
Supporting Information

Modulating Photoinduced Charge Separation in Metal-Azolate Frameworks

Ting-Ting Liu¹, Tian-Fu Liu², Xin-Ping Wu^{1}, Xue-Qing Gong^{1*}*

¹Key Laboratory for Advanced Materials and Joint International Research Laboratory for Precision Chemistry and Molecular Engineering, Feringa Nobel Prize Scientist Joint Research Center, Centre for Computational Chemistry and Research Institute of Industrial Catalysis, School of Chemistry and Molecular Engineering, East China University of Science and Technology, 130 Meilong Road, Shanghai, 200237, China

²State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, China

*Corresponding Authors:

Xin-Ping Wu: xpwu@ecust.edu.cn

Xue-Qing Gong: xgong@ecust.edu.cn

Table of Contents

Section S1. Cell parameters (Table S1)	S2
Section S2. Tests on k -point mesh (Figure S1)	S3
Section S3. The real and imaginary parts of the complex dielectric functions (Figure S2 and Discussion)	S4
Section S4. Missing-linker defect formation energies (Figure S3 and Figure S4)	S5-S6
Section S5. Coordinates (in the format of <i>VASP</i> POSCAR) of the metal–azolate frameworks studied in this work	S7-S76

Section S1. Cell parameters

Table S1. PBEsol-D3-calculated primitive cell parameters for the metal–azolate frameworks studied in this work and available experimental data¹⁻³

	Calculated						Experimental ^a					
	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)
PCN-601(Ni–Pz)	15.4436	15.4436	15.4436	90.000	90.000	90.000	15.4292	15.4292	15.4292	90	90	90
PCN-601(Ni–Vtz)	15.3591	15.3887	15.4176	90.018	89.978	90.214	–	–	–	–	–	–
PCN-601(Ni–Ttz)	15.3832	15.3832	15.3832	89.943	89.997	90.003	–	–	–	–	–	–
PCN-601(Co–Pz)	15.4073	15.4198	15.4505	89.914	90.010	90.002	–	–	–	–	–	–
PCN-601(Co–Vtz)	15.2954	15.3471	15.4006	89.966	89.974	90.237	–	–	–	–	–	–
PCN-601(Co–Ttz)	15.3135	15.3795	15.4144	89.933	89.978	90.006	–	–	–	–	–	–
PCN-602(Ni–Pz)	22.0904	22.1649	22.0905	90.178	89.965	89.984	21.5592	21.5592	21.5592	90	90	90
PCN-602(Ni–Vtz)	21.7332	21.7722	21.7526	90.232	89.959	89.975	–	–	–	–	–	–
PCN-602(Ni–Ttz)	21.5637	21.5973	21.5192	90.081	89.997	90.032	–	–	–	–	–	–
MFU-1(Co–Pz)	15.7904	15.7904	15.7904	90.000	90.000	90.000	15.9630	15.9630	15.9630	90	90	90
MFU-1(Co–Vtz)	15.7904	15.7904	15.7904	90.000	90.000	90.000	–	–	–	–	–	–
MFU-1(Co–Ttz)	15.7904	15.7904	15.7904	90.000	90.000	90.000	–	–	–	–	–	–

^aExperimental unit cell parameters were converted to primitive cell parameters.

References

- (1) Wang, K.; Lv, X.-L.; Feng, D.; Li, J.; Chen, S.; Sun, J.; Song, L.; Xie, Y.; Li, J.-R.; Zhou, H.-C. Pyrazolate-based porphyrinic metal–organic framework with extraordinary base-resistance. *J. Am. Chem. Soc.* **2016**, *138*, 914–919.
- (2) Lv, X.-L.; Wang, K.; Wang, B.; Su, J.; Zou, X.; Xie, Y.; Li, J.-R.; Zhou, H.-C. A base-resistant metalloporphyrin metal–organic framework for C–H bond halogenation. *J. Am. Chem. Soc.* **2017**, *139*, 211–217.
- (3) Tonigold, M.; Lu, Y.; Bredenkotter, B.; Rieger, B.; Bahnmüller, S.; Hitzbleck, J.; Langstein, G.; Volkmer, D. Heterogeneous catalytic oxidation by MFU-1: A cobalt(II)-containing metal–organic framework. *Angew. Chem., Int. Ed.* **2009**, *48*, 7546–7550.

Section S2. Tests on k -point mesh

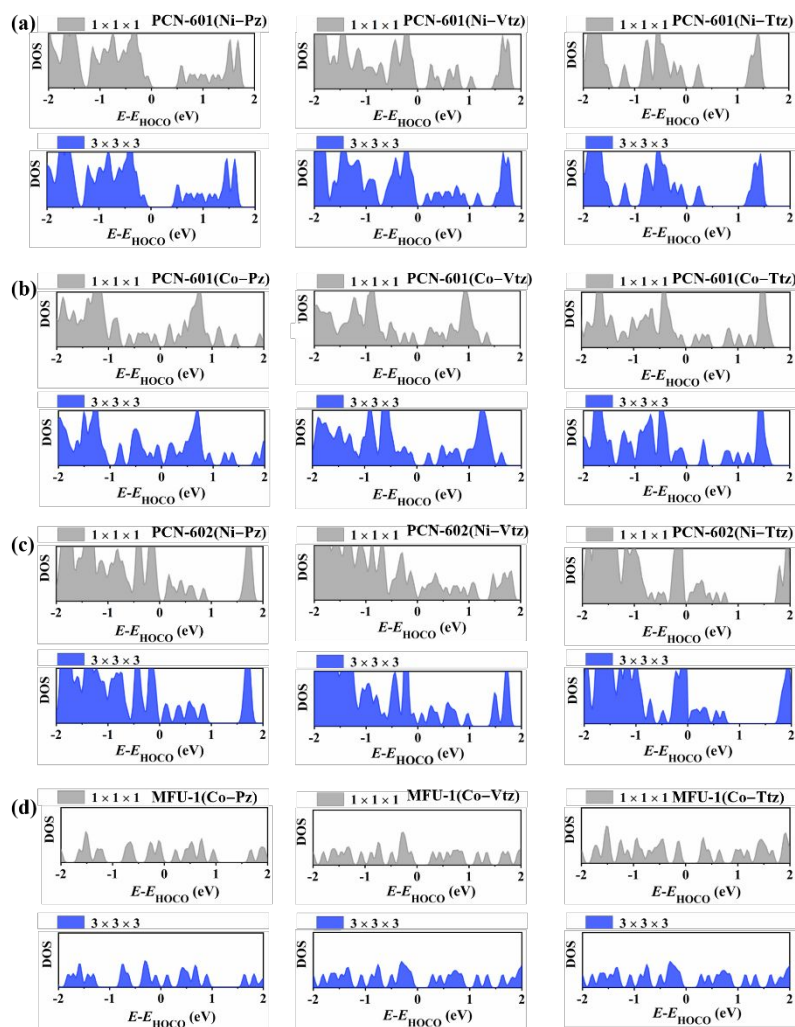


Figure S1. Calculated total density of states (DOS) of (a) PCN-601(Ni-X), (b) PCN-601(Co-X), (c) PCN-602(Ni-X), and (d) MFU-1(Co-X) (X = Pz, Vtz, or Ttz) using the PBEsol functional and different k -point meshes ($1 \times 1 \times 1$ or $3 \times 3 \times 3$). Only the spin-up manifolds are shown.

Section S3. The real and imaginary parts of the complex dielectric functions

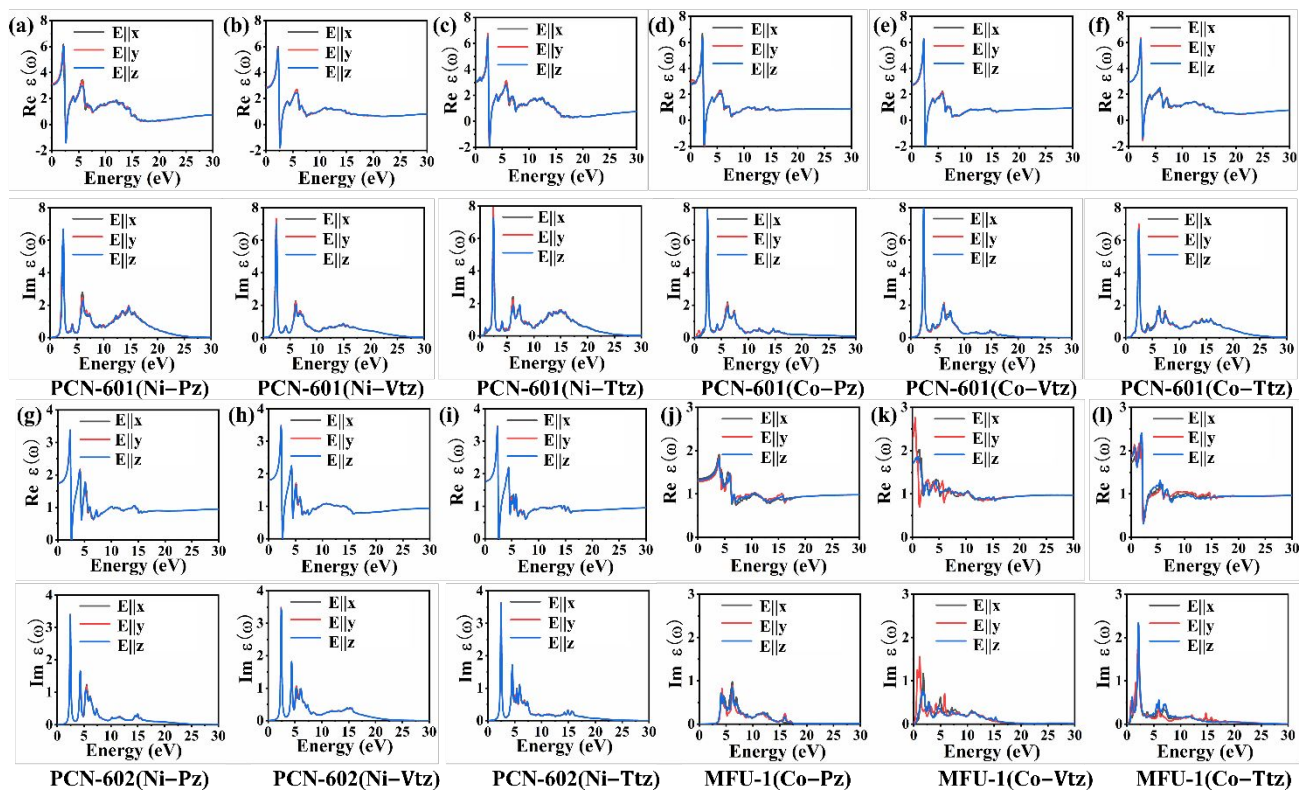


Figure S2. The calculated real (Re) and imaginary (Im) parts of the complex dielectric functions for (a) PCN-601(Ni-Pz), (b) PCN-601(Ni-Vtz), (c) PCN-601(Ni-Ttz), (d) PCN-601(Co-Pz), (e) PCN-601(Co-Vtz), (f) PCN-601(Co-Ttz), (g) PCN-602(Ni-Pz), (h) PCN-602(Ni-Vtz), (i) PCN-602(Ni-Ttz), (j) MFU-1(Co-Pz), (k) MFU-1(Co-Vtz), and (l) MFU-1(Co-Ttz).

Discussion on Figure S2

For the studied MAFs, the real and imaginary parts of the complex dielectric functions in the x-, y- and z-directions ($E||x$, $E||y$, and $E||z$) are summarized in Figure S2. The results show that the dielectric functions of most MAFs studied are isotropic essentially, and only the MUF-1 series have slightly anisotropic dielectric functions. Therefore, the optical properties were calculated by averaging the components along the x-, y- and z-directions.⁴

(4) Lu, C.-L.; Zhang, L.; Zhang, Y.-W.; Liu, S.-Y.; Mei, Y. Electronic, Optical Properties, Surface Energies and Work Functions of Ag_8SnS_6 : First-principles Method. *Chinese Phys. B* **2015**, *24*, 017501.

Section S4. Missing-linker defect formation energies

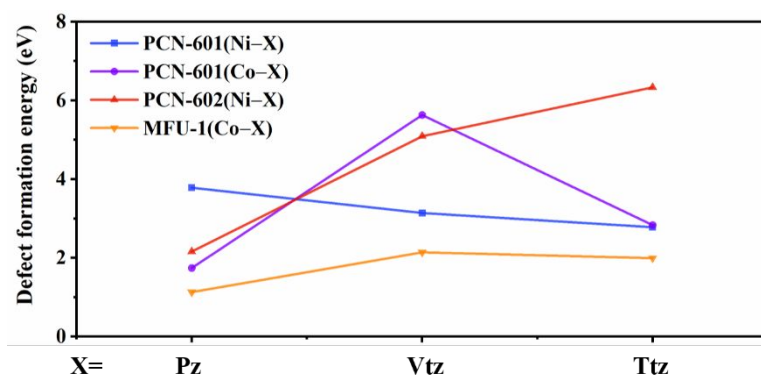


Figure S3. HSE06-calculated missing-linker defect formation energies of the metal–azolate frameworks studied in this work.

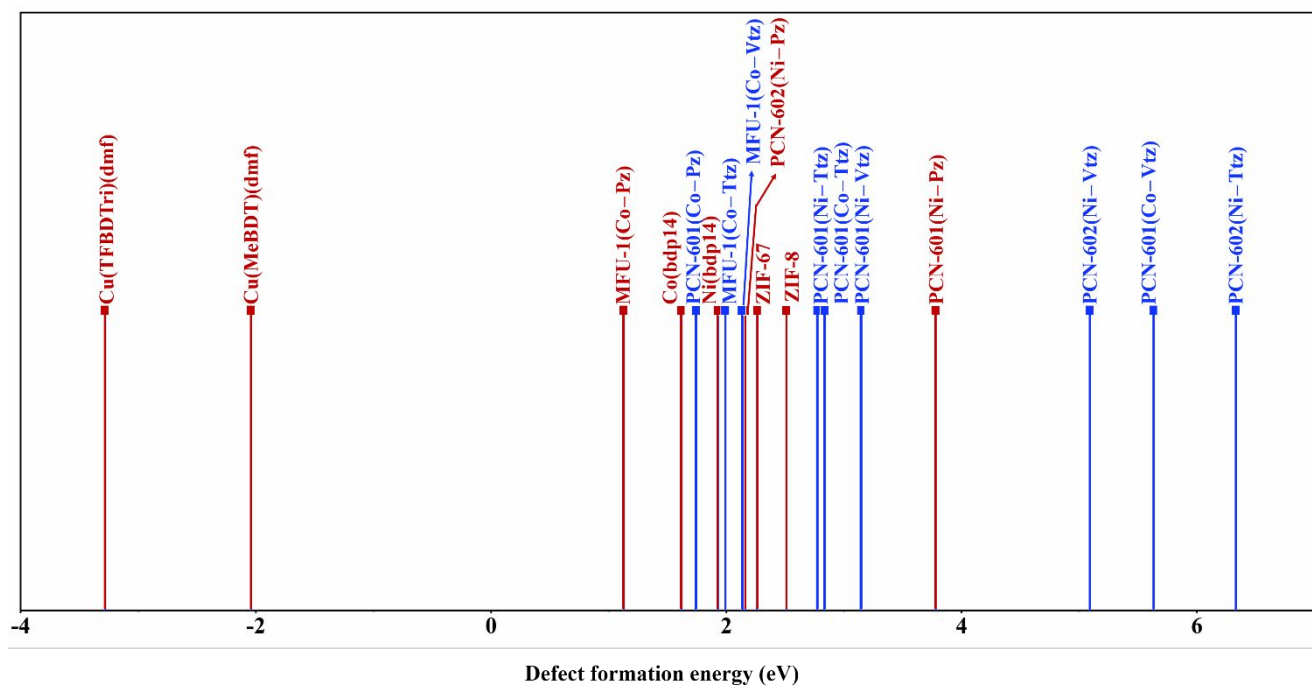


Figure S4. HSE06-calculated missing-linker defect formation energies of the hypothetical (blue) and a few experimentally synthesized (red) metal-azolate frameworks.

Section S5. Coordinates (in the format of VASP POSCAR) of the metal–azolate frameworks studied in this work

PCN-601(Ni–Pz)

1.0000000000000000

15.4435997009000001 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.4435997009000001 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.4435997009000001

Ni O C N H

11 6 96 36 56

Direct

0.9072629404118402 0.0968106901639203 0.1033388884647195

0.0947818037572716 0.9042706002562824 0.0977169950609422

0.0917901294743402 0.9032500544624398 0.8967014798034754

0.9050782289109449 0.0965685047439777 0.9024159014611044

0.4998860384175998 0.0002493054116144 0.5000641607355902

0.0012903451068667 0.4998892680957567 0.5000990160563958

0.0950235867043219 0.0954342890632418 0.9023685847190066

0.9071704592052043 0.9032612348644875 0.8965087742869926

0.9046872037261267 0.9034956297599024 0.0979132598290775

0.0917719508480346 0.0965409600899534 0.1035465404475318

0.4993557176261803 0.4999103408703220 0.0001095961957844

0.8470281684031491 0.9999749455775984 0.0000077886364593

0.9994544247457995 0.8780943894022144 0.9990579709296696

0.1513886757414511 0.9998807682025941 0.0001092292948144

0.9996508635748995 0.1218604642449037 0.0011119385478935

0.9994665877540143 0.0015444435018637 0.1306710945576839

0.9996396003720136 0.9983767548138687 0.8694730074953796

0.7763017039211206 0.0693258881059506 0.2513381874956977

0.0722417357509144 0.7717565481869855 0.2444350302647393

0.2473919254857648 0.0684257948577454 0.7754517660817086

0.0725921104108096 0.2274360862199387 0.7551586468951328

0.2467905420233265 0.9310580404155004 0.2250335543282063

0.9282761801265025 0.2501440911987203 0.2264799444819019

0.7766763712290796 0.9319210197521315 0.7477707777503113

0.9281991686721796 0.7498234944767574 0.7735609631597669

0.7412510843475388 0.2103694004991539 0.0698369263303249

0.2170244739940514 0.7466357566574260 0.0604936225131993
0.7534645574748779 0.9302380221629747 0.2259082247287054
0.9290223962205175 0.7706162674366084 0.2445306628138582
0.2222447120530404 0.9301452918183912 0.7476300086925249
0.9293897722468998 0.2298285077091933 0.7563160213464499
0.7544118010754772 0.0709631454126267 0.7740630803899791
0.0715746934338242 0.7497696663843740 0.7741446197797757
0.2217101238139065 0.0692961213914955 0.2531409076085538
0.0716448186228291 0.2501124293406676 0.2259362376553469
0.2579802957839448 0.7898006603938583 0.9302407391024516
0.7820102234198458 0.2536065479662142 0.9395518117946509
0.7240215842865325 0.9996391163505152 0.2764739335572912
0.0009771088131245 0.7335876056822030 0.2855423326095305
0.6562945730691183 0.9992658681359856 0.3430611745021537
0.0015019766830306 0.6646365796193052 0.3509963693370324
0.2757448361290145 0.9993893444996047 0.7237257887228594
0.0012942257650437 0.2662127938006122 0.7146582530642434
0.3434887293601960 0.9999862508121495 0.6571582932049864
0.0016601688503997 0.3351621217566816 0.6491986240321310
0.2749693338185466 0.9998686171896196 0.2771204257894695
0.0001398179409904 0.2883925237544318 0.2663067474658263
0.3428405643972354 0.9990102050715208 0.3435885011023743
0.0006792876690582 0.3519417880914020 0.3366546440803688
0.7248530664299295 0.0020870602035714 0.7228937449021586
0.0000566293938604 0.7114290030408128 0.7338502175817325
0.6569347747485850 0.0029961323743635 0.6564941666893560
0.0005519952196664 0.6478362685256656 0.6635391378828714
0.7239643787956425 0.2737669942700478 0.0073733041627548
0.2749150122655948 0.7262100150311142 0.9926150151666064
0.6572690600691047 0.3424102090387393 0.0078722397282505
0.3414731154127253 0.6574128637950238 0.9921617964303096
0.5699283507894606 0.9982457926114421 0.3181640786739521
0.0013683880962034 0.5795015216618467 0.3223762688554501
0.5434950766242039 0.0000132822728887 0.2289430651310340
0.0011280713373338 0.5572666147689134 0.2319363115115607
0.4298696332512861 0.0019128465596268 0.6820265061771948
0.0011861441161827 0.4202893687566132 0.6778232337999484

0.4563846866895460 0.0008091289602348 0.7712423741628243
0.0007903203852209 0.4425232177705993 0.7682591092376612
0.4291355322218422 0.9985456008324505 0.3183879835783330
0.0007538670411265 0.4391521318318965 0.3159965147222792
0.4552996869840555 0.0004009567948415 0.2290896506219866
0.0006881827394452 0.4692751331443645 0.2279554983448620
0.5706567256420456 0.0033224142962496 0.6816998268315970
0.0005344400362048 0.5606444628040350 0.6841956972433820
0.5445891828973899 0.0017278717511502 0.7710307450534586
0.0003147903251630 0.5305256964814618 0.7722424203782197
0.0013822199803926 0.3223169399912393 0.4213950482750803
0.3181838742595104 0.9987283079043578 0.4300619634347100
0.0018448997414851 0.2316923478740449 0.4429256296332724
0.2289378242746452 0.9977102881087205 0.4565389965130748
0.0012724359874667 0.6774437598458647 0.5787872006811838
0.6815966579707222 0.0023648978200868 0.5700647477891252
0.0016294534121499 0.7680798490072931 0.5572747466776775
0.7708598007291911 0.0029439736673851 0.5435989138370019
0.0019476922072315 0.3148493163482655 0.5618087148600992
0.3184841515981560 0.9987468152243721 0.5707769949892736
0.0022143930257030 0.2270989335423792 0.5309472406097484
0.2291238530446691 0.9981986023133018 0.5446285571068756
0.0017066154469134 0.6849520124141009 0.4383862877071039
0.6813260862591406 0.0007172767427974 0.4293999861304982
0.0019037956777197 0.7726922350966916 0.4692604510573517
0.7707031732438381 0.0013835866445717 0.4555469861562074
0.6821305654613781 0.4292645379620978 0.0038141545726447
0.4284978501149723 0.6820653893812434 0.9910084644691821
0.7713205466971971 0.4559964355078634 0.0025804707695087
0.4552598419549483 0.7712109002746388 0.9923281085264151
0.3165836815473639 0.5705683805280160 0.9962428223365194
0.5702537917362136 0.3177522645957609 0.0089539522286657
0.2274078879657964 0.5438118200028867 0.9973209537706254
0.5435769404058206 0.2285989279025245 0.0073395468750164
0.6820941045012816 0.5707127915595791 0.9959416466657984
0.5701531247409051 0.6821089639251170 0.9909091722148702
0.7712912178007514 0.5440323977737052 0.9967590985821317

