12265   0.74587
0.21032   0.11906   0.69908
0.72736   0.71861   0.55909
0.70103   0.68606   0.62686
0.26971   0.71737   0.56464
0.64355   0.68898   0.31191
0.64854   0.69198   0.70678
0.61996   0.66173   0.76713
0.72511   0.64903   0.61174
0.60932   0.59239   0.80752
0.64234   0.62469   0.74664
0.69498   0.61860   0.66849
0.76409   0.78497   0.56264
0.78979   0.81707   0.63399
0.84713   0.81098   0.70132
0.87693   0.84068   0.76211
0.61604   0.65862   0.25089
0.29492   0.68501   0.63492
0.76143   0.85338   0.63376
0.88663   0.90909   0.81290
0.75836   0.54313   0.74889
0.85053   0.87732   0.75520
0.91499   0.56046  -0.05071
0.84237   0.56712  -0.08578
0.80712   0.59874  -0.02039
0.79204   0.88340   0.69220
0.82264   0.43802  -0.01175
0.85550   0.81256   0.31301
0.85032   0.41841   0.87890
0.27356   0.28252   0.56176
0.87739   0.45275   0.06815
0.30098   0.31488   0.62864
0.35751   0.30927   0.69856
0.38721   0.33968   0.75580
0.27343   0.35136   0.62156
0.39503   0.40850   0.80182
0.35214   0.69031   0.70333
0.36130   0.37629   0.74266
0.74298   0.65266   0.34343
0.26969   0.28319   0.43616
0.30375   0.38201   0.67670
0.76575   0.21609   0.43847
0.79329   0.18369   0.36968
0.85856   0.18671   0.32864
0.29761   0.31559   0.36791
0.88864   0.15649   0.27055
0.75838   0.14998   0.34913
0.88927   0.09010   0.19655
0.38012   0.66022   0.76496
0.61673   0.59173   0.18281
0.85476   0.12218   0.25644
0.78943   0.11906   0.29570
0.36249   0.31208   0.32521
0.26746   0.71667   0.43884
0.29318   0.68406   0.36941
0.35441   0.68862   0.31243
0.38357   0.65857   0.25225
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0.38786   0.59099   0.19168
0.35274   0.62303   0.25014
0.79921   0.48065   0.74630
0.79287   0.34599   0.65137
0.55002   0.34743   0.72346
0.60304   0.29103   0.62557
0.74093   0.59456   0.27877
0.23630   0.90922   0.71042
0.29245   0.85386   0.61250
0.06599   0.83999   0.78077
0.11872   0.78556   0.67108
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0.79387   0.65086   0.37632
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0.22753   0.35550   0.57196
0.43139   0.33597   0.81081
0.56671   0.66046   0.21138
0.37881   0.28070   0.70478
0.73354   0.24630   0.28242
0.61555   0.71537   0.32398
0.77138   0.91214   0.68849
0.71499   0.85816   0.58635
0.92208   0.83640   0.81405
0.86915   0.78252   0.70260
0.24804   0.74915   0.28050
0.71071   0.58937   0.65132
0.76762   0.64415   0.55357
0.57883   0.66590   0.82941
0.62919   0.72083   0.71864
0.23557   0.09160   0.70529
0.29130   0.14749   0.61083
0.06468   0.15997   0.77937
0.11708   0.21507   0.67235
0.69454   0.40920   0.36364
0.75316   0.35437   0.45743
0.57071   0.33201   0.17007
0.62322   0.27657   0.27577
0.22630   0.91106   0.31985
0.28008   0.85648   0.42369
0.07897   0.83597   0.17830
0.12952   0.78136   0.28985
0.26680   0.59060   0.30034
0.21143   0.64567   0.39961
0.43141   0.66167   0.20743
0.37955   0.71615   0.31820
0.74233   0.75158   0.71829
0.76333   0.09204   0.28414
0.70672   0.14773   0.37802
0.93931   0.15857   0.23652
0.88584   0.21316   0.34410
0.25755   0.24926   0.72041
0.22108   0.08991   0.32388
0.27818   0.14552   0.41795
0.06576   0.16335   0.20322
0.11946   0.21877   0.30646
0.71667   0.51602   0.16519
0.57479   0.49843   0.57466
0.28721   0.52229   0.86164
0.41955   0.49819   0.41949
0.50979   0.49863   0.35719
0.57724   0.46983   0.36160
0.49698   0.50087   0.64427
0.41890   0.47328   0.63447
0.36272   0.44476   0.00131
0.50175   0.55377   0.25482
0.50030   0.55513   0.74892
0.64716   0.44791   0.99559
0.30498   0.50095   0.01452
0.29640   0.52652   0.14125
0.08051   0.02479   0.37914
0.21772   0.02174   0.86367
0.19756   0.99894   0.00467
0.99602   0.00198   0.35609
0.78417   0.02145   0.13534
0.80480   0.99937   0.99527
0.92231   0.02541   0.62077
0.00631   0.00226   0.64358
0.13891   0.05521   0.00751
0.86370   0.05545   0.99349
0.00126   0.94452   0.24991
0.00055   0.94483   0.74902
0.21122   0.97548   0.14002
0.92202   0.99056   0.41866
0.79109   0.97668   0.85727
0.08026   0.99032   0.58166
0.27067   0.40820   0.28817
0.21230   0.35237   0.37908
0.44376   0.33985   0.23352
0.38881   0.28518   0.33830
0.76236   0.25208   0.72156
0.76883   0.91095   0.29796
0.71254   0.85600   0.39834
0.93316   0.83922   0.20867
0.88030   0.78495   0.31941
0.25430   0.75159   0.72127
0.27179   0.59022   0.69020
0.21870   0.64500   0.58589
0.42520   0.66382   0.81759
0.37549   0.71842   0.70480
0.75292   0.75204   0.27771
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0.72926   0.14557    0.57423
0.93671   0.16426    0.80357
0.88324   0.21982    0.70052
0.24485   0.25113    0.27919
0.73765   0.40462    0.73030
0.72534   0.53303    0.67757
0.73396   0.56702    0.79488
0.80582   0.55231    0.71011
0.84077   0.57248    0.81684
0.83102   0.62630   -0.03829
0.80795   0.59364    0.07672
0.75517   0.60078   -0.04921
0.79393   0.41648    0.03966
0.71097   0.47181    0.12096
0.81065   0.40572    0.82497
0.87744   0.43910    0.82296
0.88474   0.39556   -0.09492
0.90351   0.42882    0.11073
0.91386   0.46899    0.01540
0.85740   0.47130    0.13891
0.93825   0.53362    0.77841
0.99574   0.52374    0.89426
0.91736   0.50069    0.89468
0.90893   0.57539    0.13883
0.97080   0.54123    0.10280
0.88570   0.52768    0.10485
0.94978   0.60510   -0.17244
0.93966   0.62045   -0.02122
0.00761   0.59093   -0.06130
0.43953   0.40004    0.12400
0.93876   0.10120    0.88042
0.36767   0.55806    0.79451
0.56510   0.60152    0.88304
0.13111   0.05659    0.78142
0.06698   0.09966    0.87803
0.62645   0.55866    0.78027
0.43666   0.39938    0.88164
0.86981   0.94313    0.78823
0.93359   0.90012    0.11609
0.37980   0.44318    0.22931
0.93365   0.89956    0.88186
0.38040   0.44228    0.77077
0.43579   0.60035    0.12427
0.87036   0.05625    0.21905
0.93528   0.09961    0.12522
0.36950   0.55705    0.21376
0.87369   0.94375    0.21870
0.56652   0.39709    0.10676
0.13179   0.94249    0.21106
0.06775   0.89933    0.11588
0.61121   0.43912    0.23642
0.19331  -0.00049    0.11049
0.94158   0.00258    0.34846
0.69338   0.49174    0.16634
0.44431   0.50284    0.34627
0.80728   0.99910    0.10505
0.06407   0.00046    0.34886
0.30889   0.50102    0.11404
0.56524   0.49676    0.35122
0.80932   0.00049    0.88804
0.06078   0.00274    0.65124
0.30800   0.49951    0.89426
0.55337   0.50409    0.65073
0.19476   0.99924    0.89328
0.93836   0.00096    0.65072
0.43286   0.49915    0.65505
0.00181   0.96088    0.17987
0.50269   0.47041    0.13108
0.99923   0.02918    0.13451
0.50453   0.53891    0.18162
0.00027   0.96114    0.81915
0.50092   0.47174    0.86624
0.00330   0.02943    0.86653
0.49812   0.53987    0.82138
0.07445   0.97081   -0.00077
0.60417   0.46215    0.99626
0.90265   0.03920    0.99513
0.42912   0.52912    0.00454
0.92763   0.97094   -0.00003
0.40158   0.46115    0.00102
0.09992   0.03898    0.00572
0.57674   0.53024    0.99751
0.56870   0.60095    0.11597
0.12038   0.05762    0.23355
0.06390   0.10066    0.12308
0.63642   0.55804    0.20416
0.56406   0.40184    0.86559
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S78

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0.12856    0.94358    0.78009
0.06798    0.90000    0.88159
0.62306    0.44575    0.76222
0.43161    0.60110    0.89046
0.88384    0.05831    0.76666
0.69681    0.50139    0.86052
0.80480    0.53246    0.93890
0.77889    0.46733   -0.04863
0.76925    0.50491    0.85074
0.91201   -0.00029    0.15594
0.50081    0.56945    0.00247
0.08783   -0.00007    0.16089
0.59153    0.49986    0.15479
0.00139    0.06907    0.00103
0.50225    0.43126    0.99706
0.41627    0.49929    0.16314
0.41067    0.50066    0.84540
0.91462    0.00036    0.83886
0.09035   -0.00019    0.84364
0.58614    0.50101    0.83943
0.00093    0.93071    0.99891
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POSCAR file for gd_p5_prime

POSCAR file from zrtcpb-gd-ipa-c.res: C: 146 F: 1 H: 126 O: 66 P: 1 ZR: 12
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  34.8920000000000
    0.5792995890490465   -0.0000450140396845    0.0007649282407427
   -0.0000781726227076    1.0082675674799713    0.0000166934211398
    0.0004256087542374    0.0000053656439079    0.3214078049098053
146 1 126 66 1 12
Direct
  0.79291    0.88334    0.30188
  0.65046    0.62488    0.24106
  0.26326    0.64927    0.63617
  0.29154    0.61779    0.30907
  0.39813    0.34302    0.27580
  0.23203    0.78318    0.43673
  0.20694    0.81555    0.36643
  0.15270    0.80970    0.29092
  0.12430    0.83984    0.23014
  0.23378    0.85220    0.37469
  0.26588    0.34914    0.34294
  0.11441    0.90876    0.18588
  0.71676    0.62405    0.27510
  0.14918    0.87666    0.24441
  0.38297    0.59169    0.82156
  0.20478    0.88257    0.31561
  0.39946    0.40935    0.20063
  0.72384    0.28140    0.43577
  0.69768    0.31384    0.36820
  0.64504    0.30857    0.28880
  0.61768    0.33938    0.22998
  0.72397    0.35047    0.38332
  0.61073    0.40850    0.18867
  0.88606    0.84302    0.25211
  0.64239    0.37598    0.25005
  0.69615    0.38142    0.32591
  0.34966    0.62383    0.76047
  0.36435    0.37720    0.25877
  0.29800    0.38018    0.29210
  0.74204    0.24809    0.37615
  0.24914    0.74945    0.37834
  0.25629    0.24981    0.62157
  0.74261    0.75294    0.61936
  0.25252    0.75118    0.62371
  0.20690    0.18498    0.63104
  0.75602    0.25212    0.62171
  0.75172    0.75224    0.37420
  0.24858    0.25111    0.37554
  0.29134    0.61877    0.69613
  0.76780    0.78551    0.43567
  0.22977    0.21818    0.43673
  0.20165    0.18574    0.37094
  0.14386    0.19108    0.30430
  0.11352    0.16052    0.24889
  0.22956    0.14932    0.37687
  0.23384    0.78396    0.56251
  0.10582    0.09176    0.20234
  0.13991    0.12398    0.26080
  0.19853    0.11850    0.32389
  0.79512    0.81782    0.36789
  0.20747    0.81666    0.63094
  0.14325    0.81334    0.67691
  0.11398    0.84348    0.73650
  0.24236    0.85053    0.64907
  0.11331    0.90999    0.80710
  0.23383    0.21752    0.56230
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0.14773	0.87795	0.74770
0.21224	0.88138	0.70456
0.76274	0.85289	0.35893
0.73013	0.28326	0.56105
0.14247	0.18800	0.67621
0.70174	0.31633	0.62541
0.63315	0.31681	0.64363
0.60287	0.34789	0.69653
0.88933	0.91028	0.18936
0.73924	0.34781	0.66061
0.73029	0.71949	0.43236
0.60645	0.41232	0.78568
0.64022	0.38001	0.72546
0.70844	0.38009	0.70629
0.85495	0.87847	0.24939
0.77448	0.21881	0.56198
0.92284	0.57669	-0.18163
0.93963	0.54707	0.61883
0.95155	0.50761	0.80072
0.11302	0.15754	0.73414
0.80307	0.18667	0.62809
0.85875	0.19236	0.70011
0.88910	0.16180	0.75555
0.77707	0.14987	0.61695
0.70570	0.68699	0.36087
0.89842	0.09272	0.79776
0.86463	0.12500	0.73895
0.80795	0.11915	0.67055
0.24174	0.15103	0.64799
0.11298	0.09079	0.80443
0.14677	0.12304	0.74449
0.21141	0.11994	0.70168
0.72501	0.71989	0.55792
0.69778	0.68762	0.62525
0.26918	0.71739	0.56534
0.63956	0.68778	0.32461
0.64851	0.69431	0.71110
0.61936	0.66431	0.77171
0.71841	0.65017	0.60439
0.60511	0.59487	0.80677
0.63838	0.62700	0.74601
0.68815	0.62010	0.66245
0.76382	0.78580	0.56131
0.78972	0.81784	0.63259
0.84666	0.81149	0.70081
0.87669	0.84112	0.76158
0.61258	0.65736	0.26320
0.29391	0.68500	0.63614
0.76185	0.85428	0.63174
0.88712	0.90959	0.81160
0.80058	0.44773	0.77112
0.85084	0.87789	0.75392
0.91315	0.54056	0.74507
0.83967	0.52916	0.73603
0.79328	0.55973	0.69099
0.79264	0.88420	0.69028
0.85454	0.46804	0.08948
0.85659	0.81302	0.31198
0.88440	0.43097	1.04575
0.27523	0.28270	0.56039
0.90524	0.49978	0.08397
0.30235	0.31516	0.62717
0.35745	0.30952	0.70066
0.38677	0.34001	0.75814
0.27570	0.35180	0.61673
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0.27175	0.28327	0.43475
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0.76741	0.21685	0.43687
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0.86185	0.18578	0.33683
0.30048	0.31558	0.36700
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0.75831	0.15167	0.34160
0.88937	0.09027	0.19580
0.37874	0.65985	0.76620
0.61718	0.59237	0.18152
0.85546	0.12231	0.25668
0.78876	0.12049	0.28854
0.36679	0.31277	0.33167
0.26752	0.71660	0.43956
0.29358	0.68374	0.37167
0.35538	0.68792	0.31642
0.38484	0.65755	0.25841
0.26111	0.64869	0.36364

