Electronic Supplementary Information (ESI)

The true atomistic structure of a disordered crystal: A computational study on the photon upconverting material β-$NaYF_4$ and its Er^{3+}-, Tm^{3+}-, and Yb^{3+}-doped derivates

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1 β-$NaYF_4$ 2x2x2 Supercell

To accurately represent the influence of the cation disorder on the F^- sites (and thereby on the potential cationic doping sites), initially, a 2x2x2 supercell of β-$NaYF_4$ was created. The structures shown in Figure S1 represent such a supercell with one possible Na^+/Y^{3+} distribution at the 1f sites.

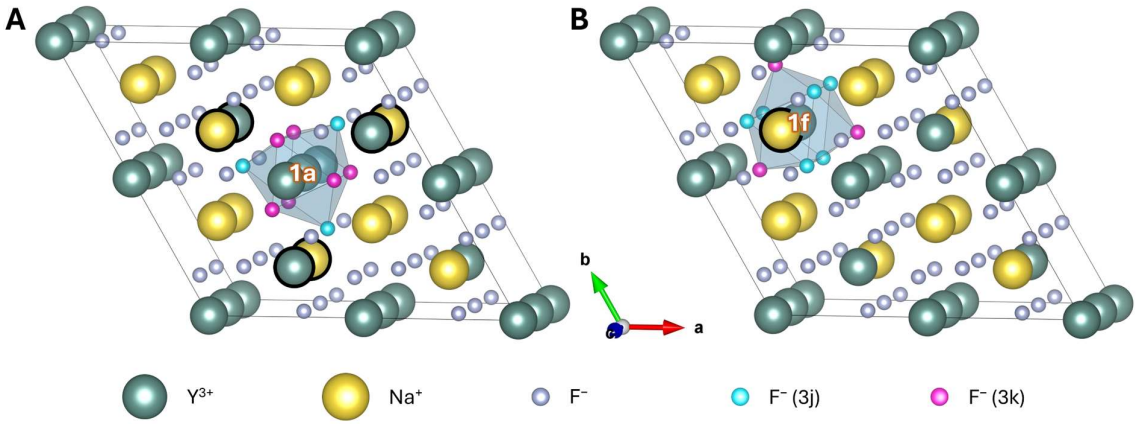

Figure S1. 2x2x2 supercell of β-$NaYF_4$ with the composition $Na_{12}Y_{12}F_{48}$. Highlighted are a potential (A) 1a and (B) 1f doping site (white labels), and their first anionic (F^- ions of the blue prism that are highlighted in cyan and pink) as well as cationic (Na^+ and Y^{3+} ions marked with a thick black line) coordination spheres.

This distribution is very similar to the one reported to be the most probable based on experimentally derived X-ray diffraction patterns. However, in this work, we aim to address structural disorder, which means that all possible surroundings of each Y^{3+} ion (potential Ln^{3+} doping site) should be represented by configurations. The 2x2x2 supercell is not large enough to represent all possible (and required) Na^+/Y^{3+} distributions at the 1f sites. Specifically, for the 1f doping site (Figure S1B), the positions of the six 3j F^- are heavily influenced by the two neighbouring 1f cations along the c-axis. For the 2x2x2 supercell shown, this means that, due to the periodic boundary conditions, the Y^{3+} at the 1f site has two Na^+ as neighbouring ions along the c-axis. When creating a second configuration of this supercell by exchanging Na^+ for Y^{3+} at this neighbouring 1f site, both neighbouring ions will correspond to Y^{3+}. To instead account for such configurations in which one neighbouring cation is Na^+ and the other is Y^{3+}, at least a 2x2x4 supercell is required (Figure 2B).

As for the 1f site, similar considerations made for the 1a site (Figure S1A) required a 2x2x4 supercell (Figure 2A). The reason for this is that three of the nine F^- around the 1a site are located at 3j sites (Figure 1B). Each of these three sites is considerably influenced by the distribution of Na^+ and Y^{3+} within a set of two closest 1f sites (large black circles in Figure S1A). In a 2x2x2 supercell eight such 1f sites exist, and the composition of the crystal remains stoichiometrically correct only if exactly four of these are occupied by Na^+ and the other four by Y^{3+}. If instead six or five of the closest 1f sites are to be of the same type, additional 1f positions must be created to counterbalance the above average occurrence of either Na^+ or Y^{3+}. In a 2x2x4 supercell, a total of 16 1f sites are available. By manipulating the12 1f sites closest to the central site, all required configurations could be created without changing the stoichiometric ratio of the crystal.