0.5433920369018850 0.7712343783983755 0.9922356658574145
0.3166383467624314 0.4290907245759854 0.0041397893131503
0.4285978243873458 0.3176411953661500 0.0091063278436252
0.2274581613795661 0.4557817822689287 0.0031318073745510
0.4554450163691826 0.2285202993066378 0.0074240552170295
0.7413964438649998 0.7894821437652624 0.9299387113709017
0.2170011114890258 0.2531771846873880 0.9398786817678015
0.7817610872691816 0.7465133638506174 0.0604292715250594
0.2582617739794060 0.2096273113421105 0.0699331549388233
0.7239009045199936 0.7262118439984278 0.9924722364983936
0.6571997780238732 0.6575416765797542 0.9919547566595597
0.2750389980137271 0.2734079426046279 0.0077108539831698
0.3415561325378604 0.3422614541452162 0.0081627881889546
0.8324155652832630 0.0426470444384464 0.1901708750327700
0.0437565545530987 0.8267809280162268 0.1831062777929162
0.1816330895407745 0.0415965922939350 0.8258049836775854
0.0441385930266236 0.1727119041048297 0.8167705255530251
0.1812906822232634 0.9581002668887422 0.1744590095097536
0.9559381848701491 0.1927155847190960 0.1671731209769476
0.8326229408186023 0.9578715301748630 0.8094358766458996
0.9558911078825787 0.8073623030455295 0.8327467562363609
0.8049254956021272 0.1569446401125631 0.0409693476883959
0.1704578542088910 0.8167792770026026 0.0399258931535371
0.8186999668150250 0.9573180836694490 0.1749843960353701
0.9565174188796419 0.8260779026040481 0.1831262852049917
0.1665391567461825 0.9567611350209901 0.8092360698946024
0.9569252411775722 0.1741710810760608 0.8174890429677788
0.8192375245539907 0.0431660254493664 0.8251085008312629
0.0434250690396851 0.8072901471957366 0.8331142938733720
0.1662460927596285 0.0429189362689755 0.1911931941303138
0.0434784080136694 0.1927359646292288 0.1668292389676296
0.1946532783188886 0.8435874700842589 0.9592098541669429
0.8290294979756609 0.1837892029392876 0.9602372301432922
0.4996243161467220 0.9976468594148216 0.3733219484952883
0.0011945348708551 0.5067462286010667 0.3742466590276408
0.5001302718611100 0.0031630620024856 0.6268129519927115
0.0010314840244376 0.4930421965046463 0.6259570092267168

0.0015673681037285 0.3736618836926553 0.4944472332750038
0.3733886675617839 0.9990972088141135 0.5003070354331101
0.0014537849403169 0.6261190858505472 0.5057377892536579
0.6264029580673167 0.0012369008365312 0.4998400730636590
0.6271181102692793 0.4999729989659372 0.9999834879928926
0.4993446798955503 0.6271033789847849 0.9911972232235371
0.3716034296213095 0.4998540434923768 0.0001821708232796
0.4993978308036446 0.3726783789499351 0.0089425095081168
0.8049720497505959 0.8429834929702409 0.9588789583126669
0.1705220823773601 0.1829509111982901 0.9603146412406574
0.8288317436922910 0.8162984160570517 0.0397540900886000
0.1948752657758774 0.1559132543029094 0.0409171496239082
0.0000169123761466 0.5726968307427072 0.8288157246757919
0.5895227956555402 0.0005035752128464 0.8254518717797907
0.0013382912733348 0.6042443964608992 0.1792754006254071
0.5881955173753397 0.0017299687697943 0.1743373449959620
0.0009397254240113 0.3955801712419955 0.8209267383567465
0.4118119891283030 0.9985440127520562 0.8259256546865572
0.0004534216867498 0.4271084945848003 0.1713632348072238
0.4104819560365058 0.0024386853201364 0.1745985997918140
0.4115819942203984 0.8265150246424326 0.9950167089062631
0.8265489948126543 0.4121732168284638 0.0058063541970128
0.4118287307243875 0.1731578337382942 0.0045254943491813
0.1722790040355022 0.4119118042408090 0.0065784601564403
0.5871431797809805 0.8264960374779307 0.9948189428048835
0.8264911983819232 0.5878474468392483 0.9931125688826938
0.5873806035770812 0.1734107852092777 0.0043991235936147
0.1721870501113472 0.5876423829712607 0.9938378835597277
0.1744909651815831 0.9985099255378245 0.5892944679917349
0.0026374825828199 0.1702683431765948 0.5728081982171247
0.8256534811316882 0.0043913430832774 0.5880799125642540
0.0016021119995671 0.8204442058937005 0.6045961456434483
0.1741352461119945 0.9968985812696118 0.4120712225175183
0.0018293176103228 0.1793128776783632 0.3956237339689253
0.8253403162747404 0.0005588103986653 0.4108615859333966
0.0021336399681786 0.8295200619083047 0.4273927579407228
0.1415347206165336 0.2356427224364737 0.7422204686281830

0.2708336787071843 0.1350276489147291 0.7780034875845132
0.8594309893428473 0.2618271472641425 0.2369696795523595
0.2702394615018946 0.8644678670260006 0.2222864683550583
0.8593535613740499 0.7381799927275807 0.7630415187219128
0.7764523903201095 0.8654809891549320 0.7237686624465596
0.1412215615220020 0.7629054676401097 0.2567568639073912
0.7762877015455132 0.1359323513655681 0.2748494715466379
0.7118345681230309 0.2001011020272259 0.1333015353944731
0.2081509103135772 0.7141153409686964 0.1226440266690219
0.2874707548760185 0.8001157983672158 0.8668156247818501
0.7907347372484139 0.2861759034491982 0.8774053310165542
0.1405606351415187 0.2617433855006865 0.2359292091220624
0.2206533025145632 0.1354705014806115 0.2778543598455130
0.8602369678030612 0.7605621470707433 0.2569606734823680
0.7312030358748984 0.8632089741462678 0.2245296218866102
0.8605854626589817 0.2404420187379657 0.7444478859642842
0.2211823083885491 0.8639395942689205 0.7230221941663686
0.1404987686618639 0.7381490854117274 0.7641410256142649
0.7324726726498270 0.1380936923455209 0.7758847746032771
0.9995736494325485 0.8145265772307155 0.9990655728803688
0.8078435579590817 0.0506311236182881 0.0187764601452969
0.9999083310687098 0.1854223549561880 0.0010983030166187
0.1908227997838594 0.9493262921366536 0.9810710790701975
0.7122040941162240 0.7995962631242435 0.8663467051752392
0.2079686804596292 0.2858868839174562 0.8778533114046567
0.2878559697023775 0.1991046975512276 0.1332672982296970
0.9994981724251986 0.0031935390653501 0.8060884574994134
0.9993609437158071 0.9967887192887375 0.1940680758795068
0.7903237081137817 0.7141057803416118 0.1226823061666380
0.1907141143071627 0.0506164931209980 0.0192189990881175
0.8078415047539664 0.9493650598902903 0.9811724820646504

PCN-601(Ni-Vtz)

1.00000000000000

15.3590911132135393 -0.0290492976047072 0.0018100799285105
-0.0284099855532523 15.3886794289407476 -0.0106652920264335

0.0040985085436716 0.0058198812461109 15.4176280897781712

Ni O N C H

11 6 48 84 44

Direct

0.9054629089021802 0.0964577891384693 0.1051633456731409
0.0934993811246869 0.8987538303759237 0.0989408035747985
0.0928607200988978 0.8996401973102550 0.8971914131971772
0.9024982541142705 0.0958798824881555 0.8985417592166556
0.4976530198710449 0.0113087963485512 0.5003245634394418
0.0102117703246947 0.4999141605875792 0.5003483704736880
0.0968064351747202 0.1016488323585847 0.8946309747737260
0.9030546513271247 0.8988191297934023 0.8999078389961852
0.9015767561714227 0.9012644702912525 0.1021629873163619
0.0912383510330841 0.0978637365523056 0.1050345645725841
0.4987077202043579 0.4960063059731112 0.9937206910065868
0.8409426874835191 0.9949856937332484 0.0009904987981670
0.9969506901292391 0.8733596765924716 0.0009772739310492
0.1559130101041930 0.9920440425260182 0.0016985022577458
0.9966967069949533 0.1221804086954208 0.0022184407623698
0.9975012635341685 0.9999387086857610 0.1319082826358837
0.9969454918097185 0.9954314768325645 0.8697668918588946
0.7694105703310257 0.0749259183434106 0.2451426709084075
0.0729819217294292 0.7592153139956821 0.2332814566433044
0.7634294064644678 0.0708361184419317 0.7625367938867171
0.0700010102285233 0.7591549004151616 0.7644552309491601
0.2301288963508625 0.0714279952030381 0.2413499855567522
0.0733448272264781 0.2500601493426515 0.2262789735639572
0.7745936376372811 0.2456881547825418 0.9331165921741018
0.7474923040754931 0.7770185401584229 0.9297710757178379
0.2237910722611289 0.2485130680157894 0.9359907733982098
0.2391924289740999 0.0711752437568123 0.7654590530127336
0.0688694006394428 0.2344355824698994 0.7556757694098053
0.2509380705867628 0.7771541299704339 0.9277573196058171
0.8251487861222486 0.0420548163241889 0.1886681276751503
0.0394340167099898 0.8158388402821402 0.1784663204279582
0.1790118021271496 0.0414944794432870 0.8187341894338971
0.0397740923529284 0.1791212600981353 0.8140429276706840

0.1715132772593293 0.9528588403202320 0.1853209758468068
0.9540640824436792 0.1867310035399754 0.1775036395079894
0.8212615794122655 0.9516500096916545 0.8168122671896469
0.9522822708021863 0.8048737879478409 0.8320813403156677
0.8069010367740361 0.1587204819479950 0.0420996452759539
0.1721503910519147 0.8120468207700497 0.0431169372104421
0.8158663213365216 0.9556446307074822 0.1807083537453238
0.9537869456909291 0.8256540050172632 0.1901065299277960
0.1721294814964622 0.9541666646670990 0.8145080652306191
0.9524934598030939 0.1759914922580208 0.8156981025616048
0.8205779969279874 0.0391690171555368 0.8178306365871819
0.0391679271476448 0.8117531118571506 0.8243465623168831
0.1712738711355613 0.0403798556423709 0.1869813545833594
0.0412912476225173 0.1922313892783620 0.1718373810772320
0.1901505157736239 0.8301249142533607 0.9588643058623418
0.8234254381942137 0.1807063069717501 0.9582747113316827
0.4966599078191081 0.0104288046743051 0.3734900334756830
0.0157140648427969 0.5044996210674526 0.3739333076103009
0.4985981999069793 0.0095032577169150 0.6269313240233316
0.0073795035881474 0.4952515028210627 0.6266437211212832
0.0074852793470939 0.3732560578730286 0.4961109261773018
0.3706285185639615 0.0108952927012922 0.5005538005479053
0.0102419451245908 0.6268068248818395 0.5046396371907136
0.6248256955305607 0.0145074539667220 0.5001419095727186
0.6264367390269925 0.4953558045077315 0.9924472037515031
0.4986313020320168 0.6230444941373818 0.9844392413730390
0.3711187849678197 0.4965008120833261 0.9954278844046556
0.4987979850834492 0.3690280274255926 0.0016515371560217
0.8069864096977284 0.8307754779600245 0.9626862637075533
0.1736769047172473 0.1834142291383216 0.9588375124494348
0.8239709223648148 0.8121385385563258 0.0467673153612509
0.1880525636088848 0.1597998169261032 0.0426810463384939
0.2326040527684654 0.9264363262944428 0.2418642231774939
0.9283469205008430 0.2432242328841099 0.2386476229885304
0.7611745133674148 0.9258672804398245 0.7585442905454798
0.9255703758559690 0.7442540428476576 0.7750704371069475
0.7436542865405116 0.2127416437521248 0.0707975721761613

0.2222546296761720 0.7448164821927321 0.0661710775661177
0.7512160991550942 0.9315220391640011 0.2345295279596016
0.9302401108278744 0.7732637657113273 0.2560399468774364
0.2305822512454583 0.9263470254831958 0.7558889618217677
0.9230083887376708 0.2317719531224895 0.7555260814040210
0.7219566373876845 0.0068352048314395 0.2757736235472024
0.0056742707402577 0.7307709854408344 0.2831167176910014
0.6541648736698775 0.0135648586147425 0.3429902254844848
0.0131527814007555 0.6624256615196629 0.3491457777473599
0.9970615792131312 0.2687451331641668 0.7176693536841228
0.3410690515036734 0.0072149538454767 0.6577166907859748
0.0028290423434427 0.3373185827048459 0.6515272521189885
0.2699316316127351 0.0014437725664536 0.2773546074707625
0.0039916950899794 0.2834432436732683 0.2693395196908455
0.3388470909869881 0.0081365869820260 0.3437839307535597
0.0110292952971065 0.3487747106180379 0.3384497756067972
0.7246652850735913 0.0013189495941788 0.7238851989682615
0.6563598709576866 0.0088328569412042 0.6569434704598081
0.0065231316152534 0.6509486043400869 0.6623185017211739
0.7233441904602884 0.2682515422735960 0.0021726600125973
0.6568307675456779 0.3376648894804077 0.9985811878646871
0.3405005303350066 0.6542661687539493 0.9875445869365791
0.5673203749617173 0.0103684210888062 0.3181254257076205
0.0171155673979300 0.5768286623280616 0.3211388425805239
0.5405821679783500 0.0073799726684882 0.2287934116195203
0.0194635443194215 0.5534452494428734 0.2308090801573286
0.4279739474856754 0.0074597576499897 0.6823169768291066
0.0056921976447981 0.4228934987564585 0.6793869014243512
0.4546258765271745 0.0052479627926871 0.7716622399141144
0.0057627288599491 0.4460504302680022 0.7697809377242208
0.4256468598277010 0.0077591653462221 0.3185024145495703
0.0159805926336034 0.4358895573140131 0.3163372866306702
0.4519610489009978 0.0056360275490590 0.2290812263161897
0.0188237200822599 0.4650786524157269 0.2278492165360149
0.5695295432567278 0.0079750296660421 0.6819834730640224
0.0072261233853368 0.5637118772004399 0.6843152891991693
0.5431746486824167 0.0055116964447777 0.7714592560942890

0.0067731456633311 0.5343232041268280 0.7728768467272928
0.0078040742778356 0.3205497688108352 0.4237988216364599
0.3146422378913840 0.0112452184369261 0.4304589434774684
0.0050853084039204 0.2299634562173836 0.4468255260915086
0.2250331261602199 0.0128585192518642 0.4575217520322283
0.0081619342582897 0.6794740451179493 0.5770200566435477
0.6807664422948605 0.0134828386523296 0.5703302692023229
0.0071695597935886 0.7700108337369684 0.5540937758335787
0.7703343866859527 0.0162619700194213 0.5433329605200470
0.0040901909295812 0.3153731712545991 0.5644141466573274
0.3156615427875593 0.0104751002133483 0.5713994548816430
0.0027376700809825 0.2267697103383384 0.5349393041651496
0.2256422069802539 0.0123532471345911 0.5456788839746949
0.0103925824342141 0.6846774215309210 0.4362676459178019
0.6797989145308847 0.0166243701880617 0.4293098549947558
0.0085396221051397 0.7732731593538844 0.4658845382031629
0.7697739391048586 0.0183665209790149 0.4551010076026074
0.6819309503004689 0.4245735747646648 0.9939374029975880
0.4278434028928118 0.6785857586237043 0.9818679104343033
0.7716011312118738 0.4514411019743818 0.9924347277953629
0.4552359443755876 0.7678628053046950 0.9765503274126814
0.3156815932869179 0.5672280343290197 0.9932436887604297
0.5694162917500236 0.3134203763957899 0.0017526236170724
0.2259305455181746 0.5402049088168610 0.9955327546528423
0.5420098518612519 0.2239617571612413 0.0037243482212830
0.6819030968574893 0.5663295967838238 0.9907865277263852
0.5699877459446583 0.6781636080191902 0.9822197750081259
0.7716456107255780 0.5398677349406995 0.9907384809905437
0.5438024846312786 0.7676646507947424 0.9769553578452346
0.3155599135313878 0.4255795598956453 0.9993576933136765
0.4274788294636949 0.3139876183193735 0.0043809575045017
0.2258523460869455 0.4519137369709227 0.9993556090523370
0.4535391794953441 0.2243272063315516 0.0054246660369870
0.7738709548360134 0.7438761516689780 0.0680716222467126
0.2507337615618255 0.2133106924753037 0.0740973419920365
0.7248059202857817 0.7215278111090058 0.9942571465184642
0.6569988499028057 0.6532184562517500 0.9872165610361634

0.2732716315562698 0.2695832248001935 0.0066729733237096
0.3403820990965087 0.3387940596158359 0.0038339547888668
0.2728967346672206 0.0006443846606388 0.7247314199509205
0.0001617394418858 0.7155956284934248 0.7320717186726924
0.2727442484912643 0.7225654416682872 0.9932361461427490
0.0079310473115584 0.5772030726740880 0.8291364729951951
0.5882899815040687 0.0050391020183440 0.8260036621433571
0.0219750901088460 0.5999148837484469 0.1775236612982241
0.5851395705566986 0.0074930577609535 0.1737325819723310
0.0059980497490955 0.3991970444877495 0.8227508047225172
0.4095955633972181 0.0045187379655545 0.8262992561905307
0.0205615466968183 0.4220240279016494 0.1717265301850901
0.4069431819336629 0.0039913763264465 0.1744600338848201
0.4109378939733830 0.8227927010094973 0.9719095928602712
0.8266632074016940 0.4069840518152645 0.9916488848156533
0.4086474882767632 0.1693888623641584 0.0055936011212836
0.1708399596843790 0.4070395830217564 0.0008558896227555
0.5886580480127890 0.8225108295271966 0.9725807769258310
0.8270147311461145 0.5843167778399376 0.9879671387462139
0.5859315376455285 0.1685878982253115 0.0020744765475342
0.1707860185770116 0.5844829753690419 0.9928808846418988
0.1711201085824641 0.0141395987132711 0.5908769560408729
0.0014402187006510 0.1705872568624116 0.5779458350252824
0.8255709186903815 0.0171215874769857 0.5876928278988984
0.0065961436553224 0.8232328416916204 0.6007536019049198
0.1698378620740044 0.0151457986904830 0.4132022587155575
0.0063625788786226 0.1767628596378330 0.4001670826296362
0.8245611592808899 0.0214918812717286 0.4102543085891810
0.0094177394111554 0.8298511351699247 0.4233420810719792
0.8602566958189328 0.2502137850013213 0.2570733566472185
0.2446487381308771 0.8578251630462432 0.2542203931507103
0.8573914455884122 0.7254308951133481 0.7689405728156871
0.7471832129682738 0.8575077359398975 0.7464109631041822
0.7184370748777908 0.2080557163469408 0.1368083483991498
0.2195214266572663 0.7174640261757190 0.1314082031505066
0.8635980299712926 0.7687507395023090 0.2798210651671198
0.7294635220594188 0.8643626366585622 0.2408044827649434

0.8535716282806689 0.2408746627503291 0.7444204117042688
0.2379350823080841 0.8574716128214774 0.7411653909400400
0.9967932132350370 0.8095722204235045 0.0012593287347826
0.8053117669495862 0.0479622877277137 0.0186574195220430
0.9971674205689212 0.1859967323202767 0.0010190907798417
0.1986636113743003 0.9459363008085191 0.9833340954631424
0.2724646106451161 0.2083004767473824 0.1412991431698387
0.9970381236990207 0.9973611643182210 0.8061137863012533
0.9988713294102709 0.9957438968014003 0.1954411693026472
0.7746775637103127 0.7149158242043470 0.1325709292650572
0.1906018908468852 0.0457526164819626 0.0184595462922061
0.7987370833281418 0.9477363047497462 0.9835469313070391

PCN-601(Ni-Ttz)

1.000000000000000

15.3832152091274299 -0.0004577519605166 0.0003327916590714

-0.0004572582969094 15.4233052093468341 0.0076089546768056

0.0003326138987746 0.0076223690992198 15.4302537385151961

Ni O N C H

11 6 60 72 32

Direct

0.9018190354046993 0.1025762899307168 0.1080338672149423

0.0980564849185157 0.8973817290547572 0.1044099843271908

0.0966230657516149 0.8976081043824280 0.8918437311822416

0.9003106299017176 0.1024100395562471 0.8974422590218722

0.4994913761939941 0.9998505327874270 0.5001411876429245

0.0015305245845596 0.4990675435425018 0.5009982293012101

0.0993287842649480 0.1014381525466490 0.8976812205973062

0.9024762144010126 0.8977440959897507 0.8915385948670931

0.9012565708331977 0.8969978164181569 0.1048673110130736

0.0969829363304768 0.1021095700765855 0.1080668704907950

0.4993933144248786 0.5010674596401188 0.9981518327512120

0.8371415196275080 0.0028370203136774 0.9999428027206605

0.9990931189455381 0.8735890682844740 0.0011210541462603

0.1617977279081302 0.0014743293420381 0.0005796740506909

0.9994786783925491 0.1264385502197527 0.0006325084508205

0.9991590585425882 0.0010511679503225 0.1329350793663693
0.9995017929893777 0.9977542259928924 0.8682051243485276
0.7662139839457964 0.0709337393160467 0.2473294887531452
0.0735304492677926 0.7649871434011715 0.2471172286816952
0.2452159448643698 0.0722447602034109 0.7669018159558689
0.0740115845136557 0.2326152491399398 0.7543399570438112
0.2434980155895587 0.9265890585509524 0.2351087445567259
0.7683184894777426 0.9293475070678596 0.7508477891685530
0.7476190676469869 0.2263919988615939 0.0725914400043592
0.7562178321537942 0.9263309492098770 0.2357357432432110
0.2303551457840740 0.9285076336936697 0.7504324725318483
0.7557481035294060 0.0735000084673274 0.7652755549370411
0.0730784027387728 0.7495405114758853 0.7670286298030007
0.2311260132962474 0.0708324571232524 0.2488818305295908
0.0732590413379626 0.2487413043567628 0.2347743964665838
0.2538117136195481 0.7797336053963519 0.9278552950211321
0.7712945482120830 0.2511975683153693 0.9312578926862471
0.7449636195252296 0.7803559473717172 0.9278620665276449
0.2269204306879118 0.2514158970324303 0.9319676023412100
0.2530974503401424 0.2241662431281242 0.0724261894663272
0.8227442875069286 0.0424003654046246 0.1897693743266373
0.0434501456944503 0.8194160625003803 0.1884336069465604
0.1835690598731787 0.0432802769653975 0.8187406587339083
0.0439050052629284 0.1784814401079586 0.8133105268477436
0.1825293757498727 0.9557052031252695 0.1825396196612417
0.9561989046672679 0.1913544570149952 0.1797891348335767
0.8243583125007348 0.9578060335932150 0.8089358318563740
0.9559963960998701 0.8064996454954709 0.8224467072776633
0.8082913350202929 0.1728143148293810 0.0432359816015548
0.1762274912733020 0.8124297957019451 0.0424411380486731
0.8168767958717922 0.9556226259644873 0.1828746938336963
0.9564823356058483 0.8184736188792670 0.1883179645842219
0.1748275702072846 0.9570376211039573 0.8089731350438285
0.9569561615361621 0.1801413128000604 0.8140623233392077
0.8169680215849553 0.0443313685872155 0.8175000326298374
0.0432199231323054 0.8065130085904642 0.8230613599965011
0.1752551602085290 0.0422444560567143 0.1907065178129557

