

Computational settings

All DFT calculations were performed using VASP. The PBE exchange-correlation functional was used in conjunction with the projector augmented wave approach. All structures were optimized to their local minima using the conjugate gradient algorithm as implemented in VASP. Optimization and other electronic settings are given below.

Settings

Parameter	INCAR setting	value
Cutoff energy	ENCUT	500
Precision	PREC	High
Smearing type	ISMEAR	0 (Gaussian smearing)
Smearing width	SIGMA	0.0005
Electronic convergence threshold	EDIFF	1E-5
Ionic relaxation threshold	EDIFFG	1E-4

K-point grid

For all calculations, only the Γ -point was used.

Geometries

Below, the geometries of the optimized structures are given. These geometries are represented as POSCAR/CONTCAR files. Further information with regard to the structure of these files is provided in the link below: <http://cms.mpi.univie.ac.at/vasp/guide/node59.html>.

Overview of obtained energies and molecules structures

System	Electronic Energy [eV]
UPy	-252.666
NaPy	-259.303
K ₂ CO ₃	-33.965
Product	-369.544
diUPy	-507.276
UPy-NaPy	-513.399
NaPy + K ₂ CO ₃	-293.652
diUPy + K ₂ CO ₃	-541.583
UPy-NaPy + K ₂ CO ₃	-547.663
diNaPy + K ₂ CO ₃	-553.408
Product + K ₂ CO ₃	-404.589
diNaPy + product + K ₂ CO ₃	-923.720
diUPy + product + K ₂ CO ₃	-912.445

	Reaction energy	Cumulative reaction energy
Pathways	[kJ/mol]	[kJ/mol]
UPy + UPy → diUPy	-187.183	
diUPy + K ₂ CO ₃ → diUPy•K ₂ CO ₃	-32.820	-220.003
diUPy•K ₂ CO ₃ + product → diUPy•K ₂ CO ₃ -product	-126.877	-346.881
UPy + NaPy → UPy-NaPy	-137.695	
UPy-NaPy + K ₂ CO ₃ → UPy-NaPy•K ₂ CO ₃	-28.686	-166.381
NaPy + K ₂ CO ₃ → NaPy•K ₂ CO ₃	-36.972	
NaPy•K ₂ CO ₃ + NaPy → diNaPy•K ₂ CO ₃	-43.591	-80.563
diNaPy•K ₂ CO ₃ + product → diNaPy•K ₂ CO ₃ •product	-73.914	-154.476
Product + K ₂ CO ₃ → product•K ₂ CO ₃	-103.937	

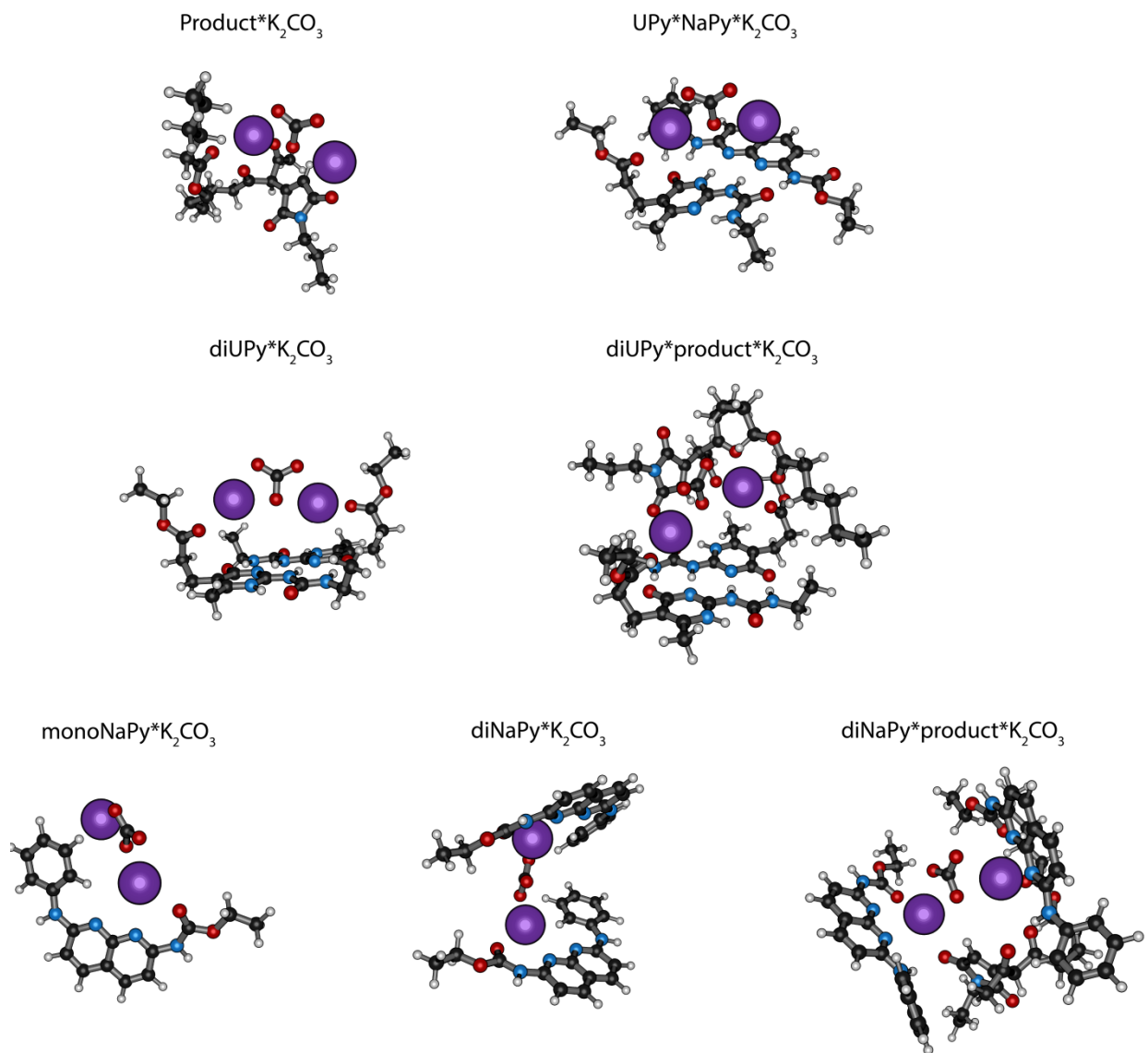


Figure 1: Optimized geometry as obtained from DFT calculations for the various phase-transfer catalysts.