2 $LiYF_4$ 3x3x1 Supercell

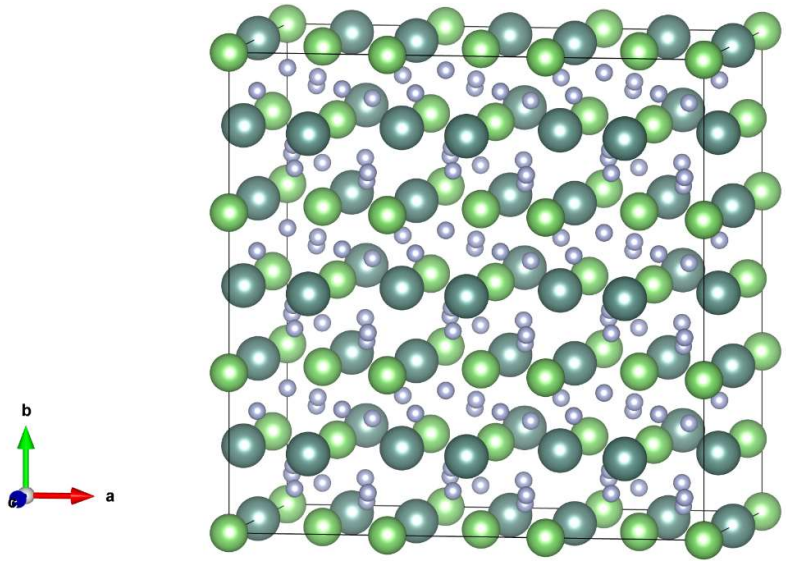

Figure S2. 3x3x1 supercell of $LiYF_4$ with the composition $Li_{36}Y_{36}F_{144}$. Dark green spheres represent Y^{3+}, light green spheres Li^+, and small grey spheres F^-.

3 Additional Structural Parameters for β-$NaYF_4$ doped with Er^{3+}, Tm^{3+}, and Yb^{3+}

Table S1. Results of the structural optimisations for three times 16 different configurations of doped β-$NaYF_4$. For the configurations doped with 4.2 % Er^{3+}, Tm^{3+}, or Yb^{3+} lattice energies relative to the most stable configuration of the respective column (ΔE) and deviations of the lattice parameters from the experimental values ($Dev._{LP}$) are being displayed.

		4.2 % Er^{3+}		**4.2 % Tm^{3+}**		**4.2 % Yb^{3+}**	
Site		ΔE	$Dev._{LP}$	ΔE	$Dev._{LP}$	ΔE	$Dev._{LP}$
	Config.	($kJ \cdot mol^{-1}$)	(%)	($kJ \cdot mol^{-1}$)	(%)	($kJ \cdot mol^{-1}$)	(%)
1f	1	0.1	0.77	0.2	0.77	0.1	0.76
	2	2.4	0.83	2.2	0.83	1.9	0.83
	3	3.4	0.90	3.4	0.90	3.3	0.91
1a	4	6.5	0.78	6.6	0.78	6.5	0.78
	5	4.6	0.85	4.9	0.86	4.6	0.86
	6	3.4	0.88	4.1	0.91	3.9	0.88
	7	1.8	0.89	2.2	0.89	1.9	0.90
	8	1.8	0.92	2.0	0.92	1.8	0.93
	9	1.2	0.86	1.3	0.86	1.2	0.85
	10	0.0	0.76	0.0	0.76	0.0	0.77
	11	1.6	0.86	2.9	0.87	2.5	0.88
	12	1.9	0.92	2.2	0.92	1.7	0.93
	13	2.3	0.86	1.9	0.86	1.9	0.88
	14	4.8	0.88	4.7	0.89	4.7	0.91
	15	4.2	0.84	4.5	0.85	4.0	0.85
	16	8.3	0.76	7.4	0.76	7.7	0.79

4 $LiYF_4$ Input File

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   &SMEAR  T
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   &MIXING  T
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5 β-$NaYF_4$ Input File

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  0.1435604600000000E+00 1  0.3460149228000000E+02
  0.1299322400000000E+00 1 -0.1427746168000000E+02
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  &END SUBSYS
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6 $LiYF_4$ Optimised Structure