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0.38897   0.59002   0.19842
0.35386   0.62202   0.25707
0.71686   0.44668   0.90534
0.79304   0.34746   0.64794
0.54967   0.34798   0.71520
0.60368   0.29225   0.61570
0.74618   0.59851   0.25757
0.23827   0.90844   0.71585
0.29366   0.85275   0.61821
0.06406   0.84120   0.77385
0.11617   0.78669   0.66373
0.79700   0.65509   0.35646
0.28578   0.41133   0.66370
0.23097   0.35604   0.56385
0.43002   0.33628   0.81547
0.56117   0.65773   0.23291
0.37807   0.28085   0.70948
0.73857   0.24713   0.27866
0.60916   0.71260   0.34652
0.77237   0.91303   0.68622
0.71558   0.85919   0.58394
0.92158   0.83667   0.81410
0.86823   0.78293   0.70270
0.24878   0.74892   0.28057
0.70187   0.59065   0.64317
0.75840   0.64466   0.54114
0.58058   0.66893   0.83841
0.63207   0.72353   0.72737
0.23754   0.09284   0.71088
0.29300   0.14890   0.61688
0.06294   0.15958   0.77090
0.11529   0.21464   0.66378
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0.76675   0.35442   0.44139
0.57614   0.33608   0.16844
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0.27790   0.85686   0.42883
0.08137   0.83577   0.17229
0.13173   0.78108   0.28340
0.26727   0.58997   0.30643
0.21142   0.64561   0.40130
0.43289   0.66044   0.21419
0.38065   0.71543   0.32161
0.74035   0.75286   0.71706
0.76095   0.09437   0.27097
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0.94337   0.15658   0.25055
0.89055   0.21127   0.35838
0.25816   0.24971   0.71927
0.21926   0.08981   0.32974
0.27636   0.14534   0.42382
0.06841   0.16411   0.19633
0.12215   0.21957   0.29903
0.71472   0.52634   0.13334
0.57443   0.50132   0.56995
0.28811   0.52285   0.86836
0.42952   0.50165   0.43058
0.50463   0.49865   0.35730
0.58862   0.47290   0.36333
0.49845   0.50158   0.64103
0.41727   0.47371   0.63330
0.36417   0.44479   0.00347
0.50441   0.55410   0.25469
0.49771   0.55632   0.74870
0.64826   0.45103   0.98107
0.30618   0.50057   0.00851
0.29448   0.52421   0.14700
0.08020   0.02513   0.37863
0.21849   0.02186   0.86372
0.19783   0.99915   0.00553
0.99566   0.00230   0.35528
0.78414   0.02162   0.13296
0.80511   0.99979   0.99333
0.92331   0.02607   0.61981
0.00718   0.00270   0.64271
0.13925   0.05554   0.00713
0.86405   0.05591   0.99187
0.00130   0.94493   0.24909
0.00133   0.94532   0.74797
0.21094   0.97549   0.14009
0.92158   0.99105   0.41754
0.79153   0.97736   0.85430
0.08114   0.99068   0.58116
0.27203   0.40708   0.27710
0.21341   0.35117   0.36680
0.44963   0.34097   0.24607
0.39389   0.28644   0.34991
```

```
0.75973   0.25312   0.71917
0.76901   0.91121   0.29639
0.71314   0.85607   0.39685
0.93412   0.83993   0.20800
0.88157   0.78547   0.31845
0.25317   0.75174   0.72146
0.26878   0.59049   0.69300
0.21668   0.64548   0.58835
0.42399   0.66322   0.81848
0.37541   0.71794   0.70481
0.75502   0.75221   0.27661
0.78869   0.09022   0.66107
0.73197   0.14555   0.56514
0.93280   0.16560   0.81170
0.87908   0.22109   0.70924
0.24653   0.25126   0.27785
0.73701   0.40559   0.72854
0.77434   0.42084   0.78811
0.78843   0.45673   0.67974
0.85417   0.44254   0.77961
0.83798   0.50454   0.67512
0.80796   0.57003   0.60197
0.79285   0.58425   -0.24762
0.74245   0.54853   0.68452
0.84044   0.46396   0.18432
0.72447   0.48518   0.06206
0.84877   0.40738   1.04940
0.90318   0.43345   0.95372
0.92654   0.42383   1.10403
0.94713   0.49273   0.14294
0.92457   0.50314   -0.00735
0.88404   0.52707   0.11360
0.94532   0.48132   0.74791
0.00488   0.51424   0.80360
0.93475   0.50164   0.89238
0.90173   0.60175   -0.22701
0.97613   0.58214   -0.16871
0.89966   0.57431   -0.09295
0.93214   0.52181   0.56189
0.91583   0.57163   0.57517
-0.00672  0.55282   0.62220
0.44322   0.40006   0.12437
0.93891   0.10177   0.87974
0.36550   0.55779   0.79649
0.56194   0.60376   0.88497
0.13174   0.05697   0.78110
0.06737   0.10005   0.87707
0.62108   0.56136   0.77654
0.43697   0.39978   0.88152
0.87054   0.94364   0.78659
0.93377   0.90061   0.11478
0.38314   0.44311   0.22920
0.93398   0.89999   0.88079
0.38035   0.44272   0.77141
0.43508   0.59972   0.12761
0.86996   0.05641   0.21700
0.93558   0.09978   0.12491
0.37229   0.55588   0.22279
0.87368   0.94421   0.21710
0.57104   0.39966   0.10570
0.13166   0.94271   0.21115
0.06787   0.89962   0.11534
0.62493   0.44213   0.22204
0.19344   0.99964   0.11060
0.94134   0.00292   0.34727
0.70075   0.49969   0.13325
0.45015   0.50050   0.35174
0.80738   0.99935   0.10241
0.06384   0.00078   0.34837
0.31144   0.50013   0.11596
0.57210   0.49831   0.34332
0.80992   0.00105   0.88555
0.06158   0.00307   0.65070
0.30801   0.49951   0.89904
0.55284   0.50519   0.64698
0.19510   0.99951   0.89336
0.93913   0.00154   0.64952
0.43136   0.49963   0.65300
0.00182   0.96126   0.17900
0.50477   0.47095   0.12974
0.99933   0.02954   0.13348
0.50512   0.53895   0.18196
0.00087   0.96157   0.81824
0.50141   0.47240   0.86548
0.00389   0.02986   0.86575
0.49643   0.54075   0.82055
0.07477   0.97118   0.99875
0.60525   0.46354   -0.00787
```

```
0.90296   0.03963   0.99362
0.42889   0.52912   0.00544
0.92802   0.97138  -0.00146
0.40300   0.46120   0.00159
0.10023   0.03934   0.00531
0.57549   0.53126  -0.00408
0.56771   0.60142   0.11814
0.12030   0.05792   0.23337
0.06422   0.10094   0.12235
0.63822   0.55870   0.19949
0.56462   0.40206   0.86442
0.12923   0.94389   0.77986
0.06832   0.90037   0.88090
0.62128   0.44619   0.75801
0.42841   0.60095   0.89402
0.88460   0.05898   0.76496
0.70879   0.50773   0.84706
0.81614   0.51766   0.85284
0.79183   0.47833   1.03539
0.76711   0.48188   0.87987
0.91206   0.00010   0.15443
0.50004   0.57010   0.00264
0.08786   0.00029   0.16062
0.59156   0.50057   0.15292
0.00165   0.06958   0.00008
0.50398   0.43163   0.99458
0.41684   0.49941   0.16169
0.41181   0.50064   0.84442
0.91514   0.00091   0.83732
0.09098   0.00022   0.84322
0.58775   0.50289   0.83586
0.00131   0.93110   0.99807
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POSCAR file for gd_product

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POSCAR file from zrtcpb-gd-ipa-c.res: C: 146 F: 1 H: 126 O: 66 P: 1 ZR: 12
  34.8920000000000
    0.5792995890490465  -0.0000450140396845   0.0007649282407427
   -0.0000781726227076   1.0082675674799713   0.0000166934211398
    0.0004256087542374   0.0000053656439079   0.3214078049098053
146 1 126 66 1 12
Direct
  0.79297   0.88394   0.30048
  0.64648   0.62649   0.24419
  0.26460   0.64925   0.63616
  0.29169   0.61759   0.30786
  0.40070   0.34367   0.27711
  0.23225   0.78304   0.43504
  0.20727   0.81548   0.36490
  0.15396   0.80962   0.28732
  0.12568   0.83983   0.22666
  0.23335   0.85225   0.37547
  0.26677   0.34765   0.33482
  0.11505   0.90886   0.18461
  0.71489   0.62871   0.25898
  0.14977   0.87673   0.24308
  0.38759   0.59201   0.81538
  0.20448   0.88268   0.31643
  0.39883   0.40907   0.19371
  0.71903   0.27934   0.43139
  0.69464   0.31206   0.36300
  0.64506   0.30718   0.27745
  0.61850   0.33844   0.21977
  0.71945   0.34868   0.38496
  0.60933   0.40781   0.18811
  0.88684   0.84365   0.25508
  0.64110   0.37499   0.24705
  0.69248   0.38004   0.32843
  0.35329   0.62403   0.75565
  0.36499   0.37681   0.25374
  0.29788   0.37877   0.28264
  0.73983   0.24642   0.37282
  0.25008   0.74947   0.37650
  0.25790   0.25008   0.62044
  0.74225   0.75353   0.62025
  0.25223   0.75088   0.62198
  0.20689   0.18548   0.63031
  0.75005   0.25079   0.61924
  0.74972   0.75353   0.37459
  0.25023   0.25089   0.37438
  0.29389   0.61881   0.69465
  0.76700   0.78647   0.43665
  0.23025   0.21835   0.43625
  0.20184   0.18585   0.37109
  0.14624   0.19147   0.29898
  0.11600   0.16093   0.24327
  0.22767   0.14909   0.38261
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0.23337   0.78365   0.56081
0.10652   0.09195   0.20110
0.14035   0.12415   0.26017
0.19678   0.11834   0.32909
0.79500   0.81870   0.36914
0.20675   0.81638   0.62891
0.14154   0.81376   0.67048
0.11246   0.84399   0.72996
0.24267   0.84966   0.65078
0.11352   0.90998   0.80543
0.23433   0.21794   0.56169
0.14746   0.87788   0.74529
0.21283   0.88065   0.70605
0.76246   0.85363   0.35776
0.72281   0.28121   0.55688
0.14032   0.18688   0.66467
0.69427   0.31449   0.61904
0.62580   0.32065   0.61433
0.59795   0.35278   0.66565
0.88993   0.91062   0.18907
0.73418   0.34125   0.67628
0.72747   0.72096   0.43269
0.60764   0.41323   0.78031
0.63866   0.38033   0.71739
0.70685   0.37442   0.72240
0.85547   0.87900   0.24984
0.77166   0.21795   0.56057
0.92594   0.56629   0.97039
0.93023   0.58390   0.75452
0.94740   0.51689   0.81631
0.11112   0.15630   0.72233
0.80106   0.18621   0.62751
0.85428   0.19267   0.70467
0.88559   0.16243   0.76019
0.77822   0.14890   0.61151
0.70160   0.68872   0.36195
0.89918   0.09317   0.79709
0.86441   0.12520   0.73888
0.80993   0.11857   0.66554
0.24383   0.15294   0.65673
0.11393   0.09078   0.80270
0.14738   0.12312   0.74238
0.21392   0.12154   0.70948
0.72347   0.72082   0.55827
0.69778   0.68792   0.62493
0.26961   0.71725   0.56343
0.63312   0.68638   0.34569
0.65127   0.69385   0.71609
0.62414   0.66332   0.77708
0.71772   0.65062   0.59876
0.61137   0.59399   0.81053
0.64283   0.62621   0.74753
0.69008   0.61999   0.65856
0.76350   0.78644   0.56230
0.78961   0.81834   0.63365
0.84594   0.81184   0.70336
0.87607   0.84147   0.76386
0.60588   0.65599   0.28462
0.29522   0.68498   0.63390
0.76232   0.85492   0.63122
0.88746   0.91001   0.81139
0.80077   0.46008   0.76231
0.85088   0.87836   0.75449
0.90937   0.55339   0.84384
0.83420   0.54571   0.83195
0.79032   0.57948   0.85973
0.79319   0.84483   0.68955
0.78270   0.42217   0.06505
0.85707   0.81386   0.31552
0.82078   0.40003   -0.02786
0.27771   0.28265   0.55860
0.82536   0.43251   0.17110
0.30530   0.31529   0.62417
0.35984   0.30980   0.69897
0.38949   0.34048   0.75498
0.27958   0.35203   0.61062
0.39906   0.40954   0.79463
0.35379   0.69015   0.69853
0.36532   0.37723   0.73609
0.74239   0.66033   0.31450
0.27425   0.28294   0.43309
0.30970   0.38290   0.66491
0.76623   0.21582   0.43530
0.79566   0.18345   0.36951
0.86406   0.18351   0.34981
0.30298   0.31514   0.36473
0.89423   0.15342   0.29134
0.75798   0.15263   0.32982
```

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0.38229   0.66010   0.75968
0.61358   0.59388   0.18541
0.85676   0.12190   0.25727
0.78862   0.12145   0.27733
0.37018   0.31343   0.33454
0.26845   0.71657   0.43763
0.29424   0.68369   0.36945
0.35506   0.68796   0.31071
0.38382   0.65755   0.25154
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0.38753   0.58985   0.19260
0.35309   0.62192   0.25235
0.67022   0.42593   1.01456
0.78775   0.33654   0.68069
0.54419   0.35673   0.66635
0.59430   0.29962   0.57007
0.74644   0.60566   0.22593
0.23977   0.90727   0.72027
0.29455   0.85133   0.62292
0.06179   0.84220   0.76415
0.11355   0.78762   0.65413
0.79614   0.66254   0.32548
0.29067   0.41181   0.65342
0.23546   0.35624   0.55605
0.43237   0.33681   0.81327
0.55253   0.65413   0.26901
0.37980   0.28106   0.71025
0.73844   0.24538   0.27515
0.60139   0.70878   0.38242
0.77351   0.91377   0.68419
0.71651   0.85992   0.58209
0.92054   0.83696   0.81744
0.86696   0.78315   0.70645
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0.70440   0.59074   0.63748
0.75521   0.64571   0.53004
0.58730   0.66739   0.84762
0.63533   0.72292   0.73648
0.24199   0.09545   0.72579
0.29639   0.15202   0.63291
0.05939   0.15723   0.75128
0.11134   0.21236   0.64435
0.71009   0.40888   0.34692
0.75969   0.35233   0.44894
0.57900   0.33550   0.15386
0.62597   0.27857   0.25980
0.22338   0.91162   0.32773
0.27667   0.85699   0.43160
0.08346   0.83572   0.16715
0.13357   0.78091   0.27798
0.26757   0.58971   0.30676
0.21292   0.64536   0.40393
0.43108   0.66055   0.20459
0.38016   0.71555   0.31400
0.74101   0.75320   0.71801
0.75984   0.09651   0.25062
0.70431   0.15275   0.34386
0.94737   0.15351   0.27235
0.89346   0.20767   0.38111
0.25972   0.25013   0.71815
0.21595   0.08941   0.33909
0.27262   0.14473   0.43476
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0.58474   0.47253   0.36529
0.50668   0.50342   0.64083
0.42447   0.47508   0.62585
0.36557   0.44486   0.99456
0.50219   0.55373   0.25397
0.50412   0.55694   0.74872
0.64768   0.44807   0.98075
0.30720   0.50082   0.99180
0.29226   0.52321   0.13892
0.08124   0.02529   0.37726
0.21943   0.02164   0.86248
0.19865   0.99917   0.00459
0.99656   0.00249   0.35426
0.78462   0.02158   0.13148
0.80593   0.00026   0.99277
0.92436   0.02638   0.61877
0.00804   0.00289   0.64168
0.14020   0.05559   0.00595
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0.21379	0.34879	0.35555
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0.75220	0.25197	0.71686
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0.71250	0.85687	0.39413
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0.88215	0.78639	0.32384
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0.21717	0.64538	0.59110
0.42831	0.66364	0.80970
0.37767	0.71812	0.69769
0.75245	0.75366	0.27695
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0.73513	0.14386	0.55496
0.92754	0.16684	0.82010
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0.83377	0.48057	0.71810
0.82523	0.53655	0.73819
0.79987	0.60357	0.79928
0.79796	0.58902	0.95237
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0.86554	0.41568	0.94387
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0.84511	0.40664	0.21360
0.86722	0.45039	0.14174
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0.93828	0.50719	0.72402
0.00114	0.52164	0.82570
0.93288	0.49385	0.87774
0.90431	0.59436	0.99069
0.98006	0.56863	0.98144
0.90703	0.54571	0.03646
0.91723	0.57561	0.66241
0.90678	0.61154	0.77372
0.98437	0.58801	0.75781
0.44270	0.39985	0.11760
0.93952	0.10226	0.87939
0.37036	0.55803	0.79054
0.56733	0.60271	0.88736
0.13311	0.05702	0.78016
0.06814	0.10010	0.87479
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0.87122	0.94408	0.78587
0.93433	0.90083	0.11450
0.38128	0.44269	0.22082
0.93436	0.90038	0.88055
0.38456	0.44338	0.76355
0.43302	0.59944	0.12046
0.87085	0.05624	0.21528
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0.87437	0.94463	0.21614
0.57060	0.39944	0.10302
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0.62195	0.44127	0.22490
0.19424	0.99976	0.10968
0.94239	0.00317	0.34622
0.69824	0.50202	0.18179
0.44562	0.49922	0.34854
0.80813	0.99950	0.10025
0.06493	0.00091	0.34723
0.31148	0.49989	0.10662
0.56785	0.49784	0.34479
0.81095	0.00187	0.88357
0.06248	0.00323	0.64980
0.31028	0.50035	0.88878
0.55997	0.50765	0.64864
0.19587	0.99942	0.89254
0.94006	0.00180	0.64834

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0.43771   0.50081   0.64930
0.00264   0.96144   0.17796
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0.50323   0.53881   0.18078
0.00164   0.96175   0.81717
0.50539   0.47316   0.86427
0.00489   0.03003   0.86467
0.50189   0.54094   0.81961
0.07551   0.97126   0.99768
0.60738   0.46358   0.99556
0.90395   0.03990   0.99238
0.43038   0.52920   0.00037
0.92884   0.97163   0.99736
0.40424   0.46140   0.99414
0.10112   0.03944   0.00410
0.57726   0.53104   0.99969
0.56444   0.60264   0.12079
0.12074   0.05812   0.23244
0.06541   0.10112   0.12035
0.63387   0.56023   0.20564
0.56845   0.40300   0.86317
0.12980   0.94386   0.77865
0.06861   0.90037   0.87937
0.62106   0.44720   0.75103
0.43352   0.60134   0.88670
0.88629   0.05938   0.76347
0.69958   0.50259   0.87046
0.81847   0.51572   0.91254
0.75386   0.45728   0.02123
0.76367   0.48076   0.89464
0.91297   0.00027   0.15319
0.50170   0.57015   0.00108
0.08866   0.00042   0.15947
0.58907   0.50004   0.15680
0.00249   0.06979   0.99867
0.50558   0.43188   0.99199
0.41471   0.49944   0.15610
0.41630   0.50095   0.83826
0.91588   0.00122   0.83598
0.09179   0.00026   0.84224
0.59329   0.50291   0.84017
0.00181   0.93123   0.99715
```