UPy

1.00000000000000

25.839050000000003	0.000000000000000	0.000000000000000
0.000000000000000	15.768689999999994	0.000000000000000
0.000000000000000	0.000000000000000	15.860910000000005

C H N O

13 20 4 4

Direct

0.5302223380125974	0.5897418510245399	0.5579642941534960
0.4408275458047811	0.5761641247028775	0.5627532702150951
0.4897962650304894	0.4485057265857404	0.5582407309246775
0.5341006477660208	0.4958625518186784	0.5573708781209570
0.4855766117304298	0.3536974245999975	0.5565730496035418
0.5878528223919727	0.4593853750801225	0.5555507522165817
0.6131801746856200	0.4676819541864686	0.4684014709720871
0.6674228975582520	0.4316786781221301	0.4656848746765190
0.7430297483244744	0.4178533223554134	0.3803084822017430
0.7616772752985326	0.4442021508411448	0.2936816208503610
0.3441696569756012	0.5738980516345269	0.5678555233317379
0.2496500389623651	0.5943149595125561	0.5699566569584088
0.2276659587159536	0.5844573637558982	0.4810348478172259
0.4072494112033427	0.4596354678901906	0.5625602030717423
0.4668107562373480	0.3300580404195692	0.6143131714762778
0.4618212788779009	0.3329196295131170	0.5027754303030967
0.5235253391330515	0.3234967835283503	0.5512594929775554
0.6115565455114914	0.4951597383298638	0.6008750367582969
0.5884734038060445	0.3928571868365358	0.5758140961598142
0.5902130204084332	0.4350050318215674	0.4195995140067523
0.6147187562688120	0.5347845516845192	0.4496367987704734
0.7669557896694397	0.4448965223934056	0.4309881200565810
0.7429618542835162	0.3485531845419170	0.3883931974280290
0.7610515137280589	0.5134904444725751	0.2866703029067784
0.8016555193127762	0.4223128442132841	0.2843428228986913
0.7375134567777166	0.4164139073439800	0.2438499826030409
0.2504587557229962	0.5326998067216351	0.6021667626497460

0.2255484118528384	0.6373594933067317	0.6078383982839370
0.2517467656841026	0.5411188432322281	0.4436716449722964
0.2256188138798527	0.6457119783123418	0.4480983689356092
0.3947449331260930	0.6786371978914404	0.5686241650639920
0.3079321903076931	0.6903045278717151	0.5643909662065895
0.1883083093546710	0.5580861418993759	0.4838204668862575
0.4808031048509798	0.6263072226993630	0.5616259951806137
0.4425103567263999	0.4901344722413303	0.5609540608409763
0.3919966574385758	0.6143802887009997	0.5659384608889620
0.3025094825519579	0.6270597634171241	0.5716258126615128
0.6903618467621815	0.4489780997771213	0.3902146717727340
0.6886182558933741	0.3919539891879395	0.5220729967793472
0.3397922511221780	0.4952271431084556	0.5672928341403541
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NaPy

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27.5969799999999985 0.000000000000000 0.000000000000000

0.000000000000000 15.713029999999998 0.000000000000000

0.000000000000000 0.000000000000000 12.950260000000001

C H N O

17 16 4 2

Direct

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0.5032056640048232 0.6071196706179176 0.5247353371806034

0.5507239694348788 0.6406816230416632 0.5316311262478014

0.5901042832296379 0.5875661587884784 0.5248035258820120

0.4604202788388274 0.6561431234773837 0.5315581788128967

0.4156728055186947 0.6176654276361274 0.5248606768282117

0.4149796821492416 0.5278720484880255 0.5111038457249881

0.3247375985469181 0.5095403039793651 0.5045550261765258

0.2435360079180717 0.4594667856868077 0.4920274977609621

0.2169075729822502 0.3759680379986019 0.4783175181003763

0.6686620526097456 0.4514122327432464 0.4936243392290279

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0.7005501463745472 0.3925480565001853 0.5394015639130011

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0.7745154225388705	0.3539074748653216	0.5622288706668974
0.8087468693793114	0.4733950441301741	0.4577736930183660
0.6065471096831299	0.3790427031545893	0.5145715609693292
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0.4541930770372510	0.4790714649870845	0.5051789847928536
0.3719867842287072	0.4814157229139271	0.5023902864893043
0.6187253587027883	0.4398154642415844	0.5072012334119514
0.3107041357939369	0.5828081344868001	0.5159203732905737
0.2950701996988913	0.4405785525537570	0.4916638386666209

Product

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0.000000000000000	0.000000000000000	15.293298000000001

C	H	N	O
22	33	1	6

Direct

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0.2721896069119079	0.3290510145152973	0.4636836487490287
0.2418009483846503	0.3384664232035741	0.3746007082597282
0.1732245449984393	0.3545369010993046	0.3845992740678214
0.5102146733766181	0.3374074723295760	0.4225470663874170
0.5281836762711323	0.3715672536221275	0.4974476836892618
0.5688626851906533	0.3077397725384002	0.4053770758206313
0.5861613776630198	0.2716218732655596	0.4703109863067345
0.5357811300597204	0.4192229242201361	0.4661099001131040
0.5566271540749772	0.4539130685005152	0.5337430491462557
0.5446275457454296	0.5015313270475026	0.4994231492575493
0.5730010727049530	0.5392108361903958	0.5553786453366630
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0.5740709563137578	0.6623555026267419	0.5362169438144589
0.6204594114628685	0.6964238840401366	0.5725695245266007
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K2C03

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0.000000000000000 0.000000000000000 12.492649999999994

C O K

1 3 2

Direct

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0.4991685870727470 0.5758799294495438 0.4120560474378590