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F	1.1531382368313590E+000	1.7313208782292868E+000	6.2947319896955998E+000
F	1.1531368037439831E+000	1.4723646761785778E+001	7.2005323315403507E+000
F	1.1531393295560568E+000	1.2125179670953392E+001	6.2947323126395895E+000
F	1.1531402198761038E+000	9.5267163389628156E+000	7.2005371387886106E+000
F	1.1531372897497005E+000	6.9282499185051698E+000	6.2947344574010131E+000
F	1.1531368884843798E+000	4.3297854009970749E+000	7.2005356606464455E+000
F	1.4453288778038293E+000	8.6715241347430994E-001	8.9662635469468277E-001
F	1.4453286020945291E+000	3.4656170296416882E+000	1.8024324853167402E+000
F	1.4453273572890963E+000	6.0640775881969224E+000	8.9662968006694443E-001
F	1.4453237039574289E+000	8.6625395120700581E+000	1.8024293650635446E+000
F	1.4453245157990220E+000	1.1261003069737557E+001	8.9662883429558171E-001
F	1.4453248604251208E+000	1.3859474199296884E+001	1.8024262361574102E+000
F	1.7313157667949699E+000	4.0437948487200019E+000	4.5014834484771482E+000
F	1.7313180485568149E+000	1.4453350390328219E+000	8.9937912393469261E+000
F	1.7313179133315644E+000	9.2407192626638412E+000	4.5014855921699768E+000
F	1.7313176865752793E+000	6.6422622307970771E+000	8.9937900917154447E+000
F	1.7313160125006393E+000	1.4437656350547581E+001	4.5014804055390716E+000
F	1.7313145165679735E+000	1.1839189064013544E+001	8.9937827800216414E+000
F	3.4656134963116667E+000	1.4145466125024681E+001	8.9937845860586716E+000
F	3.4656108639340979E+000	1.1531420065453706E+000	4.5014786703248237E+000
F	3.4656085869869480E+000	8.9485403772873440E+000	8.9937895748975620E+000
F	3.4656106551587511E+000	1.1546998578553929E+001	4.5014836445373234E+000
F	3.4656141071165569E+000	3.7516083085679348E+000	8.9937889150048633E+000
F	3.4656146920689768E+000	6.3500709564295210E+000	4.5014825207746085E+000
F	4.0437912844904336E+000	8.6715052630096157E-001	7.2005328187977149E+000
F	4.0437921837254347E+000	3.4656180895960582E+000	6.2947307389758222E+000
F	4.0437927323303517E+000	6.0640840467975448E+000	7.2005351326764391E+000
F	4.0437859295156713E+000	8.6625467114807844E+000	6.2947325171116262E+000
F	4.0437880828361310E+000	1.1261009634958929E+001	7.2005348891947207E+000
F	4.0437894241031058E+000	1.3859477911002934E+001	6.2947282316287305E+000
F	3.7516059920334848E+000	1.7313192288747117E+000	1.8024311600995055E+000
F	3.7515998858977189E+000	1.4723640560427970E+001	8.9662408208849298E-001
F	3.7515965686484454E+000	1.2125170901303472E+001	1.8024310389324911E+000
F	3.7516002042219236E+000	9.5267091571925278E+000	8.9662698908914806E-001
F	3.7516025139423661E+000	6.9282469683642978E+000	1.8024318188446711E+000
F	3.7516068180246265E+000	4.3297874844461015E+000	8.9663032199174608E-001
F	4.3297824257572666E+000	4.0437931143487704E+000	3.5956799585922088E+000
F	4.3297825773766565E+000	1.4453339131408434E+000	9.8995909904385240E+000
F	4.3297818829614982E+000	9.2407191440286720E+000	3.5956824697423531E+000
F	4.3297797698031504E+000	6.6422633419557657E+000	9.8995916782536302E+000