0.0433649626416681 0.1916844496756482 0.1788043881485351
0.1925279672552875 0.8321013935657078 0.9583564686161736
0.8219879186079453 0.1880151945228334 0.9578135073017009
0.4993049107883465 0.9977582299489143 0.3731625322059031
0.0012659222049436 0.5041461865376107 0.3744816281051584
0.4997293876452247 0.0021544948085008 0.6271212629767362
0.0015203380298558 0.4939931002532774 0.6275251614104533
0.0019653801542319 0.3723064257897022 0.4971114574310107
0.3722163834282171 0.9995783591293872 0.5002979777810808
0.0017670608723321 0.6258056107676424 0.5049033457043350
0.6266872401291863 0.9999377727364092 0.4999722184236788
0.6271558061677709 0.5013497515084140 0.9982200324685664
0.4993563336419555 0.6281642518693005 0.9913115447621905
0.3715661285543490 0.5008208880982536 0.9981426167236691
0.4994792582353540 0.3739976568218566 0.0048643025707023
0.8063899288441192 0.8325861406696689 0.9583893501631735
0.1770659590733459 0.1874709406743449 0.9581624498520398
0.8224207688069711 0.8129592834500059 0.0425591835326316
0.1921934461878649 0.1707792788640035 0.0430571055340323
0.9272659329550876 0.2482346125609283 0.2364540119451206
0.9270831166301505 0.7494562840809493 0.7659479514781893
0.2256932443338471 0.7476096259161125 0.0669097914959735
0.9275324275055041 0.7633548154230567 0.2469412367909456
0.9280561151035016 0.2354615543747656 0.7556016381462598
0.7726524376598221 0.7483663286612270 0.0670140843223592
0.7254455335411905 0.9983858959963712 0.2754741878547620
0.0008846908551661 0.7306106300645183 0.2827406859067594
0.6568276153211201 0.9981854935254901 0.3428318197424076
0.0014652455740176 0.6619318258845439 0.3494943786383971
0.2735570556577400 0.0005555429884794 0.7247369573274511
0.0014089310055851 0.2675795681163038 0.7192468931678064
0.3421644650272171 0.0008639323624067 0.6574152900777648
0.0019915051558996 0.3362376837699728 0.6525053323128489
0.2729967719448609 0.9985259123275441 0.2760129081128326
0.0005651491337417 0.2831325370988935 0.2701004081819747
0.3416636147193017 0.9983916952540000 0.3432870935856656
0.0012393207122301 0.3486844239293205 0.3394362582573223

0.7262163947684357 0.0016780884983802 0.7241668359117668
0.0003826704965704 0.7148476983061016 0.7319849642147460
0.6573798321856330 0.0019026300242473 0.6570123073940053
0.0010760842743522 0.6493964171626416 0.6625811154138930
0.7253873826731549 0.2748241386957559 0.0029426241956187
0.2736659053981612 0.7274638092443411 0.9953065547397060
0.6576332409289876 0.3437506407733437 0.0032179392523304
0.3411767706660029 0.6584203571375227 0.9934824120731847
0.5700219592832312 0.9973114132124437 0.3178689446608161
0.0011982298519726 0.5764147306442879 0.3216528881765512
0.5432969399830512 0.9967623075579155 0.2285781283439974
0.0012233939683739 0.5530622465610548 0.2314150107310979
0.4289908426736702 0.0023506699176821 0.6823866840947872
0.0016352452413457 0.4217312994180986 0.6803446291894915
0.4557327387428032 0.0031725025483453 0.7716898684889273
0.0015178945696732 0.4450494117007437 0.7705681896853420
0.4284200498674053 0.9974843640499813 0.3181073731265869
0.0011540495919675 0.4357103907723214 0.3170322645727595
0.4549038165301411 0.9969029963785161 0.2287279468665204
0.0011505521749982 0.4650003274217624 0.2285288763454858
0.5706157015206585 0.0028098982764533 0.6821992183268861
0.0011903965079298 0.5623967028608803 0.6849878394786728
0.5441239028937943 0.0034832225098000 0.7715634227504893
0.0012253514926854 0.5331025839080112 0.7734704527708232
0.0019517891466876 0.3200036912794388 0.4246852138087434
0.3167328017805033 0.9993365780931214 0.4298491942721299
0.0028013689318982 0.2295565375225763 0.4475314940533224
0.2271442759747870 0.9991452144790642 0.4564956499519539
0.0017978466236315 0.6781009277795533 0.5773441316850807
0.6821729430453871 0.0005273006113384 0.5704130526666447
0.0025631398468065 0.7685387982265013 0.5545267211832368
0.7717612913788230 0.0005612896945522 0.5437335895404800
0.0024626020266396 0.3142868880479028 0.5653916827465153
0.3169856377079512 0.9995337299088192 0.5709172898423489
0.0031501812635568 0.2260141702726486 0.5355544188506229
0.2272894767983402 0.9991177250462044 0.5445776323929223
0.0020982752258476 0.6838530485182162 0.4366309253423637

0.6819217356974292 0.9995736855015807 0.4293339783536041
0.0028193662214093 0.7720928016826676 0.4665047380703058
0.7715989238805889 0.0000599214711059 0.4556615990186543
0.6825712796677195 0.4305510297411459 0.9992001127849548
0.4282818417733267 0.6832156266699840 0.9893624992487560
0.7721287880574010 0.4572914479103289 0.9983846952665374
0.4549451373233921 0.7725139684107774 0.9850850792654953
0.3161186156055749 0.5715786022834379 0.9971803944997930
0.5705675709735374 0.3189622410422714 0.0069255881670287
0.2265552959974499 0.5447408257090345 0.9977814190584766
0.5439522128308312 0.2296727253425033 0.0113341488937593
0.6825298557342450 0.5721951391324680 0.9973058917194209
0.5702528840512144 0.6835111182464715 0.9892846339171513
0.7721219798068546 0.5454621773420101 0.9977532410133421
0.5432683144169985 0.7726894443592371 0.9849760308696460
0.3162303260079682 0.4299304587242219 0.9993392338947658
0.4285998914525919 0.3186772324300264 0.0071735067632375
0.2266339770138686 0.4565677522322460 0.9986618953812894
0.4556128337494414 0.2294791850710283 0.0115036193941620
0.7247874690439033 0.7282184722485283 0.9953355886920434
0.6574058607238840 0.6590194933861611 0.9935040531509642
0.2739309551372031 0.2740073619507015 0.0033376464770001
0.3414101602436048 0.3431666230098429 0.0035672066629147
0.0012811819838348 0.5755746189043620 0.8298591501093568
0.5887175645528586 0.0042183934742752 0.8264179689557025
0.0014418309920217 0.5992596762970734 0.1779572207101410
0.5876927285257878 0.9963020997742049 0.1735603411396269
0.0017425251577805 0.3988296767851196 0.8240063834436953
0.4113250751249140 0.0035651254737417 0.8267046965858214
0.0013028479932657 0.4225129446137785 0.1721495210493131
0.4103157159393831 0.9965842009519505 0.1738649610333383
0.4107353373491449 0.8275374352407567 0.9815462637858445
0.8273977973082651 0.4131110751886240 0.9982364634291656
0.4115961466002815 0.1742654246053874 0.0148830293791633
0.1714247669061848 0.4123018395389693 0.9989204014222466
0.5872803204823356 0.8278755381007556 0.9813082141944207
0.8274182604551896 0.5896011797941156 0.9975829140789685

0.5882443154004449 0.1746730391921645 0.0144979458860277
0.1711951434091148 0.5887992117440959 0.9976863352646177
0.1721821589946870 0.9985977888482580 0.5889277101075550
0.0040702781228390 0.1693651709292325 0.5778008485294066
0.8270436860465864 0.0009822062562108 0.5878614833060070
0.0030183234062235 0.8217027420184166 0.6009648035981385
0.1718755287721336 0.9990832531632208 0.4123412653092231
0.0032762017795775 0.1763991991034786 0.4010850332471207
0.8266842126619167 0.0002260677449826 0.4112822050275753
0.0035252703376969 0.8287677628385168 0.4242838510893208
0.9991355331035336 0.8098859522166038 0.0009680309856961
0.7957090628683616 0.0498320824764846 0.0166950576659062
0.9998272285799956 0.1901295552067523 0.9999899998711328
0.1992842958848087 0.9510840229477679 0.9829165418800301
0.9995998529611185 0.0024853524912771 0.8046947614735132
0.9992849873458027 0.9983053386407263 0.1965471808274586
0.2025359402461220 0.0490612624814659 0.0179143187408641
0.8003544484144243 0.9517821991114843 0.9826890925275080

PCN-601(Co-Pz)

1.0000000000000000

15.4073208992425528 -0.0003842405026543 -0.0014287547008697
-0.0003856718123548 15.4198846678561470 0.0114734406709560
-0.0014334324322517 0.0114674858759425 15.4504926056439622

Ni O C N H Co

3 6 96 36 56 8

Direct

0.4998249074878132 0.0007337071103279 0.5004659481374603
0.0018642774051258 0.5004352810651298 0.4994589831650487
0.4991712985785455 0.4993322570751957 0.9998932423839264
0.8493996093646814 0.9949660270237217 0.0034399902251607
0.9990787804261956 0.8726882408972401 0.0138455206087542
0.1475291120141122 0.0004343667789968 0.9987007689474652
0.0001034705977503 0.1277851579828209 0.9868460417800904
0.0015622574837266 0.9908457438338942 0.1280901554709075
0.0014652659046632 0.0103079820834040 0.8721128871567103

0.7790005484437685 0.0635991607783453 0.2512351153887522
0.0721253023447446 0.7748153115404577 0.2411832409705994
0.2431141859609554 0.0739773436409408 0.7768156827846298
0.0739899290105939 0.2265637555817861 0.7586123819287280
0.2427698223579853 0.9250506484776935 0.2237711784102530
0.9279914150690445 0.2555154187955750 0.2268508825333768
0.7784471976257095 0.9383316305168918 0.7491575242348247
0.9272126002699466 0.7466089063121117 0.7709928527115224
0.7486260450660041 0.2150880274858764 0.0696867514071968
0.2228765930582526 0.7553459864388969 0.0684459244796045
0.7585077279871371 0.9240997054378752 0.2262432114161612
0.9285858885802227 0.7740812695263770 0.2414140987194813
0.2192809704150775 0.9357795810416007 0.7476807458304506
0.9303781107919917 0.2269158713061614 0.7577598754724875
0.7584331200563597 0.0775871527476966 0.7760831567269193
0.0712682442559824 0.7442312870760119 0.7735271387721170
0.2194218007625395 0.0632739353288443 0.2531181385073111
0.0720807866867190 0.2553168319179733 0.2265879931641024
0.2504963412761398 0.7842304503192352 0.9309586461633899
0.7759495624128263 0.2440631634797938 0.9322061460742503
0.7269214864591831 0.9932048342904025 0.2764969322436528
0.0007275098789563 0.7373948164964759 0.2831899513526253
0.6576269461487669 0.9934613013183693 0.3430097405001931
0.0015342106954321 0.6683730690674921 0.3494499269701734
0.2730405467962456 0.0056725922082066 0.7245491829014767
0.0025792457171789 0.2635548954390146 0.7160536908041024
0.3421073397962289 0.0062609301727576 0.6579774377518177
0.0028608846173839 0.3324554257025980 0.6496321982037188
0.2729062626153151 0.9931874158733365 0.2762502782198126
0.0001637207491711 0.2925697114507884 0.2671686469734667
0.3420905717081553 0.9928950374758543 0.3428217588246980
0.0007908339052776 0.3553977786061893 0.3375706183560325
0.7267610485433238 0.0092572995028348 0.7248016572605422
0.9994150652976330 0.7083120132890670 0.7317882707656764
0.6576877691948013 0.0094029944528700 0.6580416985084270
0.0002033969143298 0.6455388139674483 0.6613470966198349
0.7245234095017281 0.2716106207851894 0.0026967053992308

0.2738359828110788 0.7271488943324016 0.9977529172880182
0.6575246594529887 0.3410269931035970 0.0033019758199018
0.3407461841437112 0.6575048354342812 0.9968531262493414
0.5707010343605603 0.9923964940470569 0.3187382080390861
0.0027062852082977 0.5829028316778704 0.3219260029246058
0.5440585705665768 0.9917606168057986 0.2297256959383773
0.0033382134882487 0.5601089420105296 0.2318631084908560
0.4290098972884380 0.0089392925413989 0.6821689952707786
0.0036090590348437 0.4179758158081981 0.6769550713837162
0.4556934475539620 0.0107522078020637 0.7711589783924566
0.0037459610185380 0.4408657743542435 0.7669622064324244
0.4289860710428144 0.9921060055263027 0.3185901702095322
0.0018992375587388 0.4424024998819576 0.3166020197909063
0.4557188861415042 0.9915625196950870 0.2296005095995497
0.0026702768568470 0.4721070376575653 0.2284410173763902
0.5707156292766769 0.0105929071973208 0.6821026568327611
0.0017349170609009 0.5585125655486607 0.6822295222889423
0.5440074539834185 0.0118481793537910 0.7711221390773133
0.0022597971575635 0.5288516227298672 0.7703620782987954
0.0006409831594709 0.3246856622401211 0.4217266982111028
0.3185117972176386 0.9963709892321688 0.4296925482267113
0.9997746152524414 0.2336405121662750 0.4414353907518773
0.2292747773157870 0.9968073547522849 0.4564351028094507
0.0000493952306542 0.6764084552860297 0.5772990021837572
0.6811991580571473 0.0046826308920345 0.5712097588056295
0.9994846550200052 0.7674778850115160 0.5575281194783415
0.7704141007147101 0.0030699335841859 0.5444890667303994
0.0016339498754760 0.3139972191801377 0.5619528145292705
0.3184548038383355 0.0023837423742705 0.5711040011369946
0.0004603772205130 0.2270764691588951 0.5292183406105408
0.2292617225073386 0.0009913410946041 0.5443008873483137
0.0007691130904561 0.6869053673763759 0.4371342055831917
0.6811503292735068 0.9973174772072255 0.4299079141906290
0.9998677715355697 0.7738533157173606 0.4697687126293246
0.7703562877671004 0.9978439940222970 0.4567186958965337
0.6816523387668383 0.4281839506700678 0.0011236994265218
0.4280727593837099 0.6811511540410251 0.9948918293906246

0.7707856558624755 0.4551300994451495 0.0003620327795630
0.4551607727507658 0.7702918548650999 0.9948041163109309
0.3167140889713522 0.5703631838567986 0.9993488862423234
0.5702132955841961 0.3175637585319393 0.0046185704061159
0.2275515084037636 0.5433508495313362 0.0004483175828369
0.5432264335724497 0.2284320221490930 0.0042913994484692
0.6815512026978041 0.5701211570542597 0.9975653738913124
0.5701713087791944 0.6810389786104096 0.9944403742550207
0.7707784724156994 0.5433332709458014 0.9976366280500244
0.5433677721635419 0.7702169582445748 0.9945592062576978
0.3168531614608554 0.4283455597736108 0.0023822821074759
0.4282542193967913 0.3176292143261250 0.0049967947254714
0.2276764615369942 0.4551205023470004 0.0028744860289365
0.4550201637066706 0.2284592268331096 0.0045517820006467
0.7481599125179486 0.7834814410754873 0.9303573693146561
0.2228529022181860 0.2443021389741702 0.9326029457988838
0.7760965880220567 0.7535804084811488 0.0674411007458602
0.2510954230162739 0.2138999611788819 0.0695980539571579
0.7245510375173581 0.7263684598902600 0.9968596465566435
0.6574047468153950 0.6571851715631993 0.9957423257612703
0.2741875480289977 0.2716245750954585 0.0033050685861369
0.3410379690859671 0.3412721129150214 0.0041986737818078
0.8369054103242064 0.0386169790153303 0.1904643557181060
0.0437292042123900 0.8290401831817960 0.1787160061348771
0.1763539727471652 0.0456442616465367 0.8262222481225763
0.0453577016158917 0.1724102312832727 0.8212515891656196
0.1763593288944563 0.9537979837009090 0.1740173181716997
0.9557832791901930 0.1990649620249130 0.1664597372981191
0.8361734151886608 0.9622525294965953 0.8103777639717578
0.9550157435204198 0.8021781231069056 0.8321178236030491
0.8103251769313502 0.1587681982706357 0.0415420337941868
0.1737720891676631 0.8236893226504662 0.0446032624476018
0.8245077127143006 0.9525070525617778 0.1758853071578343
0.9562839700764201 0.8287613404835525 0.1788556598350652
0.1620833175228213 0.9602857613886897 0.8091391754720476
0.9575941677315356 0.1726374422842767 0.8206694267703938
0.8241207365651633 0.0481308237030831 0.8264072977476999

0.0431013834000922 0.8007718442793319 0.8335486958169085
0.1623207077840974 0.0390897197570013 0.1914127632503408
0.0439038336618012 0.1990068494619806 0.1663732255867174
0.1897610017176774 0.8415411071316470 0.9592602363049636
0.8261296957606987 0.1765925639752552 0.9562532824450543
0.4998064423710247 0.9933447574888774 0.3741859800156888
0.0021636018183031 0.5101206441238588 0.3746302988850161
0.4998688231587067 0.0084786691997962 0.6266412621851885
0.0026119452490718 0.4907425625024189 0.6242358524679119
0.0015599283324121 0.3747488786958328 0.4954874336449393
0.3740348894834042 0.9997585350749176 0.5003980860839192
0.0009086541460235 0.6262050875109466 0.5035729177855259
0.6255782172697053 0.0011723039524085 0.5005564514891532
0.6259509497126672 0.4991432804180818 0.9994929808231987
0.4990796584284851 0.6255247224954132 0.9949506863954909
0.3724168805003245 0.4993734733536996 0.0004655988406483
0.4992463424980613 0.3731628344632796 0.0045900652815689
0.8095771404122161 0.8398728318810669 0.9587514371448123
0.1737990533599429 0.1759178325066131 0.9559554692731211
0.8257878079654901 0.8214739228606689 0.0439376408371928
0.1901032954543211 0.1570684362853072 0.0409774052493788
0.0016338768367277 0.5715351137749494 0.8264676893351108
0.5888536750430831 0.0124663026170779 0.8256745943500334
0.0038688184623439 0.6071616734006611 0.1792139730682081
0.5890160274439609 0.9926838847354418 0.1752515215461230
0.0042025047054253 0.3938641984438007 0.8196833468742426
0.4109594893072526 0.0103007507691686 0.8257525941284101
0.0025548276657261 0.4294618260189438 0.1723374987357928
0.4109500078655728 0.9924822228119936 0.1750121640865174
0.4107038860956180 0.8252368237685417 0.9958946104122006
0.8256039529725996 0.4104194868915414 0.0019245443420459
0.4105289402847134 0.1735517392762063 0.0035665814404524
0.1729440901704038 0.4103402744571909 0.0046962002997688
0.5878437691189689 0.8251268990368459 0.9953326912521732
0.8256129436034172 0.5879683207482600 0.9957752246787024
0.5876962706308291 0.1735363701323536 0.0031517685362275
0.1726207789098524 0.5879090254509691 0.9993663045218497

0.1743375903488626 0.0031963742545145 0.5886188447788854
0.0004419732514975 0.1693906620764238 0.5700884585764072
0.8252118458032811 0.0055446452431198 0.5889197652882103
0.9989579321291941 0.8187828389540854 0.6059150091638941
0.1744477147301069 0.9942854544018331 0.4120207907824494
0.9989708379246380 0.1825912200419353 0.3927593173285686
0.8250834699189227 0.9947160270348405 0.4122553733328189
0.9996421174681132 0.8314587467972316 0.4287417950858909
0.1429753628170900 0.2356643380051793 0.7459956039172937
0.2661827994816761 0.1407268694718695 0.7805597731455407
0.8591248192144860 0.2671590475826449 0.2380920061731118
0.2656860748614278 0.8582746377950699 0.2198560493860953
0.8583995259056110 0.7359350540513319 0.7584401681535411
0.7767713813509829 0.8717765899237122 0.7253459942825842
0.1411198456573075 0.7659485595875282 0.2538931531805844
0.7778606720327872 0.1304168740383034 0.2743999710222980
0.7250204335296928 0.2119022975159979 0.1362171119177589
0.2200182106082664 0.7288766832384539 0.1338919087628270
0.2738108361748743 0.7871276618313132 0.8643232963108289
0.7782856288019389 0.2703167580400461 0.8666659124432883
0.1410231331155245 0.2668658640079329 0.2376527441640803
0.2193682399629182 0.1294245300706649 0.2780878685763497
0.8597873341270983 0.7642115379898229 0.2544301570912140
0.7366839263203175 0.8568713428014476 0.2240534171963731
0.8615357269085422 0.2366449300355384 0.7445694098602758
0.2190150372153568 0.8695822141546827 0.7228494073655796
0.1401621479474642 0.7319490136064104 0.7631565873504584
0.7369426590461217 0.1448591795974608 0.7787961104727970
0.9990821041851987 0.8089947770159327 0.0109954869916038
0.8126109319741985 0.0446651698790035 0.0273528413908011
0.9998766166295994 0.1915232637854558 0.9901352293239540
0.1861406625004776 0.9524997197096425 0.9727187548802689
0.7243704287795296 0.7872193072467937 0.8639200478391729
0.2199024417023665 0.2709563055392010 0.8672452285282475
0.2749891941587066 0.2099106840201443 0.1359777275864360
0.0008790776579204 0.0116458714505896 0.8084511751276793
0.0013062422066454 0.9896549773571977 0.1918069354109306