0.5037822108678575 0.4253561842001508 0.4104025529180418

0.5008529215319999 0.6618193869186236 0.5758620556015537

0.4929001741320436 0.3372375275313080 0.5725934128466259

diUPy

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C H N O

26 40 8 8

Direct

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0.4135882113415008	0.6553052412436196	0.5599886343764159
0.4595315268066463	0.7553210704311637	0.5687696535887348
0.3654712296831705	0.6830985863807968	0.5592411833883726
0.3433831601618014	0.6833709600664142	0.4729184909479263
0.2953091945416522	0.7123929985983342	0.4718583251413093
0.2265939057304762	0.7273818376837037	0.3904440562303523
0.2079428473474657	0.7091324749835202	0.3066514456677301
0.5842057696935236	0.5994161828843451	0.5669733638864946
0.6692888951315731	0.5882146288224573	0.5702600526119561
0.6926914484603915	0.5925580849430088	0.4855684709723929
0.5826135736800140	0.4071464357188819	0.5526718639059763
0.5012399970416692	0.4006582959397920	0.5569734635634980
0.5448114155862042	0.3081635651548435	0.5519405452871319
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0.5399017374678613	0.2404195732525479	0.5501156328622544
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0.7063023732907209	0.2938105686973662	0.4618627558569223
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0.4816781704760016 0.7719934594186876 0.5180388583858248
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0.3658043903138842 0.7294873816816478 0.5839055031872693
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0.4695265087505771 0.3191489320221593 0.5566937738325197
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0.5177096054873727 0.2263938060232140 0.4979817020342172
0.5738196737136304 0.2177575744278639 0.5442901541875826
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0.3294916673346311 0.3705955107961736 0.4389239029805976

0.3084112282874734	0.4466238769190992	0.4458476463515196
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0.2728245308179827	0.3852684605709152	0.4803222384461456
0.4599975001407166	0.5608094150804347	0.5585962796991237
0.4964009277459422	0.6566618705171452	0.5648745710242695
0.5412474858865791	0.5679764080633172	0.5628704576390724
0.6220640419055267	0.5633003736174299	0.5665278803097895
0.5392628841344539	0.4350536195656815	0.5560779684226489
0.5028882756594055	0.3390625583008853	0.5548525620996517
0.4580705619885778	0.4277662160489259	0.5599340747150674
0.3772752027605140	0.4325502495055399	0.5631677086294112
0.2732163321455815	0.7012437708819249	0.3989820428460548
0.2781074747636895	0.7423827524463281	0.5275835464358664
0.5858668970411968	0.6563918442905943	0.5711888754275526
0.3800446049530611	0.5571033294060175	0.5522023015735544
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0.7255082433501306	0.2656061183632689	0.5172836015290642
0.4132939268257990	0.3392853690030361	0.5617868896032983
0.6192176515004981	0.4390632035920460	0.5510477869518455

UPy-NaPy-complex

1.00000000000000

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0.000000000000000	22.116499999999985	0.000000000000000
0.000000000000000	0.000000000000000	16.005520000000006

C	H	N	O
30	36	8	6

Direct

0.5542509230248575	0.6278153833545995	0.5428688530820676
0.4724452462607681	0.6393760515168804	0.5435393498084637
0.4769572985783725	0.7033068973288070	0.5559673936979052
0.5227798206319277	0.7279319174361394	0.5625467708536285
0.5613040631208203	0.6912106577485355	0.5556160039204233
0.4355673343871223	0.7380632925300222	0.5622399363556986
0.3922336359624581	0.7110142478117281	0.5556000626503392
0.3906931843145960	0.6474938436302283	0.5415703255672459
0.3036135451582360	0.6420625652055897	0.5382416739892770
0.2226011410740952	0.6165662657171583	0.5298717317094059
0.1922172334126397	0.5606172942411872	0.5222231749694054
0.6396542715712136	0.6035630947489701	0.5298758807952174
0.6559911312832830	0.6498394254405183	0.4770068106407156
0.6727240697665874	0.5675016473176721	0.5724200706811693
0.7041981818785078	0.6607536455260300	0.4691976449710995
0.7208064197830150	0.5783886243888847	0.5634132071559286
0.7369024277612690	0.6253770070319756	0.5124234783888747
0.5457358738453029	0.4392987771315010	0.5422129904358899
0.4629711957209275	0.4415616534606674	0.5098939978758383
0.5018007952916659	0.3494320416072290	0.5048893654682551
0.5444653032207929	0.3749547630984775	0.5268864523232411
0.4951821118265286	0.2832626757238885	0.4868279872098887
0.5909048568101767	0.3423209580071086	0.5325123204343861
0.6206422238205330	0.3536721029108615	0.4539715247231941
0.6686560720019795	0.3241567722547098	0.4565071582170297
0.7416870802771250	0.3157032852673224	0.3834643275501076
0.7639768731793566	0.3391784247209717	0.3039484099304247

0.3777251040870280 0.4601076709633615 0.4789472631710407
0.3232840263306662 0.3789071834837317 0.4411046679969834
0.2941236138074992 0.3612590852390000 0.5176840821812158
0.3496924458128806 0.5719664911804274 0.5142010440826531
0.5268767211339226 0.7763224348685357 0.5742065882534076
0.5968213836260785 0.7088665535415444 0.5624697723048034
0.4383391601489736 0.7867978062239739 0.5723273179986863
0.2158975750059484 0.6490610337079374 0.4791522862777406
0.2169300192663476 0.6403229134237776 0.5893947740077705
0.1549139944250538 0.5735182908531903 0.5261649731928534
0.1980317539773084 0.5376755028641624 0.4622690445619042
0.1997441247875079 0.5284824500526238 0.5727989658727909
0.6309967932573666 0.6763540515222314 0.4405299592323763
0.6601458546493545 0.5308485125599950 0.6121627739839007
0.7162539334740337 0.6967972979596859 0.4278347690655545
0.7458805149437610 0.5499911712621808 0.5970120731551809
0.7745245613642479 0.6340186636211705 0.5059044421514532
0.5847033845060600 0.5434250368298207 0.5490550630016233
0.3594665706905821 0.7360603556419983 0.5601073675034031
0.4736952234521018 0.2623841764652039 0.5362855202332634
0.4756801373375218 0.2777518022255409 0.4280147173428180
0.5284060725192431 0.2584220156308743 0.4823720265703449
0.6103845555367462 0.3592008516049005 0.5870951213364148
0.5861171651942013 0.2936013917897932 0.5420161095751745
0.6023730472542913 0.3370374357291215 0.3976889941538729
0.6256330438886940 0.4025029747315722 0.4442284535995491
0.7616187909296220 0.3289504907612466 0.4394878280352723
0.7386049950919035 0.2661234191852715 0.3838400582897633
0.7668337393912411 0.3886909638465501 0.3048920361903681
0.7995585204072840 0.3202591593983101 0.2972916146164148
0.7433214778306545 0.3259908430106727 0.2488750843519159
0.3050525098165927 0.4144192181725715 0.4056803955922394
0.3278819404955389 0.3398092763294439 0.3993903513466439
0.2892815631074963 0.4004190173302231 0.5589823093617990
0.3112786608175785 0.3250247604938818 0.5534962983660395