POSCAR files for meoh solvent

POSCAR file for gb_solvent

```
POSCAR file from zrtcpb-gb-meoh-c.res: C: 141 F: 1 H: 116 O: 66 P: 1 ZR: 12
  34.8920000000000
    0.5792995890490465   -0.0000450140396845    0.0007649282407427
   -0.0000781726227076    1.0082675674799713    0.0000166934211398
    0.0004256087542374    0.0000053656439079    0.3214078049098053
141 1 116 66 1 12
Direct
  0.79241   0.88298   0.30290
  0.23283   0.21726   0.56326
  0.73099   0.71857   0.43334
  0.70676   0.68618   0.36127
  0.64528   0.68996   0.30521
  0.61745   0.65966   0.24429
  0.85509   0.81246   0.31282
  0.74089   0.65174   0.34983
  0.61573   0.59195   0.18317
  0.64952   0.62447   0.24179
  0.71167   0.62073   0.29409
  0.88497   0.84232   0.25296
  0.20628   0.18472   0.63220
  0.23449   0.78393   0.56323
  0.20821   0.81656   0.63199
  0.14565   0.81232   0.68428
  0.11602   0.84241   0.74362
  0.24129   0.85127   0.64389
  0.11285   0.90964   0.80754
  0.14773   0.87763   0.74871
  0.21078   0.88193   0.69970
  0.76184   0.85266   0.36010
  0.73065   0.28259   0.56355
  0.14340   0.18844   0.68354
  0.70250   0.31539   0.62969
  0.63451   0.31479   0.65399
  0.60392   0.34578   0.70685
  0.88923   0.90969   0.19058
  0.73920   0.34764   0.66043
```

0.60562	0.41111	0.78904
0.64010	0.37877	0.73020
0.70784	0.37972	0.70631
0.85440	0.87791	0.25031
0.77450	0.21805	0.56255
0.11389	0.15794	0.74114
0.80337	0.18595	0.62825
0.86207	0.19116	0.69236
0.89218	0.16055	0.74785
0.77437	0.14977	0.62459
0.89771	0.09196	0.79834
0.86442	0.12426	0.73881
0.80502	0.11895	0.67804
0.23968	0.15008	0.64305
0.11202	0.09047	0.80462
0.14596	0.12280	0.74533
0.20921	0.11904	0.69677
0.72743	0.71856	0.55926
0.70089	0.68608	0.62709
0.26964	0.71729	0.56499
0.64694	0.69192	0.70391
0.61811	0.66171	0.76407
0.72599	0.64918	0.61484
0.60884	0.59246	0.80755
0.64158	0.62477	0.74616
0.69542	0.61873	0.67071
0.76394	0.78497	0.56273
0.78978	0.81705	0.63391
0.84736	0.81099	0.70061
0.87718	0.84070	0.76132
0.29485	0.68494	0.63519
0.76131	0.85330	0.63392
0.88660	0.90906	0.81265
0.79959	0.54009	0.74860
0.85058	0.87728	0.75484
0.90409	0.51364	0.03526
0.84830	0.54159	0.01735
0.83064	0.56364	0.12834
0.79195	0.88333	0.69224
0.75992	0.40934	0.07813
0.27300	0.28272	0.56101
0.30047	0.31512	0.62769
0.35788	0.30967	0.69541
0.38756	0.34008	0.75266
0.27215	0.35146	0.62275
0.39437	0.40871	0.80148
0.35231	0.69017	0.70304
0.36079	0.37656	0.74172
0.26926	0.28323	0.43533
0.30247	0.38212	0.67783
0.76665	0.21615	0.43755
0.79365	0.18360	0.36903
0.85781	0.18706	0.32298
0.29724	0.31552	0.36683
0.88762	0.15679	0.26481
0.75940	0.14943	0.35290
0.88909	0.08993	0.19573
0.38036	0.66004	0.76434
0.85460	0.12205	0.25531
0.79021	0.11852	0.29900
0.36132	0.31152	0.32076
0.26757	0.71659	0.43910
0.29338	0.68398	0.36982
0.35440	0.68862	0.31216
0.38359	0.65857	0.25197
0.26118	0.64885	0.36171
0.38796	0.59092	0.19187
0.35295	0.62297	0.25049
0.26482	0.64901	0.63477
0.29124	0.61833	0.30453
0.39247	0.34179	0.26470
0.23242	0.78321	0.43733
0.20708	0.81548	0.36708
0.15063	0.80981	0.29681
0.12204	0.83987	0.23604
0.23584	0.85172	0.37002
0.26436	0.35018	0.35218
0.11443	0.90843	0.18580
0.14906	0.87636	0.24489
0.38548	0.59173	0.81864
0.20673	0.88201	0.31073
0.39607	0.40922	0.20029
0.72287	0.28067	0.43843
0.69441	0.31262	0.37241
0.64249	0.30637	0.29188
0.61255	0.33674	0.23496
0.71712	0.34986	0.39112
0.60234	0.40619	0.19633

```
0.63353   0.37382   0.25932
0.68605   0.38029   0.33747
0.35188   0.62387   0.75810
0.36088   0.37701   0.25771
0.29646   0.38109   0.30070
0.74092   0.24747   0.37796
0.24910   0.74950   0.37849
0.25484   0.24970   0.62228
0.74414   0.75177   0.62062
0.25322   0.75105   0.62382
0.75696   0.25138   0.62302
0.75012   0.75187   0.37543
0.24684   0.25086   0.37636
0.29349   0.61859   0.69414
0.76651   0.78507   0.43693
0.22872   0.21783   0.43764
0.20078   0.18540   0.37159
0.14129   0.19045   0.30966
0.11104   0.15992   0.25402
0.23042   0.14940   0.37249
0.10539   0.09147   0.20219
0.13929   0.12372   0.26099
0.19951   0.11858   0.31925
0.79369   0.81745   0.36894
0.81098   0.47135   0.83027
0.79267   0.34802   0.64391
0.55125   0.34516   0.72979
0.60572   0.28952   0.63031
0.73615   0.59299   0.29167
0.23534   0.90960   0.70654
0.29150   0.85430   0.60835
0.06733   0.83950   0.78554
0.11997   0.78502   0.67593
0.79073   0.64917   0.38692
0.28149   0.41077   0.67301
0.22560   0.35545   0.57502
0.43238   0.33648   0.80605
0.56960   0.66223   0.19963
0.37980   0.28123   0.69992
0.73652   0.24657   0.28058
0.61889   0.71707   0.31214
0.77121   0.91206   0.68874
0.71480   0.85804   0.58671
0.92249   0.83648   0.81287
0.86956   0.78257   0.70144
0.24839   0.74907   0.28073
0.71167   0.58953   0.65486
0.76981   0.64440   0.55990
0.57599   0.66585   0.82415
0.62682   0.72068   0.71356
0.23406   0.09143   0.70139
0.28993   0.14736   0.60749
0.06498   0.16043   0.78246
0.11734   0.21563   0.67583
0.70250   0.40956   0.35206
0.75992   0.35458   0.44840
0.57229   0.33267   0.17116
0.62493   0.27729   0.27707
0.22784   0.91062   0.31576
0.28160   0.85607   0.41982
0.07743   0.83604   0.18229
0.12824   0.78146   0.29368
0.26742   0.59039   0.30189
0.21203   0.64543   0.40134
0.43129   0.66173   0.20671
0.37939   0.71621   0.31744
0.74232   0.75158   0.71837
0.76471   0.09120   0.29058
0.70839   0.14689   0.38505
0.93745   0.15912   0.22709
0.88451   0.21390   0.33478
0.25706   0.24959   0.71996
0.22148   0.09014   0.32127
0.27840   0.14574   0.41571
0.06463   0.16323   0.20510
0.11831   0.21865   0.30840
0.71579   0.51748   0.15564
0.57568   0.49651   0.57830
0.28717   0.52263   0.86264
0.41964   0.49831   0.41983
0.51027   0.49825   0.35703
0.57779   0.46955   0.36060
0.49466   0.50074   0.64448
0.42023   0.47263   0.63527
0.36229   0.44475   0.00205
0.50181   0.55359   0.25475
0.50013   0.55491   0.74834
0.64688   0.44795   0.99411
```

```
0.30474   0.50102    0.01564
0.29641   0.52649    0.14243
0.08078   0.02476    0.37827
0.21747   0.02188    0.86303
0.19742   0.99904    0.00305
0.99632   0.00188    0.35556
0.78424   0.02130    0.13514
0.80471   0.99923    0.99545
0.92201   0.02554    0.62087
0.00589   0.00226    0.64311
0.13868   0.05523    0.00652
0.86350   0.05528    0.99310
0.00135   0.94453    0.24971
0.00062   0.94481    0.74851
0.21120   0.97560    0.13922
0.92230   0.99088    0.41895
0.79083   0.97664    0.85697
0.07990   0.99051    0.58067
0.27213   0.40878    0.29273
0.21323   0.35307    0.38332
0.44223   0.33898    0.22699
0.38691   0.28427    0.33116
0.76180   0.25229    0.72032
0.76887   0.91096    0.29754
0.71241   0.85617    0.39847
0.93296   0.83902    0.20876
0.87973   0.78479    0.31923
0.25414   0.75153    0.72157
0.27143   0.59019    0.69091
0.21821   0.64505    0.58719
0.42562   0.66357    0.81651
0.37575   0.71825    0.70429
0.75226   0.75211    0.27773
0.78349   0.09042    0.67448
0.72696   0.14610    0.57937
0.93808   0.16385    0.79830
0.88469   0.21945    0.69530
0.24456   0.25098    0.27869
0.73569   0.40567    0.72599
0.78236   0.53082    0.66015
0.77956   0.56860    0.76733
0.85406   0.54068    0.74949
0.91488   0.49730   -0.04635
0.89144   0.49344    0.10698
0.94938   0.52904    0.06107
0.86028   0.56163   -0.05576
0.87313   0.58090    0.15758
0.81742   0.54391    0.20121
0.78856   0.58283    0.11199
0.72131   0.39154    0.12230
0.71976   0.46268    0.08940
0.79672   0.41972    1.14784
0.78173   0.39129    1.00339
0.43981   0.39992    0.12393
0.93834   0.10113    0.87978
0.36766   0.55789    0.79374
0.56417   0.60163    0.88217
0.13064   0.05668    0.78062
0.06647   0.09967    0.87747
0.62673   0.55877    0.78180
0.43572   0.39951    0.88158
0.86970   0.94308    0.78790
0.93368   0.89997    0.11607
0.38011   0.44297    0.22953
0.93355   0.89954    0.88172
0.37983   0.44254    0.77056
0.43566   0.60028    0.12399
0.87035   0.05608    0.21866
0.93505   0.09941    0.12426
0.36969   0.55698    0.21422
0.87378   0.94362    0.21856
0.56721   0.39738    0.10680
0.13207   0.94234    0.21041
0.06780   0.89917    0.11575
0.61412   0.43958    0.23331
0.19318   0.99961    0.10968
0.94190   0.00244    0.34802
0.69337   0.49310    0.16470
0.44437   0.50267    0.34642
0.80724   0.99892    0.10482
0.06439   0.00038    0.34828
0.30883   0.50101    0.11496
0.56540   0.49639    0.35001
0.80913   0.00040    0.88783
0.06042   0.00266    0.65071
0.30772   0.49973    0.89501
0.55338   0.50448    0.65136
0.19467   0.99932    0.89257
```

```
0.93804   0.00101   0.65026
0.43351   0.49875   0.65417
0.00195   0.96080   0.17948
0.50266   0.47025   0.13115
0.99922   0.02911   0.13404
0.50430   0.53883   0.18132
0.00012   0.96109   0.81871
0.50017   0.47161   0.86631
0.00302   0.02937   0.86583
0.49778   0.53975   0.82100
0.07442   0.97077   -0.00134
0.60384   0.46225   0.99450
0.90247   0.03905   0.99470
0.42892   0.52901   0.00465
0.92755   0.97083   -0.00035
0.40118   0.46111   0.00155
0.09973   0.03898   0.00493
0.57661   0.53025   0.99662
0.56816   0.60116   0.11520
0.12028   0.05768   0.23289
0.06370   0.10070   0.12246
0.63507   0.55827   0.20526
0.56313   0.40112   0.86647
0.12843   0.94355   0.77968
0.06796   0.90000   0.88148
0.62046   0.44495   0.76006
0.43118   0.60091   0.89064
0.88315   0.05826   0.76637
0.69694   0.49942   0.84712
0.78773   0.52151   0.98392
0.72903   0.44133   0.02539
0.76810   0.50765   0.85617
0.91215   -0.00041   0.15554
0.91437   0.00025   0.83853
0.41029   0.50065   0.84613
0.41625   0.49918   0.16359
0.50207   0.43111   -0.00305
0.00114   0.06894   0.00040
0.59120   0.49999   0.15393
0.08790   -0.00011   0.16016
0.50071   0.56940   0.00212
0.09000   -0.00021   0.84304
0.58559   0.50073   0.83769
0.00094   0.93069   -0.00135
```

