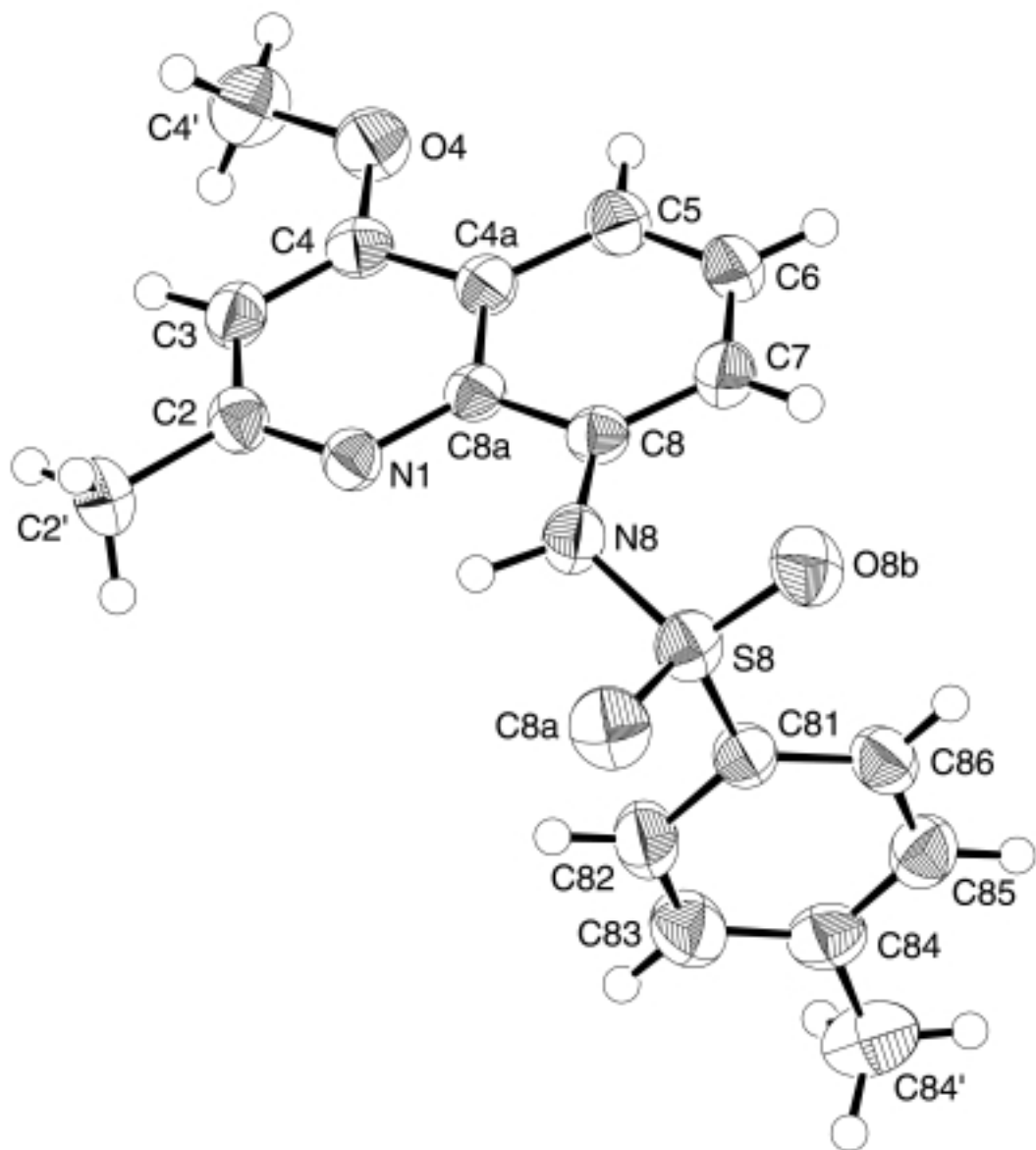


- SUPPLEMENTARY MATERIAL -

Figure S(2)	
Table S(1)	Crystallographic Information File for 4-methoxy isomer of $C_{18}H_{18}N_2O_3S$
Table S(2)	Structure Factors for 4-methoxy isomer of $C_{18}H_{18}N_2O_3S$
Table S(3)	Crystallographic Information File for 5-methoxy isomer of $C_{18}H_{18}N_2O_3S$
Table S(4)	Structure Factors for 5-methoxy isomer of $C_{18}H_{18}N_2O_3S$



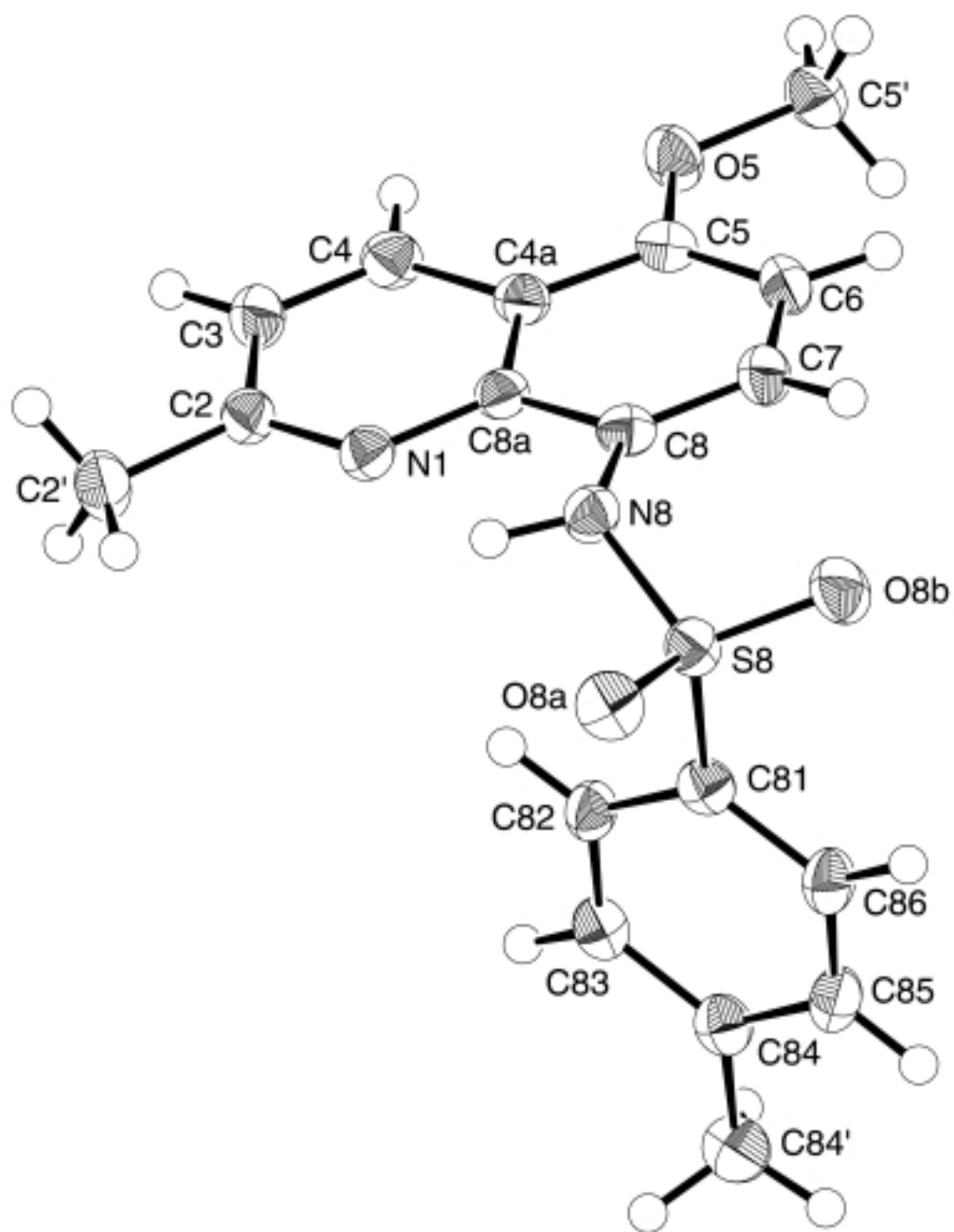


Table S(1)
Crystallographic Information File for 4-methoxy isomer of C₁₈H₁₈N₂O₃S

```

#####
data_[C18H18N2O3S] - 4-methoxy isomer
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;
SIR92 (Altomare et. al., 1994)
;
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'teXsan for Windows version 1.05 (MSC, 1997)'

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_cell_angle_gamma             90
_cell_volume                  1640(1)
_cell_formula_units_Z         4
_cell_measurement_temperature 293
_cell_measurement_reflns_used 19
_cell_measurement_theta_min   19.0
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_symmetry_Int_Tables_number    14
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loop_
_symmetry_equiv_pos_as_xyz
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' -x,1/2+y,1/2-z '
' -x, -y, -z '
' +x,1/2-y,1/2+z '
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_exptl_crystal_density_diffn   1.387
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The scan width was (1.05+0.35tan\q)\% with an \w
scan speed of 32\% per minute
(up to 5 scans to achieve I/\s(I) > 20).