0.4270184682259027	0.5236652925326186	0.5131140897835061
0.3987629672484415	0.3732611651177751	0.4694581877762488
0.2591465738842000	0.3451482557644810	0.4983761097874768
0.5046387645711305	0.5182652884691108	0.5364135635752002
0.5109603475831598	0.6027661432262645	0.5381159449218469
0.4293870190408388	0.6125649984772917	0.5362406508902000
0.3482239656489545	0.6173850632691025	0.5319563833946406
0.5916816887448906	0.5891515581607353	0.5385269511749688
0.5035296717510389	0.4705613893909971	0.5314099762598494
0.4611466455744362	0.3825232773736164	0.4976592946650143
0.4237787655274560	0.4774341129843616	0.5014103838795465
0.3700465484957996	0.4012662311050810	0.4620729971388903
0.2930531252671565	0.6947448815434106	0.5532375977180193
0.2713965023545217	0.5972858975723069	0.5253973774296852
0.6946638376358870	0.3415423997402826	0.3891765280440319
0.6828385305035799	0.2892925248528041	0.5100902278148223
0.3465791930644677	0.4997758305455008	0.4753124286419336
0.5821020925486747	0.4676020722120570	0.5633602567417718

NaPy-K2CO3-complex

1.00000000000000

26.389109999999987 0.000000000000000 0.000000000000000

0.000000000000000 21.427600000000018 0.000000000000000

0.000000000000000 0.000000000000000 12.003890000000002

C H N O K

18 16 4 5 2

Direct

0.5952384039500223 0.5814712490833359 0.5318848807235581

0.5079831852091904 0.5905097187969771 0.5239966716130631

0.5108746858688343 0.6570512662872964 0.5370340205414420

0.5593108255225874 0.6844355448688543 0.5516198259235517

0.6013679092264220 0.6472942395387511 0.5490722259733798

0.4657392203463085 0.6921173043411960 0.5330683511588998

0.4203352532825756 0.6619653173816091 0.5168216100316777

0.4209101849584350 0.5959417666671381 0.5063350617733385

0.3555910528884483 0.5091579563872372 0.5060250996987287

0.2788075315372938 0.4501955269666126 0.5057440923420260

0.2224673178182871 0.4625253219659174 0.4965067935409635

0.6535568207416532 0.4859979337818394 0.5116249733999986

0.6198440911007691 0.4357135738381261 0.5220612675842986

0.7052243352214639 0.4738850913603165 0.4902021755686193

0.6377824463462420 0.3745018359159719 0.5126762166534032

0.7227460764083105 0.4129100166532313 0.4805809994402322

0.6891017994629640 0.3627459381851379 0.4921777004596159

0.5220072348758155 0.3032486354907115 0.4321518302532161

0.3448809739881897 0.6000283662784065 0.4722047711217855

0.5624333275826429 0.7347848233834936 0.5636551417203355

0.6392286563492201 0.6669691349759569 0.5594420372087400

0.4672992957464028 0.7427513874635401 0.5426745488564910

0.2895824136120445 0.4331002450937603 0.5887304007697234

0.2920396731721746 0.4160105734981913 0.4439254362207982

0.2016097075438922 0.4190203630727968 0.5120571806698968

0.2101634633793929 0.4972666007496473 0.5581414803365821

0.2123021523152161 0.4794764947337488 0.4130966481867049

0.5800667066477311	0.4449979889447049	0.5373855356920966
0.7316316031927999	0.5129170796186884	0.4813932921633224
0.6111374561001278	0.3356524693202991	0.5204879755508519
0.7628909306724594	0.4046825026743799	0.4644692069747569
0.7028775085730212	0.3148389707493351	0.4866666698194841
0.6709045814458986	0.5775214809069062	0.5254682536176317
0.3846657986268201	0.6875802202653178	0.5135527815357757
0.5501536941380021	0.5536252585645827	0.5225045055327951
0.4624448801700402	0.5609628936009881	0.5100742641028561
0.3729993818167527	0.5690272498090958	0.4883373234429246
0.6402713769221455	0.5489739313244519	0.5239494670521735
0.3798736118675199	0.4635388586048781	0.5357111998245030
0.3046192617154595	0.5092218985418525	0.4857987416963083
0.4894622736744723	0.3023210207668575	0.5115135486776909
0.5236044392820901	0.3528684244737507	0.3640262299953342
0.5548659521343690	0.2588320722284201	0.4162311318700945
0.4734567779118368	0.4200608996703373	0.5005561833892630
0.5956657266536329	0.3112805531753610	0.2583722472910489