POSCAR file for gb_p5

POSCAR file from zrtcpb-gb-meoh-c.res: C: 141 F: 1 H: 116 O: 66 P: 1 ZR: 12
```
  34.8920000000000
    0.5792995890490465  -0.0000450140396845   0.0007649282407427
   -0.0000781726227076   1.0082675674799713   0.0000166934211398
    0.0004256087542374   0.0000053656439079   0.3214078049098053
141 1 116 66 1 12
Direct
  0.79262   0.88305   0.30283
  0.23321   0.21729   0.56198
  0.73143   0.71852   0.43318
  0.70687   0.68600   0.36191
  0.64493   0.68971   0.30748
  0.61683   0.65944   0.24682
  0.85533   0.81245   0.31045
  0.74101   0.65159   0.34976
  0.61489   0.59197   0.18393
  0.64918   0.62435   0.24252
  0.71170   0.62066   0.29360
  0.88503   0.84247   0.25105
  0.20656   0.18474   0.63088
  0.23456   0.78429   0.56240
  0.20822   0.81693   0.63114
  0.14539   0.81273   0.68243
  0.11565   0.84274   0.74193
  0.24145   0.85156   0.64430
  0.11272   0.90987   0.80722
  0.14756   0.87790   0.74818
  0.21086   0.88218   0.70019
  0.76227   0.85260   0.35967
  0.72979   0.28343   0.55975
  0.14350   0.18841   0.68156
  0.70168   0.31668   0.62402
  0.63455   0.31544   0.65513
  0.60421   0.34659   0.70778
  0.88910   0.90997   0.19004
  0.73745   0.34998   0.64648
  0.60612   0.41268   0.78536
  0.63947   0.38037   0.72408
  0.70605   0.38214   0.69176
  0.85447   0.87810   0.24960
```

```
0.77280   0.21853   0.56171
0.11400   0.15799   0.73958
0.80165   0.18644   0.62816
0.86006   0.19177   0.69312
0.89068   0.16123   0.74826
0.77358   0.15001   0.62347
0.89752   0.09244   0.79746
0.86384   0.12472   0.73818
0.80475   0.11924   0.67645
0.24016   0.15016   0.64291
0.11227   0.09066   0.80437
0.14628   0.12292   0.74490
0.20973   0.11920   0.69705
0.72716   0.71897   0.55904
0.70013   0.68688   0.62771
0.26908   0.71757   0.56436
0.64597   0.69349   0.70348
0.61617   0.66369   0.76402
0.72532   0.64989   0.61832
0.60540   0.59455   0.80810
0.63955   0.62663   0.74845
0.69461   0.61989   0.67628
0.76393   0.78531   0.56145
0.78979   0.81745   0.63244
0.84716   0.81129   0.69968
0.87700   0.84093   0.76072
0.29369   0.68514   0.63475
0.76145   0.85376   0.63257
0.88661   0.90932   0.81216
0.79436   0.53295   0.76956
0.85060   0.87758   0.75412
0.91843   0.52890   0.01828
0.84883   0.54434   0.00653
0.82664   0.56634   0.11549
0.79209   0.88372   0.69123
0.78082   0.42746   0.02813
0.27346   0.28273   0.55998
0.30059   0.31511   0.62700
0.35729   0.30957   0.69655
0.38689   0.34002   0.75368
0.27262   0.35152   0.62056
0.39446   0.40878   0.80004
0.35107   0.69013   0.70297
0.36060   0.37657   0.74115
0.26987   0.28336   0.43428
0.30277   0.38220   0.67588
0.76637   0.21657   0.43648
0.79372   0.18386   0.36900
0.85835   0.18712   0.32495
0.29812   0.31568   0.36605
0.88829   0.15686   0.26697
0.75925   0.14983   0.35139
0.88923   0.09022   0.19572
0.37844   0.65986   0.76462
0.85490   0.12228   0.25568
0.79014   0.11891   0.29776
0.36270   0.31187   0.32212
0.26670   0.71676   0.43851
0.29223   0.68394   0.36981
0.35374   0.68816   0.31353
0.38290   0.65782   0.25476
0.25960   0.64894   0.36184
0.38674   0.59024   0.19503
0.35182   0.62233   0.25359
0.26306   0.64939   0.63413
0.28970   0.61810   0.30637
0.39391   0.34207   0.26565
0.23214   0.78347   0.43656
0.20682   0.81577   0.36645
0.15084   0.81005   0.29504
0.12227   0.84013   0.23430
0.23516   0.85211   0.37062
0.26498   0.35017   0.34946
0.11417   0.90877   0.18556
0.14879   0.87671   0.24450
0.38259   0.59166   0.81935
0.20603   0.88244   0.31153
0.39690   0.40928   0.19803
0.72412   0.28150   0.43432
0.69760   0.31362   0.36573
0.64394   0.30791   0.28880
0.61550   0.33844   0.23016
0.72403   0.35033   0.37774
0.60701   0.40760   0.18880
0.63988   0.37520   0.24859
0.69482   0.38104   0.32135
0.34937   0.62384   0.75833
0.36192   0.37710   0.25635
```

0.29714	0.38104	0.29776
0.74208	0.24802	0.37534
0.24837	0.74967	0.37773
0.25521	0.24971	0.62116
0.74379	0.75230	0.61988
0.25318	0.75142	0.62315
0.75456	0.25202	0.62086
0.75122	0.75159	0.37465
0.24727	0.25104	0.37517
0.29108	0.61883	0.69382
0.76715	0.78500	0.43562
0.22912	0.21797	0.43637
0.20115	0.18553	0.37040
0.14187	0.19062	0.30790
0.11150	0.16006	0.25262
0.23052	0.14945	0.37218
0.10540	0.09157	0.20195
0.13942	0.12379	0.26053
0.19948	0.11860	0.31934
0.79417	0.81736	0.36749
0.80221	0.46434	0.79838
0.79038	0.35097	0.62530
0.55240	0.34546	0.73631
0.60619	0.28953	0.63724
0.73678	0.59311	0.28986
0.23556	0.90977	0.70786
0.29187	0.85454	0.60974
0.06675	0.83980	0.78301
0.11959	0.78550	0.67317
0.79092	0.64891	0.38648
0.28210	0.41090	0.67004
0.22650	0.35557	0.57152
0.43140	0.33640	0.80789
0.56858	0.66198	0.20356
0.37886	0.28105	0.70221
0.73883	0.24699	0.27781
0.61836	0.71674	0.31542
0.77137	0.91244	0.68783
0.71490	0.85856	0.58554
0.92211	0.83654	0.81266
0.86915	0.78283	0.70084
0.24745	0.74919	0.27997
0.71227	0.59066	0.66629
0.76959	0.64471	0.56480
0.57349	0.66825	0.82255
0.62639	0.72243	0.71141
0.23479	0.09167	0.70252
0.29056	0.14748	0.60802
0.06491	0.16052	0.78019
0.11726	0.21552	0.67306
0.71383	0.40998	0.33248
0.76803	0.35454	0.43249
0.57321	0.33479	0.17050
0.62354	0.27923	0.27863
0.22689	0.91109	0.31754
0.28065	0.85651	0.42120
0.07801	0.83618	0.17972
0.12881	0.78162	0.29082
0.26544	0.59028	0.30385
0.21010	0.64584	0.40029
0.43088	0.66069	0.21026
0.37908	0.71564	0.31867
0.74161	0.75228	0.71761
0.76434	0.09172	0.28805
0.70793	0.14744	0.38200
0.93848	0.15912	0.23082
0.88525	0.21383	0.33800
0.25730	0.24961	0.71886
0.22134	0.09013	0.32203
0.27841	0.14578	0.41573
0.06519	0.16346	0.20347
0.11912	0.21888	0.30584
0.71544	0.52266	0.14616
0.57454	0.50080	0.57096
0.28743	0.52319	0.86503
0.42498	0.50044	0.42849
0.50077	0.49857	0.35716
0.58346	0.47199	0.36397
0.49917	0.50157	0.64108
0.41709	0.47357	0.63269
0.36245	0.44478	0.00014
0.50095	0.55388	0.25479
0.49831	0.55614	0.74825
0.64869	0.45234	0.98287
0.30441	0.50058	0.00305
0.29228	0.52423	0.14335
0.08061	0.02493	0.37840
0.21765	0.02193	0.86291

0.19734	0.99913	0.00381
0.99605	0.00208	0.35564
0.78422	0.02162	0.13488
0.80472	0.99953	0.99490
0.92202	0.02587	0.62056
0.00605	0.00254	0.64277
0.13870	0.05546	0.00636
0.86346	0.05575	0.99249
0.00108	0.94481	0.24948
0.00051	0.94504	0.74827
0.21095	0.97569	0.13933
0.92187	0.99115	0.41864
0.79087	0.97685	0.85669
0.08007	0.99057	0.58087
0.27249	0.40859	0.28827
0.21357	0.35300	0.37920
0.44404	0.33930	0.22946
0.38862	0.28480	0.33428
0.75809	0.25309	0.71836
0.76894	0.91100	0.29813
0.71289	0.85596	0.39835
0.93291	0.83921	0.20644
0.87995	0.78476	0.31585
0.25424	0.75191	0.72090
0.26854	0.59055	0.69043
0.21654	0.64566	0.58610
0.42370	0.66313	0.81695
0.37504	0.71806	0.70410
0.75378	0.75158	0.27696
0.78370	0.09060	0.67174
0.72647	0.14601	0.57748
0.93638	0.16487	0.79911
0.88215	0.22019	0.69712
0.24506	0.25119	0.27748
0.73301	0.40887	0.70424
0.77207	0.52562	0.68307
0.77534	0.56114	0.79554
0.84854	0.53413	0.75851
0.93161	0.51113	0.94078
0.92272	0.51137	0.09949
0.95451	0.55233	0.02445
0.84557	0.56288	0.92749
0.86142	0.58970	0.13466
0.82515	0.54747	0.19426
0.77725	0.57896	0.10211
0.74259	0.41038	0.07494
0.71781	0.48098	0.08082
0.81718	0.43817	1.09810
0.80459	0.40867	0.95720
0.44033	0.40003	0.12112
0.93830	0.10155	0.87882
0.36500	0.55778	0.79423
0.56142	0.60359	0.88474
0.13082	0.05684	0.78057
0.06668	0.09989	0.87710
0.62136	0.56102	0.77827
0.43660	0.39967	0.87897
0.86978	0.94335	0.78750
0.93355	0.90031	0.11543
0.38073	0.44303	0.22712
0.93349	0.89977	0.88134
0.37954	0.44259	0.76948
0.43338	0.59981	0.12515
0.87046	0.05634	0.21829
0.93513	0.09967	0.12405
0.36942	0.55618	0.21883
0.87360	0.94388	0.21807
0.56801	0.39876	0.10470
0.13173	0.94269	0.21022
0.06754	0.89955	0.11541
0.61976	0.44113	0.22449
0.19307	0.99970	0.10957
0.94167	0.00267	0.34784
0.69688	0.49701	0.15010
0.44618	0.50099	0.35011
0.80725	0.99926	0.10445
0.06411	0.00062	0.34813
0.30924	0.50010	0.11258
0.56790	0.49771	0.34527
0.80919	0.00062	0.88749
0.06052	0.00292	0.65051
0.30668	0.49963	0.89554
0.55298	0.50522	0.64776
0.19455	0.99947	0.89244
0.93810	0.00136	0.64997
0.43097	0.49954	0.65219
0.00169	0.96111	0.17932
0.50188	0.47067	0.12930

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0.99908   0.02939   0.13334
0.50213   0.53883   0.18187
0.00007   0.96136   0.81837
0.50086   0.47248   0.86495
0.00305   0.02966   0.86573
0.49625   0.54065   0.82022
0.07428   0.97104   0.99845
0.60405   0.46350   0.99420
0.90234   0.03945   0.99413
0.42754   0.52912   0.00353
0.92753   0.97120   -0.00076
0.40127   0.46120   -0.00113
0.09973   0.03923   0.00472
0.57434   0.53120   0.99759
0.56615   0.60118   0.11879
0.12014   0.05776   0.23270
0.06370   0.10079   0.12223
0.63478   0.55817   0.20368
0.56411   0.40244   0.86378
0.12835   0.94378   0.77955
0.06783   0.90023   0.88115
0.62158   0.44662   0.75904
0.42798   0.60092   0.89186
0.88319   0.05867   0.76564
0.69162   0.50433   0.85875
0.80398   0.51261   0.99414
0.74148   0.45787   0.97649
0.76549   0.49686   0.87628
0.91198   0.99994   0.15528
0.91435   0.00065   0.83804
0.41128   0.50062   0.84252
0.41392   0.49939   0.15961
0.50259   0.43159   0.99357
0.00104   0.06938   -0.00013
0.58797   0.50026   0.15525
0.08767   0.00018   0.16005
0.49892   0.57002   0.00217
0.09011   0.00007   0.84287
0.58752   0.50275   0.83788
0.00080   0.93097   0.99830
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POSCAR file for gb_p5_prime

POSCAR file from zrtcpb-gb-meoh-c.res: C: 141 F: 1 H: 116 O: 66 P: 1 ZR: 12
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  34.8920000000000
    0.5792995890490465  -0.0000450140396845   0.0007649282407427
   -0.0000781726227076   1.0082675674799713   0.0000166934211398
    0.0004256087542374   0.0000053656439079   0.3214078049098053
141 1 116 66 1 12
Direct
  0.79256   0.88312   0.30281
  0.23358   0.21729   0.56195
  0.73117   0.71862   0.43384
  0.70636   0.68612   0.36276
  0.64411   0.68981   0.30948
  0.61591   0.65958   0.24884
  0.85522   0.81252   0.31044
  0.74070   0.65183   0.34940
  0.61407   0.59227   0.18472
  0.64854   0.62460   0.24313
  0.71140   0.62097   0.29287
  0.88488   0.84252   0.25086
  0.20684   0.18476   0.63087
  0.23430   0.78444   0.56221
  0.20805   0.81711   0.63090
  0.14484   0.81309   0.68075
  0.11522   0.84312   0.74040
  0.24176   0.85154   0.64542
  0.11275   0.91007   0.80693
  0.14762   0.87811   0.74795
  0.21126   0.88222   0.70126
  0.76227   0.85269   0.35984
  0.73096   0.28391   0.56008
  0.14340   0.18835   0.68001
  0.70316   0.31707   0.62520
  0.63543   0.31650   0.65180
  0.60544   0.34743   0.70615
  0.88895   0.91002   0.18966
  0.74008   0.34938   0.65478
  0.60755   0.41257   0.78952
  0.64191   0.38034   0.72954
  0.70941   0.38133   0.70328
  0.85434   0.87816   0.24932
  0.77350   0.21895   0.56170
  0.11380   0.15796   0.73801
  0.80182   0.18681   0.62833
  0.85947   0.19218   0.69540
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0.88979   0.16159   0.75076
0.77399   0.15034   0.62206
0.89718   0.09270   0.79761
0.86338   0.12503   0.73888
0.80485   0.11956   0.67541
0.24070   0.15032   0.64424
0.11226   0.09079   0.80417
0.14638   0.12301   0.74469
0.21016   0.11935   0.69826
0.72716   0.71902   0.55966
0.70031   0.68688   0.62851
0.26871   0.71772   0.56463
0.64604   0.69340   0.70404
0.61641   0.66360   0.76484
0.72579   0.64993   0.61973
0.60576   0.59453   0.80958
0.64011   0.62658   0.75003
0.69538   0.61994   0.67829
0.76389   0.78539   0.56169
0.78965   0.81757   0.63262
0.84705   0.81143   0.69978
0.87687   0.84111   0.76068
0.29330   0.68529   0.63508
0.76125   0.85386   0.63266
0.88653   0.90950   0.81175
0.82938   0.46434   0.78698
0.85044   0.87775   0.75397
0.90505   0.55728  -0.15960
0.83608   0.55044  -0.20701
0.79924   0.58684  -0.23522
0.79189   0.88387   0.69115
0.85510   0.48528   0.09456
0.27412   0.28266   0.55998
0.30127   0.31508   0.62673
0.35735   0.30956   0.69787
0.38687   0.34007   0.75478
0.27381   0.35159   0.61845
0.39475   0.40894   0.79953
0.35050   0.69034   0.70372
0.36108   0.37669   0.74055
0.27031   0.28329   0.43435
0.30385   0.38231   0.67363
0.76685   0.21697   0.43652
0.79407   0.18420   0.36910
0.85920   0.18708   0.32725
0.29842   0.31563   0.36608
0.88903   0.15676   0.26937
0.75906   0.15046   0.34965
0.88913   0.09038   0.19571
0.37790   0.66011   0.76539
0.85500   0.12246   0.25611
0.78982   0.11943   0.29629
0.36355   0.31225   0.32463
0.26638   0.71687   0.43882
0.29186   0.68398   0.37040
0.35365   0.68804   0.31502
0.38265   0.65766   0.25632
0.25889   0.64912   0.36182
0.38591   0.59022   0.19545
0.35118   0.62230   0.25439
0.26288   0.64949   0.63412
0.28885   0.61821   0.30648
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0.15134   0.81006   0.29325
0.12284   0.84012   0.23238
0.23454   0.85232   0.37159
0.26440   0.34971   0.34709
0.11408   0.90883   0.18509
0.14883   0.87679   0.24380
0.38251   0.59187   0.81944
0.20551   0.88261   0.31224
0.39605   0.40935   0.19736
0.72478   0.28192   0.43478
0.69809   0.31407   0.36664
0.64463   0.30828   0.28933
0.61588   0.33878   0.23115
0.72411   0.35084   0.37945
0.60655   0.40792   0.19067
0.63994   0.37559   0.24996
0.69481   0.38149   0.32284
0.34910   0.62403   0.75868
0.36144   0.37716   0.25614
0.29620   0.38068   0.29536
0.74253   0.24844   0.37557
0.24815   0.74975   0.37784
0.25579   0.24964   0.62114
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0.74386   0.75239   0.62027
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0.75582   0.25251   0.62094
0.75097   0.75166   0.37516
0.24750   0.25105   0.37522
0.29097   0.61895   0.69379
0.76708   0.78509   0.43590
0.22930   0.21799   0.43640
0.20124   0.18562   0.37032
0.14245   0.19088   0.30648
0.11203   0.16037   0.25104
0.23013   0.14943   0.37318
0.10530   0.09178   0.20159
0.13943   0.12399   0.26004
0.19906   0.11864   0.32009
0.79410   0.81742   0.36762
0.74808   0.44368   0.90088
0.79335   0.34985   0.63628
0.55299   0.34681   0.73065
0.60631   0.29125   0.62911
0.73677   0.59353   0.28770
0.23626   0.90968   0.70992
0.29243   0.85434   0.61183
0.06605   0.84035   0.78053
0.11872   0.78601   0.67032
0.79079   0.64921   0.38539
0.28355   0.41107   0.66631
0.22818   0.35565   0.56799
0.43088   0.33646   0.81029
0.56737   0.66206   0.20666
0.37852   0.28098   0.70510
0.73907   0.24742   0.27808
0.61743   0.71677   0.31831
0.77123   0.91260   0.68768
0.71469   0.85864   0.58562
0.92202   0.83680   0.81256
0.86906   0.78298   0.70088
0.24721   0.74921   0.28007
0.71334   0.59073   0.66880
0.77006   0.64480   0.56611
0.57360   0.66814   0.82305
0.62624   0.72230   0.71164
0.23536   0.09189   0.70469
0.29132   0.14772   0.61030
0.06444   0.16039   0.77758
0.11701   0.21537   0.67034
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0.76781   0.35512   0.43502
0.57367   0.33507   0.17137
0.62460   0.27954   0.27861
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0.07900   0.83615   0.17670
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0.26430   0.59048   0.30342
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0.43078   0.66039   0.21232
0.37927   0.71542   0.32069
0.74170   0.75243   0.71800
0.76358   0.09243   0.28526
0.70743   0.14834   0.37876
0.93958   0.15875   0.23472
0.88653   0.21357   0.34183
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0.06606   0.16383   0.20084
0.12009   0.21924   0.30360
0.71472   0.52314   0.15104
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0.28760   0.52372   0.86420
0.42362   0.50204   0.42928
0.49881   0.49858   0.35824
0.58270   0.47251   0.36621
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0.50000   0.55419   0.25526
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0.30374   0.50075   0.00042
0.29074   0.52399   0.14280
0.08026   0.02504   0.37818
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0.19725   0.99929   0.00357
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0.80460   0.99967   0.99406
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0.21067   0.97582   0.13943
0.92165   0.99127   0.41832
0.79087   0.97704   0.85592
0.08002   0.99070   0.58062
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0.21265   0.35214   0.37526
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0.75955   0.25356   0.71839
0.76895   0.91109   0.29822
0.71297   0.85610   0.39882
0.93273   0.83929   0.20609
0.87985   0.78483   0.31582
0.25398   0.75219   0.72090
0.26859   0.59063   0.69002
0.21648   0.64570   0.58577
0.42300   0.66344   0.81813
0.37429   0.71832   0.70522
0.75349   0.75160   0.27746
0.78412   0.09086   0.66954
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0.93499   0.16516   0.80308
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0.24513   0.25124   0.27755
0.73773   0.40716   0.72254
0.81905   0.43369   0.79274
0.81852   0.47350   0.69510
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0.93553   0.57255  -0.22566
0.83825   0.53250   0.71237
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0.79481   0.60449  -0.15411
0.74930   0.58069  -0.26992
0.85273   0.48583   0.19292
0.71704   0.48152   0.08571
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0.87949   0.45880   1.06562
0.43951   0.40008   0.12050
0.93805   0.10176   0.87895
0.36495   0.55798   0.79438
0.56154   0.60362   0.88568
0.13090   0.05695   0.78060
0.06655   0.10005   0.87661
0.62169   0.56095   0.78005
0.43694   0.39990   0.87839
0.86974   0.94355   0.78700
0.93343   0.90036   0.11504
0.37961   0.44307   0.22603
0.93347   0.89994   0.88085
0.37958   0.44274   0.76917
0.43233   0.59982   0.12514
0.87015   0.05650   0.21779
0.93505   0.09986   0.12410
0.36864   0.55616   0.21939
0.87345   0.94395   0.21765
0.56719   0.39902   0.10726
0.13150   0.94277   0.21003
0.06742   0.89961   0.11494
0.61923   0.44148   0.22617
0.19288   0.99987   0.10978
0.94138   0.00275   0.34739
0.69637   0.49744   0.15421
0.44461   0.50056   0.35081
0.80713   0.99936   0.10377
0.06386   0.00070   0.34791
0.30849   0.50014   0.11152
0.56671   0.49807   0.34655
0.80907   0.00084   0.88678
0.06058   0.00311   0.65027
0.30616   0.49993   0.89437
0.55317   0.50486   0.64874
0.19453   0.99956   0.89270
0.93809   0.00159   0.64959
0.43086   0.49989   0.65226
0.00150   0.96123   0.17880
0.50088   0.47085   0.13029
0.99890   0.02955   0.13309
0.50115   0.53901   0.18261
0.00004   0.96156   0.81809
0.50063   0.47251   0.86535
```