F 4.3297804953140648E+000 1.4437655459607795E+001 3.5956783640543932E+000
F 4.3297814351389450E+000 1.1839192280620315E+001 9.8995848277621867E+000
F 6.0640774014438525E+000 1.4145468079644814E+001 9.8995874110209261E+000
F 6.0640764877519420E+000 1.1531429783323670E+000 3.5956776664477852E+000
F 6.0640768515391699E+000 8.9485390320561038E+000 9.8995893506891495E+000
F 6.0640760490491443E+000 1.1546999494342494E+001 3.5956830012410399E+000
F 6.0640761747068508E+000 3.7516078608734005E+000 9.8995885607817513E+000
F 6.0640779314716990E+000 6.3500695512908738E+000 3.5956779998505115E+000
F 6.6422542353459910E+000 8.6714896533934793E-001 8.9662453705084055E-001
F 6.6422537948326204E+000 3.4656126861600356E+000 1.8024267695132743E+000
F 6.6422556239267339E+000 6.0640789615249098E+000 8.9662444412741527E-001
F 6.6422574656662006E+000 8.6625442531211618E+000 1.8024276621136319E+000
F 6.6422561765224382E+000 1.1261009007149717E+001 8.9662763206958096E-001
F 6.6422550773618712E+000 1.3859475598222657E+001 1.8024300980365584E+000
F 6.3500668501775070E+000 1.7313195443586329E+000 6.2947315669656732E+000
F 6.3500654287420071E+000 1.4723648142384972E+001 7.2005305957187913E+000
F 6.3500655140770297E+000 1.2125177329863071E+001 6.2947303534220183E+000
F 6.3500640886225490E+000 9.5267171217836761E+000 7.2005352547280852E+000
F 6.3500664950288490E+000 6.9282524362541160E+000 6.2947339297017786E+000
F 6.3500680414554918E+000 4.3297842142279395E+000 7.2005355564157369E+000
F 6.9282472908630144E+000 4.0437932874235782E+000 4.5014803116187725E+000
F 6.9282449909869896E+000 1.4453318748006589E+000 8.9937854822129299E+000
F 6.9282416325513640E+000 9.2407259709738039E+000 4.5014847042893749E+000
F 6.9282428385197248E+000 6.6422649223018846E+000 8.9937863921049956E+000
F 6.9282439214003286E+000 1.4437657413117554E+001 4.5014814500442162E+000
F 6.9282439956869988E+000 1.1839193229173533E+001 8.9937856922701265E+000
F 8.6625433571666264E+000 1.4145469056290416E+001 8.9937887925423485E+000
F 8.6625418017602716E+000 1.1531410731483989E+000 4.5014811658884701E+000
F 8.6625430133955170E+000 8.9485384459431145E+000 8.9937867627107124E+000
F 8.6625447297416294E+000 1.1547001074958811E+001 4.5014837445688416E+000
F 8.6625422244945032E+000 3.7516085265709420E+000 8.9937877555906596E+000
F 8.6625417019366679E+000 6.3500681291949199E+000 4.5014790936880607E+000
F 9.2407209385489359E+000 8.6715278882097757E-001 7.2005368450187879E+000
F 9.2407200321731047E+000 3.4656153262546403E+000 6.2947334882874530E+000
F 9.2407205854051799E+000 6.0640802844143975E+000 7.2005351793590942E+000
F 9.2407233977249295E+000 8.6625483056545178E+000 6.2947335312665453E+000
F 9.2407243516736699E+000 1.1261014502151740E+001 7.2005371525987751E+000
F 9.2407231469357800E+000 1.3859478905525359E+001 6.2947342967191959E+000
F 8.9485303808489185E+000 1.7313183923660798E+000 1.8024257771978627E+000
F 8.9485319549526068E+000 1.4723643483890243E+001 8.9662639430995272E-001
F 8.9485320965219604E+000 1.2125178517745043E+001 1.8024292757693394E+000
F 8.9485330019244422E+000 9.5267125293137145E+000 8.9662523543198391E-001
F 8.9485315859989640E+000 6.9282467000105195E+000 1.8024265510012947E+000
F 8.9485309043710632E+000 4.3297810423020415E+000 8.9662307435966981E-001
F 9.5267101745398914E+000 4.0437928512267227E+000 3.5956773784046439E+000
F 9.5267102984351446E+000 1.4453330086227874E+000 9.8995901199932259E+000
F 9.5267131373668299E+000 9.2407249961367448E+000 3.5956813866984074E+000
F 9.5267124920534467E+000 6.6422602969352980E+000 9.8995898897123276E+000
F 9.5267100824033815E+000 1.4437656485121444E+001 3.5956784901832579E+000
F 9.5267108765571393E+000 1.1839193670439025E+001 9.8995916315481853E+000
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F 1.1261005789856426E+001 3.7516091752278564E+000 9.8995894493789400E+000
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F 1.1546996134249035E+001 4.3297846172589169E+000 7.2005358559238211E+000