0.7786729311525633 0.7270543510067640 0.1329289778976985
0.1860907654461172 0.0476676247293071 0.0258893731880434
0.8098041290883984 0.9491726210780769 0.9759173703616923
0.9108049310265329 0.1011944577465727 0.1061868148263017
0.0954546371517182 0.9050675073413785 0.0958515467798762
0.0873481630219359 0.8980998050685969 0.8935280294824892
0.9054179252456152 0.0965375915406312 0.9039838213090690
0.0956624479083956 0.0953361108499564 0.9039743462104113
0.9103734216886892 0.8988997254359958 0.8932260645076369
0.9040914465189260 0.9042003591642569 0.0966906953804880
0.0875586343078751 0.1008411234314295 0.1067073925826065

PCN-601(Co-Vtz)

1.000000000000000

15.2954914521432972 -0.0031482065986222 0.0005272681627641
-0.0604368158253322 15.3470705215819425 0.0069783928008225
0.0064179031949479 0.0021488234022314 15.4006744735619598

Ni O N C H Co

3 6 48 84 44 8

Direct

0.4914531320173694 0.0147373291835962 0.4987850169463357
0.0170807090519034 0.4951322139653698 0.5077399474027473
0.4997120457261843 0.4949055449694697 0.9858534198206783
0.8258450070266576 0.0124375078738481 0.9777089225258635
0.9903245911357459 0.8621093554379584 0.9779942457017157
0.1429530505376633 0.9461232854482304 0.0040037190151736
0.9977449156071216 0.1375424557203857 0.0163967898234887
0.9949855660674700 0.0139136684333394 0.1264657918875756
0.0181760031052107 0.9968949607007502 0.8817034566316053
0.7589295409118080 0.0816759664482944 0.2272223837162031
0.0840945781930813 0.7521917152729145 0.2351908157932527
0.7707133017669747 0.0652008153674757 0.7494013067419942
0.0793464450332166 0.7681732555872998 0.7634856297953050
0.2303118645984270 0.0752422606850587 0.2238784245860899
0.0797684822172329 0.2302570405285849 0.2445854284232638
0.7739937350523363 0.2442435428888032 0.9322629372516218

0.7548315190300130 0.7729090574060820 0.9246999602791135
0.2295912158635858 0.2350532040370723 0.9304360535773810
0.2329954477706977 0.0714749932078931 0.7779409397230950
0.0662186541842829 0.2319677075136255 0.7752120977020809
0.2295754973282769 0.7551937030040321 0.9139605880730457
0.8192231370089118 0.0474114473733565 0.1753313094876532
0.0525718655849445 0.8115102541348094 0.1816766273019184
0.1795665177071299 0.0399294911360215 0.8374876306476082
0.0361920684751453 0.1723456487521275 0.8290598393314781
0.1658274113473936 0.9540536920183555 0.1794077107292722
0.9577071665754957 0.1771954733993795 0.1889362839564441
0.8179233519940965 0.9478051685009063 0.8187279443765192
0.9567312482625425 0.8269141695787212 0.8120798910934539
0.8250233489298964 0.1781783974335340 0.0496533054326207
0.1575562211480559 0.7885130742574447 0.0342245411325592
0.8214513573139044 0.9593653219653078 0.1806914694720589
0.9651511645904449 0.8197166858537557 0.1873844495369354
0.1776431856321921 0.9510513495309425 0.8331563030086286
0.9472779294746516 0.1699761907765165 0.8269226480965344
0.8260508025482025 0.0355961742697346 0.8080582638531837
0.0448810504603685 0.8279409874073167 0.8143185245461808
0.1738420226185156 0.0416442941385995 0.1681652795113138
0.0461233538011072 0.1758135889285981 0.1873851741462005
0.1650395138593694 0.8005095154799093 0.9468392870629572
0.8297503003073388 0.1860522993058709 0.9615541310611135
0.4903151063023756 0.0200475541863767 0.3722950805946397
0.0232537900670238 0.4942278091748022 0.3814997588364122
0.4929763307931978 0.0089166947366621 0.6252040205886118
0.0148117379450738 0.4959954292082713 0.6340268651874510
0.0112570918112667 0.3688726966827858 0.5104080641839559
0.3635969525177742 0.0153767782983536 0.5016435945051683
0.0193613264806842 0.6215488626811378 0.5047885227907969
0.6192767034937390 0.0153386327648519 0.4962337454655170
0.6265925837007345 0.4988930158113263 0.9894127992532518
0.4974731192408939 0.6215371956015545 0.9782342776640007
0.3731033365951575 0.4909122437174602 0.9833242699901632
0.5015650074185771 0.3683244393643577 0.9922314265956445

0.8161505972136425 0.8253090946081727 0.9559521321510758
0.1685174421770057 0.1833417232114272 0.9615159031653278
0.8257525591644637 0.8166941706583728 0.0430111220076412
0.1709481926815926 0.1796868794440840 0.0490458897940727
0.2188155370430920 0.9322903688743409 0.2464565146429933
0.9337883634817601 0.2344086791782871 0.2507056357704656
0.7533644942212092 0.9213072201227419 0.7643294057043519
0.9334611154229364 0.7628871312269965 0.7566210747176427
0.7622097377857955 0.2337550334363954 0.0765699198198391
0.2194656160400470 0.7305973649371396 0.0568883364154829
0.7590722012876867 0.9370929866613409 0.2391085503476518
0.9393578125017044 0.7619180318488787 0.2488775127211724
0.2318634207042578 0.9263440570377739 0.7684567469964705
0.9201600966686385 0.2303921468672172 0.7692486826656193
0.7193027006666597 0.0135976745607707 0.2691057309933385
0.0138457436944392 0.7191100017087066 0.2788950335022875
0.6496603604338773 0.0209870261326586 0.3374291292317793
0.0200109210154764 0.6513945697329149 0.3469650314769979
0.9957767844633665 0.2698776199536113 0.7362710753335762
0.3337480679907188 0.0108570867610212 0.6609867842503832
0.0040903589418591 0.3384809002400644 0.6683878972534600
0.2608282871514547 0.0083696109360289 0.2743988854018866
0.0109981947536539 0.2681352289223753 0.2858010437902010
0.3297603379091356 0.0167154589352876 0.3432861375014369
0.0188523313077411 0.3359109814074230 0.3534170246125399
0.7234720540588739 0.9954952638560499 0.7202655745318935
0.6530520469571783 0.0036305079693832 0.6536235263264913
0.0187113023298693 0.6547171563785028 0.6616973538676092
0.7302754691129962 0.2755673983621989 0.0025038728138043
0.6606964951031813 0.3418015761618136 0.9955405230944265
0.3381996019523967 0.6476481127231537 0.9748612329677186
0.5611245668580054 0.0218016917606789 0.3152236001988769
0.0247803741149539 0.5640912894421106 0.3243391487857252
0.5320839837207956 0.0231024682195766 0.2266492764244745
0.0306610252172277 0.5356827836507705 0.2357847260896762
0.4223960530598134 0.0086191189608797 0.6823153192335170
0.0104359507292671 0.4259712723489741 0.6911054533928933

0.4514002921485059 0.0043246028215762 0.7708536008218516
0.0113617688051875 0.4547408431255917 0.7797829877705382
0.4175792050801519 0.0194959968314379 0.3181253240929962
0.0260838235306693 0.4222454492398455 0.3275281192536639
0.4432090456315123 0.0215249403429638 0.2283914695119762
0.0322095044985105 0.4471431696534509 0.2377801899653704
0.5655999522546296 0.0038004061945287 0.6792265641753374
0.0169609679867477 0.5681625596205322 0.6880822498158992
0.5401319304216372 0.0010326141383175 0.7689496428560716
0.0151704500420209 0.5432589352175512 0.7779029243644828
0.0111202769370209 0.3126692948476091 0.4401355864010981
0.3066242147145388 0.0163981937116375 0.4311190943625789
0.0031793378823366 0.2234250359713670 0.4671620205318447
0.2170788894910771 0.0180100020171352 0.4596395462518998
0.0200254061773180 0.6780262806070212 0.5747094607367984
0.6761197724663646 0.0108618804381422 0.5664013997430857
0.0206999264456371 0.7674529054027630 0.5471530858321785
0.7657381167610353 0.0133066879535448 0.5386985322117823
0.0041908741803454 0.3137683135432923 0.5815578932445291
0.3084857003129855 0.0149672679890713 0.5738570913344390
0.9987108562692057 0.2241303577730918 0.5552266657781075
0.2183519825405185 0.0173784596885440 0.5479402852502275
0.0187031784759455 0.6765829589851293 0.4334141003797924
0.6746399890039925 0.0191977511772379 0.4245836974464012
0.0194754734848459 0.7664774876532832 0.4589836408176993
0.7647586486284794 0.0186301243903984 0.4506139811386163
0.6837394223249476 0.4292480326698467 0.9926851585298806
0.4248431260087671 0.6750757775700862 0.9734616518693571
0.7731981714709164 0.4577689127366114 0.9942223530272969
0.4492915978915093 0.7653372294852474 0.9705880182496642
0.3158386976132306 0.5601945493834393 0.9791996139074683
0.5740162194208267 0.3146662381478080 0.9944405449720506
0.2262600770642180 0.5316217158648726 0.9800747325778474
0.5494791264619963 0.2242546602943349 0.9961300764418652
0.6812770454721928 0.5711907981233750 0.9898403872545458
0.5673198254141880 0.6795383844305078 0.9794838515109561
0.7716547937862543 0.5462758720485326 0.9925935027035635

0.5381108214174688 0.7681471128022110 0.9744595608576745
0.3183538985505763 0.4189680787727283 0.9874304762887292
0.4316572440443309 0.3104571313884819 0.9941329647276831
0.2279172050549292 0.4434326373859960 0.9853919813928442
0.4606646613559846 0.2217171101454980 0.9963489354107580
0.7677994915737258 0.7546063897182478 0.0676614594759712
0.2372372651720127 0.2307902650303788 0.0762041910739626
0.7229200927433297 0.7267507213916815 0.9935303335114511
0.6551853040587048 0.6577919426803618 0.9863960003848860
0.2743182564107229 0.2659071144770877 0.0007222299930945
0.3438524904504305 0.3326439091892155 0.9932948885504587
0.2673537488577011 0.0026475732164002 0.7327577521472293
0.0108255707828562 0.7255881825198998 0.7261834497903195
0.2657707615456744 0.7104886078485961 0.9814660131867825
0.0177390870542951 0.5893807160825091 0.8316322399781129
0.5859705413610499 0.9983779629344269 0.8230107254496914
0.0340991572363549 0.5796074956500732 0.1802682998351628
0.5758386049962638 0.0258320995176007 0.1708366325792667
0.0098269972627634 0.4108404856586105 0.8353568605072468
0.4075627085540603 0.0049571692217896 0.8266221699453808
0.0372070545524466 0.4011639590296738 0.1841799127921178
0.3972717442597826 0.0229681635674126 0.1743704639136681
0.4028483316882188 0.8187288898992406 0.9654149532615719
0.8292044871370976 0.4141581345124834 0.9952923223453141
0.4165485189340572 0.1657674519579686 0.9960857549578819
0.1736540741907788 0.3973265502689145 0.9868332158304298
0.5817592954931499 0.8244157571745845 0.9731731459953252
0.8262157858046137 0.5921395767048097 0.9920776272877205
0.5958892503059374 0.1706154571620360 0.9961288649192710
0.1700847675772508 0.5748289142201486 0.9762341459301567
0.1639294731354397 0.0195934375036657 0.5935434043892727
0.9932107982869312 0.1695784161873348 0.6002434775269450
0.8215630120025281 0.0118399535444595 0.5825758380529891
0.0230167383886979 0.8230527964078860 0.5910314892870758
0.1612838844424047 0.0210896823975730 0.4157640079882796
0.0023735159068110 0.1682839615206504 0.4226466542404523
0.8195630293131799 0.0225376484548718 0.4054958837142024

0.0203563534285891 0.8209754031695482 0.4136230478847835
0.8654677935766273 0.2467228276277353 0.2660909970236176
0.2234473183625383 0.8648843200362464 0.2683546034674578
0.8653197460701563 0.7473002201371273 0.7431083575659727
0.7325288512178076 0.8533839522418774 0.7620068892151579
0.7440338241680919 0.2384588065148634 0.1447798890382614
0.2265670598606349 0.7089362690552505 0.1239199986325445
0.8711430971637455 0.7542277255344487 0.2677062014005784
0.7456917518250421 0.8694388366275376 0.2560381042244089
0.8508609204732878 0.2402092960981648 0.7565768347986364
0.2403690784942896 0.8575030216370436 0.7532339061820252
0.9857726764699919 0.7983668244319233 0.9833563353871426
0.8027730424025279 0.0402427983116240 0.0320902667308474
0.9946824376493879 0.2013057164152841 0.0110091494105617
0.2069764510281260 0.9474891515690871 0.9987003803339789
0.2520305318417400 0.2382754140941401 0.1450038755339094
0.0194707900547684 0.0025598247167906 0.8180769379298169
0.0011374541542892 0.0076223361857402 0.1896823272322976
0.7614646172442576 0.7336572993768868 0.1349466936087751
0.1214853389028505 0.0502850081430708 0.0111623250246069
0.7781973424442299 0.9804381265315030 0.9478402773209353
0.9052755488867206 0.1015783515632265 0.1031002955163274
0.1055197875160729 0.8796389219723011 0.0983241619851754
0.0953178294520498 0.8928620689100342 0.9043240932140790
0.8869039282507458 0.0957398610028548 0.8989067901836734
0.0924967576707871 0.0991268194207748 0.9155790099286065
0.8998753345332986 0.8971516541641193 0.8965645337908228
0.9086452403583962 0.8992416482236223 0.1015182203956755
0.0914919853279699 0.1010068256646690 0.0946282715335300

PCN-601(Co-Ttz)

1.00000000000000

15.3135634413564325 -0.0003789789679859 0.0025189933674763

-0.0012740353179022 15.3795839814370012 0.0013326504760219

0.0031701859988084 0.0164697299690685 15.4144444825164317

Ni O N C H Co

Direct

0.5004093484853982 0.0014485886292732 0.5071720697774822
0.9993774645217925 0.4802801302454043 0.4942312497896069
0.5000741335814212 0.5193899223290899 0.9952919474228494
0.8786780881574643 0.0280032214205974 0.9956697788558913
0.0012055143245178 0.8685031845804829 0.0424161573550776
0.1223482091814461 0.0270491130860435 0.9961860670739640
0.0001185080427106 0.1452499773454647 0.9693767079535078
0.0009074914511942 0.9736670932671032 0.1547021954941243
0.9997342441718473 0.9539126445874899 0.9007175611415619
0.7415572750913810 0.0520803190800692 0.2369197559861647
0.0743455437533385 0.7464193420833354 0.2478897666443487
0.2407292148498001 0.0923472631720017 0.7747864613749869
0.0747061539098439 0.2239849734733284 0.7490648320197835
0.2266930593018230 0.9124152451765255 0.2559279443041049
0.7657588990355535 0.9463069538334423 0.7540213661144008
0.7407196258284898 0.2465943134024897 0.0608685897999095
0.7752772110784107 0.9113698675238808 0.2557480917524941
0.2371030678377721 0.9481918424314699 0.7551833558012504
0.7612943620195125 0.0905698302399074 0.7725663178238662
0.0716241536594424 0.7376848775459450 0.7530466641948905
0.2557526233456855 0.0545231011415552 0.2397729726065378
0.0712295778095395 0.2244022162506454 0.2320423036392967
0.2368797023823674 0.7778885982466051 0.9376206254663160
0.7721265286185854 0.2625070774094596 0.9195892008316093
0.7617263214104710 0.7791890066017260 0.9396024886328362
0.2281410855948351 0.2624079505866490 0.9216293902228259
0.2563521184665589 0.2482301633801072 0.0637198783353057
0.8035845296903048 0.0293638575177368 0.1817219002557522
0.0453569287897011 0.8072867473592069 0.1956485561225634
0.1803508466001418 0.0583506401777711 0.8255202456813109
0.0452724734149328 0.1754292429728181 0.8125308755348755
0.1776330312318422 0.9449391565396965 0.1936031963803160
0.9548268445820653 0.1716809043325682 0.1701223615881915
0.8241324053017891 0.9692792458520785 0.8127595546218132
0.9548675902121602 0.7962717842917115 0.8098292814909271

0.7997500370830650 0.1885412651013709 0.0371802701357211
0.1757211066311939 0.8306414273893665 0.0551396505125012
0.8237091534037759 0.9443769238878730 0.1931637370482093
0.9566951152172294 0.8072671047965798 0.1954236239641816
0.1782565231027746 0.9703527374373451 0.8138470576897703
0.9564157736637071 0.1755639556418629 0.8122446457649630
0.8215496253867869 0.0573924356675732 0.8238734430883241
0.0436450168152192 0.7977827628273602 0.8069948560855664
0.1949770687740155 0.0307521800675374 0.1837334489888107
0.0425673035328415 0.1687743935789925 0.1732446674493318
0.1758801987464764 0.8317741019001446 0.9663911802531331
0.8185508307375358 0.1979404507499396 0.9517349156179051
0.4999249364723255 0.9825765096850816 0.3825157708743276
0.9976049530582571 0.4826399797615011 0.3687756200761001
0.5010507045166079 0.0273128516661529 0.6306357441412231
0.9967158007750498 0.4780152874070609 0.6198127952285191
0.0029770971403593 0.3546322496293826 0.4895697067579263
0.3737169859786533 0.9999196595552959 0.5082121222988718
0.0001880692360885 0.6057648797076212 0.4987247369389891
0.6269390369963048 0.9959156080715914 0.5072571372854782
0.6269926971227946 0.5190755312422013 0.9957615380433609
0.5004419014893529 0.6455928944385505 0.0046464473071666
0.3731785586156704 0.5194332923204925 0.9953406919435182
0.4997074314136682 0.3935601093233885 0.9847454591140448
0.8232762081344376 0.8327383523440588 0.9678276410391220
0.1807313578189920 0.1984821832980614 0.9536602359514106
0.8261922254513507 0.8295947251116331 0.0564466727425739
0.1975058964574643 0.1900692325196118 0.0395955373722643
0.9256813948834832 0.2294118037462525 0.2268287404648461
0.9252765749901357 0.7351644190194193 0.7578707335227222
0.2365302062998538 0.7765567387626078 0.0826030975760190
0.9273539180592323 0.7463606390253830 0.2473722438776491
0.9275654998507221 0.2242416850054738 0.7486420184430642
0.7665649603460380 0.7745108860383070 0.0844837215171523
0.7247428267191012 0.9788578042732965 0.2821980756036595
0.0007305416004471 0.7097056672562942 0.2791648969856340
0.6576018243458464 0.9772400750320003 0.3511545718874274

0.0002551667506054 0.6398250741196918 0.3433904906824168
0.2750559360174947 0.0236807513940320 0.7313297571599406
0.0013173624320260 0.2541010150692955 0.7111741916783529
0.3433299784675015 0.0256869756424223 0.6634376491293281
0.0012994582534773 0.3211094112511006 0.6444174907756945
0.2746252763365575 0.9810971483901412 0.2838655389364249
0.9983285161482556 0.2612934193636960 0.2645912990528743
0.3418971040272325 0.9800383022052728 0.3526652138938928
0.9986852163648550 0.3272465921021137 0.3331612464194862
0.7275329146627740 0.0213351358031559 0.7294493480202959
0.9979460735164878 0.6999369426635766 0.7229229352800672
0.6589715472676687 0.0226903799032527 0.6618980343752128
0.9971532737272071 0.6329901570389040 0.6554413747225141
0.7240845623733421 0.2918070219860383 0.9876347573413682
0.2733622490287289 0.7438918363617830 0.0094737670324889
0.6578040566985166 0.3618711471118203 0.9844324098212240
0.3424313038126243 0.6766393154608750 0.0065748469149725
0.5705067439996299 0.9757901591890032 0.3269141343805657
0.9977077067565716 0.5547389490995229 0.3156238386909820
0.5433165417572283 0.9643765693265109 0.2384741486234958
0.9949601489552293 0.5317240434868040 0.2254888376624891
0.4302873731291754 0.0379818770205702 0.6857016005008916
0.9960864658923185 0.4059472277622831 0.6727401643444679
0.4576702297547257 0.0584539857193747 0.7723353119454970
0.9919453609562936 0.4286933924389302 0.7630633579307755
0.4286918645798679 0.9761940909749001 0.3277674191768867
0.9953835086078939 0.4141633232745221 0.3109806507844297
0.4546934835039451 0.9643766143875396 0.2390511087274305
0.9931017062240244 0.4434791177926627 0.2226107053338779
0.5725374544812425 0.0374763006714147 0.6847531256479371
0.9943444436311069 0.5462547473304440 0.6778043774973739
0.5464238741062033 0.0584129853820770 0.7717138657188514
0.9908920676749418 0.5168672484029884 0.7660853876010520
0.0040503093967530 0.3002994281541760 0.4184170493433612
0.3174550074204348 0.9899015051594304 0.4386467603828308
0.0091797723811666 0.2103828293363392 0.4430345211301514
0.2278291827122416 0.9914449764338258 0.4656211814211773