```
0.00296   0.02986   0.86537
0.49618   0.54076   0.82080
0.07420   0.97116   0.99826
0.60309   0.46373   0.99642
0.90230   0.03959   0.99377
0.42705   0.52926   0.00356
0.92737   0.97132   0.99873
0.40072   0.46134   0.99845
0.09954   0.03936   0.00455
0.57390   0.53136   0.99873
0.56519   0.60147   0.11991
0.11988   0.05796   0.23259
0.06366   0.10101   0.12174
0.63390   0.55845   0.20446
0.56477   0.40233   0.86656
0.12840   0.94399   0.77929
0.06779   0.90041   0.88071
0.62242   0.44651   0.76240
0.42806   0.60112   0.89161
0.88298   0.05895   0.76527
0.70424   0.49949   0.84615
0.79837   0.53151   0.88477
0.78903   0.48700   1.05078
0.77243   0.48772   0.89178
0.91179   0.00004   0.15477
0.91429   0.00084   0.83755
0.41122   0.50072   0.84242
0.41279   0.49952   0.15943
0.50219   0.43171   0.99457
0.00091   0.06957   0.99965
0.58687   0.50047   0.15694
0.08752   0.00030   0.15989
0.49844   0.57016   0.00271
0.09002   0.00021   0.84278
0.58718   0.50278   0.83927
0.00067   0.93108   0.99793
```

POSCAR file for gb_product

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POSCAR file from zrtcpb-gb-meoh-c.res: C: 141 F: 1 H: 116 O: 66 P: 1 ZR: 12
    34.8920000000000
     0.5792995890490465   -0.0000450140396845    0.0007649282407427
    -0.0000781726227076    1.0082675674799713    0.0000166934211398
     0.0004256087542374    0.0000053656439079    0.3214078049098053
141 1 116 66 1 12
Direct
    0.79340   0.88444   0.30370
    0.23349   0.21785   0.56214
    0.72854   0.72088   0.42862
    0.70415   0.68903   0.35438
    0.63809   0.69020   0.31805
    0.61060   0.65976   0.25763
    0.85603   0.81379   0.31291
    0.74308   0.65763   0.32336
    0.61353   0.59410   0.18290
    0.64808   0.62706   0.23666
    0.71480   0.62627   0.26791
    0.88568   0.84359   0.25249
    0.20642   0.18537   0.63090
    0.23336   0.78400   0.56173
    0.20708   0.81674   0.63016
    0.14310   0.81334   0.67714
    0.11383   0.84353   0.73653
    0.24176   0.85073   0.64715
    0.11292   0.91019   0.80593
    0.14732   0.87812   0.74661
    0.21163   0.88161   0.70250
    0.76307   0.85420   0.36152
    0.72915   0.28341   0.55957
    0.14204   0.18841   0.67623
    0.70105   0.31668   0.62319
    0.63255   0.31773   0.64227
    0.60307   0.34914   0.69492
    0.88933   0.91076   0.18907
    0.73932   0.34787   0.65792
    0.60904   0.41345   0.78589
    0.64124   0.38095   0.72372
    0.70936   0.38024   0.70448
    0.85502   0.87917   0.25004
    0.77341   0.21895   0.56191
    0.11252   0.15791   0.73382
    0.80179   0.18687   0.62870
    0.85792   0.19256   0.69956
    0.88833   0.16202   0.75496
    0.77534   0.15015   0.61891
    0.89758   0.09298   0.79765
    0.86351   0.12524   0.73938
```

0.80630	0.11944	0.67240
0.24114	0.15136	0.64729
0.11239	0.09107	0.80333
0.14616	0.12336	0.74368
0.21075	0.12024	0.70066
0.72195	0.72060	0.55405
0.69420	0.68804	0.61936
0.26867	0.71740	0.56426
0.64726	0.69437	0.70974
0.61955	0.66416	0.77139
0.71251	0.65051	0.59323
0.60805	0.59468	0.80922
0.63740	0.62686	0.74246
0.68341	0.62023	0.65199
0.76176	0.78635	0.56163
0.78772	0.81810	0.63419
0.84509	0.81169	0.70115
0.87552	0.84128	0.76151
0.29384	0.68502	0.63462
0.75981	0.85453	0.63435
0.88649	0.90975	0.81147
0.81509	0.45820	0.79396
0.84970	0.87807	0.75463
0.90957	0.55136	0.82860
0.83622	0.54398	0.81194
0.79642	0.58025	0.80632
0.79104	0.88442	0.69238
0.80747	0.44969	0.11060
0.27524	0.28299	0.55964
0.30280	0.31548	0.62591
0.35818	0.30979	0.69867
0.38830	0.34028	0.75480
0.27661	0.35221	0.61525
0.39854	0.40931	0.79551
0.35114	0.69029	0.70277
0.36396	0.37711	0.73794
0.27208	0.28332	0.43399
0.30732	0.38292	0.66944
0.76742	0.21699	0.43662
0.79521	0.18429	0.36978
0.86153	0.18635	0.33414
0.30052	0.31549	0.36532
0.89122	0.15604	0.27596
0.75899	0.15137	0.34472
0.88952	0.09052	0.19564
0.37945	0.66011	0.76347
0.85574	0.12253	0.25675
0.78952	0.12026	0.29146
0.36635	0.31254	0.32729
0.26706	0.71667	0.43851
0.29282	0.68379	0.37023
0.35484	0.68768	0.31557
0.38361	0.65733	0.25624
0.25955	0.64902	0.36064
0.38603	0.59006	0.19273
0.35169	0.62208	0.25291
0.26416	0.64903	0.63339
0.28925	0.61813	0.30472
0.39704	0.34266	0.26952
0.23167	0.78327	0.43595
0.20657	0.81566	0.36564
0.15190	0.80988	0.29112
0.12354	0.84002	0.23023
0.23381	0.85222	0.37291
0.26571	0.34904	0.34214
0.11420	0.90888	0.18481
0.14883	0.87678	0.24351
0.38600	0.59177	0.81527
0.20481	0.88260	0.31381
0.39728	0.40901	0.19357
0.72390	0.28151	0.43420
0.69755	0.31382	0.36638
0.64459	0.30830	0.28789
0.61624	0.33903	0.23026
0.72344	0.35054	0.38135
0.60746	0.40820	0.19171
0.64018	0.37574	0.25109
0.69448	0.38141	0.32547
0.35152	0.62382	0.75600
0.36308	0.37681	0.25320
0.29719	0.37992	0.28931
0.74270	0.24824	0.37511
0.24874	0.74957	0.37742
0.25594	0.25022	0.62112
0.73963	0.75331	0.61751
0.25194	0.75115	0.62278
0.75452	0.25229	0.62104
0.75105	0.75372	0.37269

```
0.24903   0.25106   0.37506
0.29320   0.61851   0.69182
0.76690   0.78663   0.43613
0.22984   0.21827   0.43654
0.20159   0.18582   0.37083
0.14359   0.19119   0.30481
0.11322   0.16068   0.24911
0.22960   0.14942   0.37605
0.10574   0.09199   0.20143
0.13975   0.12416   0.26022
0.19851   0.11865   0.32285
0.79491   0.81897   0.36971
0.65954   0.42533   1.02775
0.79307   0.34710   0.64479
0.54994   0.34954   0.71425
0.60245   0.29330   0.61541
0.74418   0.60078   0.24936
0.23750   0.90876   0.71298
0.29292   0.85304   0.61561
0.06409   0.84121   0.77463
0.11614   0.78661   0.66488
0.79555   0.65728   0.34780
0.28804   0.41184   0.65985
0.23163   0.35656   0.56315
0.43173   0.33643   0.81163
0.55907   0.66017   0.22806
0.37840   0.28104   0.70798
0.74003   0.24725   0.27753
0.60811   0.71519   0.33995
0.77080   0.91326   0.68879
0.71326   0.85949   0.58747
0.92077   0.83679   0.81299
0.86673   0.78313   0.70224
0.24835   0.74909   0.27967
0.69629   0.59087   0.62994
0.75048   0.64507   0.52609
0.58319   0.66864   0.84249
0.63185   0.72356   0.72967
0.23677   0.09309   0.70944
0.29235   0.14921   0.61595
0.06246   0.15994   0.77069
0.11491   0.21509   0.66412
0.71323   0.41034   0.33793
0.76669   0.35459   0.43822
0.57452   0.33557   0.16922
0.62463   0.27960   0.27573
0.22469   0.91142   0.32254
0.27822   0.85683   0.42630
0.08033   0.83598   0.17303
0.13060   0.78132   0.28438
0.26429   0.59053   0.30069
0.20973   0.64619   0.39800
0.43181   0.66003   0.21240
0.38078   0.71494   0.32205
0.73682   0.75274   0.71513
0.76219   0.09385   0.27594
0.70662   0.14994   0.36968
0.94266   0.15746   0.24558
0.88981   0.21219   0.35336
0.25761   0.25023   0.71884
0.21932   0.08996   0.32818
0.27650   0.14540   0.42263
0.06800   0.16432   0.19688
0.12179   0.21966   0.30009
0.70281   0.52925   0.19304
0.58266   0.49817   0.57888
0.29270   0.52454   0.85892
0.42289   0.50448   0.42625
0.49772   0.49839   0.35734
0.58230   0.47299   0.36725
0.50711   0.50290   0.64257
0.42497   0.47460   0.62677
0.36495   0.44468   0.99424
0.50024   0.55407   0.25463
0.50303   0.55675   0.74924
0.64851   0.44956   0.98594
0.30622   0.50062   0.98998
0.29083   0.52299   0.13858
0.08052   0.02535   0.37738
0.21810   0.02212   0.86250
0.19759   0.99937   0.00380
0.99591   0.00253   0.35464
0.78404   0.02200   0.13274
0.80485   0.00007   0.99389
0.92264   0.02642   0.61956
0.00655   0.00298   0.64196
0.13904   0.05578   0.00588
0.86377   0.05616   0.99167
```