F 1.1839184713632656E+001 8.6714854520671858E-001 8.9662409845143276E-001
F 1.1839188171999945E+001 3.4656164459868180E+000 1.8024299618219155E+000
F 1.1839186287261846E+001 6.0640771814423342E+000 8.9662733238686687E-001
F 1.1839184891349856E+001 8.6625426284388816E+000 1.8024269439971807E+000
F 1.1839187036321169E+001 1.1261010284623570E+001 8.9662388992581743E-001
F 1.1839185796181368E+001 1.3859472082369342E+001 1.8024249744417873E+000
F 1.2125177755769595E+001 4.0437928288665850E+000 4.5014832714206721E+000
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F 1.3859473173351523E+001 1.1546999038719767E+001 4.5014825977021706E+000
F 1.3859472089842804E+001 3.7516087488844563E+000 8.9937874109601363E+000
F 1.3859473261764975E+001 6.3500710796188562E+000 4.5014844680383277E+000
F 1.4145460237238620E+001 1.7313161829663606E+000 1.8024284241098563E+000
F 1.4145463512899651E+001 1.4723642587034584E+001 8.9662425452932093E-001
F 1.4145463124974867E+001 1.2125178373843953E+001 1.8024279831136765E+000
F 1.4145461008170722E+001 9.5267102837574882E+000 8.9662381259859025E-001
F 1.4145462612019076E+001 6.9282473594218414E+000 1.8024285591844160E+000
F 1.4145462494534110E+001 4.3297831033043241E+000 8.9662802498349781E-001
F 1.4437651323419271E+001 8.6715177368943053E-001 7.2005345966522203E+000
F 1.4437649378262540E+001 3.4656156511401282E+000 6.2947336585169991E+000
F 1.4437651141722355E+001 6.0640826058762052E+000 7.2005380249802409E+000
F 1.4437652537355588E+001 8.6625462612241027E+000 6.2947356488209429E+000
F 1.4437651283069114E+001 1.1261012182087908E+001 7.2005362909039148E+000
F 1.4437651888948750E+001 1.3859479200838329E+001 6.2947315594595095E+000
F 1.4723643376182999E+001 4.0437928627941089E+000 3.5956828253236202E+000
F 1.4723639049736787E+001 1.4453326212248228E+000 9.8995908956473961E+000
F 1.4723639853736614E+001 1.4437654360377497E+001 3.5956774305496464E+000
F 1.4723643835858594E+001 1.1839191511252061E+001 9.8995877964168386E+000
F 1.4723641012283322E+001 6.6422619085445014E+000 9.8995911546209676E+000
F 1.4723642348853417E+001 9.2407238109665073E+000 3.5956799322709356E+000

7 β-$NaYF_4$ Optimised Structure (configuration 10)

A 1.2056437308948636E+01 0.0000000000000000E+00 0.0000000000000000E+00
B -5.9969677559366437E+00 1.0473134435223811E+01 0.0000000000000000E+00
C 1.1946225120407898E-03 -2.5457702667339905E-03 1.4150749505173852E+01