UPy-NaPy-k2co3-complex

1.00000000000000

27.596969999999989 0.000000000000000 0.000000000000000

0.000000000000000 21.685919999999994 0.000000000000000

0.000000000000000 0.000000000000000 20.380539999999999

C H N O K

31 36 8 9 2

Direct

0.5635003229591645 0.6240726621596392 0.5573819978740805

0.4794598035752519 0.6362622019771192 0.5566663989331878

0.4841394168507788 0.7011944364528374 0.5688120413908941

0.5313289532177625 0.7259173916337858 0.5754879831411520

0.5709011461454232 0.6883377700400178 0.5695691040942124

0.4415843622218853 0.7365027216986356 0.5749592879503587

0.3968800380373825 0.7091059809165168 0.5690820257335190

0.3952616805503157 0.6447876940004603 0.5557579033173548

0.3054840666443867 0.6382201944935488 0.5558161039468715

0.2221885646322776 0.6108627389133755 0.5508347456512300

0.1915417170074173 0.5534876179880220 0.5424956501942786

0.6514148110605554 0.5996783360931035 0.5474178571627614

0.6679538864932472 0.6470551062789862 0.5059171264863129

0.6856514751972500 0.5634939885395674 0.5811951223543577

0.7174802178714131 0.6586986201230665 0.4998431019644152

0.7350765895345297 0.5751009097205800 0.5741369301921402

0.7513549927195906 0.6229900406683037 0.5338723333500488

0.5541268655351240 0.4304160955196824 0.5538159333648627

0.4697318895942948 0.4352829182409071 0.5241781831023368

0.5081000929657928 0.3401805356578448 0.5222129350558824

0.5520420801673372 0.3648342851527542 0.5418898580279335

0.4996764427813940 0.2729619468494157 0.5078131102008382

0.5973578036012985 0.3275443979848655 0.5540107030412403

0.6441961450776759 0.3481470815652031 0.5188163631538941

0.6409896592215952 0.3557901542621848 0.4454613783967825

0.6859530075917650 0.3565912568553398 0.3456242418327353

0.7338941408945313 0.3336355262184955 0.3192931940256823

0.3824584862550068 0.4559657969037794 0.4992125208594383
0.3246881718821623 0.3728603621111521 0.4756494758771457
0.2963905339613148 0.3551651965177725 0.5374514444437295
0.4931123949641276 0.5453855062511359 0.2788184490421210
0.3531916615017807 0.5683142809765197 0.5319975696873027
0.5356385077984133 0.7749345196224448 0.5864395013276853
0.6074686611484923 0.7059273416626295 0.5764337470465768
0.4444617439875911 0.7859037913906516 0.5847465867537398
0.2146964841350142 0.6454193763224453 0.5126134243564060
0.2163721122857280 0.6330808628892085 0.5986867504479133
0.1529839035706471 0.5657719653451029 0.5457497110013684
0.1979928130103946 0.5318234220616488 0.4945876537462461
0.1994988463053849 0.5195313650687577 0.5809875866697616
0.6420531942994101 0.6739003018447132 0.4773323234809915
0.6728939412258045 0.5264685444443735 0.6130299439301107
0.7296695851142195 0.6955851719379590 0.4673812510961732
0.7610744436450181 0.5467020208196062 0.6008925414220803
0.7900241923042300 0.6321463398339082 0.5286871436921748
0.5948449186237202 0.5379672532123136 0.5617616620222907
0.3631684990822202 0.7345170755942406 0.5741140130359049
0.4806170895292812 0.2509495806051543 0.5491275407766267
0.4760562534216070 0.2686348645751151 0.4647017921226530
0.5329905286518557 0.2470056021047899 0.4986800230518331
0.6055939106028201 0.3292150249570460 0.6069458510767592
0.5903712180339785 0.2788872928781682 0.5426751221146363
0.6546246660482451 0.3939206508327860 0.5377452016223246
0.6738809466911501 0.3162323815947977 0.5305732809266226
0.6548978354970448 0.3353526304868051 0.3205883693325698
0.6825513765617565 0.4069625073114103 0.3407616956641901
0.7356534279758972 0.2830560750589007 0.3194929365349573
0.7382875365857497 0.3495771385764540 0.268437764981730
0.7642687530118791 0.3517166707113161 0.3482821206940402
0.3052594738153987 0.4088747694203737 0.4483895922399977
0.3286223450674224 0.3327394048045099 0.4430409716838442
0.2913354192915170 0.3955189573444016 0.5693119617248010

0.3154666982876498 0.3193714406530638 0.5656149816492372
0.4338309035447519 0.5196857734599086 0.5263677849152149
0.4024968690310933 0.3667687614605921 0.4961045692047807
0.2604354843969603 0.3371714164091094 0.5242276362255621
0.5132820801383375 0.5122619548356313 0.5466676258954348
0.5190126448992829 0.5988700735967972 0.5518597678200647
0.4350678966690000 0.6093808010092870 0.5494260963763443
0.3515064135323417 0.6140334662637267 0.5478110010826144
0.6020561086402365 0.5845265243222201 0.5537867466328221
0.5117513184028740 0.4636602867288350 0.5419545467774078
0.4671412635351733 0.3751198788494643 0.5145432279062031
0.4299697090357213 0.4726483231335641 0.5170706760810361
0.3731589508353401 0.3957088962094038 0.4899787684291229
0.2944091365487251 0.6914448790753178 0.5696164279521508
0.2725963789083912 0.5921859988187357 0.5457931827575717
0.6833521670393758 0.3415961243689767 0.4154330641607693
0.6055905648504704 0.3752940145606133 0.4153714498283982
0.3515859495373541 0.4977805771687818 0.4930244643919644
0.5912734550779299 0.4586016114349851 0.5731136802050797
0.4859680631984827 0.5321860965995334 0.3431144402500548
0.4629840003584312 0.5823847999865206 0.2503860847783611
0.5294200303916243 0.5205461143275696 0.2491186827392512
0.5582480108447057 0.4642062773174451 0.3464654894664870
0.4131418542600331 0.5974392533332962 0.3482704545314978

diNaPy-k2co3-complex

1.00000000000000

27.116849999999995	0.000000000000000	0.000000000000000
0.000000000000000	21.613759999999992	0.000000000000000
0.000000000000000	0.000000000000000	20.743289999999982

C	H	N	O	K
35	32	8	7	2

Direct

0.5844563822556641	0.6916418799146880	0.4290191139946913
0.4993622556618078	0.6953616253332748	0.4208553426942822
0.5020100824484240	0.7204026098905822	0.3567863106817592
0.5493908369865610	0.7311792601858823	0.3300438835267993
0.5903075391935493	0.7171357802644704	0.3655162462152715
0.4577433877223808	0.7327182404257787	0.3236477294048712
0.4132946414605940	0.7206900184189635	0.3531999825661492
0.4141217414729431	0.6961358933471514	0.4166391087376644
0.3521351812513321	0.6668178005998969	0.5037267135616194
0.2782649724755765	0.6439924192103278	0.5620854856760382
0.2231076916573957	0.6446741559555564	0.5506732344675445
0.6415771655297250	0.6518192998956965	0.5190842652473967
0.6084452841105271	0.6350524809016953	0.5678127903856262
0.6924388351094262	0.6417555036321266	0.5284631077394378
0.6257024614419996	0.6081759525555638	0.6247583213493302
0.7094825287023717	0.6154957691315521	0.5855238582814991
0.6761669004935501	0.5985822815120928	0.6339326963757012
0.5160147114767879	0.5132242944748711	0.6395889480673094
0.6640235982380471	0.3487872040838536	0.5292056032729997
0.6315418768681794	0.3871226030684902	0.5633560420387707
0.7138624372268476	0.3458311742607374	0.5481402124950563
0.6482582076299767	0.4207545937791168	0.6165571367035481
0.7304811867545253	0.3800447386192360	0.6006841257105716
0.6976733425651328	0.4172826888649627	0.6354239505501859
0.6067885727057706	0.2947599949857926	0.4483833709710842
0.5215900439160456	0.2905231353682613	0.4435045666798837
0.5231039987523093	0.2512922072415970	0.3876327802875714