0.0002585730577422 0.6599159526349396 0.5700503779968003
0.6829649480194533 0.0021322807300805 0.5774488545408190
0.0017708762160709 0.7500255018355091 0.5457983083282301
0.7725199447138564 0.9916703127089264 0.5514677195981079
0.0057484930728862 0.2977869069557642 0.5584662126300302
0.3183182638964439 0.0079311136130968 0.5787309962399050
0.0103976177313356 0.2088028666844792 0.5310987669851031
0.2282896360728515 0.0014882403941883 0.5531481935217286
0.0013628129199219 0.6628389624040381 0.4298551909197386
0.6824927293509688 0.9841707116160592 0.4373620001432172
0.0022813998993456 0.7518645828365820 0.4577822751586069
0.7721945564216242 0.9815822976431718 0.4639542695621373
0.6827195145395848 0.4482695047452907 0.9915716120093307
0.4294937028917616 0.7012819523139768 0.0074515449503991
0.7725861527764764 0.4743138743912496 0.9963449661013115
0.4562753563733040 0.7905982987825411 0.0119160079297203
0.3174645211271283 0.5901335076620171 0.0005576877927922
0.5706265851284087 0.3380108318315749 0.9797326480166504
0.2274947052287715 0.5636210760536429 0.9997665616164895
0.5438099977958402 0.2489987870006800 0.9708085143859932
0.6830332841436899 0.5893871506335486 0.0027664661047382
0.5715772801610512 0.7010328250080349 0.0084598505513469
0.7728058773953990 0.5623850929456466 0.0031089084806339
0.5450139421252658 0.7904648472589457 0.0125866278985640
0.3171073607957453 0.4488205208433982 0.9920398791875655
0.4286323784767276 0.3380202967342854 0.9812137683184901
0.2273463538873486 0.4754359644267012 0.9948971204582975
0.4551936429496664 0.2489748253123309 0.9717958719867354
0.7276903308545144 0.7432591867340790 0.0117159861201870
0.6585341601062566 0.6760169325628524 0.0089047470896233
0.2748265705184352 0.2924110439910379 0.9902628889224658
0.3415684128919594 0.3621560883149328 0.9866306830784097
0.9883715208239465 0.5596951883444135 0.8223222747719703
0.5917553906346953 0.0718918062829701 0.8244898213047307
0.9946249722049458 0.5785287070928717 0.1724214499363796
0.5877490220151884 0.9560275104853204 0.1839014722960854
0.9901135674115906 0.3822942132978184 0.8164465269996199

0.4130630707115230 0.0720494540248922 0.8257335542422553
0.9911661743941949 0.4005537267237713 0.1664787473545815
0.4095709119388431 0.9560191301456342 0.1850778062642178
0.4115629890458550 0.8456903866557255 0.0138140787022820
0.8275741108354282 0.4294087526216970 0.9941850838254638
0.4102067055719232 0.1943747999193448 0.9664241554552362
0.1721210676399352 0.4308275039044176 0.9923599831226539
0.5898475049598844 0.8454460562693811 0.0150767304502324
0.8282199969980581 0.6065077975253601 0.0084760414219360
0.5885796864096946 0.1943383354520591 0.9644939939632238
0.1722158075593256 0.6081203392075238 0.0027567900092436
0.1731251440034072 0.0058408534927494 0.5975451369542313
0.0137518395427776 0.1533703295546189 0.5750745444420460
0.8279823543361857 0.9932339105182351 0.5956288338809301
0.0019681846092325 0.8040993339009148 0.5913956796220958
0.1724668864287153 0.9846214492896124 0.4217633972454777
0.0115722812275791 0.1562648525069150 0.3975695583433989
0.8270205410785110 0.9718584413700526 0.4199396365785901
0.0028342791181615 0.8076717820548680 0.4142381124821739
0.0015663094223228 0.8074470849849575 0.0242818388913122
0.8264352456160893 0.9913032098520986 0.9865768108055377
0.0002054907292219 0.2083161611510675 0.9784548945122964
0.0711649715472760 0.9875386961463377 0.9784440584026370
0.9992819482857627 0.0013043803224519 0.8565255783541446
0.0008411467691118 0.9878695041266141 0.2166715745933487
0.1754738287051225 0.9918231540329998 0.9864240368330357
0.9309117053925107 0.9897006898972478 0.9772928611390057
0.8660558889874608 0.1089028907461085 0.1083010906040442
0.0937703768328646 0.8949792588290393 0.1205904547727670
0.1097176782550662 0.8818297169251181 0.8714379952833013
0.9022496667637512 0.1140652903446764 0.8984505464731924
0.0985747169015525 0.1139802918040687 0.8992444425247186
0.8905286816321123 0.8815292256119136 0.8734278515023419
0.9082896512453829 0.8948343682927415 0.1204474885460414
0.1311519124671818 0.1081283700776865 0.1090933967055889

PCN-602(Ni-Pz)

1.000000000000000

22.0904284681838199 0.0169146969826035 -0.0119318726857240

-0.0109112046543517 22.1649481610582022 -0.0304727392508712

0.0253130448629328 -0.0384128986271493 22.0904870252601775

Ni O N C H

11 6 36 168 104

Direct

0.0707148410533591 0.0710711177102112 0.0723304651770107

0.9326482885870107 0.9255284912203336 0.0767470086972679

0.9337473220368580 0.0757156885175760 0.9222284846510220

0.0713470095598510 0.9292404405787593 0.9276223687871692

0.0668588648267132 0.0767061689385855 0.9216781865298671

0.9293428053757751 0.9293714501023445 0.9264921599006115

0.0670037481020174 0.9231638828048219 0.0769378847010316

0.9292104631417644 0.0714365842713676 0.0763171364823805

0.5006345073063088 0.4998755179039875 0.9999970903457935

0.9996381922072715 0.5004688227534828 0.4999839209215651

0.4992763167982304 0.9999027977097086 0.5001185595156201

0.0006420201217097 0.9097124586321215 0.0050803849296059

0.0004377647963949 0.0905682838116562 0.9933530952820817

0.9999549620452584 0.0003233607547628 0.9075047614471359

0.9998133620688492 0.0009998592114258 0.0924979413885154

0.8874175267881128 0.9941815570659216 0.9984801644235333

0.1137946461592279 0.0001446246750731 0.0002539957950418

0.8743786201991242 0.0324098742618801 0.8670784237820826

0.1270155447390451 0.9711763616543223 0.8690917614990354

0.1265857098330017 0.0288527806171359 0.1310489331062499

0.8743784509797905 0.9680530586858751 0.1334412555515243

0.8712501282718108 0.8716383678446391 0.0311403270535990

0.8716357106679311 0.1266185933635740 0.9698595545706468

0.1277000566797142 0.1296502969563491 0.0292957230179098

0.1280247970811814 0.8706175692557991 0.9702315178530938

0.0317532259440441 0.8713422437207612 0.8712369576137604

0.9685046768499532 0.8667416892198574 0.1327367821743053

0.0317341045313242 0.1293879208698456 0.1291490343558337

0.9689890778645491 0.1342341853929909 0.8661255064882596

0.0299375144021425 0.8651607386309621 0.1322599486191223
0.9703600522847395 0.1300168941660118 0.1297297872221534
0.0304498404439641 0.1347697122862925 0.8657854712264594
0.9701632492555206 0.8711252770496287 0.8709876480543883
0.8718988347073875 0.8709630712215599 0.9690018437272343
0.1291300770156525 0.8723440866021903 0.0321429153884978
0.1294199051306251 0.1277865696346154 0.9672923267685292
0.8717353533857946 0.1266099355183954 0.0321350426157281
0.8735732275974968 0.0297092539521202 0.1330426321418869
0.8740415684606404 0.9708390120810719 0.8674828082788082
0.1256254880456709 0.0327082402066452 0.8678077559485473
0.1257097959956042 0.9672224773285052 0.1317891724608984
0.5878353110469448 0.9999608496509396 0.5001684394830903
0.4106155645969451 0.9999509540962137 0.5000550153251524
0.5003621548214454 0.5882284491380432 0.9999175491976331
0.5009018478593532 0.4115463118299516 0.0001107909730962
0.9994801665119653 0.5013020559704913 0.5883969013983190
0.9998079103832112 0.4996931223337526 0.4116131343311480
0.9992600221235364 0.5884998261322636 0.5013779105702554
0.9998627248235721 0.4124675082526181 0.4986037514419905
0.5896253459213625 0.4997781479173042 0.0000277642565223
0.4118987993290801 0.4998837654548964 0.0000063175614926
0.4991215320172628 0.0001236970323504 0.4116294264898386
0.4994992107771807 0.9996123502482703 0.5887179811062779
0.8325687600845839 0.0509679274980286 0.8262986748208121
0.7298335491212811 0.0541235147263706 0.7276186743247095
0.6840914733746075 0.0538626684165564 0.6835201813322413
0.1690934169402425 0.9523753964502504 0.8288021934491780
0.2693602339638446 0.9474866667425204 0.7284376978340319
0.3146686782277328 0.9466678334321799 0.6839085403115561
0.1683552356176747 0.0476226818255228 0.1716203051534393
0.2689821314389533 0.0525223234454941 0.2716005390850285
0.3143680680987444 0.0533223448194846 0.3160539187508604
0.8328030394757207 0.9494235964352669 0.1743324691593386
0.7297038854724320 0.9458634228611658 0.2726619658979956
0.6839279442131172 0.9460670485172642 0.3167746436614465
0.8301300294715404 0.8301401010796710 0.0497233892201336

0.7297374149824662 0.7288748949194357 0.0533000830044088
0.6846969699798535 0.6841105544631318 0.0531937589436353
0.8301519482555619 0.1679059308269117 0.9516296037753165
0.7300346172584824 0.2692822011913307 0.9481187773017297
0.6856233350519787 0.3147262005959632 0.9477269034234084
0.1685629443656040 0.1711588645968476 0.0478463567725527
0.2705695740998735 0.2706608194745996 0.0523815605892821
0.3156837925398079 0.3154023155654855 0.0529952284226169
0.1689590705692652 0.8290118083330142 0.9519275876139304
0.2702837239958100 0.7292772147470998 0.9478193548265352
0.3151741280677456 0.6843064323877286 0.9472256179863336
0.0512362240796307 0.8299258323129095 0.8304879492574671
0.0554428343843512 0.7282198772703410 0.7302881697686416
0.0550387495657105 0.6834264290067011 0.6852418900743089
0.9485948194955256 0.8264289910122571 0.1739462660536404
0.9435119525616429 0.7262685526791230 0.2738344274648057
0.9435290647641068 0.6818316772292761 0.3188813547237430
0.0514758046405532 0.1707155660128450 0.1698455167370270
0.0560975874523635 0.2726316483802194 0.2696796086097066
0.0557021353175884 0.3174850337016650 0.3146349790745901
0.9491386186591271 0.1748587938571760 0.8252924811220979
0.9441582306006779 0.2750139014479913 0.7260385644310148
0.9441944624012351 0.3195835301760113 0.6812531736171010
0.0484535670251347 0.8238334601508441 0.1730301842471818
0.0516690090131178 0.7264036052366976 0.2735008038409035
0.0517534022307373 0.6820908895381379 0.3185017919488899
0.9517875663274680 0.1716247800671198 0.1706028875039678
0.9482470594892618 0.2717216984088182 0.2700255613997484
0.9478398160004673 0.3165069632489548 0.3149566503489183
0.0490994963654003 0.1758219984165024 0.8247751137110271
0.0523180531335186 0.2744343380701793 0.7257036678152531
0.0524544080921032 0.3189443250809134 0.6809010373293987
0.9515640790572064 0.8296131546229972 0.8300192072257673
0.9476745078796540 0.7292679278231802 0.7302898610637811
0.9472123856089354 0.6844766728125364 0.6852785097479810
0.8310142695069658 0.8295872713182249 0.9501979944466754
0.7304063449048783 0.7282969961075096 0.9457435987525855

0.6853414412243026 0.6835111464110497 0.9455634099890062
0.1706723713378651 0.8315154007539434 0.0513493652255477
0.2703685778197666 0.7284536447318359 0.0553450275397296
0.3153334937686978 0.6835232251971775 0.0548041663479637
0.1712383252635448 0.1685097141994802 0.9484517327883495
0.2710895481798374 0.2712836338162248 0.9448888046488193
0.3161756887298068 0.3160197821262472 0.9454703442537919
0.8302625910135362 0.1674195740634588 0.0510879217516589
0.7301690858260059 0.2703552268767950 0.0555853528534129
0.6856829778848024 0.3158198546845483 0.0552736030163317
0.8316786908664895 0.0486823623578729 0.1734780937545040
0.7296971585876832 0.0532397365360069 0.2726036073679552
0.6838990004423806 0.0534083249673003 0.3167008867779302
0.8322157919641029 0.9517434404500733 0.8271521681054423
0.7301765197333481 0.9467947327711741 0.7278040571229099
0.6843907432548590 0.9464231546975341 0.6836865569514430
0.1670077345801957 0.0515318133132538 0.8267065251206631
0.2702207210457601 0.0548302292726532 0.7278591280430646
0.3156310617675047 0.0540848710289694 0.6834010978513874
0.1670331134930336 0.9484938909042953 0.1729325643765094
0.2699208108518292 0.9451831068855938 0.2721690684226772
0.3152848768746992 0.9458909147321108 0.3166446667718148
0.8033926471665964 0.0011965349523422 0.7985407155026323
0.7548992053259411 0.0006653753070296 0.7516472906708387
0.6597581974870081 0.9999781773411343 0.6598086972511155
0.6105967595793658 0.9997924812123884 0.6113885727889254
0.1970098187665528 0.0019578447212965 0.7995401691022366
0.2451658655407556 0.0015549409771936 0.7523225781229073
0.3394828404262498 0.9999515354506201 0.6597304465553151
0.3883007988703184 0.9994157565950701 0.6111157193721510
0.1965303867084671 0.9980501855555275 0.2006401932482333
0.2447297616720263 0.9984548770675659 0.2478224675529859
0.3390658187342197 0.0000090271466888 0.3403987217018809
0.3878849659445223 0.0004323098351833 0.3890370296502681
0.8032980542390362 0.9991488548175411 0.2020826201744299
0.7546627204948848 0.9994362804883039 0.2488189973624060
0.6593301983321922 0.9998098938646365 0.3404770558408430

0.6102745185962206 0.9999178678276195 0.3889910085195112
0.8022583376505139 0.8009724669508813 0.9998982613318930
0.7546268901329825 0.7530555513366224 0.9995909607114228
0.6606855688646718 0.6596403340360411 0.9993105926029813
0.6118332062929426 0.6107923729785085 0.9993847033498611
0.8016837564038326 0.1964516134059764 0.0016064840018828
0.7542821643619391 0.2448069834720243 0.0019645461480522
0.6614380171496421 0.3398083020039238 0.0013315899530610
0.6125729593550275 0.3889124410170766 0.0008914724686377
0.1984876067976344 0.1985421390816597 0.9980174642235298
0.2462602855414460 0.2464116200014530 0.9983129460554494
0.3404161819938309 0.3399053029268018 0.9995316229853017
0.3895037831336268 0.3887461710527162 0.9998816237378279
0.1983510923548053 0.8015334736023334 0.0019547959016961
0.2459182572474603 0.7535350681590458 0.0018753303086143
0.3396991238969349 0.6596796393415616 0.0007268373738896
0.3888945907849433 0.6109185620349677 0.0002465424483589
0.0017118162520191 0.8010315410788422 0.8019465971423756
0.0017658987492908 0.7531120661088835 0.7546451244498016
0.0008912690468819 0.6600084052141568 0.6610839359661185
0.0004287453451823 0.6115841127895507 0.6123222100504222
0.9980022833161826 0.7970095076025316 0.2018133389002372
0.9975246757285490 0.7501689437955932 0.2494468972470187
0.9977351720342043 0.6583823515626506 0.3424189393739425
0.9982652496741906 0.6102447234962938 0.3906207442556493
0.0020488889456800 0.1998951727481852 0.1984589920284208
0.0023211804769829 0.2478576957273546 0.2456334546859082
0.0016114848392874 0.3409823120196549 0.3389069407597560
0.0012041155239970 0.3893729517439297 0.3877085273647083
0.9986822569227982 0.2035818837494432 0.7969133372174824
0.9982032717701586 0.2507807392154078 0.7498003263528972
0.9984037800221728 0.3427620234149629 0.6573955929309676
0.9987277282889693 0.3908745339359001 0.6093009386191852
0.5493615250635031 0.9997272984435455 0.6276728253508921
0.6888887855375998 0.0000584441690279 0.5308492504732385
0.4495078654139775 0.9995641448922541 0.6274480380650331
0.3096253524952601 0.9994165806782789 0.5311554730233325

0.4491738447496587 0.0002101285242020 0.3728155861933544
0.3094978074140755 0.0000864777308891 0.4695601246465344
0.5490775486914359 0.9999174010148550 0.3727439472614975
0.6888096978149747 0.0000401588993881 0.4692325536898068
0.6282820707724142 0.5497085539922253 0.9995887536952353
0.5312162884413709 0.6888281617762644 0.0003271247887113
0.6287422042988169 0.4500847838993707 0.0006376282453502
0.5319558251811571 0.3109916670960899 0.9998822780620387
0.3731600276406795 0.4499260717806592 0.0000227986705497
0.4703091527778511 0.3108129835768310 0.9995898859130392
0.3729128788641418 0.5497067928942343 0.0000257695687296
0.4695825985809847 0.6889030612426268 0.0005759512599042
0.9999488722780967 0.6275027563420537 0.5511724836418352
0.9998307765366050 0.5310777426561302 0.6898569836656350
0.9986024613087423 0.6269017468714750 0.4515925387453876
0.9992542702969658 0.5313906805365463 0.3110225670267184
0.0005410545661491 0.3733998375214611 0.4488426182106124
0.0003454625482675 0.4700078485574863 0.3101765223634274
0.9993115083017443 0.3741589147541902 0.5483969747858026
0.9991809790789929 0.4696817590028175 0.6890352532857307
0.9989362704600921 0.5496007046114855 0.3734902859038698
0.9990525959349625 0.6890216080005516 0.4704151982403388
0.0006794536242012 0.4503815637664914 0.3720537317529917
0.0003625454759160 0.3115942131346330 0.4681136232167944
0.9989555479962107 0.4514487490052872 0.6265390212724284
0.9996088500393867 0.3119902953970666 0.5297338846746342
0.9999785338944349 0.5506039661894562 0.6279532986158927
0.9997953578260237 0.6893208309708854 0.5320417373880346
0.5504257460708075 0.6268892401575670 0.9998500484604378
0.6905677360497080 0.5308914903442457 0.9998283739111784
0.4502716137259668 0.6270209396196975 0.0002425163505109
0.3108288999161459 0.5304094960210861 0.0000242267612833
0.4509138148127434 0.3726966846675737 0.9997952356444273
0.3109792574001489 0.4689762472621837 0.0000163845360106
0.5510664673399930 0.3729190341060757 0.0003125196454974
0.6908658627366933 0.4694836599863024 0.0005279829220939
0.6266274488536752 0.9999944838240324 0.4501872437643897

0.5299530282845524 0.9997765392681117 0.3106138126731253
0.6267486666140414 0.9999519714243164 0.5500893103341014
0.5300378255432818 0.9998448820775678 0.6897810347480871
0.3718626005366232 0.9994928965365020 0.5500037995190894
0.4684058156795672 0.9997175127452991 0.6896584326799413
0.3716474191110350 0.0002812503743144 0.4502641116350929
0.4683139542519257 0.0000080634829658 0.3106678337436293
0.8254882706935263 0.0990748620547421 0.8186803913804965
0.7464598822979980 0.0979437873504523 0.7437070862022779
0.6667255298996153 0.0971535017452467 0.6670399874394306
0.1774171816131869 0.9042413888637739 0.8225925645559187
0.2523124244509134 0.9041065356886762 0.7449422371118217
0.3314073036182208 0.9029620147746371 0.6676109194934838
0.1761613446082251 0.0957834359493148 0.1782306644640812
0.2520284469291951 0.0959464904601788 0.2550157412005163
0.3311397826759617 0.0970585449407153 0.3322186643170184
0.8259831295196989 0.9013210822358957 0.1820516880896577
0.7465151096481577 0.9020998604103312 0.2565987895140651
0.6667173935665645 0.9027637041479082 0.3333309692926889
0.8227555368267190 0.8231388416112537 0.0980207162761033
0.7457469974622626 0.7453955727859096 0.0973238150540112
0.6676518517801284 0.6676148686347574 0.0967552226836546
0.8230385170939698 0.1754236596325356 0.9033588181700551
0.7461010771707421 0.2522970054452784 0.9043042363171310
0.6692117841998808 0.3311464414482899 0.9039228818995326
0.1745629224201011 0.1797656029462260 0.0961329416659353
0.2540655723631460 0.2541465875699842 0.0961383100396631
0.3319961345981284 0.3317866535002949 0.0969484585960885
0.1754692963772229 0.8205286038514714 0.9036682148844690
0.2539281240980387 0.7458928589212874 0.9040735094959089
0.3316483974182773 0.6679197533304730 0.9033205998291081
0.0995682750316931 0.8228093413735635 0.8235448400233949
0.0994635780584332 0.7442653498770611 0.7466358572823495
0.0983600401632572 0.6661492059498926 0.6681893948862552
0.9002480462528126 0.8204061362587467 0.1816629509870538
0.8996898221552243 0.7425197321961292 0.2572529297838813
0.9002350352723951 0.6647900767356418 0.3361954702197707

0.0998889908689549 0.1775909054956983 0.1765441309685727
0.1000859152124889 0.2565734266812925 0.2531548290267693
0.0989490663672967 0.3349728528303046 0.3315092719570458
0.9007691775491438 0.1815946586544541 0.8181743239364039
0.9004262981585853 0.2588176115951057 0.7428878739665876
0.9009249147785638 0.3369730247982545 0.6643032292576976
0.0966556125795179 0.8155343297604460 0.1796544943163454
0.0953820496391486 0.7430739579084431 0.2569615868579902
0.0950931957676815 0.6651247904233841 0.3356079832714229
0.9035690461859005 0.1790687284245465 0.1779634533587853
0.9045876972461073 0.2546928752962927 0.2538000091891206
0.9042448363734295 0.3328763832418673 0.3321177967054751
0.0973220330402427 0.1832849862181263 0.8174331679660654
0.0959842059266194 0.2577824591648650 0.7422599479393881
0.0957641914008960 0.3359195475060019 0.6636554183186121
0.9033055263371779 0.8223070167676099 0.8225304903743904
0.9039661768117710 0.7461815600406538 0.7466149103533226
0.9035395348664892 0.6679724185026998 0.6683947504968373
0.8238002666035413 0.8224326431118243 0.9018365353526718
0.7469872258843040 0.7443866377755839 0.9018450431697858
0.6688137197672575 0.6666970145100208 0.9018491595653870
0.1788223964381714 0.8260190513737484 0.0997083821268347
0.2540091451007385 0.7442733814546187 0.0995026132102552
0.3321147233772521 0.6665003193148280 0.0982266990571645
0.1796725112936954 0.1740147691648559 0.9001115367730108
0.2547864412171421 0.2553875568288717 0.9007454305557587
0.3330872501561828 0.3328957403699846 0.9020224208946246
0.8225184233656861 0.1738342700657469 0.0994594875309431
0.7463184640784633 0.2544077537839726 0.0996886195326709
0.6693345661959569 0.3331341166531274 0.0988651152106144
0.8241433790948136 0.0968511584795522 0.1802842854905435
0.7465737278629874 0.0969377232833537 0.2566460268876938
0.6667079657374941 0.0968910900327487 0.3332262801353636
0.8250252794795614 0.9035190023945106 0.8202439776260633
0.7470511246817750 0.9031453520375550 0.7438869928358045
0.6673268251008366 0.9028716612605976 0.6672722513177192
0.1731112832710195 0.0996776444338963 0.8186501696203337