Na -3.0991034750626576E+00 8.7255508673403668E+00 2.0362000133700908E+00
Na -2.8216057271276478E+00 8.7268137878219161E+00 5.4728920595659591E+00
Na -3.1522734330892455E+00 8.7232878030521732E+00 8.6764918782534366E+00
Na -2.9285322605466177E+00 8.7249974384335811E+00 1.1942622203951792E+01
Y -2.9636936093284114E+00 5.2737508804849842E+00 -2.4579568525484536E-03
Y -3.0021139092004887E+00 5.2474826649645694E+00 3.5377792126626564E+00
Y -3.0286074422615141E+00 5.2212655313906673E+00 7.0667148650680245E+00
Y -3.0044646450413381E+00 5.2409880576806129E+00 1.0618075665042904E+01
Y 2.7676928998108814E-02 7.0066694411543997E+00 1.7640511039751179E+00
Na 2.2147865792835730E-02 6.9803603897049786E+00 5.1860830241629579E+00
Y 1.9741214221277478E-03 7.0172065465228144E+00 8.8240875052389320E+00
Na -3.2916672343578278E-02 6.9799061670760381E+00 1.2403130601026891E+01
Y 4.1205529246391759E-02 -2.1627011646898815E-03 -3.3544400549856395E-03
Y 2.0021275337053887E-03 1.2717468343624479E-02 3.5303877122026548E+00
Y 6.8745263331278852E-03 2.2196781203409947E-02 7.0766922334643576E+00
Y -2.3405740878333713E-02 7.4088766400859157E-03 1.0607344632347841E+01
Na 1.2317124267511297E-01 3.4907353013595430E+00 1.8049385008340177E+00
Na -1.0111875385510047E-01 3.4888393350823494E+00 5.3003259474844588E+00
Na 6.9445567898141367E-02 3.4907005129505229E+00 8.9666699206485294E+00
Na -9.9935885285807338E-02 3.4868752230290334E+00 1.2346494685128219E+01
Na 2.9924971335532660E+00 1.6975224982966202E+00 1.7477473058894772E+00
Y 3.0093141933466478E+00 1.7677064282492734E+00 5.3086239214342568E+00
Na 3.0201694673349042E+00 1.7442448555261099E+00 8.8511148060178435E+00
Y 3.0261466494097360E+00 1.7726088496497989E+00 1.2369775241364819E+01
Y 3.0170825822127703E+00 5.2461831089635433E+00 8.7884586607661803E-03
Y 3.0449033105368568E+00 5.2537867386949779E+00 3.5325703355186664E+00
Y 3.0280992601363423E+00 5.2239495359150734E+00 7.0832023231617347E+00
Y 3.0149281985262282E+00 5.2779897597776140E+00 1.0610204476540366E+01
Na 3.2049408242013220E+00 8.7280972484962280E+00 1.5736173393530233E+00
Na 2.9822900336753055E+00 8.7255274759991259E+00 5.2400259512628020E+00
Na 3.1538909212806230E+00 8.7259950538880364E+00 8.6199115530486647E+00
Na 2.9286929911394970E+00 8.7239904854204617E+00 1.2401969872322317E+01
Na 6.0493169376766538E+00 6.9808644807952769E+00 1.7477820392905958E+00
Y 6.0591996598359934E+00 7.0002283221529318E+00 5.3081425634270989E+00
Na 6.0487901079647655E+00 6.9794148718743347E+00 8.7942629378553079E+00
Y 6.0333280485473475E+00 6.9998433027422040E+00 1.2390943173290411E+01
Y 5.9862965973400275E+00 -2.6385011880447097E-04 -1.3243300082842109E-02
Y 6.0405677048038973E+00 9.6568469874954189E-03 3.5337705743128351E+00
Y 6.0593144228762137E+00 3.8356994520040329E-02 7.0620110520894501E+00
Y 6.0459081549306255E+00 -8.6235953132078273E-03 1.0616667585876977E+01
Na 5.9262976451905702E+00 3.4895630066648229E+00 1.4585304062565059E+00
Na 6.0977055972006706E+00 3.4898964208545711E+00 4.8953856389385866E+00
Na 5.9264307890623691E+00 3.4887262564410939E+00 9.2552243407602077E+00
Na 6.2051527056818934E+00 3.4893259640267926E+00 1.2576284638990971E+01
Y 9.0386759186532970E+00 1.7719891811044683E+00 1.7505968090580668E+00
Na 9.0471988056332329E+00 1.7442940455908142E+00 5.1861508547724284E+00
Y 9.0401647369475349E+00 1.7562278524129837E+00 8.8215454137717888E+00
Na 9.0483813158526996E+00 1.7422561488209980E+00 1.2402963816296724E+01
F -3.6996154088102351E+00 6.5423271330404891E+00 1.7512305857247310E+00
F -3.7341993558442637E+00 6.5117986585842731E+00 8.8557750195367806E+00
F -3.6456337806220658E+00 6.6545072942872316E+00 5.2945413465026991E+00
F -3.6471594244791388E+00 6.6507419165776938E+00 1.2399984155122056E+01
F -6.4162368670822800E-01 1.4104641198215093E+00 1.7493709463400291E+00
F -6.5529904129718164E-01 1.4123069299928366E+00 8.8461988207992981E+00
F -7.2502088816499843E-01 1.2861937010179649E+00 5.2978316408890365E+00
F -7.1831073927331279E-01 1.2898921741385974E+00 1.2399116761763890E+01