0.5699802713969904 0.2346547149339316 0.3627403365704279
0.6115792932912084 0.2561045873351174 0.3924662129659996
0.4782076748732153 0.2316381490607240 0.3602139815999897
0.4343472710709972 0.2505736104656666 0.387226668946110
0.4363805770273127 0.2899198554514769 0.4419635378489740
0.3767661846394623 0.3396150458141141 0.5209565655583326
0.3058955544820091 0.3861088126929673 0.5699175016105135
0.2503819825397829 0.3827014466259276 0.5628110917653704
0.3388367568897666 0.6917785613970333 0.4121982960432781
0.5526732671366305 0.7503052375756331 0.2815048510842792
0.6272678209659017 0.7247668312676765 0.3462281675288493
0.4590616608681546 0.7516248952589295 0.2748726181109007
0.2894166106598614 0.6762878221158841 0.6003540473506208
0.2918398503440695 0.5977268980611540 0.5752942251099674
0.2038016401608774 0.6306680885759985 0.5948993495608098
0.2103325759860465 0.6911887662062629 0.5374029808828590
0.2127106958611412 0.6124611130247780 0.5120285360860459
0.5693354404742199 0.6424639281715324 0.5606117300035049
0.7184907425186661 0.6541500454647413 0.4903113336558711
0.5980730336018697 0.5935521321915286 0.6601828518302717
0.7489604207480655 0.6075743198452904 0.5916980772767834
0.6894540100090925 0.5772527199158224 0.6783118464661270
0.6578870639115071 0.6883580639346314 0.4319978624640657
0.3783329161876521 0.7297502060354795 0.3289287292180450
0.5936170561789098 0.3911938913381466 0.5473885512031437
0.7394601992489769 0.3163386989884128 0.5213603704238344
0.6212669510842996 0.4492447280362729 0.6423564652926723
0.7692556601012438 0.3772647822327602 0.6145602025919521
0.7106642997446492 0.4437391870973548 0.6768574099277305
0.5723390421368697 0.2051226091217053 0.3201410393773444
0.6481868797443930 0.2443081855615695 0.3743405232561043
0.4786012327007067 0.2016348458147011 0.3178423099337909
0.6804447991749817 0.2944387984715344 0.4525679341050850
0.3989091673545402 0.2360015925772592 0.3674841983395804
0.3613646794441139 0.2994978204057975 0.4357970970547695

0.3195787494660401	0.4339931761588217	0.5673488467158665
0.3188280902361574	0.3659909925076832	0.6155189237151657
0.2327268359991486	0.4100180009531859	0.6010648781741882
0.2384159140424029	0.4013020485253271	0.5160679476843876
0.2372747635319283	0.3347696954276547	0.5668168778515297
0.5403341704934692	0.6814826055241279	0.4560749932483009
0.4548905436195156	0.6837313962053091	0.4496707777015112
0.3672773074314442	0.6845455925575410	0.4430834741864394
0.6281030656275289	0.6783905387059369	0.4597401637565755
0.6508098040508827	0.3132149586813357	0.4751461025708917
0.4777732654841396	0.3093339876960669	0.4695774944746087
0.3902689822855400	0.3095011673758731	0.4650623380444333
0.5632051126374169	0.3115609143078646	0.4730898238263669
0.3773361339448403	0.6565080410845279	0.5513643087594279
0.3016688417651095	0.6626559511273162	0.5021199605927382
0.5415572753461673	0.4666353122652737	0.6604290443530736
0.4853805639253630	0.5048603422194182	0.5904953169607238
0.5199561741318878	0.5678152364899507	0.6648288704600361
0.4026791211296564	0.3529709459644121	0.5670308654655213
0.3272320309429153	0.3516191331586588	0.5165695784967661
0.4975267244115283	0.3877573186102454	0.5862239975040511
0.4716873828313046	0.6200980474633770	0.5726529887822485

di-NaPy-k2co3-product-complex

1.00000000000000

26.1067000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	25.8878799999999991	0.0000000000000000
0.0000000000000000	0.0000000000000000	26.8407200000000010

C	H	N	O	K
57	65	9	13	2

Direct

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0.4542733405835725	0.5129501408581257	0.4089210889948137
0.4704679037893203	0.5542324332825282	0.3811687973337203
0.4249298600604058	0.5838084666512509	0.3645116285187677
0.3294746506954707	0.5738013604220576	0.3769201261535677
0.3058950026284240	0.5595344953788028	0.3264886429001630
0.2501892222185190	0.5773514433019727	0.3228147318166604
0.5227955634786969	0.5731827915264882	0.3674709998087113
0.5448004992431262	0.6100389273532937	0.4071795730945219
0.5595291031205968	0.5283469943505712	0.3559608719895871
0.5480581516357628	0.4985168827431223	0.3089371212637856
0.5634981604111630	0.6621788746622946	0.3882634919837171
0.5662823345840081	0.7042606084412345	0.4281630833381098
0.5135945239273234	0.7291992586210092	0.4392217418437905
0.5025680976866778	0.7374721847592712	0.4948655316376978
0.4920081862043113	0.6860830028185820	0.5200597373246405
0.4877057240913820	0.6519172507226748	0.6022746404022009
0.4760962654534716	0.6648528059987838	0.6560299148604837
0.4718196382125521	0.6176177666035382	0.6898202288699018
0.4589125572147310	0.6324453884073996	0.7435619911266663
0.4544598120568449	0.5860857753705934	0.7786883118717368
0.4397982689058967	0.6012783613136572	0.8318676554451382
0.4848693455905184	0.4283856516756820	0.5658631499277448
0.4251619220882530	0.3168472333947831	0.3900612691644341
0.3853877543689833	0.2919724322841291	0.4632169256373491
0.3988408324513280	0.2388832327457289	0.4555594948927104
0.4264295967516477	0.2265861737492930	0.4116822526335686