Stationary background counts were recorded at each end of the
scan, and the scan time:background time ratio was 2:1.
;

#####
# EXPERIMENTAL DATA

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_diffrn_measurement_method           \w-2\q

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      2      1     -1
      1      1     -3
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_diffrn_reflns_limit_l_min          -17
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Refinement of F^2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2, conventional R-factors R are based
on F, with F set to zero for negative F^2. The threshold expression of
F^2 > 2sigma(F^2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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_refine_ls_weighting_details
'calc w=1/[\s^2(Fo^2)+(0.0468P)^2+1.0357P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary        direct

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_refine_ls_shift/su_mean           0.000

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  _atom_site_U_iso_or_equiv
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  _atom_site_symmetry_multiplicity
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O4 O 0.22758(18) -0.0593(2) 0.40045(17) 0.0509(6) Uani 1 1 d . . .
O8B O -0.42315(18) -0.1074(2) 0.31851(17) 0.0544(7) Uani 1 1 d . . .
O8A O -0.44546(18) 0.1381(2) 0.30990(18) 0.0571(7) Uani 1 1 d . . .
N1 N -0.0666(2) 0.1604(2) 0.37746(18) 0.0362(6) Uani 1 1 d . . .
N8 N -0.2612(2) 0.0462(3) 0.34271(19) 0.0428(7) Uani 1 1 d . . .
H8 H -0.2525 0.1439 0.3587 0.064(3) Uiso 1 1 d . . .
C2 C 0.0294(3) 0.2202(3) 0.3968(2) 0.0385(7) Uani 1 1 d . . .
C2' C 0.0266(3) 0.3707(3) 0.4082(3) 0.0528(9) Uani 1 1 d . . .
H2A H 0.1015 0.4043 0.4153 0.096(4) Uiso 1 1 calc R . . .
H2B H -0.0134 0.3934 0.4651 0.096(4) Uiso 1 1 calc R . . .
H2C H -0.0101 0.4098 0.3514 0.096(4) Uiso 1 1 calc R . . .
C3 C 0.1320(3) 0.1535(3) 0.4058(2) 0.0404(8) Uani 1 1 d . . .
H3 H 0.1975 0.2010 0.4196 0.064(3) Uiso 1 1 calc R . . .
C4 C 0.1345(2) 0.0172(3) 0.3939(2) 0.0375(7) Uani 1 1 d . . .
C4A C 0.0338(2) -0.0536(3) 0.3723(2) 0.0352(7) Uani 1 1 d . . .
C4' C 0.3326(3) 0.0066(4) 0.4177(3) 0.0589(10) Uani 1 1 d . . .
H4A H 0.3913 -0.0588 0.4207 0.096(4) Uiso 1 1 calc R . . .
H4B H 0.3321 0.0544 0.4785 0.096(4) Uiso 1 1 calc R . . .
H4C H 0.3448 0.0682 0.3655 0.096(4) Uiso 1 1 calc R . . .
C5 C 0.0272(3) -0.1931(3) 0.3583(2) 0.0425(8) Uani 1 1 d . . .
H5 H 0.0913 -0.2454 0.3634 0.064(3) Uiso 1 1 calc R . . .
C6 C -0.0741(3) -0.2507(3) 0.3371(2) 0.0465(8) Uani 1 1 d . . .
H6 H -0.0778 -0.3427 0.3272 0.064(3) Uiso 1 1 calc R . . .
C7 C -0.1726(3) -0.1755(3) 0.3297(2) 0.0431(8) Uani 1 1 d . . .
H7 H -0.2406 -0.2174 0.3151 0.064(3) Uiso 1 1 calc R . . .
C8 C -0.1683(2) -0.0400(3) 0.3441(2) 0.0346(7) Uani 1 1 d . . .
C8A C -0.0645(2) 0.0242(3) 0.3650(2) 0.0330(7) Uani 1 1 d . . .
C81 C -0.3616(2) 0.0148(3) 0.1627(2) 0.0409(7) Uani 1 1 d . . .
C82 C -0.3196(3) 0.1276(4) 0.1185(3) 0.0560(10) Uani 1 1 d . . .
H82 H -0.3019 0.2034 0.1555 0.064(3) Uiso 1 1 calc R . . .
C83 C -0.3042(3) 0.1267(4) 0.0193(3) 0.0614(10) Uani 1 1 d . . .
H83 H -0.2751 0.2021 -0.0101 0.064(3) Uiso 1 1 calc R . . .
C84 C -0.3312(3) 0.0162(4) -0.0370(3) 0.0496(9) Uani 1 1 d . . .
C84' C -0.3175(3) 0.0202(4) -0.1465(3) 0.0695(12) Uani 1 1 d . . .
H84A H -0.2409 0.0379 -0.1595 0.096(4) Uiso 1 1 calc R . . .
H84B H -0.3638 0.0897 -0.1748 0.096(4) Uiso 1 1 calc R . . .
H84C H -0.3393 -0.0644 -0.1745 0.096(4) Uiso 1 1 calc R . . .
C85 C -0.3724(3) -0.0949(4) 0.0080(3) 0.0505(9) Uani 1 1 d . . .
H85 H -0.3904 -0.1703 -0.0293 0.064(3) Uiso 1 1 calc R . . .
C86 C -0.3880(3) -0.0973(3) 0.1078(3) 0.0466(8) Uani 1 1 d . . .
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O8B 0.0452(14) 0.0537(15) 0.0649(16) 0.0084(13) 0.0085(12) -0.0137(12)
O8A 0.0401(13) 0.0576(16) 0.0744(17) -0.0061(13) 0.0102(12) 0.0116(12)
N1 0.0418(15) 0.0343(15) 0.0324(13) -0.0023(11) 0.0025(11) -0.0005(12)
N8 0.0390(15) 0.0413(16) 0.0478(16) -0.0071(13) -0.0008(12) 0.0006(12)
C2 0.0456(19) 0.0361(18) 0.0339(17) -0.0024(14) 0.0048(14) -0.0033(15)
C2' 0.062(2) 0.035(2) 0.061(2) -0.0062(17) 0.0017(18) -0.0040(17)
C3 0.0401(17) 0.043(2) 0.0378(17) -0.0005(15) -0.0003(14) -0.0076(15)
C4 0.0400(17) 0.0433(19) 0.0295(15) 0.0015(14) 0.0039(12) 0.0025(15)
C4A 0.0401(17) 0.0359(18) 0.0298(16) -0.0017(13) 0.0027(13) 0.0009(14)
C4' 0.0343(17) 0.070(3) 0.072(3) 0.003(2) 0.0044(17) -0.0022(19)
C5 0.047(2) 0.0385(19) 0.0423(19) -0.0032(15) 0.0000(15) 0.0042(16)
C6 0.061(2) 0.0309(18) 0.047(2) -0.0021(15) -0.0033(17) 0.0018(16)
C7 0.0450(19) 0.041(2) 0.0428(19) 0.0000(15) -0.0030(15) -0.0075(16)
C8 0.0371(16) 0.0370(18) 0.0299(15) 0.0008(13) 0.0018(12) 0.0019(14)
C8A 0.0380(15) 0.0359(17) 0.0252(14) -0.0004(13) 0.0024(12) 0.0011(14)
C81 0.0337(16) 0.0392(18) 0.0496(19) 0.0005(16) -0.0013(14) 0.0004(15)
C82 0.071(3) 0.044(2) 0.053(2) -0.0002(18) -0.0005(18) -0.0144(19)
C83 0.078(3) 0.053(2) 0.053(2) 0.009(2) 0.004(2) -0.011(2)
C84 0.0402(18) 0.057(2) 0.052(2) 0.0011(18) -0.0014(15) 0.0121(17)
C84' 0.065(3) 0.089(3) 0.054(2) 0.000(2) -0.0025(19) 0.018(2)
C85 0.047(2) 0.047(2) 0.057(2) -0.0107(18) -0.0053(17) 0.0058(17)
C86 0.0421(19) 0.037(2) 0.061(2) 0.0034(17) 0.0000(16) 0.0021(16)

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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loop_

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S8 N8 1.630(3) . ?
S8 C81 1.762(3) . ?
O4 C4 1.353(4) . ?
O4 C4' 1.432(4) . ?
N1 C2 1.315(4) . ?
N1 C8A 1.372(4) . ?
N8 C8 1.409(4) . ?
C2 C3 1.401(4) . ?
C2 C2' 1.512(5) . ?
C3 C4 1.373(4) . ?
C4 C4A 1.420(4) . ?
C4A C5 1.408(4) . ?
C4A C8A 1.412(4) . ?
C5 C6 1.365(4) . ?
C6 C7 1.401(4) . ?