F	-1.4435674214181957E+00	5.1478959465662628E+00	1.8037991474273196E+00
F	-1.4652801214513425E+00	5.1868754155384531E+00	8.8481246168557881E+00
F	-1.5191040996638239E+00	5.1865829839440849E+00	5.2977717077429913E+00
F	-1.4939425134928279E+00	5.1875227612645904E+00	1.2351391442314068E+01
F	-4.4877614261915619E+00	1.0418458869996577E+01	1.7955628443427969E+00
F	-4.5067857837070440E+00	1.0432082593669776E+01	8.8549950621054698E+00
F	-4.4517085746233915E+00	1.0412102608813866E+01	5.2987352573563165E+00
F	-4.4442238003774435E+00	1.0384572551272134E+01	1.2348206944148341E+01
F	-1.5910384236647890E+00	7.1138616294230017E+00	1.6738082230576737E-01
F	-1.7054853478996204E+00	7.1768108485051583E+00	7.2212900725916596E+00
F	-1.6534484494954984E+00	7.1737608956181802E+00	3.3791461507506990E+00
F	-1.7003139275637507E+00	7.1773225213808951E+00	1.0476012533264903E+01
F	1.3708588638109780E+00	1.9014278077617766E+00	-1.6837956839842735E-01
F	1.3302660462716003E+00	1.9062603602512564E+00	6.9274105933562904E+00
F	1.3421624528764475E+00	1.9336283040212701E+00	3.6719393388952079E+00
F	1.3349477886089585E+00	1.9362233672681577E+00	1.0771674280726648E+01
F	3.7149554626577341E+00	2.9785520828753242E-01	-1.7885193349785156E-01
F	3.7307613755173104E+00	1.9841302904127475E-01	6.8759282175736258E+00
F	3.7307310769552764E+00	2.0552201013258792E-01	3.7259418043785377E+00
F	3.7157384732662044E+00	2.4109531568083378E-01	1.0772308854388074E+01
F	7.2116689010414936E-01	5.4407356600880217E+00	1.8226073346915619E-01
F	7.1500706360651411E-01	5.4867024909524025E+00	7.2288598188425324E+00
F	7.2115213902095632E-01	5.4800234739495650E+00	3.3718889941291876E+00
F	7.0887035306424429E-01	5.4765509263338874E+00	1.0425166199579582E+01
F	2.2976212538868004E+00	3.9682985476626937E+00	1.7930310036762565E+00
F	2.2525184582529043E+00	3.9827318023832814E+00	8.8546496728076871E+00
F	2.1277243781145785E+00	3.9725630809857488E+00	5.2971303898013247E+00
F	2.1356577346332708E+00	3.9685655949738656E+00	1.2398966269558679E+01
F	-8.6983047700233351E-01	9.2066091047970673E+00	1.7525976710093352E+00
F	-8.7202052638438965E-01	9.2062578949845282E+00	8.8476025494932742E+00
F	-6.8559749920943935E-01	9.2128029446714681E+00	5.2993207987050743E+00
F	-7.5612552602526584E-01	9.2118983646271744E+00	1.2396730170880376E+01
F	1.0070379654992516E+00	8.3795687720008978E+00	1.7255514362977167E-01
F	1.0003750661289981E+00	8.3825530525581673E+00	7.2272715021884784E+00
F	1.0006076310773844E+00	8.3788377875417126E+00	3.3700756489939163E+00
F	9.6370884171211513E-01	8.3459938977241706E+00	1.0475967805641483E+01
F	4.0500891467783120E+00	3.1521042137403925E+00	-1.7493675366197861E-01
F	3.9198099568099893E+00	3.1011624758210838E+00	6.9255410593765623E+00
F	4.0041931882408734E+00	3.1361515712075709E+00	3.7235688675386203E+00
F	4.0000887639191802E+00	3.1534704663801487E+00	1.0774191396871027E+01
F	2.3817452812901569E+00	6.6567638302192389E+00	1.7544659288545998E+00
F	2.3674660130494254E+00	6.6708280632893295E+00	8.8479191801361914E+00
F	2.3337618075620141E+00	6.5393898862047823E+00	5.2995280735520494E+00
F	2.2857120836234648E+00	6.5389839030449419E+00	1.2401804920684045E+01
F	5.2937612421033409E+00	1.3041427453119414E+00	1.7564569133843000E+00
F	5.3336478098838125E+00	1.3033579153755408E+00	8.8519410299453032E+00
F	5.3873216645207265E+00	1.4177763267799166E+00	5.3002227867023057E+00
F	5.3813446663855631E+00	1.4265865261149759E+00	1.2347093500883837E+01
F	1.5698046780210519E+00	1.0422444412081461E+01	1.7472170989681377E+00
F	1.5895917671699351E+00	1.0375613287876844E+01	8.8532168332461101E+00
F	1.5546458559295084E+00	1.0423695774665839E+01	5.2932080747435046E+00
F	1.5135928596577322E+00	1.0418588579471976E+01	1.2402266747507877E+01
F	4.5275011800404519E+00	5.1835913741550321E+00	1.7507339995495759E+00
F	4.5126359099028353E+00	5.1855941426593599E+00	8.8522965028941343E+00
F	4.5880838893614131E+00	5.1565352259792556E+00	5.3057419726556958E+00
F	4.5640905448108766E+00	5.1817815981520878E+00	1.2400661922279541E+01
F	4.3657166202436137E+00	7.1752273494540919E+00	-1.2176601637749769E-01
F	4.3763659896367075E+00	7.1717504639781993E+00	6.9289343758135846E+00
F	4.4014953633451697E+00	7.1395201310277647E+00	3.6707015249814647E+00
F	4.3729960518962159E+00	7.1660566929655092E+00	1.0774602171194998E+01
F	7.3334768896687539E+00	1.9516367464199027E+00	1.2024438497023203E-01
F	7.4311534042043572E+00	1.8661620114942663E+00	7.2190727917252770E+00