0.2540130651628516 0.0988240471943129 0.7439025147301308
0.3330852233005075 0.0971349459596738 0.6664059152545221
0.1735070654313162 0.9003440869888735 0.1808132854942599
0.2536745326330774 0.9011821230704768 0.2561433354365121
0.3328459943826587 0.9027980070268171 0.3334227788466180
0.7274358532210812 0.0001426113218628 0.5617005360312390
0.2713338031402159 0.9991026193969503 0.5623265014521053
0.2710864760797094 0.0003288711834557 0.4385709347496203
0.7271958166867307 0.0000844773823871 0.4381582433502729
0.5621894818074793 0.7271374608065386 0.0004410627232545
0.5630429431440689 0.2727492948831198 0.9998416708989595
0.4393721638515657 0.2724657788004023 0.9993643388380633
0.4386325735230514 0.7272744744600601 0.0009238158847893
0.0001528881680883 0.5617482711557074 0.7285398469112749
0.9988143626005055 0.5628556714550967 0.2731610816165073
0.0008185921806358 0.4393107797282099 0.2714840263488512
0.9991863673343246 0.4382413062014834 0.7269024126869823
0.9989841499000107 0.7270543916544412 0.4392055377377417
0.0007534436508436 0.2731180548650940 0.4372457316859624
0.9992871810278317 0.2740562304130734 0.5610450368647832
0.0004040641721375 0.7276163939997531 0.5631612788175104
0.7288096553358017 0.5620220728480803 0.9995996605804578
0.2722947774016191 0.5612120182523412 0.9998676709067382
0.2726008710004209 0.4380348461310248 0.0000516734251761
0.7293812998310329 0.4386750330122311 0.0008035464310936
0.5610314262822200 0.9995158497819006 0.2722210843650359
0.5610081740932387 0.0000652402774080 0.7282148263792934
0.4372129190841818 0.9997957707537211 0.7279526191968984
0.4372821202867812 0.0000863071812560 0.2722818410770103
0.1420775120210891 0.9717699922408940 0.0203683180669145
0.1399431196894838 0.0309450566532590 0.9806928282232974
0.8557984127439155 0.9646309125197376 0.0103117586236081
0.8648262030996747 0.0302955461136278 0.9838706457357276
0.0015111858029329 0.0032273535052454 0.1369208108362585
0.0004645308624944 0.9970396142458782 0.8630682658237632
0.9998529422741669 0.1345364894513494 0.9988817138686485
0.0003950358091984 0.8655647498041006 0.0007581097135585

PCN-602(Ni-Vtz)

1.00000000000000

21.7332543125591755 0.0184133228324438 -0.0108466993832868

-0.0091527108383081 21.7721676385132810 -0.0402797814190390

0.0261258691460694 -0.0480481824604645 21.7525840433166842

Ni O N C H

11 6 48 156 92

Direct

0.0719854230675452 0.0703292985188213 0.0727632118486170

0.9303852262422367 0.9255863659409655 0.0766470835891369

0.9316698235270451 0.0752806487059345 0.9201140252959519

0.0721529004794590 0.9297795934792035 0.9282051122660420

0.0665540922840719 0.0728013030956376 0.9225997191097761

0.9314807026470362 0.9281699699904564 0.9265526362547689

0.0670286207552024 0.9248781987177352 0.0733893078953827

0.9276614413008417 0.0748041487308129 0.0784107123958009

0.4997995451853754 0.4994463888065468 0.0033760431768144

0.9970259560066523 0.5006596476974394 0.4998385512513792

0.4997132221370393 0.0032819330325324 0.5002087103385477

0.0014501415922510 0.9087922911699735 0.0017346240482325

0.0027392817085996 0.0895151464590782 0.9960285367080886

0.0009925851652284 0.0025032098183644 0.9048203241594734

0.0013416241133584 0.9984751771276521 0.0927716576510065

0.8852758128317717 0.9927055569700940 0.9995936594592791

0.1165845405700310 0.0002235458018873 0.0013361476361737

0.8732701589630594 0.0304291734875477 0.8659544122705896

0.1276189947130320 0.9695795542439853 0.8688715576149590

0.1281423134415931 0.0281276401164305 0.1316280864561108

0.8745653451192013 0.9678678862080261 0.1327368474978812

0.8693176557173032 0.8707739445301073 0.0301142414152409

0.8725732459722266 0.1260730623992643 0.9675056770012063

0.1285150908168191 0.1299145079409882 0.0292435218934202

0.1284342044003566 0.8705482235455193 0.9687852474313701

0.0335776285741787 0.8715224024463737 0.8705793309113758

0.9688318851939002 0.8665946942420248 0.1322373871934346

0.0336546727931335 0.1282272460299296 0.1289655559653582
0.9700485206880884 0.1351942825126571 0.8661787737717859
0.0306280872000642 0.8651864835935967 0.1278399992093426
0.9716114813996839 0.1319545708208878 0.1309880830828192
0.0318685637731519 0.1313712402130847 0.8661901535812291
0.9719117401090145 0.8701162013635013 0.8699576879116364
0.8761671779166917 0.8677032478423854 0.9679240856342943
0.1293538297996975 0.8700744380690537 0.0309764686740976
0.1315233545829670 0.1222437948135777 0.9670426962781988
0.8705076418223143 0.1287953808317681 0.0305588715655247
0.8717624411244174 0.0302055704827637 0.1343448617511740
0.8770094466641467 0.9682829252329554 0.8659798521740285
0.1268716164534922 0.0314782327709793 0.8662487925235851
0.1275440686271097 0.9659046614293771 0.1284035562830397
0.5894198155480979 0.0028339973819769 0.5005275066819621
0.4099636766208619 0.0034855464478483 0.4998010046777281
0.4999611261163395 0.5892340518010144 0.0034130139669273
0.4997109159624102 0.4098439660661271 0.0027756329670012
0.9973959224248290 0.5012739502685548 0.5894209644052850
0.9970078831097524 0.5000136109248956 0.4102734894550224
0.9963994182047102 0.5901653753795628 0.5004076638877919
0.9972674502841770 0.4111974370872318 0.4992757388538038
0.5896404552217831 0.4994556587638641 0.0032101701478524
0.4098487034105034 0.4993721454922877 0.0036208723952456
0.4996291008620162 0.0032422274483039 0.4105900368992366
0.4998950719215287 0.0033532519528876 0.5899823178703016
0.8311786440946847 0.0496568310721557 0.8267068787754468
0.1686987165363973 0.0477859169137673 0.1722619720601344
0.8270416116147885 0.8312879170722738 0.0491025637585381
0.1674714633469421 0.1722918517411216 0.0478896163031521
0.9486519979068930 0.8272960633333355 0.1735482224390807
0.9503641158801273 0.1763469488336113 0.8266117259842289
0.9531951836725270 0.1732248528261451 0.1712503529606195
0.9507240452534305 0.8294043479302644 0.8299218816014147
0.1697892399730350 0.8294929382003033 0.0518437478720060
0.8293354191645506 0.1692638653606835 0.0490033574597533
0.8303330313375525 0.0491248155712256 0.1744337774793223

0.1675175189926605 0.0520865415512759 0.8258600592272387
0.7322634375985615 0.0563730342987796 0.7307654195176383
0.6857542656721520 0.0570093847799598 0.6862511359688668
0.1701151602394901 0.9499814964417652 0.8282676373487163
0.2704909736017171 0.9492666179911495 0.7305180839845491
0.3162351489853563 0.9496144855543847 0.6854544869636996
0.2683424355712276 0.0555254662926004 0.2681011429473514
0.3139430805271388 0.0564428261055951 0.3135934533555371
0.8331753412690048 0.9467124604845125 0.1734801980957030
0.7309332376993396 0.9458827681621855 0.2717319679133112
0.6848456022416869 0.9468953796281241 0.3165423780865524
0.7322029334966516 0.7309817259135514 0.0559804796100067
0.6862562847124778 0.6858338084652118 0.0567845805286424
0.8309757741409030 0.1669188855788164 0.9465668954386075
0.7310337092811139 0.2686301599618943 0.9457369552785977
0.6858115889256737 0.3144571953461295 0.9466986192845184
0.2672168710106178 0.2679539803240374 0.0551256116500056
0.3123539630910628 0.3139519699180866 0.0560423915720349
0.1697168277885552 0.8285656768039118 0.9496206860757610
0.2702998808040675 0.7304750380463432 0.9495177610696430
0.3157174442754140 0.6850216162531311 0.9499421170048947
0.0531723981406955 0.8297855182947416 0.8290464552394283
0.0529262044047272 0.7286184464825212 0.7318208789502236
0.0520848188151746 0.6833478262163837 0.6862275678476593
0.9410824322327187 0.7283946230930738 0.2689030802469858
0.9406249404113893 0.6836571102686122 0.3148586635644293
0.0558933148512253 0.1691097085588282 0.1698939112050510
0.0571886821448615 0.2707096864941079 0.2699334487924858
0.0556865025501594 0.3160735148574361 0.3155565344508418
0.9433943167963790 0.2713237459829969 0.7287163977257478
0.9428315919575283 0.3166558808369899 0.6834358927168296
0.0510892696831462 0.8228084854176672 0.1677524572863689
0.0517140823637590 0.7283217628162006 0.2707208893874622
0.0511441752620954 0.6836249016725802 0.3164469791286706
0.9466302930566215 0.2690332933223161 0.2677598882200272
0.9452723208630687 0.3144531186103734 0.3133927834031525
0.0529577534485739 0.1717253015081894 0.8245851390774774

0.0542052691003860 0.2734067771773852 0.7285454244768843
0.0534587710094172 0.3185799624690731 0.6833022365118353
0.9424521497776013 0.7330069735412508 0.7303212619095376
0.9417360680239284 0.6876467929306926 0.6845691010425341
0.8368175173290808 0.8245622737052329 0.9473482619509568
0.7308983356649676 0.7293705080028872 0.9458531826115859
0.6851171455631899 0.6841886174222580 0.9467898177119309
0.2677684363205728 0.7302827179714271 0.0596651951173754
0.3132794059532316 0.6846585668409872 0.0600246518141816
0.1746809646470453 0.1618607692480083 0.9462655381633880
0.2699309639844216 0.2679402772702915 0.9450206275789625
0.3151090317968297 0.3137153644307915 0.9461054723602587
0.7312384186229934 0.2666726894243183 0.0558964448580355
0.6858904156848666 0.3125690467232687 0.0566573352231217
0.7319829715960680 0.0562510632070712 0.2704037738149054
0.6857854218696815 0.0570816991499328 0.3152961586443013
0.8358073345578205 0.9474793472665795 0.8246668623773843
0.7317776905677746 0.9461962639088171 0.7284738422748376
0.6854798287328308 0.9469345266723863 0.6839064810038096
0.2668834550292729 0.0594623633590601 0.7287891736678134
0.3127536275378162 0.0597059918900555 0.6835881726402491
0.1699232768373733 0.9455466666120529 0.1688064643363418
0.2689881273086101 0.9454263818343236 0.2701064355513196
0.3145257350435173 0.9464565368682258 0.3154505277934803
0.8060792731147330 0.9988450321901752 0.7994252198143599
0.7566598770560233 0.0008187629970422 0.7529585261528382
0.6613289566433593 0.0024124570316815 0.6614961638775441
0.6120915332749561 0.0028033806276682 0.6127556746683354
0.1959485693910565 0.0019778117036253 0.8005158801083070
0.2444799528150767 0.0041259058780270 0.7532560281246958
0.3384879598073667 0.0048756335753879 0.6607821187579148
0.3875745226346439 0.0045444511029800 0.6119896230956101
0.1962963577736261 0.9971954012414557 0.1973043669523307
0.2446052407773038 0.9998334325523643 0.2450757999938062
0.3382886577148199 0.0020506379882121 0.3384759552891978
0.3873355597550372 0.0028630473173266 0.3875536446490884
0.8045675317167067 0.9981646758457643 0.2003556794706896

0.7558164350742516 0.0004628390831627 0.2475516038937613
0.6612096788340622 0.0025366875713360 0.3395489349191365
0.6120211524913586 0.0030459216129870 0.3883406032080217
0.8049778925419844 0.8011612391212566 0.9985121008593012
0.7560861492230231 0.7538522544775290 0.0004023279627532
0.6616087247070297 0.6608986707963069 0.0022916164177644
0.6123946717255961 0.6118399745159522 0.0029091298388835
0.8032908764500561 0.1950176172570934 0.9979339727812118
0.7551541859016808 0.2432959679060218 0.0002352412550763
0.6616788516739405 0.3377229361747069 0.0022147935714543
0.6124010673499498 0.3870140086267284 0.0028122889939795
0.1975501814706604 0.1944537379260254 0.9971216731647488
0.2448427254252863 0.2434138092752605 0.9994304820389459
0.3378641930449078 0.3379656047403685 0.0016956947727138
0.3870445419537560 0.3871286793698090 0.0025104976113255
0.1966086793621926 0.8021054485055998 0.0018799763379533
0.2449016985036607 0.7543396262065016 0.0042703522431324
0.3384656537542554 0.6607322934149948 0.0052805272880931
0.3875233994511760 0.6116564467271601 0.0049980832184389
0.0008646631700842 0.8025908012170717 0.8028450237967846
0.9982155813960034 0.7546198317230548 0.7550211769606179
0.9964125166407953 0.6618616758270335 0.6614012590753191
0.9962329374024890 0.6131209988466395 0.6123596431265739
0.9991680289259364 0.7985216944758093 0.1973429351994511
0.9967987320568881 0.7516552391811615 0.2457352194244038
0.9955641621649036 0.6602765652242866 0.3395256310847330
0.9956796385578173 0.6118360165321448 0.3883506484686521
0.0048344080081932 0.1980114326857318 0.1971829655891852
0.0027462098471531 0.2460836153658477 0.2449242220598933
0.9996492445529910 0.3391023460316376 0.3383416786425570
0.9983159982049301 0.3880461349261495 0.3872891196034942
0.0013335597522186 0.2008079021750646 0.7992639960069425
0.9992473094556402 0.2487184768191923 0.7521270107066798
0.9977338820418993 0.3409824014531182 0.6597580364505973
0.9973441347947940 0.3894441662245285 0.6111752695791210
0.5502193089800542 0.0029395963833920 0.6295658560443087
0.6921605961224770 0.0020751674070780 0.5317457840520774

0.4493165345392569 0.0037520110538480 0.6291753843158219
0.3072674098657870 0.0032941646094429 0.5311950206692941
0.4493096641730006 0.0030936111411748 0.3709839488879112
0.3072518088716478 0.0026797112337533 0.4686208413626147
0.5502378833172088 0.0031956060115661 0.3713679236826337
0.6921138339147959 0.0020973758663345 0.4691791695749430
0.6290974084109848 0.5499261754641438 0.0031906685903493
0.5311631175301770 0.6917908704419844 0.0022610545218100
0.6291295501171561 0.4489442401239714 0.0030283648795972
0.5310153406470448 0.3073112884240246 0.0019792466339723
0.3702741681953441 0.4490139502812482 0.0030055727263729
0.4683897427378270 0.3073640715911381 0.0018532907983513
0.3705109070797050 0.5498860779777530 0.0044260364754649
0.4685353991491965 0.6917312375142757 0.0031008076949774
0.9961359981101339 0.6298588263718159 0.5507061144381353
0.9980345404219264 0.5324146002867352 0.6922161354447809
0.9961735288353992 0.6291365428487268 0.4499841527680104
0.9964795788876515 0.5312802543602118 0.3077507437248101
0.9978295857009698 0.3715065145550867 0.4490132273701946
0.9975626730371090 0.4687871369656023 0.3075251255381843
0.9969687212772911 0.3721257121430597 0.5496108035477647
0.9984561759353952 0.4698916021364141 0.6918529030559384
0.9962400049099855 0.5502641633077587 0.3711033517873332
0.9961138654593853 0.6924148856941983 0.4688906663913031
0.9978008858406326 0.4497004051686133 0.3706663277641127
0.9976202034402775 0.3084577379901958 0.4681942330732696
0.9978740078927473 0.4509806425171163 0.6285090196687548
0.9969558795158946 0.3087881868976297 0.5307518435483587
0.9972353894221797 0.5515407226082090 0.6291117987890331
0.9960645888407882 0.6929049362347541 0.5314700605081057
0.5504466995689512 0.6286654917396461 0.0027464118965881
0.6923399888819404 0.5306730782291282 0.0031489922576000
0.4494067206669854 0.6285674076811603 0.0039397400758432
0.3071904154070069 0.5308944688613408 0.0040496898404072
0.4491008281191924 0.3704719201711342 0.0023822540073581
0.3070564623588865 0.4683653231155134 0.0030926970888814
0.5503045732460876 0.3704208638294944 0.0025534749544889

0.6923515528575237 0.4681587363256412 0.0030083409919541
0.6288441731081562 0.0026355749225999 0.4501128053715107
0.5314099570187452 0.0030705835204472 0.3080899718391024
0.6288878811836724 0.0026095670362736 0.5509264770524069
0.5308450384651948 0.0027467213707340 0.6927101657396193
0.3705792984278844 0.0038994916518789 0.5502545595966311
0.4682237536934082 0.0033532609437756 0.6924551411387654
0.3704799781707280 0.0029467099761860 0.4493889607592223
0.4688004659777008 0.0029560559943604 0.3078669993871870
0.7504915822742362 0.0997472752562558 0.7487845911901374
0.6679145844107666 0.1011832472799767 0.6700334726148185
0.1793041141310354 0.9012913737362709 0.8215153561312434
0.2546559884399358 0.9049173645720288 0.7481869422565097
0.3353069530603463 0.9059904566015788 0.6688035202873053
0.2506396138288949 0.0989024180352871 0.2498433126528639
0.3312534541591106 0.1007452982916988 0.3303368266509210
0.8275774703781664 0.8973955841685211 0.1799391276767892
0.7478464681261769 0.9013225456431968 0.2552144283268944
0.6667601075278213 0.9034314187497969 0.3343124384081761
0.7503900114299213 0.7490581543712409 0.0993955333486340
0.6690503837189752 0.6693947339657313 0.1011484797858202
0.8251259329283442 0.1729843596357412 0.8971544204256432
0.7479937254433153 0.2523582799708208 0.9010406259559574
0.6686440388592843 0.3325125132798874 0.9029763653715648
0.2488844935228514 0.2503970444482135 0.0985884860688699
0.3284996217737586 0.3316040544719883 0.1004552218049213
0.1773525960123976 0.8199121336407273 0.9009076652945822
0.2542412923910859 0.7477931078446005 0.9050800634408063
0.3341228150344051 0.6678163251999933 0.9062076643298269
0.1018855386913131 0.8222520458489768 0.8202541124652285
0.0974972815144355 0.7437893253379855 0.7499374567670785
0.0955699137351615 0.6641511055938309 0.6692562132269373
0.8976934308130993 0.7458300133218287 0.2502352122634690
0.8965413053708104 0.6662756548179800 0.3320555618397592
0.1054193998857258 0.1740780029410089 0.1760954857791717
0.1018764933423171 0.2539343567129464 0.2535162811616729
0.0990533291735503 0.3341240028669432 0.3339080110621708

0.9000279929114541 0.2527287983056468 0.7464213999597220
0.8988609009343875 0.3337649689933357 0.6657267110413869
0.0999362360123754 0.8122542867742197 0.1710535064995824
0.0961084600003943 0.7455294252898597 0.2542270739131851
0.0947381691738300 0.6663315970434880 0.3348505833429343
0.9036111188073406 0.2504322166088429 0.2491860270508823
0.9007565571908955 0.3314281636571721 0.3300630670809070
0.1019830827924508 0.1757382862417387 0.8152322612216949
0.0986274350271756 0.2570620836410669 0.7458602536147794
0.0969296531544686 0.3370649348082253 0.6657766528230624
0.8990517789888699 0.7521622181365046 0.7475738573347002
0.8975507036243187 0.6717494269751754 0.6662476955330163
0.8349282834275655 0.8131215815962847 0.8985568696882282
0.7472971676880249 0.7458324644903342 0.9011620481040410
0.6670273236767059 0.6665886531974792 0.9031207906902736
0.2491604014873019 0.7477546306670888 0.1031685895996048
0.3297181496784347 0.6671601881292304 0.1042482860288061
0.1863491249910041 0.1628250733152825 0.8975393642264393
0.2537265007310481 0.2510543075206400 0.9003209333545072
0.3331523980525475 0.3311766431645538 0.9024654890903605
0.7486958840991136 0.2484566140704985 0.0994627854551311
0.6686823368967012 0.3294086128803499 0.1010316175434554
0.7502525108121461 0.0995533892269691 0.2524934869453119
0.6683854421850413 0.1013113699724215 0.3322617550473410
0.8316308897166351 0.8984326346364426 0.8154579072931227
0.7491272115644989 0.9016831693491554 0.7442929324055285
0.6675954969301472 0.9033239620595950 0.6659998879114823
0.2476407796276092 0.1028835008333786 0.7456624531180864
0.3290573452723251 0.1037081960697961 0.6654760335349721
0.1788305338643283 0.8965439445558445 0.1734645622944484
0.2519235288891934 0.9008349730522269 0.2539385631060611
0.3321160284456610 0.9029101545054274 0.3334472662982861
0.7311473270175028 0.0018312778585852 0.5632758050025188
0.2682388932476698 0.0031916937653236 0.5627099052531719
0.2682834673772234 0.0019683442574063 0.4371077929815570
0.7309369020841103 0.0016820480364430 0.4374396378667882
0.5626311847044860 0.7307563091374760 0.0013262082363212