C7 C8 1.369(4) . ?
C8 C8A 1.419(4) . ?
C81 C86 1.378(4) . ?
C81 C82 1.384(5) . ?
C82 C83 1.379(5) . ?
C83 C84 1.377(5) . ?
C84 C85 1.372(5) . ?
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loop_

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O8A S8 N8 104.24(14) . . ?
O8B S8 C81 108.33(15) . . ?

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O8A S8 C81 108.76(15) . . ?
N8 S8 C81 106.28(14) . . ?
C4 O4 C4' 118.0(3) . . ?
C2 N1 C8A 117.1(3) . . ?
C8 N8 S8 127.1(2) . . ?
N1 C2 C3 124.1(3) . . ?
N1 C2 C2' 116.8(3) . . ?
C3 C2 C2' 119.2(3) . . ?
C4 C3 C2 119.0(3) . . ?
O4 C4 C3 125.1(3) . . ?
O4 C4 C4A 115.1(3) . . ?
C3 C4 C4A 119.8(3) . . ?
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C8A C4A C4 116.2(3) . . ?
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C7 C8 N8 125.3(3) . . ?
C7 C8 C8A 120.3(3) . . ?
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N1 C8A C4A 123.8(3) . . ?
N1 C8A C8 116.9(3) . . ?
C4A C8A C8 119.2(3) . . ?
C86 C81 C82 120.2(3) . . ?
C86 C81 S8 121.4(3) . . ?
C82 C81 S8 118.4(3) . . ?
C83 C82 C81 119.4(3) . . ?
C84 C83 C82 121.3(4) . . ?
C85 C84 C83 118.6(3) . . ?
C85 C84 C84' 121.4(4) . . ?
C83 C84 C84' 120.0(4) . . ?
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C81 C86 C85 119.1(3) . . ?

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Table S(2)

Structure Factors for 4-methoxy isomer of C₁₈H₁₈N₂O₃S

#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	13	5	0	4.89	0.35	23.62	0	-1	2	1	155.93	141.17	7.11	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	14	5	0	0.31	-14.00	22.56	0	0	2	1	1.41	10.79	3.30	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	0	6	0	1744.22	1636.16	66.91	0	0	2	1	776.98	730.36	26.26	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	1	6	0	1.39	5.50	11.87	0	2	2	1	87.09	72.31	5.28	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	2	6	0	6.92	5.53	12.29	0	3	2	1	1898.79	1840.18	55.38	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	3	6	0	90.67	98.63	8.98	0	4	2	1	121.26	108.96	7.37	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	4	6	0	1123.20	1087.81	54.96	0	5	2	1	0.24	4.86	11.39	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	5	6	0	40.86	44.79	8.21	0	6	2	1	1438.58	1572.89	60.08	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	6	6	0	318.83	349.25	18.12	0	7	2	1	613.14	595.17	29.16	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	7	6	0	17.40	1.87	18.44	0	8	2	1	7.77	6.66	12.71	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	8	6	0	0.09	-20.08	20.08	0	9	2	1	239.47	240.96	15.51	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	9	6	0	27.73	5.99	14.35	0	10	2	1	301.31	296.73	17.12	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	10	6	0	44.76	55.61	12.00	0	11	2	1	110.25	100.11	13.58	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	11	6	0	0.73	20.27	20.50	0	12	2	1	43.53	59.02	11.46	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	12	6	0	3.73	-10.59	23.88	0	13	2	1	6.60	19.69	22.46	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	13	6	0	5.82	23.33	24.62	0	14	2	1	54.07	18.92	28.42	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	1	7	0	735.57	731.03	34.11	0	15	2	1	3.14	16.38	31.09	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	2	7	0	1037.16	1051.00	54.00	0	-15	3	1	17.92	1.32	17.38	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	3	7	0	1359.48	1188.08	60.66	0	-14	3	1	6.77	-27.35	27.35	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	4	7	0	455.74	448.52	23.20	0	-13	3	1	5.91	4.12	21.75	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	5	7	0	686.28	654.28	30.06	0	-12	3	1	19.84	14.80	20.21	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	6	7	0	1600.56	1700.49	77.97	0	-11	3	1	237.77	251.13	17.38	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	7	7	0	390.95	365.11	19.86	0	-10	3	1	472.71	501.59	25.68	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	8	7	0	33.41	42.80	11.49	0	-9	3	1	145.54	144.55	11.94	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	9	7	0	37.29	44.50	11.94	0	-8	3	1	590.39	553.46	28.74	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	10	7	0	35.96	76.46	13.07	0	-7	3	1	1474.70	1507.73	63.46	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	11	7	0	38.88	-44.18	44.18	0	-6	3	1	1262.05	1258.43	54.16	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	12	7	0	16.10	21.69	26.00	0	-5	3	1	361.34	372.10	19.47	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	13	7	0	3.01	-19.76	25.20	0	-4	3	1	42.51	68.61	6.76	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	0	8	0	658.63	653.61	33.31	0	-3	3	1	1013.55	962.15	37.78	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	1	8	0	513.03	439.80	21.82	0	-2	3	1	1096.55	1117.48	40.26	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	2	8	0	92.57	74.24	10.97	0	-1	3	1	277.52	268.61	13.23	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	3	8	0	446.81	455.54	22.98	0	0	3	1	603.17	564.46	17.75	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	4	8	0	718.50	699.30	36.46	0	1	3	1	0.15	5.47	3.77	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	5	8	0	55.97	54.74	11.13	0	2	3	1	167.39	218.86	41.58	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	6	8	0	2.29	-22.98	22.98	0	3	3	1	7.70	5.79	10.46	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	7	8	0	5.75	1.58	14.19	0	4	3	1	4.38	2.03	7.47	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	8	8	0	144.87	13.58	14.87	0	5	3	1	581.99	534.99	23.36	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	9	8	0	5.56	-22.91	22.91	0	6	3	1	1746.54	1717.19	66.36	