0.00137	0.94521	0.24842
0.00087	0.94553	0.74710
0.21085	0.97571	0.13870
0.92179	0.99155	0.41739
0.79110	0.97763	0.85428
0.08052	0.99110	0.57995
0.27118	0.40683	0.27484
0.21353	0.35112	0.36800
0.44818	0.34054	0.23782
0.39359	0.28622	0.34487
0.75761	0.25336	0.71856
0.76993	0.91244	0.29830
0.71372	0.85766	0.40021
0.93344	0.84026	0.20751
0.88050	0.78608	0.31897
0.25255	0.75168	0.72052
0.27136	0.59007	0.68748
0.21765	0.64500	0.58553
0.42464	0.66370	0.81578
0.37434	0.71843	0.70476
0.75528	0.75412	0.27524
0.78673	0.09055	0.66381
0.72982	0.14589	0.56825
0.93239	0.16579	0.81022
0.87856	0.22125	0.70768
0.24720	0.25108	0.27737
0.73849	0.40505	0.72999
0.82135	0.42861	0.82312
0.78759	0.45818	0.70915
0.86359	0.47166	0.77998
0.93795	0.52460	0.83317
0.91726	0.56692	0.91299
0.92975	0.56882	0.75537
0.82849	0.52774	0.72805
0.81048	0.59737	0.72780
0.80513	0.59756	0.88692
0.74336	0.57344	0.80136
0.78382	0.43268	0.18135
0.72996	0.48982	0.13042
0.82771	0.47631	0.14672
0.84767	0.43291	0.06970
0.44106	0.39983	0.11719
0.93831	0.10202	0.87928
0.36950	0.55775	0.78934
0.56468	0.60345	0.88698
0.13119	0.05726	0.77992
0.06673	0.10028	0.87597
0.62738	0.56116	0.78484
0.44081	0.40027	0.87430
0.87001	0.94380	0.78634
0.93346	0.90093	0.11412
0.38015	0.44267	0.22132
0.93360	0.90012	0.88010
0.38421	0.44318	0.76428
0.43189	0.59970	0.12133
0.87013	0.05665	0.21688
0.93557	0.10002	0.12438
0.36900	0.55595	0.21679
0.87380	0.94472	0.21660
0.56906	0.39948	0.10658
0.13167	0.94282	0.20972
0.06753	0.89977	0.11447
0.61939	0.44169	0.22857
0.19333	0.99987	0.10930
0.94161	0.00319	0.34677
0.69624	0.50149	0.18694
0.44355	0.49977	0.34883
0.80716	0.99966	0.10233
0.06411	0.00096	0.34747
0.31022	0.49968	0.10652
0.56561	0.49834	0.34678
0.80958	0.00131	0.88542
0.06098	0.00333	0.64980
0.30961	0.50021	0.88820
0.56044	0.50697	0.65110
0.19480	0.99974	0.89209
0.93851	0.00185	0.64893
0.43813	0.50037	0.65000
0.00182	0.96150	0.17821
0.50180	0.47069	0.13008
0.99934	0.02981	0.13281
0.50150	0.53907	0.18163
0.00041	0.96179	0.81737
0.50552	0.47324	0.86578
0.00345	0.03009	0.86499
0.50118	0.54091	0.82048
0.07459	0.97138	0.99767
0.60693	0.46421	0.99913

```
0.90269   0.03988   0.99325
0.42910   0.52918   0.00069
0.92779   0.97162   0.99799
0.40350   0.46131   0.99421
0.10001   0.03958   0.00414
0.57642   0.53150   0.00115
0.56378   0.60254   0.11959
0.12026   0.05813   0.23228
0.06418   0.10120   0.12137
0.63315   0.56052   0.20615
0.56841   0.40321   0.86648
0.12881   0.94410   0.77860
0.06796   0.90060   0.87985
0.62341   0.44740   0.75802
0.43149   0.60113   0.88746
0.88381   0.05923   0.76470
0.70083   0.50330   0.86808
0.81475   0.52175   0.91120
0.75676   0.45658   0.02429
0.76593   0.48374   0.90372
0.91214   0.00043   0.15396
0.91463   0.00114   0.83686
0.41614   0.50071   0.83864
0.41299   0.49946   0.15652
0.50477   0.43192   0.99332
0.00141   0.06982   0.99927
0.58701   0.50029   0.15877
0.08789   0.00049   0.15955
0.50005   0.57017   0.00156
0.09053   0.00045   0.84215
0.59367   0.50314   0.84278
0.00108   0.93134   0.99717
```