0.5626279714913665 0.2684206313522779 0.0017712306605091
0.4367118904249310 0.2685475876811552 0.0015485114428770
0.4369248086650401 0.7306250353464634 0.0026892513435683
0.9983327134697220 0.5638481189583260 0.7313326659335715
0.9956777307137727 0.5628703671714845 0.2689598387632373
0.9978988946485430 0.4371490473019648 0.2685471348410857
0.9990398855247875 0.4381823917177314 0.7305031855842259
0.9959388355049441 0.7309779923387225 0.4370885323307334
0.9978252137781638 0.2694810453563932 0.4365957831304854
0.9965507314460638 0.2700697393947991 0.5624124238482651
0.9959626749987436 0.7321084973225780 0.5628372280176066
0.7312477704574931 0.5622660284520435 0.0034800001903079
0.2682296366502115 0.5624641720039421 0.0043615510484614
0.2680828169645366 0.4368589334729904 0.0026645636661158
0.7312868124398122 0.4365461338326142 0.0029432962035969
0.5633056954278217 0.0029488240757942 0.2693902407397744
0.5622692616061187 0.0022784744219138 0.7317894588106029
0.4365128479146634 0.0033286857751946 0.7312772601852515
0.4372843031692355 0.0028026263515670 0.2689067456747267
0.1480950798152989 0.9748010107380978 0.0220667770315686
0.1395065352899039 0.0347071737400171 0.9810961855412685
0.8513611415783089 0.9638279176381062 0.0090512553949367
0.8651869425732386 0.0328519567750050 0.9905278847495609
0.0022411274824634 0.0000023303430012 0.1379391336210034
0.0013005896532192 0.9981738785650833 0.8598183889204165
0.0021650016481303 0.1345288914225051 0.9994239612152995
0.0006436164697377 0.8637490076118226 0.9988836179211802

PCN-602(Ni-Ttz)

1.00000000000000

21.5637266168798192 0.0075555598790846 -0.0181274903189451

-0.0197247215773522 21.5972862028175356 -0.0108550128697872

0.0191201795382385 -0.0196639325279889 21.5192550551036490

Ni O N C H

11 6 60 144 80

Direct

0.0721431484644199 0.0732875068025365 0.0745662739140371
0.9287605102718430 0.9262643418199730 0.0765326991231916
0.9287578524899160 0.0739763820772623 0.9238798147740184
0.0719508728351599 0.9269826845352753 0.9258216125829009
0.0690874893463231 0.0748876987777507 0.9236583328198336
0.9303622894814367 0.9270532869148411 0.9244779564494010
0.0690125929054020 0.9255433263711339 0.0767217641485445
0.9304273899252422 0.0731886552568994 0.0758755846988137
0.5000931301617726 0.5000084691041451 0.0000033683454532
0.9999861966229133 0.5000374404196819 0.5000598579449473
0.4999551515836842 0.9999978868790294 0.5000348364734606
0.0003311515516344 0.9091603331081544 0.0008662007088063
0.0005208964929295 0.0912366626271961 0.9996590609433298
0.9991490234708564 0.0002953523592453 0.9056091030866753
0.9994199818112222 0.0004784681309715 0.0951562622382909
0.8792300036597283 0.9991364005931729 0.0007588136668133
0.1199362380906237 0.9994562408304262 0.9998200291568509
0.8717374055112259 0.0313826721283661 0.8673413752306232
0.1282280227853718 0.9690712472085110 0.8677638013150641
0.1285079825269690 0.0312134402710313 0.1323618991163471
0.8718793996827614 0.9687830357385465 0.1332780551905444
0.8705166756821541 0.8700076531794778 0.0319009489073636
0.8705957560460362 0.1300844896596161 0.9682145303342509
0.1292743823682940 0.1308117846073884 0.0316239336244024
0.1289622200324487 0.8690384940528375 0.9685806824727337
0.0322874462708498 0.8687630272427498 0.8688799024136671
0.9678844692722279 0.8676285687845038 0.1324439429631283
0.0323535057795397 0.1315606258684738 0.1313752876498526
0.9678138626639523 0.1325726104344795 0.8678284637970251
0.0301972987894104 0.8676700506994166 0.1322722207989173
0.9700936497899306 0.1316417699305461 0.1310263659145008
0.0301347519776982 0.1325916284013928 0.8680318094976371
0.9700444818639511 0.8687466560973860 0.8690553104680276
0.8707366802252920 0.8702660188277989 0.9685741463610498
0.1303666211124224 0.8709737561916668 0.0316892510730682
0.1302828840035986 0.1292383671725972 0.9685159967204484
0.8701350950696920 0.1291616846708621 0.0314940765184915

0.8721468469682847 0.0313531656951369 0.1331085905785585
0.8721805719728337 0.9688287494495853 0.8672122617276088
0.1279801056364036 0.0317117484920431 0.8678279809359992
0.1280367616822602 0.9685987622378818 0.1324312338181599
0.5903779462419294 0.9999926663273655 0.5000298382228507
0.4095682456037366 0.0000104701508903 0.5000363907387921
0.5000665196791729 0.5902659231052780 0.9999707497555974
0.5001043711227666 0.4097371259941056 0.0000280091051579
0.9999906889432637 0.5001434533688069 0.5905027615347649
0.9999891887862944 0.4999378828677976 0.4095839874318301
0.9999824355650517 0.5901193789576240 0.5001988759409954
0.999990623677562 0.4099411395790256 0.4999174758694309
0.5906139336507223 0.5000061043117512 0.0000045520965912
0.4095271798712261 0.5000205849729085 0.0000081086015271
0.4999497463207945 0.0000168740421884 0.4094473358315511
0.4999370754963977 0.9999697945027961 0.5906013494108819
0.8298319791949424 0.0518247629235091 0.8279447640192998
0.1698478574789419 0.9485780029501569 0.8280745157912719
0.1702486955648155 0.0516877555210797 0.1719536789087783
0.8299245568199680 0.9483727619015596 0.1726456335735307
0.8296555585882572 0.8293835776720186 0.0520698217430891
0.8300431216395765 0.1709031677935897 0.9480145269000673
0.1696425395863201 0.1717365623593778 0.0519668686640173
0.1691825174893467 0.8280350230336637 0.9482302744880968
0.0529461070136108 0.8281227354723626 0.8282063024686366
0.9472507136505399 0.8270404609177220 0.1729858377780857
0.0529543874471656 0.1721641154485880 0.1721257949850639
0.9472029760206695 0.1730179840676271 0.8271659208339130
0.0513978392391579 0.8272277510686763 0.1725806657471338
0.9488356256635626 0.1721078006329506 0.1714737649722125
0.0513493345674050 0.1729338436276535 0.8276181518733097
0.9488192461451206 0.8282622593208444 0.8285787134530267
0.8299354293771302 0.8296633019940671 0.9478582428236564
0.1717547896494125 0.8308221743799606 0.0523713056500199
0.1715318152424459 0.1695107986870639 0.9477961307541278
0.8291377157934221 0.1696144903858610 0.0522074608172147
0.8302683698716251 0.0522010830195043 0.1724790572207411

0.8304841014547506 0.9479994305391202 0.8276322825656450
0.1696126596246188 0.0524079390417143 0.8280363224144054
0.1696491764853221 0.9478689263736015 0.1721922044831672
0.7317838341512797 0.0556659775566146 0.7324233796145023
0.6859735789914865 0.0555793425817726 0.6865457178409002
0.2679375848024605 0.9445238830432743 0.7324272252968314
0.3138093592739679 0.9444976787504444 0.6865875797648542
0.2682311035236538 0.0556599922908489 0.2677380115346750
0.3140591660440748 0.0555985000181352 0.3135821006079880
0.7316844174666741 0.9444321114617722 0.2677247396473845
0.6858688517578599 0.9444832990009715 0.3135763952003927
0.7325109397302043 0.7324135201771256 0.0557473713313286
0.6866637461897938 0.6866028022593582 0.0556578970962249
0.7324786388394600 0.2675786634675248 0.9442810086829425
0.6866769425629329 0.3134128582824971 0.9443658590818416
0.2677530761136069 0.2677696657727608 0.0557103585397840
0.3135616292512040 0.3136290803869173 0.0556445561291667
0.2676566632192845 0.7322259582511990 0.9443108248260899
0.3134698865589129 0.6863912838705133 0.9443704527492827
0.0562581915388307 0.7313776801531233 0.7314806302277574
0.0559634061783498 0.6854763683761220 0.6857643441639567
0.9437070327332435 0.7307141221382238 0.2690914554207566
0.9440077937710143 0.6849712244596731 0.3147523304684370
0.0562552095362747 0.2688453283811256 0.2686907687214273
0.0559148500256441 0.3146986918185775 0.3144050469411681
0.9437504343733494 0.2691915146890054 0.7309316489439652
0.9440611534087324 0.3149592889969384 0.6852933749889800
0.0559248000287482 0.7308800481011204 0.2688700411982055
0.0558029177282791 0.6851256760377638 0.3145742479975198
0.9441427115766743 0.2686457499099930 0.2684983822754035
0.9441700502681130 0.3145468268734248 0.3142418720631568
0.0559647562805594 0.2690906205057146 0.7310994734491771
0.0558499946850475 0.3148741015183276 0.6854265796327965
0.9441905228737966 0.7314818302886295 0.7316859099290909
0.9442196335171644 0.6855675136112893 0.6859368669948864
0.7323824600017659 0.7322366276430188 0.9437710981218430
0.6865025240052205 0.6864422762377345 0.9440298162668483

0.2677550726937099 0.7321996599077707 0.0562739067388094
0.3135497762472284 0.6863627879196201 0.0559980992814531
0.2678338625177048 0.2677846422605228 0.9437000971761123
0.3136104620977775 0.3136709618430018 0.9439721950546769
0.7322974900058483 0.2677475172874608 0.0562108087380082
0.6865003880343963 0.3135725490200585 0.0559548951878668
0.7314988438123962 0.0562399602554891 0.2679015910080977
0.6856630787914568 0.0559667891415145 0.3137358828019075
0.7315984860539544 0.9438937802729086 0.7322439346620868
0.6857570281829268 0.9441378256612154 0.6863951669064505
0.2681349128489430 0.0562579226646989 0.7323081694371325
0.3140205438971435 0.0559178028633696 0.6864945014674575
0.2682205621930720 0.9439027159521771 0.2677314584583925
0.3140613278963897 0.9441666484941535 0.3135699767591404
0.8044160449371134 0.9997997144257269 0.8033519940416980
0.7554296199763684 0.9997572996641395 0.7559188926085767
0.6620869715438786 0.9998916481467717 0.6625660451255797
0.6129346616905451 0.9999308989742559 0.6131878375722764
0.1953335424425688 0.0005574815092118 0.8034730801039487
0.2442638261921033 0.0004714258546059 0.7559363650877202
0.3376998947382006 0.0001168231720996 0.6625832739811841
0.3869504713215761 0.9999904418680075 0.6132453815984036
0.1955877776054820 0.9996898984973228 0.1966155148544360
0.2444859351432740 0.9997424785339177 0.2441463036465166
0.3378098195624233 0.9999358637937164 0.3374981673465953
0.3870031415386990 0.0000144364225321 0.3868451347020070
0.8043058348684653 0.0004221233929087 0.1969302913892577
0.7552969389170556 0.0003972846505391 0.2442599578567055
0.6620157611511033 0.0001659935170935 0.3375114623993554
0.6128953052299622 0.0000732507018810 0.3868692709637287
0.8047345862024571 0.8042738489165586 0.9997943101813576
0.7563207624578538 0.7560156107288236 0.9997290505133520
0.6625695749775602 0.6624778367370254 0.9998932986746638
0.6132591522218362 0.6130412391375941 0.9999573104535813
0.8045772104431776 0.1955523616955901 0.0002831170653224
0.7562238648533679 0.2438921519112824 0.0002804791422690
0.6625690034822043 0.3375515459352698 0.0001057656606136

0.6132852936559559 0.3869763558038173 0.0000387085881357
0.1956667468784090 0.1958008464321779 0.9997108280955374
0.2440223125254946 0.2440235413305345 0.9996730429955747
0.3375572293257747 0.3376263887702535 0.9998702314298171
0.3868858815166760 0.3870392551227937 0.9999713305231381
0.1955284660789047 0.8042188360287241 0.0004496515713157
0.2439097710600748 0.7559892629200888 0.0003389875597932
0.3375121289333265 0.6624000598364148 0.0001128326155140
0.3868474372024124 0.6129882314536559 0.0000179976751298
0.0007182029576782 0.8031437050398367 0.8033440549153639
0.0003159628830360 0.7549958511752877 0.7551759668835629
0.0000261545915876 0.6617692556355408 0.6622420050192304
0.9999538592328889 0.6126979511938089 0.6131400904745448
0.9994703931513484 0.8021819388459619 0.1976703554149282
0.9997528707111343 0.7541716729099903 0.2455959623145887
0.9999680893036995 0.6614342248877279 0.3382544161944381
0.0000172909028748 0.6124551371161644 0.3872740840730842
0.0007231430697487 0.1971287997349123 0.1968530499487642
0.0003091335647838 0.2451769126613996 0.2450654586278915
0.9999947636257076 0.3383189839648821 0.3379361177127578
0.9999477245565558 0.3874023143114300 0.3869680321687952
0.9994456304053827 0.1978472188284712 0.8024253792923730
0.9997839190453135 0.2457615102870818 0.7544087615101773
0.0000163261294972 0.3385568095081766 0.6617947373741515
0.0000628909481151 0.3875858809508870 0.6128356700461950
0.5507398570409379 0.9999491939263763 0.6303681188587973
0.6939302755976939 0.9999565185838577 0.5316359520783536
0.4491453323980039 0.9999683494027494 0.6304056724034268
0.3060172801843706 0.0000210372565590 0.5316529314166942
0.4491762197715659 0.0000175727655574 0.3696462284167126
0.3060284884548778 0.0000402492058740 0.4684008507028423
0.5507299010077134 0.0000346732844108 0.3696667917670453
0.6939227126351568 0.0000081363699280 0.4683859923281659
0.6303267478184438 0.5508364171693216 0.9999809601911309
0.5316344257759127 0.6936343460045080 0.9999651288327840
0.6303391270722898 0.4492116272421285 0.0000018284659618
0.5315659063184626 0.3063750109987637 0.0000562614699646

0.3697998365014783 0.4492138824707013 0.9999976636198653
0.4684566788705311 0.3064065949733532 0.0000303354359019
0.3697727771106898 0.5507795776500828 0.0000308317160815
0.4685277759649651 0.6935887081014300 0.9999568671244035
0.9999753386346271 0.6298064576754143 0.5509952354748151
0.0000059939388350 0.5316986322639465 0.6943126532416599
0.0000066325920045 0.6297273692086378 0.4494240929373206
0.9999831730531312 0.5313732587257292 0.3058409392867745
0.9999656329899693 0.3702524911424234 0.4490888004374511
0.9999704513865311 0.4683623752538963 0.3057830077611925
0.0000409069219316 0.3703230270849431 0.5506731107907257
0.0000267481159071 0.4686896846032980 0.6942294086012382
0.0000015767310302 0.5505238142964828 0.3698483545224960
0.0000069183577978 0.6934379744661143 0.4686644318816633
0.9999768191379275 0.4493120619080244 0.3697436256807691
0.9999668696260997 0.3065686568092190 0.4681823161577228
0.0000260914291133 0.4495440814153824 0.6302424762686627
0.0000061377273113 0.3066144383880598 0.5314199103078892
0.9999831568288755 0.5507685555637707 0.6303581001236012
0.9999996199055872 0.6935008685345352 0.5318969880246200
0.5509448775297798 0.6299581627222324 0.9999632899825244
0.6941387702445354 0.5315912442966351 0.9999727009751851
0.4492011052554901 0.6299051269842550 0.9999707228218142
0.3059708187416206 0.5314505383379213 0.0000411284564024
0.4492047192694173 0.3700921106549728 0.0000055355567383
0.3059879659265334 0.4684162841031281 0.0000252792828945
0.5509452143733498 0.3700489452839051 0.0000553749211534
0.6941379337494951 0.4685487172138494 0.9999728582405396
0.6300876470726564 0.0000247362044945 0.4491365029273098
0.5315395953181650 0.0000337830621859 0.3057031108496773
0.6301045529363520 0.9999514643760037 0.5509004738289178
0.5315291783087659 0.9999672417024499 0.6943173280980375
0.3698366690128054 0.9999988055339273 0.5509256702717522
0.4683942877843350 0.9999644631580722 0.6943459186136707
0.3698575437913831 0.0000353606567742 0.4491503575490228
0.4684074071464153 0.0000246120151175 0.3056872023714519
0.7500061086719469 0.0995664085005430 0.7503395984983570

0.6683533294309782 0.0996383580753459 0.6685483381955848
0.2497816034352454 0.9006453664140750 0.7503738008312197
0.3314917060940061 0.9003675089748526 0.6686768476833791
0.2500916366368529 0.0995418827943837 0.2498758178093752
0.3317966576438707 0.0996784024331205 0.3316088495856278
0.7499201256125474 0.9005589556484495 0.2497941177453598
0.6682088431986699 0.9004181029980316 0.3315836954358886
0.7504706060440753 0.7503778227326379 0.0998673275951063
0.6691068753050331 0.6689350385000168 0.1000354349268662
0.7503869093348854 0.2496542845844303 0.9001309691474333
0.6691317560764816 0.3310910420822779 0.8999930352512280
0.2498677631745423 0.2498735862381167 0.0998305429707145
0.3311934497011890 0.3314467374756020 0.0999797471905737
0.2498055580810217 0.7500596643341382 0.9001593054023829
0.3311284460558994 0.6686378058390545 0.9000313555503823
0.1002365922224655 0.7494028888373450 0.7494599343276249
0.0999386383786245 0.6674857344157417 0.6677244794205066
0.8998137120849847 0.7487989627907865 0.2511030407244661
0.9000762025064404 0.6669278726015975 0.3328346838440908
0.1002358283407006 0.2508309717806441 0.2507660287988429
0.0998394950058099 0.3327756602252805 0.3325164294908944
0.8998534196719916 0.2510865487519851 0.7489471987747152
0.9001196784804861 0.3329902176270707 0.6672612162134968
0.0997740874626558 0.7490612872548468 0.2508293179010153
0.0998144156900622 0.6672238526260728 0.3325657559428450
0.9001960118776537 0.2505519020663272 0.2505187046840121
0.9001479157072509 0.3325117673427087 0.3322406699127853
0.0998402061207386 0.2509684684751647 0.7491132257342130
0.0998496626214802 0.3328347980483315 0.6674067477652628
0.9002408344589412 0.7495656895237275 0.7496447220615750
0.9001436890510064 0.6676797038941800 0.6679425178474361
0.7501852572836469 0.7501163007067149 0.8996040420891234
0.6687848099309690 0.6686403005218011 0.8997421595688309
0.2499269300635873 0.7500308018854511 0.1004833071028273
0.3312288403222041 0.6685548962328411 0.1002550292710751
0.2499812697802852 0.2499399198737322 0.8995005047486089
0.3313117667873371 0.3315448530004588 0.8997269508613428

0.7500990280091244 0.2499123359908921 0.1003930756666733
0.6688203302487210 0.3313851073149792 0.1002461747337051
0.7496801885887763 0.1001495036539808 0.2500907515243611
0.6678776160692763 0.0999434045979015 0.3318690083719389
0.7497062422296636 0.8999486676969326 0.7499788581512661
0.6679604758546560 0.9001337882527736 0.6682301066707197
0.2500661860131288 0.1002480074062788 0.7501073215001171
0.3318059843409245 0.0998947597459434 0.6684076514307336
0.2500547970506659 0.8999486420123759 0.2498859873971568
0.3317950066568400 0.9001722479562986 0.3316242632034019
0.7331236831042673 0.9999364901728143 0.5636361286974036
0.2668183899313945 0.9999710746848578 0.5636522395895653
0.2668579617603797 0.0000568023191292 0.4363764200066598
0.7330989420232612 0.0000336536235466 0.4363553076349689
0.5635279816479226 0.7328174709727264 0.0000092839829477
0.5634007700428043 0.2671685754908424 0.0000174078535906
0.4364938938608773 0.2672793481942151 0.0000045616558992
0.4366211026437625 0.7327292823595428 0.9999800164181707
0.9999832215345350 0.5636866965723755 0.7335332953437117
0.9999805169235998 0.5632825904104308 0.2666367291564526
0.9999766272272481 0.4363602887885989 0.2665791596283000
0.0000218756713082 0.4367352444357664 0.7333981384995241
0.9999926406354120 0.7324743642104465 0.4366151547254304
0.9999717044025545 0.2674633347376130 0.4361025162647181
0.0000147618141781 0.2675333636730244 0.5634149660205452
0.9999724442588445 0.7326412618939031 0.5639329996144724
0.7333456388164237 0.5634811494255985 0.9999672526263623
0.2667463657401044 0.5632735440837067 0.0000148312702279
0.2667839876051161 0.4365296951231343 0.0000316659341593
0.7333399423634859 0.4366978377257880 0.9999723088688199
0.5635181033194172 0.9999886380320220 0.2664473904908107
0.5635060030478556 0.9999950388610586 0.7335774017144985
0.4364414767519875 0.9999981525706687 0.7336109695533892
0.4364681928140826 0.9999904621538320 0.2664143299310879
0.1474424355615795 0.9667479481580372 0.0168699215574435
0.1481140464557456 0.0315183399420675 0.9827825548411724
0.8510872964612872 0.9628584367837476 0.9989033809907539

0.8514802257392304 0.0354554946848182 0.0051154365108772
0.9997810571534842 0.0012694108613331 0.1408109710555436
0.9993421792553860 0.9996484655060698 0.8599449986456520
0.0002408223593378 0.1367477854637897 0.0003825384727065
0.9998298771336138 0.8636588169416441 0.0002855174227250

MFU-1(Co-Pz)

1.0000000000000000

15.7903995514000002 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.7903995514000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.7903995514000002