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	10	8	0	6.60	23.17	12.04	0	7	3	1	1298.24	1208.04	56.80	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	11	8	0	0.01	-18.83	21.46	0	8	3	1	11.77	11.77	16.36	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	12	8	0	4.76	14.90	33.21	0	9	3	1	724.97	691.29	34.50	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	9	9	0	377.00	403.89	21.62	0	10	3	1	903.43	879.25	41.54	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	10	9	0	1417.04	1323.27	54.26	0	11	3	1	447.23	524.15	24.84	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	11	9	0	131.32	151.54	14.09	0	12	3	1	0.07	15.58	20.60	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	12	9	0	2.07	-27.06	27.06	0	13	3	1	70.28	70.96	14.38	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	13	9	0	27.51	3.22	14.93	0	14	3	1	78.86	85.95	17.06	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	14	9	0	90.14	98.05	14.03	0	15	3	1	27.52	-41.58	41.58	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	15	9	0	64.31	89.75	13.42	0	-14	4	1	32.08	32.31	13.32	o							
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	2	1	0	1997.77	2040.15	53.84	0	8	9	0	10.45	-3.64	33.98	10.84	o						
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	3	1	0	2191.25	2234.35	61.66	0	9	9	0	4.66	-31.63	31.63	-12	4	1	0.01	-29.73	29.73	o	
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	4	1	0	1608.11	1596.03	50.94	0	10	9	0	127.97	138.86	20.31	0	-11	4	1	1.77	-5.34	14.09	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	5	1	0	1279.14	1259.72	47.53	0	11	9	0	2.83	-4.92	21.43	0	-10	4	1	18.26	25.52	9.62	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	6	1	0	227.86	230.25	11.36	0	10	0	0	9.81	1.32	16.22	0	-9	4	1	729.23	690.39	35.59	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	7	1	0	123.11	114.88	9.46	0	1	10	0	319.34	322.38	20.21	0	-8	4	1	259.40	318.81	15.70	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	8	1	0	278.45	299.50	15.38	0	2	10	0	5.86	9.14	15.96	0	-7	4	1	163.40	196.14	14.19	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	9	1	0	5.76	-1.42	15.16	0	3	10	0	133.10	131.52	15.48	0	-6	4	1	222.23	267.16	13.81	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	10	1	0	4.57	-19.95	19.95	0	4	10	0	159.69	155.49	16.28	0	-5	4	1	20.45	46.21	6.37	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	11	1	0	2.89	0.29	18.70	0	5	10	0	82.42	93.03	14.42	0	-4	4	1	11.13	4.12	11.97	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	12	1	0	9.91	-23.14	23.14	0	6	10	0	36.77	47.05	12.87	0	-3	4	1	556.48	592.93	30.67	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	13	1	0	101.01	39.87	19.30	0	7	10	0	12.84	12.84	12.84	0	-2	4	1	185.29	214.16	14.50	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	14	1	0	5.92	19.57	20.40	0	8	10	0	55.43	53.97	14.42	0	-1	4	1	1358.84	1552.43	53.80	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	15	1	0	7.17	4.89	29.80	0	9	10	0	0.01	-31.31	31.31	0	0	4	1	109.74	102.46	5.13	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	0	2	0	28527.15	25134.90	555.14	0	1	11	0	59.01	63.20	13.87	0	1	4	1	219.33	247.75	12.04	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	1	2	0	11306.08	10937.07	248.30	0	2	11	0	87.55	105.04	14.64	0	2	4	1	107.75	154.85	8.53	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	2	2	0	6742.90	7191.77	169.36	0	3	11	0	28.86	-4.02	29.09	0	3	4	1	0.11	5.57	9.62	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	3	2	0	4279.20	4483.86	113.37	0	4	11	0	47.88	35.49	14.83	0	4	4	1	361.28	329.31	17.92	o
#	h,k,l, Fo-squared, Fo-squared, sigma(Fo-squared) and status flag	4	2	0	4492.94	4541.46	118.45	0	5	11	0	68.54	75.91	15.09	0	5	1					

2	6	1	18.80	-16.57	16.57	0	12	1	6.62	18.07	14.88	-14	4	2	36.30	-41.13	41.13	0		
3	6	1	91.75	95.77	9.43	0	1	12	1	19.23	-31.47	31.47	-13	4	2	73.75	73.27	15.45	0	
4	6	1	221.56	238.26	13.23	0	2	12	1	11.49	14.80	30.51	-12	4	2	0.87	-27.06	27.06	0	
5	6	1	745.28	703.33	33.72	0	3	12	1	71.78	94.71	17.67	-11	4	2	8.40	5.89	20.18	0	
6	6	1	353.38	322.93	17.92	0	4	12	1	22.78	8.56	29.80	-10	4	2	582.22	575.64	29.25	0	
7	6	1	242.07	252.48	16.25	0	5	12	1	2.90	-25.58	33.92	-9	4	2	530.05	576.76	27.64	0	
8	6	1	386.64	368.43	20.56	0	13	1	1.47	0.74	13.47	-8	4	2	406.44	379.02	19.15	0		
9	6	1	326.51	371.65	20.63	0	-15	0	2	22.81	29.73	13.77	-7	4	2	47.18	67.00	9.11	0	
10	6	1	66.94	9.53	25.04	0	-14	0	2	14.82	18.50	22.33	-6	4	2	186.75	179.31	11.94	0	
11	6	1	9.81	19.21	10.72	0	-13	0	2	79.16	88.14	15.93	-5	4	2	788.81	712.30	29.83	0	
12	6	1	59.02	16.22	0	-12	0	2	0.60	-24.04	24.04	-4	4	2	2759.28	3061.76	94.38	0		
13	6	1	0.93	-25.26	25.26	0	-11	0	2	1931.38	1742.26	865.27	-3	4	2	1618.13	1794.35	63.10	0	
-13	7	1	1.21	-44.22	44.22	0	-10	0	2	2398.34	2147.18	92.61	-2	4	2	23.99	22.62	5.44	0	
-12	7	1	2.47	17.15	10.43	0	-9	0	2	264.02	264.81	15.54	-1	4	2	431.15	398.52	19.37	0	
-11	7	1	97.81	135.80	15.70	0	-8	0	2	21.31	42.61	7.34	0	4	2	1185.95	1148.67	31.56	0	
-10	7	1	18.59	-9.81	22.98	0	-7	0	2	237.03	273.56	13.64	0	4	2	634.27	746.99	33.50	0	
-9	7	1	4.95	10.36	18.02	0	-6	0	2	294.60	229.76	11.71	0	2	4	186.63	217.67	11.65	0	
-8	7	1	43.20	58.18	11.68	0	-5	0	2	94.44	96.86	7.30	0	3	4	538.82	516.07	22.37	0	
-7	7	1	6.11	0.87	17.28	0	-4	0	2	128.77	187.93	9.69	0	4	2	1.18	3.70	10.43	0	
-6	7	1	220.95	225.03	16.70	0	-3	0	2	2998.25	3203.77	83.64	0	5	4	0.77	-9.43	11.46	0	
-5	7	1	66.95	51.07	11.13	0	-2	0	2	2287.71	2286.74	60.31	0	6	4	2	40.37	27.39	6.95	0
-4	7	1	428.89	387.58	20.02	0	-1	0	2	2179.65	2398.57	60.34	0	7	4	2	611.78	604.18	30.47	0
-3	7	1	32.86	32.86	7.79	0	1	0	2	1412.12	1355.90	37.71	0	8	4	2	981.72	1048.91	43.48	0
-2	7	1	93.44	107.84	10.30	0	2	0	2	1264.59	1397.58	41.22	0	9	4	2	966.58	955.94	43.41	0