0.4397998143953846 0.2648962620792693 0.3787667656744235
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0.3457544709252040 0.2731905801922659 0.5376494615432303
0.3031631484552743 0.3378071903514182 0.5940591617757679
0.2662541940639754 0.3825949229444933 0.6626969260443322
0.2438711341198091 0.3704586589760294 0.7133783918807710
0.4687951399424674 0.3591171350361383 0.3173257901281978
0.5168677397121678 0.3346186199602821 0.3181053642837514
0.4545899280612348 0.3878328606049539 0.2750597451098916
0.5492526796184199 0.3378792624570105 0.2768678269825524
0.4875166488852933 0.3913773958244216 0.2342808856111653
0.5348511751470235 0.3661089875538640 0.2347269287628240
0.7135311226922059 0.5335915219344697 0.4795397528786023
0.6944536510351349 0.5008135943781152 0.5576240052818437
0.7470505200632303 0.4876072616351597 0.5665182377723030
0.7830851603312016 0.5003322924503258 0.5290646372752668
0.7670801320459101 0.5235781640003342 0.4858480083188139
0.7591096690603840 0.4616827655404812 0.6113370548169873
0.7208466934526995 0.4506179086950081 0.6448542162751781
0.6698892988216021 0.4666410253502254 0.6332891628566251
0.5830145092453820 0.4750183881466395 0.6720677901745381
0.5007957331530966 0.4535423586269264 0.7050592623300417
0.4808202132301017 0.4288110695821098 0.7523290891585307
0.7223548824554592 0.5742332691431337 0.3956977214214914
0.7616860180302140 0.6103450308910908 0.4042406735645470
0.7094752694321884 0.5615492057633530 0.3462777523172380
0.7879614407744826 0.6323249803902203 0.3642558551389161
0.7355491715219743 0.5843004384067250 0.3065739387427943
0.7751409777506171 0.6195510096798100 0.3152001742672274
0.3283739333177347 0.6160028971381546 0.3819881596774393
0.3076563191870213 0.5556883410143872 0.4073283644281772
0.3082587157589557 0.5173618214886033 0.3215303798893118
0.3289053079616401 0.5773166817691242 0.2967036457456906
0.2335023024427009 0.5675615460749759 0.2864409255305880

0.2263678896654114 0.5591042325980760 0.3517122120994012
0.2470766631712822 0.6194691793807297 0.3275480419712128
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0.5641228984731205 0.4594823638209380 0.3112246122123628
0.5069209990882526 0.4968996242658787 0.3008833382399629
0.5667099958150554 0.5188161924364948 0.2776819325387985
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0.6018648924852315 0.6542581902130701 0.3723372045684059
0.5935794163218781 0.7341756195742647 0.4162641762956755
0.5823576027886468 0.6869837018332964 0.4622020500166741
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0.5107757197114884 0.7664319140081592 0.4196442127990855
0.4693259675151897 0.7632036456067072 0.4995521412752487
0.5353652847587357 0.7565582514835143 0.5130520273416344
0.5237592124006342 0.6587262800685663 0.5155009898337218
0.4575159641334696 0.6676920489963162 0.5043596887341606
0.5065886419726718 0.6910778058213525 0.6691623213799112
0.4407485315229171 0.6881302322888599 0.6567644829496870
0.4421201682739235 0.5915384758770249 0.6750095830783286
0.5078000860045612 0.5954919708249182 0.6883318787116687
0.4884169639034491 0.6591385073981469 0.7580196086663271
0.4225619707133761 0.6543330029913011 0.7442488236110215
0.4258557884026156 0.5588318085977971 0.7636874763403552
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0.4371475881192810 0.5673651559798258 0.8563930403740235
0.4682341001870536 0.6277790595496752 0.8481124107807794
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0.2105919872083669 0.3446923434800960 0.7102245543477936

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0.5604029595623781 0.3686267991859049 0.2026805254671167
0.4159303879576149 0.3902238510010228 0.3673419972785897
0.3446824872763540 0.1924197665855029 0.5622693293880169
0.6388485925921927 0.4234372515213183 0.6901417627582748
0.8234307649868902 0.4905210980908381 0.5344052612306857
0.7939045626517798 0.5321823769442506 0.4559537938033130
0.7987442477299729 0.4506473133907010 0.6189388587254269
0.4841994440007697 0.4365110493139452 0.6710764880534009
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0.4390974429160981 0.4341832288094978 0.7543210188670203
0.4886592438986402 0.3871151565714670 0.7528107470225487
0.4979742296444292 0.4463073090296303 0.7857401573623704
0.7708974235214222 0.6217636794116099 0.4423057223273895
0.6792696627622571 0.5332594909018167 0.3397130731870502
0.8183208669666494 0.6602901262529041 0.3715904496238522
0.7252234233843119 0.5738067485333004 0.2684878838469193
0.7956862767267322 0.6369759594564378 0.2840736404429202
0.6566320608362077 0.5443552774428060 0.4288049357430484
0.7288820216374641 0.4308621512188118 0.6798850060489493
0.4764924084953857 0.4842419248739402 0.4292557014682012
0.3822698807063367 0.5572401926102293 0.3827643730738147
0.3986845880419473 0.3296321907043234 0.4307504373075721
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0.3195967569109155 0.2888654210338838 0.5804316348458721
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0.6786634339204273 0.5231647266302638 0.5145530602442727
0.6570897337147610 0.4907539578267938 0.5915773460868282
0.6320798160304449 0.4544202573654100 0.6679429496693620
0.6944989893115093 0.5521739939251953 0.4350854957094223
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0.3676608812985143	0.4813831048171862	0.4278326562429384
0.5482987965452841	0.5967328136239811	0.4508167942376071
0.5968507546929519	0.5181905090496247	0.3818982655974177
0.4830956793898090	0.6945336233384558	0.5729287965485070
0.4997429288607008	0.6093365266709224	0.5864088171169396
0.4813985801179798	0.4521136332859403	0.5227084355732327
0.4442466388147916	0.4096222352932771	0.5866662842691803
0.5290363527553986	0.4252170835488693	0.5870974035099016
0.3048140119633793	0.3774480038299375	0.5695886227139696
0.2832275048434254	0.3340009957917084	0.6410340815815352
0.5684160702409432	0.5156069912126668	0.6537117846623685
0.5558936659531677	0.4440188107225342	0.7029952059436081
0.5559809629907424	0.5190305088427355	0.5500729525435718
0.3843402981081405	0.4176349895696141	0.5085766425192744

diUPy-k2co3-product-complex

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C	H	N	O	K
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Direct