H C O Co N

48 48 1 4 12

Direct

0.5745847552839223 0.6755990165550827 0.1876535686882903

0.6529812042989249 0.5984904427358089 0.1644562861945715

0.6447795144714092 0.6413031320185638 0.2688931472293916

0.5703751698900419 0.3144118800496045 0.7870714731305526

0.6365418659136068 0.3828891218547241 0.8462933899135905

0.6556472209498168 0.3688589216536045 0.7361229851087359

0.6311519702588484 0.4788916025514567 0.9257118791250960

0.3610699008460188 0.5210805157383476 0.9217094165363804

0.1961174530471794 0.4244932019788905 0.3243065979485422

0.1623222718290478 0.3540503321724273 0.4052833231948014

0.2694884472665322 0.3511930207905749 0.3680894858359096

0.2100840195885354 0.5881182417134099 0.6811893141358567

0.1610279717156828 0.6490304169973626 0.6000989465929649

0.2709809050089476 0.6635206966658131 0.6234329182805141

0.9272480103547451 0.5307289178137253 0.3675666324301190

0.9260127142607999 0.4627696087691078 0.6322643654820510

0.3669913336444139 0.0776488487604610 0.5022421061203346

0.6810736879889916 0.2114781988178791 0.5890560071135340

0.6013002977681126 0.1529881084688256 0.6429459792820964

0.6169986637424216 0.2624988396587256 0.6668331826296665

0.6400965770899418 0.0794163963125669 0.5023420979870536

0.3225807747867293 0.7898788100307002 0.5806051135450971

0.4000886425441834 0.8524067920758114 0.6332752130615447
0.3851824017495034 0.7445633003592107 0.6630817939402576
0.3680114514226176 0.9214657549245189 0.4955868839490876
0.6409604494871459 0.9230064597313046 0.5052936396835861
0.3158677778561483 0.4205380349021368 0.2122991741488676
0.3939316374226820 0.3605757696394534 0.1574909025876607
0.3751232364214800 0.3422536000543133 0.2677998476130270
0.3602857576194936 0.5279705087534978 0.0779475363478426
0.6284549188511903 0.4777382866686537 0.0816885310225004
0.3227090258759304 0.5836633992685023 0.7994502639064507
0.4042533685697336 0.6521770251761154 0.8365054223745148
0.3733960256513953 0.6531295078778712 0.7272137908445870
0.4241610576691031 0.2212500751877187 0.3181287620436919
0.3715834507793829 0.1497033583286793 0.3870473207744141
0.3370781330215991 0.2569214320334652 0.3809421219704632
0.5865388485455583 0.7822444853425736 0.3189965938426482
0.6437822116633214 0.8465492699629991 0.3913272788676707
0.6695776782320451 0.7370900046448625 0.3807679328683022
0.0824629923708713 0.5383701906790463 0.3702974310566489
0.0818928194721806 0.4648404251525307 0.6329130242316552
0.8205438468817334 0.3275088876695378 0.5818655458339705
0.8173683886624659 0.4007167338153579 0.6674917887247744
0.7223271111481040 0.3508010790988507 0.6325578955523810
0.8031466890348824 0.6751996203866923 0.4196054708648091
0.8327481231027321 0.5992793926018152 0.3419937934132307
0.7251059684095509 0.6293609030572966 0.3515717633081294
0.5706404293026992 0.4874834542768127 0.9584638467124051
0.4206009002562396 0.5126080436710367 0.9562639495453098
0.9601176285262341 0.5175966249964858 0.4270751840839324
0.9595483475280275 0.4789752441650847 0.5738032877676034
0.4276940399123674 0.0440373564792722 0.5000185784111153
0.5798630407687853 0.0449251263302841 0.5019263924812805
0.4282391091672437 0.9558863384852572 0.4981154196966244
0.5803625746826881 0.9567126495592291 0.5017838842039239
0.4198250364096694 0.5153545462816425 0.0445262174737238
0.5696270598663276 0.4889378418407304 0.0464977148910535
0.0481766155824701 0.5206424667816378 0.4280208577461835

0.0477616508940883 0.4812839881486539 0.5747108919469923
0.3792436919544784 0.3914227233807566 0.2184207380288967
0.4453513347305744 0.4548966531801923 0.2399250513438957
0.6082175547817954 0.6199337762533688 0.2135634682420999
0.5474719612657850 0.5522840336383936 0.2379167533006807
0.6056349011867610 0.3748975913645367 0.7844354773821252
0.5479434914266292 0.4464660624873957 0.7636751239028357
0.3843560868679887 0.6123116029856490 0.7826766784158963
0.4492056365560089 0.5473136322581880 0.7623207005369110
0.2160312256960708 0.3931871473948618 0.3836413643619210
0.2406908311362770 0.4552115619251182 0.4499065216107070
0.2200421274111122 0.6161211573903600 0.6178078801885150
0.2420657165030846 0.5513471384341244 0.5531421432984374
0.7831578634008380 0.6160494242828491 0.3879176690519586
0.7649225113907718 0.5476696654498383 0.4500277607900216
0.7826521621701517 0.3785874604486423 0.6110121791886414
0.7644415180237303 0.4475671943074175 0.5494900973100911
0.3933620149584129 0.2156078855987786 0.3807742275891144
0.4529597085712069 0.2382295072413143 0.4500603407718131
0.6163136004543759 0.2153970012312598 0.6154169051617302
0.5527292050369752 0.2382949245291996 0.5498906924900311
0.3866681049857306 0.7883837732867747 0.6088221022111142
0.4523544079395379 0.7631736427164029 0.5463590201943589
0.6170146437801804 0.7828828655130025 0.3820503757880900
0.5551428896195034 0.7616619631545163 0.4497408618052816
0.4946797384056367 0.5042249319584826 0.1845591527910670
0.4942639542077458 0.5031787658708211 0.0917490837134665
0.4973766299354310 0.4965095812662241 0.8178663745862096
0.4960052776453452 0.4983489903706158 0.9107050047380838
0.1870951584255280 0.5036389928104228 0.5019328615941490
0.0942330747809450 0.5026546172031772 0.5019537664218774
0.8198193394650346 0.4971849218574675 0.4995600886075380
0.9128387335069164 0.4975158538372995 0.5000595997029293
0.5029253310577531 0.1836509391100378 0.4999718773597124
0.5034750051712038 0.0908927828019799 0.5004808892078856
0.5043544954571146 0.8170360631206393 0.4977923705635590
0.5045592207291563 0.9098322671886692 0.4986147390809208

0.5036782146413614 0.5001442136479852 0.5007004448828383
0.4314366845586548 0.4300565151215210 0.4306643321603403
0.5737523600026933 0.5701745496073727 0.4293609663590061
0.5728529161802740 0.4291590900305948 0.5719640709619043
0.4333648881686187 0.5715947469470422 0.5712442886364784
0.4682271295243723 0.4718212099565164 0.3207410506261041
0.5308874398255057 0.5324555167104421 0.3195764906522029
0.5315490038940354 0.4672780000409489 0.6822061090220757
0.4708417618594751 0.5297656442274175 0.6814455628542149
0.3222498355489734 0.4721603747252345 0.4696960225325526
0.3230975867392445 0.5322076626254599 0.5328878083588577
0.6835924730445697 0.5291828147326214 0.4694807918279977
0.6833070487466983 0.4674958694712572 0.5307656762125319
0.4717033032607887 0.3195994893834637 0.4694648154498822
0.5329644660319346 0.3195082759241288 0.5313885253603843
0.4720073163298366 0.6815307019533563 0.5293693248221700
0.5350454576406491 0.6807017175292671 0.4692094836499123

MFU-1(Co-Vtz)

1.000000000000000

15.7903995514000002 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.7903995514000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.7903995514000002

H C O Co N

48 42 1 4 18

Direct

0.5683261576690910 0.6702468930656877 0.1899602624978272

0.6516102048015782 0.5963612183044376 0.1666004800641190

0.6379794254075435 0.6352820200253646 0.2730101565822096

0.5654327869211286 0.3191952829256053 0.7838050762684219

0.6326465419839522 0.3864582638923935 0.8458681760145055

0.6516648848056050 0.3746828307522989 0.7336399919734049

0.6343037094641844 0.4798139456453399 0.9268633902626817

0.3626860764113289 0.5176761463921835 0.9221690328274548

0.1974597449266540 0.4254291780021617 0.3218784149616880

0.1626861000853310 0.3572944038098100 0.4047090959473039

0.2706390374922591 0.3540835268526692 0.3692502072410235
0.2122307901119527 0.5841876726630559 0.6799897025706301
0.1615998988704987 0.6429421837897920 0.5966780609674061
0.2730618848502502 0.6574632668922931 0.6177171757045556
0.9270299931187012 0.5265753364825798 0.3688275550241968
0.9264793982300503 0.4635471364401127 0.6359437218665889
0.3687395254203807 0.0771932393543935 0.5035397907794490
0.6793347633639613 0.2122400418817705 0.5867219275578250
0.5969209621457523 0.1535914431437391 0.6392341467538358
0.6116439474380897 0.2652938660943320 0.6613212392852077
0.6427995358140066 0.0782283267194472 0.5036878789968995
0.3212912920153173 0.7877737915402960 0.5800076346525245
0.3996193968831392 0.8519570679084651 0.6299868501679455
0.3879245376184031 0.7435479788393309 0.6600871766513805
0.3695975667785447 0.9222679742118274 0.4948026113121813
0.6435243391852623 0.9236229821126045 0.5028068592772570
0.3132947514117461 0.4213635622694554 0.2141607010230189
0.3932742185367317 0.3651961187178827 0.1576180215299914
0.3766370361068780 0.3450381452092515 0.2680087900388557
0.3616733160456107 0.5260176024765926 0.0768989805484850
0.6318222469768173 0.4820490423266577 0.0808341971000672
0.3204624956082753 0.5821984801892199 0.7979943238490321
0.4045588787921801 0.6474464116104173 0.8357333732484165
0.3751120123856850 0.6496243457574806 0.7259797531099750
0.4248568916140840 0.2261120485733343 0.3203807508863008
0.3747904833183853 0.1506276034714773 0.3872758228631454
0.3371292774016794 0.2571743326869154 0.3846295260152459
0.5803634955556589 0.7780054093494186 0.3235122983791783
0.6389564923696796 0.8462110106948444 0.3931810409542322
0.6665396397312406 0.7361638433353903 0.3854209053183340
0.0810464556142563 0.5353248428574773 0.3716052032922050
0.0804807208237506 0.4692960790890552 0.6371974421030089
0.8218775966606202 0.3335698124603255 0.5763759385060183
0.8133645389775310 0.4039729772900316 0.6657242915461694
0.7190978804084622 0.3555678624613350 0.6232563666723934
0.8034475904476324 0.6722322004495922 0.4206443277200620
0.8310954624253668 0.5974812201133304 0.3409034338821186

0.7230575141602529 0.6281137432958985 0.3538736875418067
0.5731364913296133 0.4882381453234217 0.9585082880540696
0.4227038905640228 0.5104556963655824 0.9562084729625511
0.9594415238246796 0.5153145002179116 0.4290271335431370
0.9590295017496402 0.4798653801107235 0.5769390956324827
0.4296766932129685 0.0440325942865627 0.5007862390096065
0.5820239267893257 0.0447070503579141 0.5023106745661252
0.4301441966756059 0.9560914913065659 0.4975522312319427
0.5825006201977914 0.9565725321479732 0.4997214704634843
0.4218001546383903 0.5141964340399383 0.0442039492415702
0.5722853221562616 0.4919633631613323 0.0464785608420755
0.0472558544154182 0.5190388911010970 0.4300679304376942
0.0471018920050454 0.4842621791068993 0.5781561283346903
0.3778299562070941 0.3948084933138176 0.2190219748130673
0.4427004745129111 0.4593027076579830 0.2406678269702525
0.6048404558100842 0.6157134648038252 0.2147357781453465
0.6026575220315209 0.3787620886763463 0.7834989573280424
0.3833182210168360 0.6083672776430831 0.7817812530749890
0.4467553938683793 0.5421159829828994 0.7613999613570215
0.2164493398166272 0.3959858326672574 0.3824252006646773
0.2405652048741516 0.4591297610366070 0.4476444602296041
0.2207520006872983 0.6110827639085841 0.6158415605857357
0.7824314436563427 0.6138976456651193 0.3879963302764651
0.7820948661891904 0.3823915572475443 0.6069482533846227
0.3944719413643725 0.2173511439225138 0.3829145490936838
0.4536725513935096 0.2394741801890277 0.4525216804702410
0.6140636973422602 0.2155853279172462 0.6121069073175605
0.3863314704974030 0.7877125025135285 0.6059617467156286
0.4510080668986944 0.7629882866335649 0.5424542850366691
0.6136793810889287 0.7817325250688256 0.3851961903807890
0.4942465650146417 0.5044350533527933 0.1851696616320027
0.4965735472044273 0.5044631763402236 0.0928932935452522
0.4969121533543088 0.4954154440818357 0.8170839457014338
0.4983138744175548 0.4969573824556122 0.9093950687169965
0.1871151531906818 0.5040278143911507 0.5015111888543373
0.0946311460695313 0.5041700104237066 0.5048011984888632
0.8186183780277858 0.4969143329130148 0.4993184421654462

0.9110085386040936 0.4963571892349918 0.5025435045735946
0.5031926710977004 0.1843759448119400 0.5005002070158966
0.5057187200289448 0.0919252799847854 0.5019567310559836
0.5038069768883844 0.8165607090548406 0.4965428868540016
0.5064898201914971 0.9087893257241575 0.4965638257711618
0.7637856012632724 0.5450089598648660 0.4490984384288552
0.5096586967623509 0.5018747286536183 0.5039480630694086
0.4372897904153419 0.4359140406474751 0.4366214145170986
0.5756193788723181 0.5758784487365745 0.4240768219050324
0.5797367821844830 0.4232345280616059 0.5786373648244592
0.4331868978407485 0.5712348861397984 0.5702501744140775
0.5509219330189410 0.4507540975222852 0.7641018414543339
0.7641140634024879 0.4507237284726031 0.5501758256584210
0.5504559691674018 0.5466596285210414 0.2373605159772438
0.2413835219970437 0.5479507958946499 0.5540317871627352
0.5535910434918634 0.2374963609473753 0.5482863454713396
0.5586412765718052 0.7623135479074818 0.4548039745416332
0.4672137904252267 0.4753602258522491 0.3220681565298662
0.5329808402735381 0.5306923782686965 0.3219994074028847
0.5332420944980996 0.4670535633976556 0.6794630093891598
0.4691700459187231 0.5243937426909469 0.6797539893443840
0.3227957003809223 0.4756454253218863 0.4687122181415688
0.3246643327988963 0.5313038000961754 0.5338375961456947
0.6816383169758353 0.5268625037429899 0.4691201186900997
0.6799195115097376 0.4680579030047269 0.5314501503029021
0.4741581618773836 0.3212842018800828 0.4725392859042188
0.5357545221041207 0.3214937016106134 0.5322128466351757
0.4729640159939166 0.6806119706062717 0.5274708358366240
0.5382424871661513 0.6784323145882851 0.4712269433773599

MFU-1(Co-Ttz)

1.0000000000000000

15.7903995514000002 0.0000000000000000 0.0000000000000000

0.0000000000000000 15.7903995514000002 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.7903995514000002

H C O Co N

Direct

0.5635729594554419 0.6631446982705143 0.2095832450358941
0.6447921888423451 0.5997864177780059 0.1602932437426290
0.6496969842318805 0.6220274886754495 0.2715926006440341
0.5638413492150249 0.3347165633314901 0.7899879679017943
0.6442502053259815 0.3981386703531840 0.8399788260135637
0.6495963800614248 0.3785580754800790 0.7285930034666848
0.3605458643316410 0.5125296465691989 0.9262767698143435
0.6366700699703784 0.4911015465196726 0.9252150580713376
0.2056874666047932 0.4186574611814109 0.3188429600835789
0.1614799559274473 0.3639909057172304 0.4087918274934523
0.2732610137793330 0.3551620521965262 0.3847172964132923
0.2105825597475288 0.5859921453382739 0.6809162044888453
0.1636593549404921 0.6390204294712376 0.5914547459585933
0.2763036661824643 0.6483194649315038 0.6117775122286844
0.9243775617083685 0.4898724950303972 0.3623523724153586
0.9242058711397334 0.5095989599532942 0.6382014816164769
0.3632571125918673 0.0751775902546541 0.5016238404326714
0.6806566730167276 0.2137315506398494 0.5852328718601854
0.5926596549940584 0.1633927176796846 0.6377361834380721
0.6110456922858774 0.2758217460012560 0.6507508840219529
0.6396062970805474 0.0762175139958430 0.5046422766787515
0.3208576517380308 0.7913803002290365 0.5817433107298982
0.4096937555944891 0.8415285590158774 0.6328989095663857
0.3894643118928158 0.7298606060993365 0.6488542475013048
0.3636001966451232 0.9244477103323945 0.5021909335178520
0.6400896945469796 0.9253084456049550 0.4994789157382229
0.3187430727992790 0.4149795644706771 0.2113822812037256
0.4086404145580573 0.3638196185773310 0.1633068966372306
0.3887544377167629 0.3519341504800337 0.2758077268540688
0.3611738968237290 0.5072219113448710 0.0777032149686789
0.6371825591670870 0.4912532111498464 0.0763337054415061
0.3174671405253520 0.5820589078262799 0.7927022080834263
0.4073796511308601 0.6356140890883282 0.8384255734445745
0.3847870496287200 0.6455288352892694 0.7264373802926087
0.4343120472284880 0.2112533623800701 0.3338948875370846

0.3578008917873134 0.1590881069159238 0.4005298041061138
0.3480304259648719 0.2702269596879674 0.3797686209377247
0.5721478239069810 0.7834710854531721 0.3326468892805181
0.6480482258102782 0.8359820055366782 0.3995582654333276
0.6557341308431646 0.7237894372401144 0.3827253036233458
0.0760455302882903 0.4878226459418755 0.3623235627654324
0.0760357575619608 0.5138295865715250 0.6381014332959580
0.7908020153477651 0.3372495162988542 0.5638337290484117
0.8402536861567071 0.3992613975133921 0.6458499373381485
0.7286600816627384 0.3782223206322115 0.6501539492239772
0.7910767553749594 0.6616147743617162 0.4346631390276059
0.8426823070318648 0.5980981972016579 0.3553550467596196
0.7315412652644255 0.6186168343560112 0.3469739844202593
0.4220800590588709 0.5067243639731203 0.9579747546871786
0.5751881649772344 0.4942730526282446 0.9573504505781401
0.9569756202531252 0.4963001726391383 0.4233877026193511
0.9569276089789724 0.5037004999200718 0.5771789348553114
0.4251165171932385 0.0435957077908782 0.4998041155007158
0.5779710361680159 0.0441496356499442 0.5032233814965394
0.4253418472008477 0.9563626635647964 0.5017161809246602
0.5782437556609921 0.9569493720535718 0.4987435426428632
0.4222517367591365 0.5028203081331952 0.0448413160006211
0.5757129976920865 0.4963474753834305 0.0442745221690757
0.0438016194746211 0.4936518156296970 0.4235478312175971
0.0437276291148692 0.5073154903361186 0.5769618662719438
0.3852667143694788 0.3956628339453161 0.2210261337295236
0.6069844123184467 0.6086023028763279 0.2181398096987550
0.6063653299144676 0.3900822949803313 0.7821046492891313
0.3835224111352957 0.6023883485462065 0.7817182713384554
0.2176806709910579 0.3978074929888393 0.3845460292003935
0.2206153341799677 0.6056830974662901 0.6145451961428208
0.7837662038241646 0.6065949578848162 0.3915798491801681
0.7824336611425622 0.3914328535378075 0.6077566489340072
0.3933314868797950 0.2181575499744284 0.3905116404615541
0.6143422699597991 0.2218570331207843 0.6061043270688629
0.3870865787448494 0.7826587450916662 0.6027486857076312
0.6115402960324943 0.7773399574210273 0.3905054019498593

0.4999164188085601 0.4989050882967305 0.1841145294901096
0.4992050852540899 0.4987573499069171 0.0949499353645180
0.4988650274881721 0.4997830237573240 0.8177555095787739
0.4985107170871714 0.5005941021142633 0.9068625938129458
0.1829934748553370 0.5011374764044731 0.5001510496102384
0.0939617504826629 0.5007108127810014 0.5002768359000598
0.8181217930848987 0.4995298783053101 0.5002574331334912
0.9067975551956380 0.4997571608014724 0.5003022551162317
0.5008305023865560 0.1847968475380739 0.5010906461261726
0.5014580824036656 0.0948495375738716 0.5016909368528317
0.5017404323630927 0.8155639764817479 0.4985125733455646
0.5018427645984218 0.9055628127257975 0.4994148173545128
0.5000528310650054 0.5001405477912257 0.5001490668102662
0.4259520731093289 0.4265165274264291 0.4269151484887104
0.5750573930140135 0.5722410083648697 0.4273941680415163
0.5741782473039052 0.4279024657411838 0.5732869435589834
0.4265120726656448 0.5740154627036631 0.5736686766226100
0.4652003713027000 0.4775055267318891 0.3237193692574962
0.4397489708856597 0.4661914637358819 0.2394107303147379
0.5353780400024704 0.5231923329893107 0.3232082706893920
0.5618532829172906 0.5318230877271688 0.2381426938871769
0.5341747977380891 0.4761549244426746 0.6781166360790252
0.5605208261281760 0.4666119831837676 0.7632740203317070
0.4647243803721111 0.5228002405981513 0.6778385417074304
0.4389059392920132 0.5330800000413021 0.7623364892877689
0.3220867598644475 0.4773378642318562 0.4650193423678246
0.2375297538683228 0.4668362648878670 0.4401692594151712
0.3225213020906850 0.5236702214654727 0.5343723952845636
0.2382850668559868 0.5354025315754498 0.5595818411215205
0.6792659386921400 0.5219774786243718 0.4648519823308987
0.7639467679560568 0.5300429146279058 0.4371748300681446
0.6789930293125934 0.4777808117870066 0.5353945727076379
0.7636581818465444 0.4688526724010273 0.5630857165670307
0.4662722696548300 0.3247028746344895 0.4738811816198591
0.4409326746807167 0.2389625332422227 0.4652125705684256
0.5340511026221080 0.3253548581665626 0.5252496147270449
0.5582198095903053 0.2405641503107816 0.5372685758765172

0.4668864599685207 0.6755804103456882 0.5252908990645153
0.4428962372161607 0.7610540163878028 0.5346288791318372
0.5350684355404667 0.6749149664254759 0.4745195005695635
0.5612561669808969 0.7599639402173963 0.4643630735546367