-1	7	1	58.84	59.76	9.89	0	3	0	2	220.88	240.26	11.75	0	10	4	2	47.37	-15.64	19.44	0
0	7	1	79.27	77.27	9.32	0	4	0	2	3023.99	2801.20	801.64	0	12	4	2	171.39	185.00	26.39	0
1	7	1	481.79	439.06	21.79	0	5	0	2	5654.06	5651.70	148.06	0	12	4	2	613.98	627.61	34.05	0
2	7	1	382.49	403.50	20.95	0	6	0	2	3248.87	3268.07	100.66	0	13	4	2	254.38	249.91	21.91	0
3	7	1	1587.81	1544.35	68.12	0	7	0	2	38.66	10.84	13.97	0	14	4	2	0.02	-30.47	30.47	0
4	7	1	693.03	626.19	28.67	0	8	0	2	7.79	13.07	13.61	0	-14	5	2	26.00	35.46	14.77	0
5	7	1	335.35	347.09	18.31	0	9	0	2	3985.22	3664.33	124.25	0	-13	5	2	0.01	-20.40	27.77	0
6	7	1	1125.26	1158.19	48.30	0	10	0	2	1960.76	1719.76	85.96	0	-12	5	2	0.47	-26.39	26.39	0
7	7	1	3.14	5.18	18.86	0	11	0	2	164.52	166.69	14.51	0	-11	5	2	87.30	77.88	13.74	0
8	7	1	0.14	-18.50	18.50	0	12	0	2	78.68	75.27	12.90	0	-10	5	2	1.90	-25.16	25.16	0
9	7	1	121.13	115.14	14.96	0	13	0	2	63.89	66.48	12.39	0	-9	5	2	42.29	33.02	11.07	0
10	7	1	13.77	5.53	24.13	0	14	0	2	17.19	-20.72	20.72	0	-8	5	2	239.89	204.73	15.25	0
11	7	1	17.14	27.61	13.29	0	15	0	2	133.74	134.06	17.96	0	-7	5	2	25.87	17.76	8.01	0
12	7	1	4.62	-2.22	19.98	0	-15	0	2	6.84	38.29	12.61	0	-6	5	2	467.30	502.04	26.53	0
13	7	1	33.20	3.28	38.10	0	-14	1	2	9.16	15.32	12.49	0	-15	5	2	439.88	516.01	26.39	0
-12	8	1	49.43	71.60	12.87	0	-13	1	2	6.75	-27.96	27.96	-4	5	2	0.81	-15.80	15.80	0	
-11	8	1	9.40	-4.67	19.47	0	-12	1	2	35.60	42.41	11.49	-3	5	2	2349.53	2540.96	82.70	0	
-10	8	1	0.86	8.37	21.11	0	-11	1	2	51.40	27.74	11.20	-2	5	2	331.99	370.91	19.57	0	
-9	8	1	19.15	-23.85	36.91	0	-10	1	2	37.50	3.44	23.65	-1	5	2	311.83	326.00	15.01	0	
-8	8	1	55.84	60.40	13.74	0	-9	1	2	171.86	154.50	13.19	0	5	2	1921.98	2062.99	7.18	0	
-7	8	1	37.49	37.49	11.17	0	-8	1	2	150.25	124.25	10.94	0	2	5	2	4.89	7.18	12.26	0
-6	8	1	649.25	712.59	67.34	0	-7	1	2	0.39	9.07	10.07	0	2	5	2	2.96	4.89	7.18	0
-5	8	1	380.29	365.08	21.21	0	-6	1	2	2.96	2.90	12.32	0	3	5	2	463.55	458.76	23.52	0
-4	8	1	743.35	677.90	32.24	0	-5	1	2	0.33	-0.58	5.79	0	4	5	2	215.22	225.36	12.65	0
-3	8	1	65.11	72.79	11.26	0	-4	1	2	103.62	123.18	7.30	0	5	5	2	45.61	46.08	8.17	0
-2	8	1	14.44	22.27	8.30	0	-3	1	2	1102.20	1003.66	35.59	0	6	5	2	14.39	10.10	14.29	0
-1	8	1	1011.26	100.85	11.39	0	-2	1	2	361.09	371.52	17.80	0	7	5	2	431.33	377.89	19.66	0
0	8	1	1051.26	1036.50	40.00	0	-1	2	2	6.00	14.90	3.06	0	8	5	2	8.56	6.22	6.22	0
1	8	1	648.76	635.62	33.08	0	0	2	2	133.47	133.28	4.54	0	9	5	2	75.55	81.54	12.23	0
2	8	1	205.03	204.09	15.32	0	1	1	2	136.01	150.09	7.79	0	10	5	2	360.92	340.53	20.63	0
3	8	1	191.04	183.62	14.48	0	2	1	2	2852.99	2809.15	73.34	0	11	5	2	50.45	11.71	27.35	0
4	8	1	211.76	216.44	16.99	0	3	1	2	312.35	324.15	14.35	0	12	5	2	23.54	-11.49	30.22	0
5	8	1	1214.51	1110.59	50.27	0	4	1	2	11.78	9.01	4.63	0	13	5	2	5.44	27.45	12.52	0
6	8	1	136.55	118.71	14.35	0	5	1	2	3.41	3.44	9.17	0	14	5	2	43.68	7.08	37.84	0
7	8	1	20.47	20.05	11.17	0	6	1	2	308.87	307.09	15.61	0	-13	6	2	32.66	45.21	14.13	0
8	8	1	209.89	230.89	18.79	0	7	1	2	76.12	53.48	8.27	0	-12	6	2	6.77	-4.89	15.06	0
9	8	1	95.68	105.58	14.16	0	8	1	2	124.35	108.74	10.27	0	-11	6	2	15.95	-2.67	26.74	0
10	8	1	5.34	-28.96	30.41	0	9	1	2	329.97	316.01	17.44	0	-10	6	2	236.27	253.39	17.89	0
11	8	1	0.49	-24.94	28.45	0	10	1	2	31.30	45.82	9.59	0	-9	6	2	65.57	52.90	12.07	0
12	8	1	22.83	22.88	28.16	0	11	1	2	48.41	51.46	11.46	0	-8	6	2	112.25	139.18	12.32	0
-1	8	1	15.19	26.58	34.01	0	12	1	2	139.01	154.95	14.90	0	-7	6	2	62.75	58.15	15.75	0
-10	9	1	16.58	3.77	24.91	0	13	1	2	17.64	-12.04	26.32	0	-6	6	2	652.67	627.35	32.53	0
-9	9	1	27.91	6.31	25.20	0	14	1	2	2.13	14.16	24.42	0	-5	6	2	146.99	159.61	12.16	0
-8	9	1	0.30	-15.93	21.95	0	15	1	2	65.79	109.06	15.99	0	-4	6	2	165.51	185.26	12.81	0
-7	9	1	14.39	8.40	23.72	0	-15	2	2	12.55	-0.74	21.14	0	-3	6	2	15.84	18.15	7.02	0
-6	9	1	49.39	38.26	13.58	0	-14	2	2	46.80	70.60	15.12	0	-2	6	2	33.75	28.90	7.05	0
-5	9	1	16.35	16.35	21.69	0	-13	2	2	2.68	4.92	19.53	0	-1	6	2	719.95	699.91	30.70	0
-4	9	1	11.80	11.10	19.28	0	-12	2	2	206.48	213.96	17.35	0	0	6	2	319.75	344.12	20.76	0
-3	9	1	32.52	-16.12	20.40	0	-11	2	2	0.21	7.18	8.46	0	1	6	2	27.13	23.88	6.82	0
-2	9	1	66.59	44.60	11.87	0	-10	2	2	258.87	271.28	16.								

6	8	2	1.27	-22.40	22.40	6	2	3	16.28	16.06	5.63	-9	7	3	7.05	34.24	10.14	o	
7	8	2	89.22	105.29	13.35	o	7	2	3	33.72	42.16	7.50	-8	7	3	39.15	12.55	17.47	o
8	8	2	2.92	-5.66	20.79	o	8	2	3	102.47	91.78	11.07	-7	7	3	174.96	193.40	15.48	o
9	8	2	15.55	22.46	8.56	o	9	2	3	38.95	25.58	8.62	-6	7	3	434.01	456.28	24.59	o
10	8	2	21.72	7.59	28.45	o	10	2	3	13.67	1.26	21.01	-5	7	3	833.99	846.46	39.52	o
11	8	2	29.20	-41.54	41.54	o	11	2	3	57.24	47.24	11.84	-4	7	3	815.44	683.02	35.27	o
12	8	2	41.09	3.41	33.02	o	12	2	3	61.59	41.16	13.16	-3	7	3	14.04	5.99	10.36	o
-11	9	2	0.19	-28.80	28.80	o	13	2	3	3.54	-8.14	17.96	-2	7	3	151.92	153.92	12.00	o
-10	9	2	48.70	64.94	14.42	o	14	2	3	22.89	35.37	13.13	-1	7	3	34.77	16.38	17.86	o
-9	9	2	24.21	2.93	25.10	o	15	2	3	66.85	91.49	15.83	0	7	3	30.12	37.21	6.03	o
-8	9	2	34.20	10.68	27.10	o	-15	3	3	0.01	-12.04	25.94	-1	7	3	247.41	235.14	14.87	o
-7	9	2	2.20	10.10	20.95	o	-14	3	3	11.41	-6.69	12.16	0	7	3	527.03	535.96	25.55	o
-6	9	2	5.00	29.57	11.49	o	-13	3	3	103.85	124.86	14.61	0	7	3	280.24	291.90	16.51	o
-5	9	2	6.31	25.16	9.81	o	-12	3	3	197.74	175.45	17.44	0	7	3	0.24	11.20	16.38	o
-4	9	2	33.19	36.36	11.33	o	-11	3	3	14.68	-7.40	18.54	0	7	3	577.85	600.51	28.51	o
-3	9	2	120.34	112.86	15.03	o	-10	3	3	5.38	12.26	18.99	0	7	3	12.52	4.67	19.21	o
-2	9	2	1.34	1.61	10.52	o	-9	3	3	191.83	192.08	14.64	0	7	3	199.50	189.44	15.25	o
-1	9	2	128.65	134.80	14.32	o	-8	3	3	290.59	258.44	15.64	0	7	3	7.74	-20.82	22.14	o