POSCAR file for gd_solvent

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POSCAR file from zrtcpb-gd-meoh-c.res: C: 144 F: 1 H: 122 O: 66 P: 1 ZR: 12
  34.8920000000000
    0.5792995890490465  -0.0000450140396845   0.0007649282407427
   -0.0000781726227076   1.0082675674799713   0.0000166934211398
    0.0004256087542374   0.0000053656439079   0.3214078049098053
144 1 122 66 1 12
Direct
  0.79244   0.88301   0.30309
  0.64941   0.62460   0.24158
  0.39252   0.34185   0.26530
  0.23238   0.78326   0.43720
  0.20701   0.81554   0.36700
  0.15059   0.80989   0.29664
  0.12204   0.83994   0.23578
  0.23573   0.85179   0.37004
  0.26427   0.35008   0.35228
  0.11437   0.90851   0.18583
  0.14898   0.87644   0.24488
  0.38542   0.59170   0.81854
  0.71178   0.62092   0.29313
  0.20658   0.88210   0.31092
  0.39587   0.40923   0.20041
  0.72281   0.28072   0.43867
  0.69410   0.31271   0.37293
  0.64206   0.30646   0.29260
  0.61204   0.33684   0.23579
  0.71676   0.34998   0.39152
  0.60199   0.40628   0.19666
  0.63305   0.37394   0.25993
  0.68573   0.38043   0.33771
  0.88502   0.84238   0.25304
  0.35183   0.62385   0.75801
  0.36073   0.37700   0.25788
  0.29625   0.38099   0.30062
  0.74113   0.24756   0.37809
  0.24918   0.74956   0.37835
  0.25457   0.24970   0.62240
  0.74428   0.75175   0.62064
  0.25306   0.75105   0.62374
  0.75673   0.25126   0.62321
  0.75009   0.75189   0.37539
  0.20621   0.18471   0.63210
  0.24711   0.25080   0.37637
  0.29344   0.61860   0.69401
  0.76655   0.78508   0.43691
  0.22885   0.21778   0.43759
  0.20089   0.18535   0.37155
  0.14134   0.19038   0.30975
  0.11111   0.15985   0.25410
  0.23053   0.14934   0.37243
  0.10546   0.09140   0.20236
  0.13934   0.12365   0.26117
```

0.23438	0.78393	0.56314
0.19956	0.11850	0.31944
0.79377	0.81746	0.36899
0.20809	0.81655	0.63186
0.14550	0.81235	0.68402
0.11588	0.84247	0.74324
0.24124	0.85124	0.64379
0.11288	0.90965	0.80750
0.23273	0.21725	0.56325
0.14770	0.87765	0.74854
0.21079	0.88191	0.69967
0.76189	0.85267	0.36019
0.73052	0.28253	0.56385
0.14333	0.18840	0.68343
0.70256	0.31533	0.63031
0.63449	0.31494	0.65379
0.60406	0.34596	0.70669
0.88918	0.90975	0.19060
0.73955	0.34735	0.66254
0.73092	0.71861	0.43331
0.60574	0.41113	0.78955
0.64056	0.37871	0.73177
0.70850	0.37937	0.70962
0.85442	0.87796	0.25045
0.97924	0.51802	1.03385
0.88094	0.47849	0.96201
0.89201	0.50505	1.16808
0.77440	0.21795	0.56270
0.11390	0.15788	0.74099
0.80336	0.18583	0.62834
0.86204	0.19106	0.69256
0.89219	0.16047	0.74815
0.77452	0.14960	0.62454
0.70662	0.68626	0.36120
0.89792	0.09187	0.79841
0.86459	0.12415	0.73886
0.80528	0.11879	0.67785
0.23971	0.15010	0.64297
0.11214	0.09045	0.80462
0.14607	0.12277	0.74532
0.20936	0.11906	0.69686
0.72746	0.71857	0.55926
0.70096	0.68609	0.62714
0.26963	0.71731	0.56489
0.64496	0.69000	0.30581
0.64717	0.69197	0.70432
0.61837	0.66177	0.76461
0.72597	0.64917	0.61469
0.60879	0.59249	0.80757
0.64168	0.62481	0.74641
0.69542	0.61874	0.67074
0.76400	0.78496	0.56274
0.78982	0.81704	0.63392
0.84730	0.81095	0.70086
0.87716	0.84067	0.76148
0.61712	0.65971	0.24485
0.29485	0.68495	0.63510
0.76140	0.85330	0.63377
0.88668	0.90905	0.81257
0.79966	0.53994	0.74768
0.85065	0.87727	0.75478
0.90350	0.51327	0.03476
0.84823	0.54155	0.01668
0.83100	0.56371	0.12769
0.79204	0.88333	0.69211
0.75936	0.40979	0.07327
0.85519	0.81250	0.31289
0.27290	0.28271	0.56119
0.30041	0.31509	0.62787
0.35785	0.30963	0.69556
0.38753	0.34003	0.75287
0.27215	0.35145	0.62287
0.39436	0.40867	0.80169
0.35235	0.69015	0.70290
0.36078	0.37651	0.74189
0.26937	0.28318	0.43547
0.30253	0.38211	0.67787
0.74095	0.65190	0.34909
0.76671	0.21617	0.43760
0.79370	0.18359	0.36908
0.85795	0.18699	0.32342
0.29730	0.31548	0.36706
0.88778	0.15669	0.26542
0.75937	0.14945	0.35268
0.88917	0.08987	0.19608
0.38034	0.66001	0.76426
0.85466	0.12199	0.25557
0.79017	0.11853	0.29883

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0.61553   0.59209   0.18311
0.36145   0.31155   0.32130
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0.29346   0.68405   0.36969
0.35450   0.68866   0.31209
0.38364   0.65858   0.25196
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0.38785   0.59094   0.19172
0.35293   0.62301   0.25043
0.26480   0.64903   0.63467
0.29122   0.61840   0.30450
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0.79300   0.34768   0.64566
0.55122   0.34558   0.72832
0.60550   0.28982   0.62931
0.73645   0.59325   0.29000
0.23545   0.90954   0.70673
0.29147   0.85424   0.60831
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0.11982   0.78505   0.67571
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0.28171   0.41080   0.67279
0.22558   0.35547   0.57525
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0.73711   0.24676   0.28065
0.61845   0.71705   0.31329
0.77129   0.91205   0.68866
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0.57642   0.66591   0.82508
0.62712   0.72074   0.71409
0.23435   0.09149   0.70174
0.28997   0.14743   0.60738
0.06494   0.16032   0.78214
0.11724   0.21558   0.67574
0.70228   0.40972   0.35183
0.75964   0.35473   0.44857
0.57187   0.33277   0.17177
0.62445   0.27739   0.27768
0.22761   0.91073   0.31622
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0.07756   0.83611   0.18168
0.12817   0.78155   0.29348
0.26737   0.59047   0.30189
0.21206   0.64554   0.40132
0.43138   0.66168   0.20677
0.37953   0.71623   0.31735
0.74261   0.75152   0.71839
0.76455   0.09125   0.29002
0.70830   0.14694   0.38452
0.93770   0.15898   0.22811
0.88470   0.21380   0.33542
0.25648   0.24962   0.72010
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0.57546   0.49639   0.57807
0.28697   0.52246   0.86270
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0.51052   0.49819   0.35716
0.57775   0.46949   0.36019
0.49516   0.50077   0.64453
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0.50007   0.55484   0.74828
0.64719   0.44813   0.99478
0.30472   0.50096   0.01564
0.29633   0.52645   0.14240
0.08073   0.02485   0.37815
0.21756   0.02184   0.86290
0.19748   0.99899   0.00377
0.99632   0.00184   0.35590
0.78419   0.02134   0.13510
0.80473   0.99919   0.99569
0.92217   0.02558   0.62115
0.00589   0.00221   0.64310
0.13876   0.05527   0.00676
0.86362   0.05539   0.99311
0.00133   0.94456   0.24982
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0.27176	0.40863	0.29228
0.21312	0.35291	0.38343
0.44240	0.33913	0.22807
0.38711	0.28432	0.33182
0.76129	0.25209	0.72056
0.76888	0.91099	0.29785
0.71241	0.85613	0.39838
0.93298	0.83909	0.20873
0.87989	0.78485	0.31930
0.25378	0.75149	0.72149
0.27141	0.59019	0.69063
0.21817	0.64509	0.58713
0.42556	0.66352	0.81655
0.37591	0.71820	0.70401
0.75208	0.75214	0.27768
0.78389	0.09022	0.67403
0.72710	0.14588	0.57942
0.93795	0.16382	0.79901
0.88467	0.21935	0.69555
0.24518	0.25090	0.27867
0.73662	0.40511	0.73076
0.78218	0.53079	0.65928
0.77971	0.56844	0.76686
0.85413	0.54051	0.74822
0.86067	0.56152	0.94361
0.87373	0.58082	0.15658
0.81770	0.54402	0.20066
0.78907	0.58302	0.11155
0.72398	0.39035	0.11830
0.71942	0.46293	0.08952
0.79705	0.41809	0.14002
0.78392	0.39359	0.00127
0.88441	0.48504	0.86264
0.91736	0.45405	0.97404
0.83397	0.46056	0.96388
0.92303	0.47801	1.16460
0.91268	0.53464	1.18621
0.84490	0.50001	1.22180
1.01597	0.51507	0.95719
1.01163	0.49553	1.07791
0.98862	0.54883	1.06038
0.43953	0.39993	0.12392
0.93855	0.10106	0.87982
0.36752	0.55787	0.79373
0.56418	0.60167	0.88231
0.13067	0.05666	0.78039
0.06669	0.09965	0.87766
0.62652	0.55881	0.78139
0.43565	0.39944	0.88187
0.86982	0.94307	0.78774
0.93360	0.90003	0.11603
0.37993	0.44297	0.22981
0.93357	0.89953	0.88175
0.37982	0.44247	0.77067
0.43557	0.60029	0.12385
0.87040	0.05602	0.21903
0.93516	0.09933	0.12465
0.36948	0.55701	0.21402
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0.56697	0.39743	0.10701
0.13202	0.94241	0.21046
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0.94191	0.00235	0.34822
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0.06440	0.00043	0.34842
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0.80919	0.00036	0.88802
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0.30766	0.49961	0.89507
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0.93815	0.00101	0.65028
0.43339	0.49878	0.65451
0.00190	0.96082	0.17958
0.50262	0.47031	0.13125
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0.00016	0.96110	0.81880

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0.50016   0.47162   0.86634
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0.90249   0.03908   0.99487
0.42886   0.52900   0.00467
0.92756   0.97085   0.99977
0.40113   0.46109   0.00152
0.09984   0.03899   0.00508
0.57673   0.53034   0.99662
0.56794   0.60129   0.11519
0.12038   0.05762   0.23300
0.06377   0.10064   0.12268
0.63483   0.55841   0.20539
0.56286   0.40120   0.86639
0.12850   0.94356   0.77969
0.06801   0.90002   0.88150
0.62050   0.44494   0.76005
0.43118   0.60089   0.89042
0.88335   0.05818   0.76649
0.69686   0.49954   0.84611
0.78733   0.52188   0.98315
0.72777   0.44180   0.02446
0.76802   0.50766   0.85562
0.59118   0.50006   0.15383
0.00125   0.06891   0.00051
0.50195   0.43119   0.99711
0.41615   0.49915   0.16374
0.41025   0.50061   0.84607
0.91443   0.00024   0.83869
0.91212   0.99960   0.15574
0.50060   0.56936   0.00213
0.00094   0.93072   0.99862
0.08786   0.99990   0.16022
0.09016   0.99980   0.84304
0.58552   0.50071   0.83790
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POSCAR file for gd_p5

POSCAR file from zrtcpb-gd-meoh-c.res: C: 144 F: 1 H: 122 O: 66 P: 1 ZR: 12
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      0.5792995890490465   -0.0000450140396845   0.0007649282407427
     -0.0000781726227076   1.0082675674799713   0.0000166934211398
      0.0004256087542374   0.0000053656439079   0.3214078049098053
144 1 122 66 1 12
Direct
   0.79249   0.88302   0.30317
   0.64969   0.62476   0.23955
   0.39310   0.34213   0.26766
   0.23223   0.78348   0.43705
   0.20691   0.81578   0.36695
   0.15098   0.81004   0.29549
   0.12247   0.84009   0.23458
   0.23528   0.85211   0.37114
   0.26401   0.34992   0.35091
   0.11432   0.90869   0.18601
   0.14898   0.87666   0.24486
   0.38275   0.59161   0.81981
   0.71317   0.62159   0.28698
   0.20615   0.88242   0.31199
   0.39606   0.40938   0.20137
   0.72170   0.28081   0.44053
   0.69334   0.31292   0.37479
   0.64195   0.30676   0.29311
   0.61266   0.33719   0.23536
   0.71614   0.35015   0.39386
   0.60292   0.40660   0.19568
   0.63403   0.37425   0.25912
   0.68615   0.38065   0.33817
   0.88517   0.84249   0.25289
   0.34989   0.62383   0.75838
   0.36089   0.37711   0.25861
   0.29601   0.38089   0.29957
   0.73978   0.24770   0.37949
   0.24874   0.74979   0.37808
   0.25510   0.24952   0.62253
   0.74413   0.75187   0.62049
   0.25313   0.75131   0.62348
   0.75732   0.25154   0.62425
   0.75045   0.75183   0.37533
   0.20655   0.18457   0.63209
   0.24707   0.25084   0.37660
   0.29167   0.61880   0.69374
   0.76686   0.78504   0.43679
   0.22904   0.21777   0.43769
   0.20109   0.18533   0.37161
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| | | |
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| 0.11151 | 0.15987 | 0.25363 |
| 0.23056 | 0.14929 | 0.37312 |
| 0.10555 | 0.09142 | 0.20272 |
| 0.13951 | 0.12363 | 0.26135 |
| 0.23444 | 0.78419 | 0.56286 |
| 0.19956 | 0.11844 | 0.32018 |
| 0.79403 | 0.81744 | 0.36883 |
| 0.20810 | 0.81678 | 0.63164 |
| 0.14516 | 0.81264 | 0.68251 |
| 0.11546 | 0.84269 | 0.74187 |
| 0.24148 | 0.85136 | 0.64500 |
| 0.11279 | 0.90975 | 0.80764 |
| 0.23313 | 0.21711 | 0.56324 |
| 0.14755 | 0.87779 | 0.74846 |
| 0.21094 | 0.88200 | 0.70080 |
| 0.76201 | 0.85261 | 0.36004 |
| 0.73026 | 0.28270 | 0.56549 |
| 0.14340 | 0.18821 | 0.68243 |
| 0.70254 | 0.31552 | 0.63215 |
| 0.63391 | 0.31630 | 0.64976 |
| 0.60393 | 0.34740 | 0.70294 |
| 0.88911 | 0.90986 | 0.19072 |
| 0.74045 | 0.34649 | 0.67039 |
| 0.73082 | 0.71862 | 0.43333 |
| 0.60662 | 0.41183 | 0.79062 |
| 0.64154 | 0.37927 | 0.73358 |
| 0.71001 | 0.37875 | 0.71732 |
| 0.85447 | 0.87806 | 0.25051 |
| 0.97014 | 0.56983 | -0.06338 |
| 0.92154 | 0.50635 | 0.97785 |
| 0.90650 | 0.55823 | 0.12584 |
| 0.77464 | 0.21824 | 0.56330 |
| 0.11389 | 0.15776 | 0.74019 |
| 0.80366 | 0.18606 | 0.62846 |
| 0.86176 | 0.19135 | 0.69428 |
| 0.89189 | 0.16075 | 0.74977 |
| 0.77531 | 0.14972 | 0.62295 |
| 0.70645 | 0.68627 | 0.36098 |
| 0.89807 | 0.09207 | 0.79855 |
| 0.86481 | 0.12435 | 0.73893 |
| 0.80604 | 0.11891 | 0.67629 |
| 0.24022 | 0.15003 | 0.64416 |
| 0.11224 | 0.09047 | 0.80501 |
| 0.14626 | 0.12273 | 0.74563 |
| 0.20979 | 0.11904 | 0.69812 |
| 0.72698 | 0.71872 | 0.55913 |
| 0.69997 | 0.68641 | 0.62711 |
| 0.26940 | 0.71755 | 0.56451 |
| 0.64372 | 0.68956 | 0.30941 |
| 0.64734 | 0.69275 | 0.70647 |
| 0.61784 | 0.66273 | 0.76660 |
| 0.72341 | 0.64923 | 0.61258 |
| 0.60553 | 0.59331 | 0.80592 |
| 0.63939 | 0.62554 | 0.74613 |
| 0.69231 | 0.61904 | 0.66889 |
| 0.76415 | 0.78502 | 0.56251 |
| 0.78996 | 0.81711 | 0.63372 |
| 0.84730 | 0.81103 | 0.70105 |
| 0.87709 | 0.84075 | 0.76179 |
| 0.61604 | 0.65936 | 0.24778 |
| 0.29423 | 0.68510 | 0.63466 |
| 0.76158 | 0.85341 | 0.63344 |
| 0.88664 | 0.90916 | 0.81274 |
| 0.75740 | 0.54465 | 0.74517 |
| 0.85066 | 0.87739 | 0.75483 |
| 0.91140 | 0.54906 | -0.00703 |
| 0.84900 | 0.56210 | -0.07471 |
| 0.82125 | 0.60015 | -0.03680 |
| 0.79217 | 0.88344 | 0.69181 |
| 0.82186 | 0.44234 | -0.01716 |
| 0.85544 | 0.81256 | 0.31275 |
| 0.27334 | 0.28254 | 0.56144 |
| 0.30073 | 0.31490 | 0.62833 |
| 0.35760 | 0.30938 | 0.69744 |
| 0.38710 | 0.33979 | 0.75505 |
| 0.27271 | 0.35129 | 0.62221 |
| 0.39394 | 0.40854 | 0.80288 |
| 0.35166 | 0.69007 | 0.70273 |
| 0.36061 | 0.37631 | 0.74309 |
| 0.26952 | 0.28317 | 0.43583 |
| 0.30281 | 0.38193 | 0.67775 |
| 0.74191 | 0.65248 | 0.34430 |
| 0.76616 | 0.21640 | 0.43839 |
| 0.79336 | 0.18389 | 0.36961 |
| 0.85822 | 0.18704 | 0.32654 |
| 0.29744 | 0.31553 | 0.36755 |
| 0.88819 | 0.15677 | 0.26854 |

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0.78964   0.11904   0.29733
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0.26717   0.71687   0.43871
0.29275   0.68422   0.36950
0.35404   0.68866   0.31267
0.38309   0.65850   0.25286
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0.26365   0.64935   0.63399
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0.79428   0.34591   0.65815
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0.79243   0.65029   0.37876
0.28215   0.41064   0.67208
0.22661   0.35534   0.57316
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0.37930   0.28089   0.70273
0.73513   0.24692   0.28214
0.61626   0.71619   0.32029
0.77147   0.91217   0.68813
0.71511   0.85816   0.58610
0.92220   0.83647   0.81383
0.86933   0.78258   0.70245
0.24794   0.74935   0.28033
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0.76619   0.64403   0.55532
0.57666   0.66723   0.82854
0.62863   0.72176   0.71800
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0.06473   0.16018   0.78059
0.11716   0.21532   0.67380
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0.57253   0.33319   0.17122
0.62413   0.27774   0.27809
0.22685   0.91111   0.31810
0.28077   0.85652   0.42169
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0.12889   0.78162   0.29136
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0.21082   0.64602   0.40015
0.43095   0.66146   0.20805
0.37931   0.71615   0.31828
0.74238   0.75167   0.71822
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0.70729   0.14761   0.38105
0.93855   0.15894   0.23311
0.88532   0.21364   0.34042
0.25720   0.24936   0.72021
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0.27847   0.14561   0.41659
0.06529   0.16322   0.20416
0.11889   0.21863   0.30751
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0.08053   0.02490   0.37887
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0.80466   0.99938   0.99532
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0.00613   0.00231   0.64330
0.13883   0.05530   0.00726
0.86355   0.05554   0.99345
0.00124   0.94456   0.24987
0.00048   0.94490   0.74887
0.21122   0.97545   0.13948
0.92196   0.99075   0.41888
0.79085   0.97672   0.85727
0.08024   0.99050   0.58130
0.27122   0.40841   0.29016
0.21255   0.35258   0.38058
0.44327   0.33954   0.23157
0.38809   0.28481   0.33588
0.76258   0.25236   0.72149
0.76884   0.91097   0.29804
0.71248   0.85600   0.39810
0.93309   0.83923   0.20844
0.88023   0.78494   0.31903
0.25401   0.75175   0.72121
0.26925   0.59049   0.69029
0.21716   0.64562   0.58587
0.42421   0.66313   0.81701
0.37564   0.71801   0.70383
0.75267   0.75202   0.27764
0.78500   0.09027   0.67133
0.72832   0.14589   0.57646
0.93727   0.16416   0.80169
0.88393   0.21974   0.69866
0.24482   0.25104   0.27893
0.73905   0.40377   0.74263
0.72648   0.53411   0.67146
0.73184   0.56864   0.78840
0.80550   0.55389   0.70922
0.86133   0.56273   0.82898
0.85929   0.62252  -0.04249
0.80380   0.59876   0.05642
0.77921   0.60856  -0.09327
0.80153   0.41815   0.03480
0.71047   0.47332   0.11093
0.86165   0.45543   0.03696
0.84420   0.43060  -0.09940
0.92309   0.49797   0.88294
0.96908   0.49794   0.01809
0.88181   0.49006   1.02175
0.94860   0.54530   0.17344
0.90808   0.58912   0.14248
0.86044   0.54681   0.16516
-0.02370  0.56150   0.84219
0.01626   0.56235  -0.01650
0.96460   0.60102  -0.05972
0.43997   0.40013   0.12528
0.93859   0.10122   0.88022
0.36469   0.55779   0.79512
0.56124   0.60246   0.88148
0.13075   0.05666   0.78091
0.06675   0.09969   0.87793
0.62218   0.55965   0.77765
0.43555   0.39947   0.88274
0.86978   0.94320   0.78805
0.93356   0.90020   0.11611
0.37985   0.44308   0.23064
0.93355   0.89964   0.88193
0.37888   0.44230   0.77210
0.43484   0.60030   0.12530
0.87027   0.05629   0.21933
0.93513   0.09959   0.12519
0.36878   0.55698   0.21530
0.87359   0.94380   0.21870
0.56762   0.39773   0.10632
0.13185   0.94262   0.21081
0.06768   0.89946   0.11589
0.61454   0.44003   0.23245
0.19340   0.99952   0.11003
0.94164   0.00260   0.34850
0.69345   0.49342   0.16102
0.44441   0.50281   0.34687
0.80718   0.99914   0.10514
0.06409   0.00054   0.34883
0.30796   0.50094   0.11650
0.56547   0.49684   0.34928
0.80917   0.00049   0.88814
0.06063   0.00275   0.65106
0.30614   0.49921   0.89653
0.55064   0.50388   0.65043
0.19466   0.99933   0.89277
0.93825   0.00108   0.65056
0.43074   0.49882   0.65473
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0.00177   0.96095   0.17990
0.50230   0.47057   0.13149
0.99915   0.02921   0.13443
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0.00016   0.96121   0.81903
0.49876   0.47177   0.86611
0.00316   0.02947   0.86648
0.49518   0.53999   0.82085
0.07438   0.97090   0.99909
0.60259   0.46290   0.99387
0.90247   0.03925   0.99512
0.42759   0.52906   0.00540
0.92756   0.97104  -0.00000
0.40048   0.46109   0.00267
0.09986   0.03905   0.00551
0.57516   0.53084   0.99558
0.56738   0.60147   0.11468
0.12041   0.05759   0.23336
0.06377   0.10063   0.12313
0.63532   0.55859   0.20235
0.56307   0.40184   0.86615