F	7.3700908573120634E+00	1.9363038432004465E+00	3.3761475972474595E+00
F	7.3981611454287917E+00	1.8982406990077132E+00	1.0480773974211512E+01
F	9.7432074115863969E+00	2.3734192100095650E-01	1.7546057494284542E-01
F	9.7665025143652464E+00	1.9689488267415270E-01	7.2290516874559074E+00
F	9.7461562683690897E+00	2.3939615581518128E-01	3.3580664354504379E+00
F	9.7455155154789619E+00	2.3994521070208016E-01	1.0426173452229072E+01
F	6.7469320812438349E+00	5.4827433989947263E+00	3.6756108681244020E+00
F	6.7390791369626033E+00	5.4243415332274347E+00	1.0828712161006459E+01
F	6.7400450163356664E+00	5.4322523489956511E+00	-1.7541612916177868E-01
F	6.7599141646544307E+00	5.5333227073133884E+00	6.9182662360789058E+00
F	5.3337534913915015E+00	9.2138308881398849E+00	1.7536282788980915E+00
F	5.3260625632758556E+00	9.2078316352149514E+00	8.8472351275027403E+00
F	5.1882039557641066E+00	9.1840890679114349E+00	5.3029035964200242E+00
F	5.1591831691148569E+00	9.2064649027910832E+00	1.2397939387211515E+01
F	8.2723099070860915E+00	3.9769184928956998E+00	5.2959296507600362E+00
F	8.3390906704527001E+00	3.9710857784224429E+00	1.2400413684163414E+01
F	8.1589347256693028E+00	3.9724038423101597E+00	1.7498793822057461E+00
F	8.1414516145474067E+00	3.9402335962540582E+00	8.8510649104376480E+00
F	7.0407030816488030E+00	8.3781269986191891E+00	3.7190304314305132E+00
F	7.0103890683851668E+00	8.3433472084050262E+00	1.0773348524659545E+01
F	6.9986920168420044E+00	8.3447744413683882E+00	-1.7415865674029460E-01
F	7.0803973323468776E+00	8.3901051943809630E+00	6.9262491728249982E+00
F	1.0003910366208904E+01	3.1088628806286205E+00	3.3754918706323171E+00
F	1.0037057590204213E+01	3.1432825676067369E+00	1.0425639004683530E+01
F	1.0030885008289502E+01	3.1457084455115703E+00	1.7393274440645973E-01
F	1.0027468752057370E+01	3.1426772653612911E+00	7.2263667944613657E+00