0	9	2	325.12	306.91	13.30	o	-7	3	3	316.50	261.27	14.03	0	7	3	25.23	12.94	20.50	o
1	9	2	0.22	2.03	14.80	o	-6	3	3	359.29	362.83	17.54	0	7	3	80.18	87.88	13.84	o
2	9	2	236.39	221.40	16.70	o	-5	3	3	388.58	468.70	22.53	0	7	3	0.73	-3.93	24.78	o
3	9	2	64.61	79.16	11.91	o	-4	3	3	294.50	379.18	18.73	0	7	3	1.30	14.77	19.40	o
4	9	2	149.65	146.58	14.42	o	-3	3	3	264.98	281.22	13.19	-12	8	3	0.02	4.76	31.18	o
5	9	2	10.88	-3.99	26.74	o	-2	3	3	4074.60	4227.71	112.82	-11	8	3	6.60	-19.69	19.69	o
6	9	2	47.50	53.77	13.71	o	-1	3	3	3565.45	3319.97	92.49	-10	8	3	30.13	6.56	26.96	o
7	9	2	170.10	160.10	18.37	o	0	3	3	225.04	253.46	25.50	0	7	3	0.05	-14.42	25.00	o
8	9	2	2.29	6.66	14.48	o	1	3	3	2270.41	2232.65	66.42	-8	8	3	4.00	-13.71	24.52	o
9	9	2	21.41	43.93	13.61	o	2	3	3	854.25	782.81	33.66	-7	8	3	65.75	90.14	12.26	o
10	9	2	0.02	-19.40	25.65	o	3	3	3	55.66	69.06	6.37	-6	8	3	56.61	32.66	13.48	o
11	9	2	54.02	76.17	14.61	o	4	3	3	1620.79	1521.40	56.09	-5	8	3	7.55	6.08	12.23	o
-9	10	2	0.89	3.70	18.44	o	5	3	3	610.01	610.10	27.26	-4	8	3	4.33	25.00	8.62	o
-8	10	2	11.84	-1.67	27.80	o	6	3	3	949.26	903.71	48.72	-3	8	3	51.69	55.99	9.59	o
-7	10	2	1.47	-2.80	22.49	o	7	3	3	18.11	26.13	7.72	-2	8	3	331.61	306.87	17.89	o
-6	10	2	3.50	18.73	19.18	o	8	3	3	591.96	583.68	26.19	-1	8	3	415.44	440.87	22.14	o
-5	10	2	22.04	35.66	9.91	o	9	3	3	234.04	239.97	16.89	0	8	3	3.55	-19.33	23.07	o
-4	10	2	20.00	-24.88	31.15	o	10	3	3	39.62	45.34	10.49	0	8	3	5.78	8.66	10.49	o
-3	10	2	15.84	-29.22	10.49	o	11	3	3	96.81	110.96	14.03	0	8	3	161.51	203.60	14.55	o
-2	10	2	8.11	-2.41	20.08	o	12	3	3	93.48	106.00	13.97	0	8	3	671.73	683.79	31.47	o
-1	10	2	29.41	29.64	11.17	o	13	3	3	7.68	-27.96	27.96	-4	8	3	143.65	143.65	14.09	o
0	10	2	5.46	-9.71	14.56	o	14	3	3	81.62	96.80	16.89	0	8	3	834.15	786.45	41.22	o
1	10	2	40.46	39.07	11.62	o	-14	4	3	4.87	-30.51	30.67	0	8	3	112.32	116.72	14.74	o
2	10	2	0.14	-16.70	24.49	o	-13	4	3	6.83	-13.68	28.64	0	8	3	62.82	71.02	13.52	o
3	10	2	24.56	-8.11	19.31	o	-12	4	3	2.81	10.68	10.23	-8	8	3	6.42	1.87	18.41	o
4	10	2	31.59	23.36	13.07	o	-11	4	3	137.35	128.62	14.93	0	8	3	1.71	24.65	10.33	o
5	10	2	0.05	-26.45	26.45	o	-10	4	3	37.20	-37.20	37.20	-9	8	3	31.64	22.27	26.27	o
6	10	2	5.53	22.94	11.26	o	-9	4	3	128.84	137.18	13.48	0	8	3	4.08	13.97	13.07	o
7	10	2	1.25	16.86	11.81	o	-8	4	3	35.29	-25.55	25.55	-11	9	3	22.92	-18.70	29.83	o
8	10	2	0.17	15.58	15.83	o	-7	4	3	5.99	-9.11	10.78	-10	9	3	0.68	-26.03	26.03	o
9	10	2	3.78	-33.37	33.37	o	-6	4	3	237.89	229.02	13.10	-9	9	3	8.02	-15.29	15.29	o
-8	11	2	5.53	23.04	28.35	o	-5	4	3	271.69	231.92	12.42	-8	9	3	4.78	1.67	20.08	o
-7	11	2	104.95	96.19	20.08	o	-4	4	3	104.47	131.42	9.07	-7	9	3	17.88	-17.06	24.00	o
-6	11	2	74.46	29.41	15.41	o	-3	4	3	927.87	964.43	43.76	-6	9	3	5.72	25.65	8.59	o
-5	11	2	0.71	29.48	9.65	o	-2	4	3	76.01	76.85	7.40	-5	9	3	2.45	8.11	8.75	o
-4	11	2	0.62	-15.90	21.21	o	-1	4	3	31.29	32.63	6.31	-4	9	3	6.09	3.93	12.68	o
-3	11	2	106.75	120.10	16.99	o	0	4	3	2960.59	3039.14	63.31	0	-3	9	102.73	89.33	14.58	o
-2	11	2	9.48	15.93	17.09	o	1	4	3	373.02	446.24	20.40	-2	9	3	8.35	-18.70	18.70	o
-1	11	2	59.03	23.85	31.15	o	2	4	3	18.98	10.01	5.15	-1	9	3	160.75	149.38	14.42	o
0	11	2	69.57	75.94	28.03	o	3	4	3	101.78	115.62	9.14	0	9	3	46.62	44.56	7.61	o
1	11	2	5.12	12.61	23.72	o	4	4	3	7.02	-11.65	11.65	0	9	3	130.34	101.11	14.58	o
2	11	2	36.41	23.27	32.69	o	5	4	3	453.22	466.26	25.26	0	9	3	81.43	4.70	31.44	o
3	11	2	21.90	7.59	27.32	o	6	4	3	6.89	2.16	14.29	0	9	3	10.60	-22.98	22.98	o
4	11	2	0.30	0.55	22.65	o	7	4	3	582.39	610.65	31.57	0	9	3	82.62	82.06	14.06	o
5	11	2	32.83	51.01	13.71	o	8	4	3	196.16	209.46	14.32	0	9	3	14.94	29.90	11.07	o
6	11	2	142.45	178.31	19.18	o	9	4	3	0.04	5.15	18.02	0	9	3	18.01	33.15	10.62	o
7	11	2	0.32	10.04	22.56	o	10	4	3	101.78	115.62	9.14	0	9	3	46.62	44.56	7.61	o
8	11	2	0.34	-19.92	25.42	o	11	4	3	3.00	16.03	18.66	0	9	3	7.85	30.83	11.78	o
-5	12	2	51.81	35.14	37.43	o	12	4	3	103.87	95.38	14.61	0	9	3	15.03	39.03	12.32	o
-4	12	2	46.52	50.49	15.61	o	13	4	3	119.61	104.46	15.90	0	9	3	56.15	68.48	17.18	o
-3	12	2	6.70	-32.37	32.37	o	14	4	3	35.68	38.52	13.48	-10	9	3	11.70	8.69	30.35	o
-2	12	2	12.52	12.13	15.70	o	-14	5	3	22.41	27.84	14.67	-8	10	3	18.82	52.97	12.61	o
-1	12	2	6.54	6.34	26.45	o	-13	5	3	107.52	76.20	15.19	-7	10	3	0.16	3.96	23.27	o
0	12	2	0.09	13.28	10.56	o	-12	5	3	17.42	26.71	13.00	-6	10	3	11.03	13.48	14.45	o
1	12	2	5.82	36.36	11.39	o	-11	5	3	127.65	134.22	15.41	-5	10	3	43.42	65.20	14.06	o
2	12	2	22.90	10.91	25.26	o	-10	5	3	25.47	29.64	9.85	-4	10	3	20.84	-30.28	30.28	o
3	12	2	30.65	0.64	18.28	o	-9	5	3	22.55	28.70	9.40	-3	10	3	0.21	-23.11	25.00	o
4	12	2	100.81	138.82	17.57	o	-8	5	3	314.15	326.59	17.96	-2	10	3	83.87	96.89	13.39	o
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0	0	4	36378.67	35409.75	553.50	10	4	4	28.54	-22.78	25.81	-9	10	4	1.69	-2.96	30.15	0	
1	0	4	150.45	129.62	6.89	0	11	4	19.59	29.51	11.01	-8	10	4	4.15	-0.97	31.89	0	
2	0	4	2075.43	2146.34	63.36	0	12	4	149.05	159.71	17.51	-7	10	4	4.31	14.90	9.94	0	
3	0	4	1972.22	1773.21	58.25	0	13	4	49.37	73.05	14.67	-6	10	4	32.28	-21.27	34.14	0	
4	0	4	4257.63	4094.10	114.21	0	14	4	4.96	24.07	25.90	-5	10	4	4.82	-27.77	27.77	0	
5	0	4	493.92	453.99	21.37	-14	5	4	2.64	-33.95	33.85	-4	10	4	9.56	-5.92	21.72	0	
6	0	4	84.54	77.71	7.85	-13	5	4	18.63	-16.41	32.12	-3	10	4	17.09	7.24	24.94	0	
7	0	4	118.85	126.56	10.56	-12	5	4	62.87	48.50	13.90	-2	10	4	35.41	51.68	10.14	0	
8	0	4	1238.63	1156.39	59.92	-11	5	4	26.02	59.21	11.78	-1	10	4	128.58	106.35	15.38	0	
9	0	4	0.08	-6.40	17.31	-10	5	4	9.31	-20.43	25.87	0	10	4	118.24	110.82	10.63	0	
10	0	4	181.12	157.42	14.90	-9	5	4	354.33	337.18	19.63	0	10	4	1.75	-25.45	25.45	0	