0.12848   0.94367   0.77996
0.06794   0.90012   0.88165
0.62160   0.44565   0.76162
0.42820   0.60077   0.89235
0.88360   0.05834   0.76655
0.69338   0.50291   0.85081
0.79517   0.53493   0.94210
0.77291   0.46898  -0.04835
0.76582   0.50662   0.84875
0.59091   0.50044   0.15264
0.00123   0.06909   0.00093
0.50176   0.43145   0.99737
0.41571   0.49926   0.16428
0.40854   0.50060   0.84698
0.91450   0.00042   0.83880
0.91193   0.99978   0.15603
0.49906   0.56968   0.00218
0.00086   0.93084   0.99887
0.08777  -0.00000   0.16070
0.09029   0.99989   0.84339
0.58349   0.50134   0.83682
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POSCAR file for gd_p5_prime

POSCAR file from zrtcpb-gd-meoh-c.res: C: 144 F: 1 H: 122 O: 66 P: 1 ZR: 12
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    0.5792995890490465 -0.0000450140396845   0.0007649282407427
   -0.0000781726227076   1.0082675674799713   0.0000166934211398
    0.0004256087542374   0.0000053656439079   0.3214078049098053
144 1 122 66 1 12
Direct
  0.79240   0.88339   0.30245
  0.64862   0.62582   0.23914
  0.39752   0.34302   0.27472
  0.23146   0.78353   0.43695
  0.20649   0.81587   0.36654
  0.15202   0.80996   0.29157
  0.12350   0.84007   0.23084
  0.23349   0.85249   0.37420
  0.26589   0.34921   0.34570
  0.11372   0.90895   0.18596
  0.14858   0.87686   0.24446
  0.38045   0.59152   0.82085
  0.71450   0.62409   0.27557
  0.20444   0.88280   0.31493
  0.39843   0.40957   0.20144
  0.72318   0.28210   0.43707
  0.69680   0.31465   0.37036
  0.64554   0.30927   0.28811
  0.61787   0.34011   0.22990
  0.72142   0.35152   0.38900
  0.60905   0.40933   0.19159
  0.64092   0.37689   0.25306
  0.69339   0.38247   0.33184
  0.88561   0.84315   0.25266
  0.34704   0.62367   0.76012
  0.36375   0.37731   0.25959
  0.29768   0.38032   0.29475
  0.74150   0.24891   0.37679
  0.24828   0.74976   0.37852
  0.25621   0.24968   0.62203
  0.74231   0.75279   0.61968
  0.25137   0.75146   0.62395
  0.75704   0.25283   0.62217
  0.75150   0.75232   0.37459
  0.20675   0.18489   0.63114
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0.24922	0.25093	0.37593
0.28870	0.61877	0.69568
0.76755	0.78554	0.43633
0.23024	0.21802	0.43696
0.20203	0.18565	0.37094
0.14383	0.19110	0.30556
0.11322	0.16064	0.25011
0.23009	0.14926	0.37559
0.10536	0.09195	0.20245
0.13977	0.12411	0.26077
0.23319	0.78432	0.56276
0.19879	0.11854	0.32254
0.79478	0.81790	0.36864
0.20694	0.81705	0.63122
0.14295	0.81356	0.67810
0.11361	0.84366	0.73781
0.24154	0.85104	0.64845
0.11250	0.91028	0.80749
0.23389	0.21738	0.56255
0.14700	0.87825	0.74806
0.21128	0.88186	0.70395
0.76234	0.85294	0.35972
0.73014	0.28385	0.56233
0.14257	0.18817	0.67728
0.70162	0.31666	0.62748
0.63253	0.31883	0.63604
0.60246	0.34983	0.68967
0.88876	0.91043	0.18976
0.73986	0.34636	0.67356
0.73015	0.71949	0.43243
0.60674	0.41266	0.78895
0.64088	0.38032	0.72934
0.70972	0.37867	0.72065
0.85443	0.87858	0.24991
0.95721	0.55560	0.67572
0.93557	0.54512	0.89088
0.87569	0.59684	-0.21685
0.77521	0.21957	0.56185
0.11294	0.15779	0.73529
0.80381	0.18732	0.62740
0.85992	0.19277	0.69857
0.88991	0.16210	0.75399
0.77712	0.15065	0.61697
0.70516	0.68725	0.36031
0.89792	0.09305	0.79777
0.86460	0.12544	0.73841
0.80759	0.11983	0.67075
0.24115	0.15076	0.64709
0.11232	0.09096	0.80488
0.14623	0.12314	0.74480
0.21060	0.11976	0.70090
0.72490	0.71975	0.55796
0.69737	0.68749	0.62512
0.26749	0.71759	0.56558
0.63965	0.68906	0.32073
0.64687	0.69428	0.70850
0.61724	0.66441	0.76897
0.71889	0.65005	0.60699
0.60322	0.59509	0.80618
0.63719	0.62708	0.74601
0.68850	0.62006	0.66550
0.76350	0.78573	0.56198
0.78922	0.81778	0.63343
0.84639	0.81159	0.70116
0.87630	0.84128	0.76185
0.61200	0.65893	0.25890
0.29168	0.68508	0.63634
0.76107	0.85414	0.63285
0.88640	0.90976	0.81205
0.83282	0.44874	0.82166
0.85016	0.87798	0.75447
0.90395	0.55672	0.77267
0.85006	0.52749	0.74019
0.80670	0.53797	0.63525
0.79179	0.88414	0.69118
0.83852	0.50150	0.09862
0.85621	0.81314	0.31255
0.27520	0.28257	0.56104
0.30228	0.31501	0.62798
0.35801	0.30950	0.69998
0.38722	0.34000	0.75767
0.27495	0.35151	0.61906
0.39464	0.40885	0.80283
0.34904	0.68995	0.70461
0.36145	0.37660	0.74315
0.27202	0.28314	0.43541
0.30466	0.38223	0.67492
0.74301	0.65508	0.33281

0.76738   0.21766   0.43677
0.79475   0.18498   0.36903
0.86142   0.18658   0.33522
0.30051   0.31551   0.36784
0.89089   0.15618   0.27711
0.75807   0.15236   0.34227
0.88882   0.09074   0.19586
0.37622   0.65967   0.76644
0.85494   0.12292   0.25647
0.78841   0.12108   0.28947
0.61452   0.59343   0.18081
0.36648   0.31266   0.33050
0.26610   0.71683   0.43978
0.29201   0.68395   0.37194
0.35391   0.68801   0.31694
0.38310   0.65762   0.25862
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0.38647   0.59023   0.19753
0.35170   0.62221   0.25669
0.26083   0.64940   0.63596
0.28931   0.61809   0.30853
0.73731   0.44308   0.92452
0.79394   0.34475   0.66787
0.54864   0.35106   0.70060
0.60250   0.29561   0.60001
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0.29269   0.85342   0.61693
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0.71475   0.85898   0.58516
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0.86826   0.78309   0.70274
0.24807   0.74929   0.28075
0.70330   0.59058   0.64911
0.75981   0.64449   0.54570
0.57733   0.66916   0.83337
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0.23631   0.09250   0.70929
0.29222   0.14840   0.61513
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0.11570   0.21495   0.66545
0.71149   0.41140   0.34711
0.76296   0.35569   0.44982
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0.62629   0.28055   0.27319
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0.71152   0.52764   0.14214
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0.28647   0.52289   0.86871
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0.41572   0.47350   0.63378
0.36295   0.44468   0.00365
0.50157   0.55488   0.25461
0.49576   0.55631   0.74850
0.64790   0.45245   0.98413
0.30420   0.50036   0.00649
0.29183   0.52375   0.14733
0.07962   0.02522   0.37913

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0.00052   0.94550   0.74839
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0.92101   0.99124   0.41757
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0.27172   0.40729   0.28098
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0.44879   0.34099   0.24359
0.39355   0.28622   0.34718
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0.76839   0.91123   0.29683
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0.93365   0.84010   0.20853
0.88124   0.78559   0.31897
0.25192   0.75203   0.72169
0.26590   0.59056   0.69233
0.21424   0.64574   0.58807
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0.78771   0.09102   0.66207
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0.88081   0.22139   0.70708
0.24736   0.25107   0.27824
0.73942   0.40272   0.75186
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0.83392   0.59778  -0.15331
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0.87313   0.94433   0.21757
0.57006   0.40037   0.10754
0.13102   0.94285   0.21131
0.06717   0.89977   0.11559
0.62233   0.44303   0.22536
0.19261   0.99993   0.11096
0.94076   0.00318   0.34742
0.69822   0.50088   0.14288
0.44747   0.50141   0.35199
0.80684   0.99966   0.10321
0.06315   0.00093   0.34861
0.30957   0.49989   0.11599
0.56946   0.49952   0.34533
0.80916   0.00132   0.88624
0.06077   0.00340   0.65089
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0.30607   0.49942   0.89911
0.55143   0.50452   0.64738
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0.42980   0.49944   0.65329
0.00118   0.96148   0.17922
0.50279   0.47144   0.13056
0.99871   0.02983   0.13388
0.50253   0.53958   0.18220
0.00006   0.96182   0.81852
0.50019   0.47255   0.86600
0.00309   0.03014   0.86587
0.49452   0.54084   0.82055
0.07413   0.97137   0.99898
0.60423   0.46451   0.99417
0.90230   0.03992   0.99395
0.42711   0.52921   0.00510
0.92720   0.97160   -0.00108
0.40153   0.46129   0.00192
0.09955   0.03954   0.00551
0.57358   0.53190   0.99647
0.56496   0.60236   0.11745
0.11971   0.05813   0.23357
0.06375   0.10123   0.12263
0.63506   0.55972   0.20003
0.56442   0.40238   0.86683
0.12842   0.94418   0.78018
0.06755   0.90062   0.88124
0.62130   0.44653   0.76107
0.42593   0.60083   0.89322
0.88372   0.05936   0.76516
0.71112   0.49442   0.81414
0.80798   0.52219   0.84336
0.77674   0.49622   1.03968
0.77289   0.48274   0.88408
0.58881   0.50144   0.15485
0.00103   0.06977   0.00042
0.50303   0.43195   0.99586
0.41441   0.49973   0.16178
0.41026   0.50057   0.84443
0.91442   0.00114   0.83777
0.91155   0.00036   0.15472
0.49780   0.57056   0.00212
0.00056   0.93137   0.99837
0.08729   0.00047   0.16074
0.09006   0.00042   0.84362
0.58605   0.50330   0.83661
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POSCAR file for gd_product

POSCAR file from zrtcpb-gd-meoh-c.res: C: 144 F: 1 H: 122 O: 66 P: 1 ZR: 12
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   -0.0000781726227076    1.0082675674799713    0.0000166934211398
    0.0004256087542374    0.0000053656439079    0.3214078049098053
144 1 122 66 1 12
Direct
  0.79214   0.88385   0.30130
  0.64642   0.62600   0.24569
  0.39769   0.34425   0.27633
  0.23175   0.78336   0.43658
  0.20670   0.81578   0.36646
  0.15308   0.80985   0.28963
  0.12469   0.84000   0.22888
  0.23300   0.85251   0.37618
  0.26447   0.34796   0.33910
  0.11423   0.90897   0.18593
  0.14902   0.87688   0.24445
  0.38842   0.59220   0.81415
  0.71421   0.62690   0.26831
  0.20404   0.88288   0.31700
  0.39473   0.40968   0.19416
  0.71797   0.27963   0.43429
  0.69257   0.31226   0.36668
  0.64363   0.30707   0.28003
  0.61617   0.33820   0.22295
  0.71583   0.34912   0.39031
  0.60471   0.40761   0.19379
  0.63721   0.37493   0.25199
  0.68803   0.38032   0.33432
  0.88578   0.84351   0.25538
  0.35360   0.62422   0.75539
  0.36162   0.37742   0.25520
  0.29487   0.37926   0.28665
  0.73940   0.24698   0.37478
  0.24933   0.74980   0.37788
  0.25699   0.25007   0.62201
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0.74183   0.75333   0.62126
0.25187   0.75113   0.62330
0.75024   0.25081   0.62116
0.74884   0.75340   0.37593
0.20694   0.18531   0.63181
0.25014   0.25071   0.37587
0.29487   0.61876   0.69255
0.76615   0.78636   0.43772
0.23071   0.21803   0.43760
0.20241   0.18554   0.37219
0.14602   0.19120   0.30207
0.11552   0.16075   0.24634
0.22880   0.14884   0.38158
0.10611   0.09187   0.20281
0.14035   0.12398   0.26145
0.23309   0.78395   0.56234
0.19759   0.11813   0.32824
0.79406   0.81859   0.36997
0.20656   0.81666   0.63060
0.14166   0.81380   0.67361
0.11249   0.84402   0.73297
0.24214   0.85016   0.65111
0.11302   0.91019   0.80684
0.23432   0.21773   0.56310
0.14710   0.87811   0.74691
0.21221   0.88110   0.70641
0.76164   0.85356   0.35875
0.72210   0.28120   0.55986
0.14115   0.18753   0.67049
0.69301   0.31399   0.62360
0.62467   0.32045   0.61591
0.59624   0.35223   0.66833
0.88906   0.91056   0.18960
0.73230   0.33997   0.68573
0.72713   0.72070   0.43399
0.60609   0.41200   0.78762
0.63650   0.37909   0.72446
0.70439   0.37276   0.73334
0.85454   0.87889   0.25033
0.94128   0.57189   0.71793
0.95214   0.53776   0.90928
0.87574   0.59332   0.89537
0.77222   0.21823   0.56155
0.11164   0.15705   0.72821
0.80195   0.18643   0.62782
0.85572   0.19272   0.70392
0.88666   0.16239   0.75971
0.77840   0.14923   0.61266
0.70178   0.68844   0.36254
0.89887   0.09318   0.79821
0.86464   0.12526   0.73942
0.80982   0.11879   0.66673
0.24293   0.15211   0.65435
0.11319   0.09100   0.80457
0.14682   0.12326   0.74442
0.21267   0.12091   0.70756
0.72316   0.72055   0.55959
0.69739   0.68772   0.62662
0.26912   0.71750   0.56459
0.63411   0.68761   0.33720
0.65115   0.69352   0.71831
0.62448   0.66299   0.78001
0.71672   0.65041   0.59999
0.61238   0.59345   0.81421
0.64277   0.62586   0.74996
0.68871   0.61978   0.65905
0.76294   0.78628   0.56332
0.78915   0.81823   0.63449
0.84575   0.81184   0.70359
0.87590   0.84153   0.76382
0.60688   0.65704   0.27696
0.29478   0.68520   0.63475
0.76173   0.85478   0.63224
0.88699   0.91009   0.81186
0.81225   0.44803   0.80378
0.85050   0.87838   0.75478
0.90356   0.55895   0.82902
0.84753   0.53154   0.79106
0.79471   0.54973   0.71493
0.79263   0.88475   0.69029
0.80088   0.45626   0.12925
0.85603   0.81374   0.31596
0.27633   0.28275   0.56027
0.30365   0.31548   0.62573
0.35904   0.31020   0.69858
0.38871   0.34097   0.75403
0.27716   0.35208   0.61353
0.39761   0.40992   0.79449
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0.74195   0.65853   0.32328
0.76639   0.21634   0.43626
0.79555   0.18400   0.36981
0.86383   0.18409   0.34866
0.30107   0.31537   0.36650
0.89374   0.15385   0.29047
0.75772   0.15307   0.33147
0.88986   0.09026   0.19654
0.38138   0.66056   0.76203
0.85616   0.12219   0.25794
0.78810   0.12177   0.27907
0.61304   0.59324   0.18830
0.36792   0.31379   0.33381
0.26778   0.71689   0.43880
0.29349   0.68415   0.36999
0.35476   0.68833   0.31277
0.38329   0.65807   0.25259
0.26059   0.64922   0.36178
0.38608   0.59061   0.19070
0.35188   0.62267   0.25085
0.26525   0.64915   0.63447
0.29006   0.61845   0.30487
0.65312   0.42354   1.03459
0.78571   0.33499   0.69273
0.54256   0.35650   0.66582
0.59382   0.29997   0.56779
0.74508   0.60267   0.24236
0.23883   0.90788   0.71968
0.29384   0.85201   0.62223
0.06203   0.84210   0.76810
0.11395   0.78749   0.65834
0.79528   0.65958   0.34038
0.28783   0.41190   0.65632
0.23235   0.35611   0.56068
0.43218   0.33745   0.81095
0.55419   0.65620   0.25496
0.37963   0.28158   0.70873
0.73774   0.24619   0.27710
0.60284   0.71125   0.36670
0.77278   0.91366   0.68514
0.71576   0.85973   0.58355
0.92055   0.83709   0.81701
0.86695   0.78320   0.70653
0.24921   0.74940   0.28010
0.70175   0.59060   0.63541
0.75400   0.64537   0.53122
0.58822   0.66711   0.85146
0.63512   0.72254   0.73901
0.23984   0.09434   0.72111
0.29502   0.15060   0.62758
0.06050   0.15853   0.76018
0.11301   0.21356   0.65331
0.70473   0.40929   0.35348
0.75555   0.35304   0.45523
0.57724   0.33497   0.15605
0.62575   0.27829   0.26095
0.22312   0.91181   0.32750
0.27660   0.85726   0.43159
0.08220   0.83588   0.17002
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0.26547   0.59074   0.30185
0.21122   0.64620   0.40085
0.43093   0.66096   0.20690
0.38035   0.71573   0.31807
0.74066   0.75304   0.71902
0.75918   0.09676   0.25341
0.70413   0.15319   0.34659
0.94680   0.15392   0.27061
0.89335   0.20836   0.37880
0.25859   0.25015   0.71972
0.21713   0.08924   0.33672
0.27444   0.14449   0.43178
0.07149   0.16462   0.19108
0.12548   0.21991   0.29411
0.70224   0.52772   0.19349
0.58445   0.49760   0.58057
0.29344   0.52556   0.85529
0.42023   0.50568   0.42521
0.49499   0.49837   0.35786
0.57877   0.47240   0.36939
0.50887   0.50284   0.64326
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0.36355   0.44536   0.99269
0.49939   0.55407   0.25498
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0.30574   0.50162   0.98622
0.28944   0.52403   0.13518
0.08001   0.02526   0.37886
0.21868   0.02192   0.86405
0.19789   0.99926   0.00614
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0.78393   0.02181   0.13244
0.80515   0.00032   0.99338
0.92395   0.02662   0.62012
0.00742   0.00302   0.64283
0.13947   0.05572   0.00761
0.86430   0.05630   0.99165
0.00098   0.94519   0.24930
0.00138   0.94575   0.74786
0.21099   0.97563   0.14057
0.92128   0.99150   0.41790
0.79124   0.97839   0.85277
0.08152   0.99098   0.58143
0.26732   0.40544   0.26868
0.21172   0.34896   0.36165
0.44958   0.34312   0.24828
0.39658   0.28826   0.35506
0.75271   0.25179   0.71878
0.76815   0.91166   0.29428
0.71177   0.85687   0.39538
0.93413   0.84028   0.21245
0.88109   0.78625   0.32405
0.25227   0.75158   0.72106
0.27316   0.59027   0.68891
0.21842   0.64500   0.58775
0.42686   0.66428   0.81343
0.37549   0.71883   0.70300
0.75147   0.75352   0.27828
0.79241   0.08960   0.65424
0.73494   0.14439   0.55686
0.92890   0.16668   0.81911
0.87413   0.22176   0.71624
0.24844   0.25066   0.27817
0.73429   0.39346   0.78163
0.81478   0.41945   0.84276
0.78530   0.44628   0.71860
0.86248   0.45878   0.78697
0.87247   0.50872   0.73869
0.81652   0.56436   0.63728
0.76623   0.57026   0.76835
0.75914   0.52840   0.68250
0.78113   0.43511   0.19248
0.72745   0.48791   0.13026
0.80464   0.48435   0.17224
0.85029   0.44741   0.09855
0.96864   0.51087   0.86766
0.99647   0.55535   0.92535
0.92980   0.53095   0.99620
0.91639   0.61095   0.93082
0.84549   0.61145   0.83659
0.84438   0.58418   0.97083
0.96083   0.54727   0.66766
0.98386   0.58964   0.74420
0.91031   0.58890   0.65724
0.43831   0.40035   0.11762
0.93905   0.10222   0.88076
0.37154   0.55824   0.78824
0.56823   0.60229   0.89066
0.13215   0.05719   0.78171
0.06750   0.10029   0.87697
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0.87065   0.94413   0.78639
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0.37717   0.44338   0.22049
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0.38410   0.44381   0.76216
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0.93629   0.09986   0.12629
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0.87339   0.94452   0.21673
0.56612   0.39930   0.10842
0.13144   0.94289   0.21148
0.06778   0.89983   0.11526
0.61659   0.44107   0.23146
0.19347   0.99976   0.11100
0.94123   0.00302   0.34724
0.69477   0.50004   0.18748
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0.80725   0.99962   0.10150
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0.30973   0.50113   0.88491
0.56223   0.50642   0.65277
0.19521   0.99961   0.89371
0.93955   0.00197   0.64932
0.43968   0.50080   0.64960
0.00167   0.96146   0.17908
0.49973   0.47068   0.13125
0.99939   0.02971   0.13351
0.50068   0.53901   0.18211
0.00098   0.96189   0.81836
0.50528   0.47302   0.86618
0.00419   0.03018   0.86606
0.50312   0.54067   0.82115
0.07479   0.97137   0.99899
0.60530   0.46339   0.00149
0.90317   0.03998   0.99368
0.42939   0.52953   -0.00025
0.92798   0.97170   0.99840
0.40218   0.46193   0.99337
0.10043   0.03954   0.00567
0.57696   0.53077   0.00312
0.56399   0.60204   0.12361
0.12018   0.05798   0.23405
0.06476   0.10110   0.12246
0.63283   0.55955   0.20955
0.56547   0.40214   0.86852
0.12926   0.94405   0.77998
0.06807   0.90056   0.88068
0.62206   0.44578   0.76053
0.43430   0.60145   0.88566
0.88570   0.05938   0.76485
0.70248   0.49955   0.86742
0.81953   0.51541   0.89638
0.75516   0.45666   0.03218
0.76631   0.47892   0.90359
0.58550   0.49955   0.16116
0.00189   0.06991   0.00035
0.50287   0.43183   0.99466
0.41138   0.49998   0.15553
0.41672   0.50105   0.83756
0.91530   0.00138   0.83716
0.91203   0.00037   0.15431
0.50133   0.56997   0.00221
0.00114   0.93140   0.99822
0.08781   0.00050   0.16096
0.09115   0.00048   0.84353
0.59432   0.50208   0.84507
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