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0.4210709385320259	0.6774693503386986	0.6768646680115139
0.3774359573713323	0.6456500490451076	0.6725520387877982
0.4225314789757511	0.7365991347715196	0.6771494175648505
0.3216143706315889	0.6656150396933834	0.6686986960420037
0.2914951508265196	0.6518363000763659	0.6087864678506065
0.3206783143652160	0.6679121804518414	0.5516363585410908
0.3267161693858607	0.7298296172603552	0.4695120559901267
0.2948083806807532	0.7751319303375093	0.4438151130290305
0.5724365099023855	0.6128870364795638	0.6896903689837987
0.6685132302896865	0.6110360399560506	0.6966765130159390
0.6937672045639094	0.6193945714427191	0.6337216193670959
0.5858596612064230	0.4472071101017428	0.6740336689148891
0.4955280874466989	0.4334704224909177	0.6637088711654329
0.5527548725192131	0.3596161962484255	0.6494237663591250
0.5954728732482409	0.3913918621677429	0.6608325131426068
0.5530925693012326	0.3021837346840198	0.6333422884692463
0.6518561944723889	0.3728113064378794	0.6616027190565016
0.6864999231597885	0.3945358399446314	0.6086541730400188
0.6653746969609431	0.3801931085157919	0.5462962997186460
0.6616419931521116	0.3140076249389726	0.4685656591505155
0.6843583117116090	0.2597941918462280	0.4566716786569029
0.3991636122538692	0.4198793070097270	0.6599007221724028
0.3024439694867292	0.4203078968879761	0.6603258794979205
0.2657602576898127	0.4485932388169557	0.6155858336383304
0.4606901800928360	0.4989801237969240	0.4068803204156389

0.5097636102437105	0.3402338536784313	0.2743387493373804
0.5470550476867760	0.3758281186162149	0.2377525171665243
0.5232682572778465	0.4308725545570152	0.2256001248609996
0.5643422840834627	0.4752873386175987	0.2198371644324244
0.5858101093329021	0.4880097679580719	0.2830297684706806
0.6410065161393779	0.5493524664039147	0.3342977163877271
0.6747903048696410	0.5983191584459311	0.3280505378455950
0.6779282884031759	0.6305947003412050	0.3871813011048437
0.7135414612993599	0.6790576675774338	0.3813360157217391
0.7166675541785285	0.7117532153259299	0.4402204719944035
0.7520217400038460	0.7603498932417002	0.4341678608258662
0.4696519502656685	0.3180742526384810	0.3809886950926893
0.5165445940049136	0.3424811243616299	0.3432559258149664
0.3804286337182729	0.4201145234893683	0.4549316753653929
0.4255609063957908	0.3828248091625984	0.4594015754876575
0.4333017141626928	0.3606577667414609	0.4035782906359128
0.3941973306996807	0.3840486701842428	0.3602020857279672
0.3244942253730269	0.4546025817361360	0.3674197219424408
0.2677413364364434	0.4364141693002168	0.3792018817485143
0.2275748911868857	0.4740074370750195	0.3504578615411148
0.4918792621923014	0.2823427545903734	0.4308961981493869
0.4908675377999521	0.2238566874738528	0.4171708007041294
0.5061690643548866	0.6745448164135897	0.6853372662725866
0.4370607368578764	0.7512454546224890	0.7215443778065832
0.4499566038270358	0.7509412699744741	0.6417846250758225
0.3837856423541384	0.7540698046498964	0.6685833220403676
0.2987804413090192	0.6475362759713797	0.7061520860036480
0.3202971090965089	0.7084226397876373	0.6759416912877041
0.2865754851161890	0.6088542949098985	0.6071605433151086
0.2525401468687443	0.6707199394165740	0.6099767987229009
0.3673507928121992	0.7414782628137585	0.4810089266224825
0.3290357660319849	0.6962630799308029	0.4377716826737780
0.2928952171174526	0.8082231899605244	0.4762069979369346
0.3133648828943755	0.7892389849186705	0.4013544798629088
0.2543672770877576	0.7626663405720315	0.4329587494581000

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0.6940308847777641 0.5862079912971405 0.7254784011223897
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0.6989868417771165 0.5816797810812588 0.6096753527023090
0.5296562305409120 0.5404405130308096 0.6830138456235814
0.6165761653469642 0.5438031388036504 0.6909003278523503
0.7327359767469928 0.6380108701434863 0.6387015631557204
0.4676345065426782 0.3607609994115553 0.6463273814275773
0.5268231334130422 0.2800870122287876 0.6642284884631019
0.5383293514543765 0.2966305444571261 0.5862926058917546
0.5926279553466228 0.2850731018428432 0.6362000775593257
0.6702121201184017 0.3867856348998875 0.7043412456035233
0.6539681550702116 0.3295825630115700 0.6618571101887367
0.7266559726302823 0.3788115691609719 0.6138644514538075
0.6874900365255783 0.4376520273799709 0.6118596005658448
0.6182791181549745 0.3139209516490219 0.4699860721060458
0.6739318685218667 0.3427791399823282 0.4336665094989668
0.6719162243479364 0.2315850075185881 0.4920301332090521
0.6702725544580918 0.2453718959724814 0.4120821914533834
0.7276910293452106 0.2607523235576906 0.4555232000241721
0.3099164445894817 0.3796066035466338 0.6456230675718251
0.2841756212760750 0.4184697900424091 0.7062023059238811
0.2826798822580834 0.4486707474421724 0.5692655819832134
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0.4408158039784101 0.4922918386982889 0.6718577549525002
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0.2273301262215412 0.4284992308948320 0.6142056869717607
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0.5158223786370302 0.2980265103217024 0.2630430956329889
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0.5450949005554221 0.5107607432243639 0.2012412940970686
0.5963861396635358 0.4644756245634368 0.1879850097062686
0.6089544507502381 0.4550973874650395 0.3019932842918833

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