11	0	4	330.81	336.41	20.82	-8	5	4	424.99	416.54	21.08	0	10	4	109.82	133.71	15.48	0	
12	0	4	190.96	207.30	17.41	-7	5	4	10.15	8.30	22.81	0	10	4	6.13	6.02	22.20	0	
13	0	4	37.56	41.32	12.97	-6	5	4	33.43	24.97	7.92	0	10	4	2.07	12.16	23.33	0	
14	0	4	38.28	27.61	32.92	-5	5	4	2.26	0.77	14.00	0	10	4	25.29	53.55	12.10	0	
15	0	4	92.68	108.93	17.31	-4	5	4	0.51	4.70	11.68	0	10	4	3.12	-25.87	25.87	0	
-15	1	4	0.00	2.25	12.65	-3	5	4	664.27	622.97	28.54	0	10	4	42.27	-37.07	37.07	0	
-14	1	4	0.27	-2.03	21.43	-2	5	4	315.73	288.14	15.51	0	10	4	1.37	10.01	27.80	0	
-13	1	4	38.68	51.04	11.46	-1	5	4	16.87	24.65	6.02	0	10	4	26.27	35.27	16.32	0	
-12	1	4	10.46	8.98	21.17	0	5	4	138.88	111.86	6.48	-7	11	4	38.35	-41.29	41.29	0	
-11	1	4	77.84	71.60	11.91	0	5	4	129.53	157.52	10.62	-6	11	4	2.04	3.80	25.23	0	
-10	1	4	0.34	-13.35	16.54	0	5	4	80.15	54.03	9.01	-5	11	4	1.82	-6.73	23.49	0	
-9	1	4	72.46	66.97	10.27	0	5	4	338.12	334.03	17.67	-4	11	4	58.03	65.58	16.99	0	
-8	1	4	157.83	149.70	12.23	0	4	5	1.33	8.98	9.59	-3	11	4	6.21	25.10	12.00	0	
-7	1	4	8.65	4.25	7.14	0	5	4	913.75	886.59	37.49	-2	11	4	3.60	23.14	11.94	0	
-6	1	4	387.66	393.59	18.02	0	5	4	179.05	201.41	14.13	0	11	4	19.76	3.99	22.27	0	
-5	1	4	663.51	697.31	35.88	0	7	5	4	6.84	8.62	0	11	4	3.40	2.36	9.73	0	
-4	1	4	53.45	62.01	5.99	0	8	5	355.94	303.42	18.41	0	11	4	17.63	1.09	27.03	0	
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-2	1	4	217.37	258.02	13.23	0	10	5	4	213.11	187.58	16.57	0	11	4	4.45	-29.19	29.19	0
-1	1	4	3082.33	3291.17	87.27	0	11	5	4	6.54	-22.88	22.88	0	11	4	9.09	-7.66	24.84	0
0	1	4	2702.66	2702.66	108.83	0	12	5	4	0.03	16.35	25.71	0	11	4	0.30	17.54	10.94	0
1	1	4	3340.32	3296.74	87.59	0	13	5	4	0.01	-5.92	28.51	0	11	4	59.04	-25.84	32.57	0
2	1	4	827.23	823.26	33.53	-13	6	4	10.52	-7.47	26.29	0	11	4	1.19	3.83	13.93	0	
3	1	4	110.23	108.77	7.27	-12	6	4	4.30	-25.26	25.26	-5	12	4	37.17	24.42	32.63	0	
4	1	4	1066.80	1071.17	44.38	-11	6	4	24.88	11.87	25.52	-4	12	4	22.59	9.69	34.43	0	
5	1	4	23.01	-14.29	14.29	-10	6	4	6.00	147.58	17.31	-3	12	4	2.19	-25.45	25.45	0	
6	1	4	6.15	10.04	11.39	-9	6	4	16.28	37.68	9.85	-2	12	4	6.48	2.61	17.15	0	
7	1	4	-0.51	-0.51	12.29	-8	6	4	0.71	0.71	12.65	-1	12	4	9.47	-1.03	26.87	0	
8	1	4	62.03	61.46	9.40	-7	6	4	1.46	-20.56	21.17	0	12	4	7.25	9.57	16.25	0	
9	1	4	61.34	54.03	11.04	-6	6	4	37.23	5.86	23.01	0	12	4	0.08	8.69	23.49	0	
10	1	4	1.34	-9.24	17.51	-5	6	4	1059.13	1117.80	58.05	0	12	4	6.63	-5.05	32.44	0	
11	1	4	1.79	6.69	10.23	-4	6	4	232.69	205.63	14.16	0	12	4	28.89	26.26	33.08	0	
12	1	4	23.62	44.86	11.23	-3	6	4	0.61	12.04	13.16	0	12	4	32.00	11.87	20.43	0	
13	1	4	13.05	10.10	10.30	-2	6	4	1.13	8.12	11.13	-1	12	4	21.39	26.93	26.93	0	
14	1	4	0.00	-27.48	-27.48	-1	6	4	590.10	570.49	27.93	-14	1	5	17.91	-26.10	26.10	0	
-15	2	4	46.81	70.09	15.22	0	6	4	49.98	51.88	5.67	-13	1	5	58.72	25.04	30.83	0	
-14	2	4	83.02	125.47	14.64	0	6	4	103.15	100.37	9.69	-12	1	5	75.43	49.24	15.51	0	
-13	2	4	6.41	5.25	25.33	0	6	4	1.78	-14.55	16.19	-11	1	5	1526.09	1636.61	82.32	0	
-12	2	4	21.15	16.86	23.52	0	6	4	89.68	106.19	10.52	-10	1	5	546.34	534.25	27.96	0	
-11	2	4	14.07	1.83	21.46	0	6	4	1.86	16.89	7.43	-9	1	5	298.24	263.33	16.57	0	
-10	2	4	375.46	383.07	20.31	0	5	6	0.56	0.56	11.75	-8	1	5	187.12	174.45	12.78	0	
-9	2	4	216.57	237.46	15.83	0	6	6	4	119.01	84.02	12.29	-7	1	5	70.03	64.68	8.08	0
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-7	2	4	328.82	324.28	16.41	0	8	6	4	166.09	187.51	14.83	-5	1	5	1467.79	1482.98	58.21	0
-6	2	4	211.60	173.03	11.39	0	9	6	4	1.55	7.24	23.11	-4	1	5	184.90	152.57	9.86	0
-5	2	4	545.45	532.19	23.17	0	10	6	4	24.50	37.68	11.07	-3	1	5	6.17	2.25	5.65	0
-4	2	4	10.56	-0.68	10.56	-11	6	4	28.00	16.51	29.44	-2	1	5	821.87	945.42	37.49	0	
-3	2	4	327.71	370.10	17.15	-12	6	4	23.13	49.40	10.59	-1	1	5	12078.88	12397.08	289.30	0	
-2	2	4	6467.34	6748.14	166.56	-13	6	4	12.22	6.05	28.99	0	1	5	73.60	103.93	5.04	0	
-1	2	4	2157.10	1992.94	61.62	-12	7	4	13.30	8.17	19.63	0	1	5	590.91	539.11	27.58	0	
0	2	4	352.05	415.70	13.86	-11	7	4	3.88	23.46	26.58	0	1	5	1017.24	1009.87	39.90	0	
1	2	4	1674.11	1629.82	52.42	-10	7	4	9.29	7.24	21.82	0	3	1	5	25.14	37.01	6.18	0
2	2	4	18.31	16.35	5.63	-9	7	4	46.15	11.97	22.08	0	4	1	5	639.94	548.00	24.00	0
3	2	4	360.67	360.67	17.15	-8	7	4	58.25	74.27	15.23	0	5	1	5	1352.55	1397.64	13.97	0
4	2	4	758.39	839.09	39.10	-7	7	4	108.24	117.23	15.45	0	6	1	5	480.03	456.22	23.56	0
5	2	4	65.10	76.72	7.69	-6	7	4	1149.97	1223.06	63.14	0	7	1	5	339.77	372.23	17.31	0
6	2	4	111.57	100.14	9.49	-5	7	4	360.58	365.79	20.14	0	8	1	5	3.04	11.68	18.15	0
7	2	4	782.31	789.21	34.46	-4	7	4	656.47	706.64	36.04	0	9	1	5	597.36	526.56	28.22	0
8	2	4	260.43	296.89	16.41	-3	7	4	148.00	178.02	12.81	0	10	1	5	62.27	66.97	12.61	0
9	2	4	10.96	4.25	7.98	-2	7	4	5.66	5.66	17.63	11	1	5	84.33	98.34	12.90	0	
10	2	4	17.78	-5.73	20.40	-1	7	4	220.29	194.62	13.64	0	12	1	5	0.01	-0.61	23.46	0
11	2	4	225.75	230.73	17.51	0	7	4	248.49	222.45	15.83	0	13	1	5	78.34	80.55	15.03	0
12	2	4	222.41	208.14	19.37	0	7	4	147.88	165.50	11.81	0	14	1	5	233.17	319.06	22.91	0
13	2	4	28.33	25.74	13.29	0	7	4	356.10	370.04	18.89	-13	2	5	21.68	21.79	26.13	0	
14	2	4	0.00	11.87	15.19	0	7	4	308.36	305.00	17.22	-10	2	5	19.03	48.33	10.62	0	
-14	3	4	8.31	-33.27	33.27	0	7	4	334.31	334.64	16.31	-12	2	5	8.33	17.60	17.83	0	
-13	3	4	86.75	108.90	13.52	0	7	4	1805.12	1785.38	80.4								

12	3	5	20.24	11.23	15.22	9	8	5	1.42	18.41	11.10	0	-7	2	6	388.57	387.09	18.41	0	
13	3	5	111.25	89.62	18.09	0	10	8	5	24.39	32.57	14.77	0	-6	2	6	830.21	794.36	34.08	0
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-14	4	5	0.80	-29.06	29.06	0	-10	9	5	18.42	18.86	32.92	0	-4	2	6	38.78	30.80	7.53	0
-13	4	5	7.25	21.91	12.87	0	-9	9	5	5.35	-29.57	29.73	0	-3	2	6	1368.86	1405.88	54.71	0
-12	4	5	1.14	14.22	9.88	0	-8	8	5	26.41	15.38	15.80	0	-2	2	6	1341.43	1332.03	52.37	0
-11	4	5	27.30	38.49	11.62	0	-7	9	5	33.02	-14.64	25.42	0	-1	2	6	240.49	225.94	11.20	0
-10	4	5	499.33	475.27	24.30	0	-6	9	5	123.84	127.05	15.74	0	0	2	6	40.47	54.81	4.97	0
-9	4	5	0.86	-17.80	19.50	0	-5	9	5	27.20	-33.95	33.95	0	1	2	6	1092.00	1119.61	45.31	0
-8	4	5	113.52	103.97	12.87	0	-4	9	5	33.82	12.39	19.60	0	2	2	6	857.54	873.53	41.42	0
-7	4	5	56.97	43.02	8.88	0	-3	9	5	6.99	8.11	15.51	0	3	2	6	82.48	65.10	7.50	0
-6	4	5	11.26	21.85	6.63	0	-2	9	5	149.97	140.21	14.61	0	4	2	6	115.42	131.84	9.65	0
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-3	4	5	42.00	35.14	7.59	0	1	9	5	54.79	65.81	11.78	0	7	2	6	737.58	740.17	34.27	0
-2	4	5	433.40	407.21	18.41	0	2	9	5	9.00	-16.28	24.33	0	8	2	6	12.89	11.42	8.08	0
-1	4	5	0.08	9.43	5.21	0	3	9	5	23.63	-13.93	25.10	0	9	2	6	169.35	206.11	14.55	0
0	4	5	7.01	7.43	15.22	0	4	9	5	3.60	36.04	10.62	0	10	2	6	0.98	-2.77	20.14	0
1	4	5	49.21	44.47	6.73	0	5	9	5	34.03	45.31	12.84	0	11	2	6	22.19	11.10	23.27	0
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3	4	5	17.57	-15.83	15.83	0	7	9	5	0.00	5.37	11.42	0	13	2	6	4.47	-9.07	21.05	0
4	4	5	1.97	4.67	11.30	0	8	9	5	0.59	-33.37	33.37	0	14	2	6	14.34	-4.31	32.05	0
5	4	5	221.11	208.27	12.87	0	9	9	5	0.01	1.38	18.41	0	14	3	6	6.98	4.99	23.97	0
6	4	5	3.51	16.38	6.73	0	10	9	5	70.73	112.44	16.48	0	-13	3	6	18.43	10.75	24.30	0
7	4	5	49.26	46.79	9.49	0	-9	10	5	31.50	51.81	13.52	0	-12	3	6	18.43	-1.35	22.28	0
8	4	5	16.96	16.96	17.35	0	-8	10	5	0.84	-24.84	32.95	0	-11	3	6	18.43	-0.35	20.20	0
9	4	5	10.30	2.00	20.43	0	-7	10	5	18.21	18.12	19.79	0	-10	3	6	29.00	28.93	12.45	0
10	4	5	192.18	174.42	15.80	0	-6	10	5	63.61	52.55	14.80	0	-9	3	6	0.22	4.51	19.57	0
11	4	5	1.09	2.41	23.49	0	-5	10	5	17.73	17.73	13.00	0	-8	3	6	31.34	33.92	10.17	0
12	4	5	10.87	-31.34	31.34	0	-4	10	5	2.70	-8.98	26.74	0	-7	3	6	40.25	39.90	8.66	0
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-13	5	5	115.05	110.83	16.54	0	-2	10	5	3.64	6.60	10.72	0	-5	3	6	85.66	106.39	9.27	0
-12	5	5	51.55	79.94	14.29	0	-1	10	5	168.75	169.62	18.28	0	-4	3	6	344.25	298.28	15.99	0
-11	5	5	323.32	338.98	22.20	0	0	10	5	30.13	35.10	22.28	0	-3	3	6	27.25	42.51	7.66	0
-10	5	5	239.14	217.89	18.60	0	1	10	5	19.75	18.95	21.34	0	-2	3	6	96.46	73.08	7.66	0
-9	5	5	239.01	233.66	17.31	0	2	10	5	32.85	-7.79	32.82	0	-1	3	6	36.34	35.95	6.79	0
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0	5	5	363.59	385.13	29.34	0	-5	11	5	21.47	10.97	14.63	0	8	3	6	14.63	6.02	13.28	0
1	5	5	42.21	38.65	6.31	0	-4	11	5	0.68	45.86	11.39	0	9	3	6	2.79	-7.40	18.57	0
2	5	5	121.65	130.10	10.88	0	-3	11	5	16.05	-5.25	20.76	0	10	3	6	51.06	53.93	11.65	0
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4	5	5	0.92	-2.35	10.62	0	-1	11	5	13.81	-28.00	29.06	0	12	3	6	29.53	54.32	13.03	0
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6	5	5	2.25	4.09	12.65	0	1	11	5	0.92	-13.61	28.48	0	14	3	6	63.80	78.84	16.41	0
7	5	5	32.93	53.16	9.46	0	2	11	5	2.06	24.17	10.91	0	-14	4	6	24.97	7.14	8.20	0
8	5	5	26.11	34.88	9.62	0	3	11	5	3.92	17.63	24.75	0	-13	4	6	1.89	9.72	27.03	0
9	5	5	191.93	159.48	17.83	0	4	11	5	4.32	30.73	12.20	0	-12	4	6	15.51	14.87	15.12	0
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-11	6	5	108.83	116.97	17.02	0	0	12	5	4.72	14.01	14.05	0	-5	4	6	652.94	624.87	30.99	0
-10	6	5	37.58	26.81	14.42	0	1	12	5	1.87	-35.04	35.04	0	-4	4	6	124.26	128.01	10.20	0
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-8	6	5	313.44	270.50	19.60	0	3	12	5	0.12	6.05	28.96	0	-2	4	6	102.61	92.77	8.04	0
-7	6	5	205.22	168.08	14.80	0	-14	0	6	151.90	173.03	20.93	0	-1	4	6	1382.99	1325.92	57.15	0
-6	6	5	4.93	13.97	17.70	0	-13	0	6	0.07	-27.00	27.00	0	0	4	6	8.39	3.94	8.96	0
-5	6	5	316.95	337.66	18.76	0	-12	0	6	100.86	68.06	15.48	0	1	4	6	275.33	254.03	13.29	0
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-2	6	5	587.17	619.43	31.31	0	-9	0	6	101.11	104.58	11.94	0	4	4	6	72.85	53.13	9.72	0
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0	6	5	82.45	79.07	6.80	0	-7	0	6	30.43	33.05	9.04	0	6	4	6	378.67	382.65	18.60	0
1	6	5	134.79	114.34	11.87	0	-6	0	6	313.50	293.38	15.12	0	7	4	6	15.14	0.64	16.64	0
2	6	5	14.55	26.61	7.59	0	-5	0</												

10	6	6	6.38	4.89	20.21	o	10	1	7	218.08	251.81	18.44	o	3	6	7	6.81	14.03	16.22	o
11	6	6	12.08	24.75	25.39	o	11	1	7	0.29	-1.13	18.25	o	4	6	7	315.67	309.15	19.31	o
12	6	6	0.64	-30.70	30.70	o	12	1	7	53.69	70.80	12.78	o	5	6	7	580.90	566.56	28.41	o
-12	7	6	30.46	5.89	34.50	o	13	1	7	34.66	52.29	14.06	o	6	6	7	257.24	229.57	18.92	o
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-9	7	6	42.84	45.82	12.26	o	-13	2	7	28.15	15.35	14.93	o	9	6	7	9.90	12.04	18.15	o
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-6	7	6	26.42	8.98	11.87	o	-10	2	7	0.23	12.49	22.33	o	12	6	7	29.94	21.24	16.77	o
-5	7	6	319.54	320.06	19.28	o	-9	2	7	4.15	-6.82	22.17	o	-11	7	7	1.27	1.45	29.19	o
-4	7	6	387.75	393.79	20.56	o	-8	2	7	47.16	73.76	10.72	o	-10	7	7	16.11	24.52	25.16	o
-3	7	6	9.21	2.86	17.09	o	-7	2	7	0.95	-18.54	18.54	o	-9	7	7	0.03	2.99	23.72	o
-2	7	6	108.43	80.29	10.97	o	-6	2	7	230.05	254.70	14.55	o	-8	7	7	41.40	49.94	12.61	o
-1	7	6	359.85	319.93	18.50	o	-5	2	7	20.17	41.06	7.05	o	-7	7	7	133.84	116.88	15.12	o
0	7	6	189.77	203.31	20.88	o	-4	2	7	102.08	122.03	10.23	o	-6	7	7	313.51	318.97	21.40	o
1	7	6	89.15	-19.08	31.89	o	-3	2	7	0.09	6.02	9.69	o	-5	7	7	385.43	358.26	22.24	o
2	7	6	3.94	5.99	14.83	o	-2	2	7	360.80	385.93	18.57	o	-4	7	7	5.10	-16.12	20.92	o
3	7	6	436.22	447.27	22.69	o	-1	2	7	52.77	74.23	7.79	o	-3	7	7	10.49	10.33	14.26	o
4	7	6	47.13	14.80	26.19	o	0	2	7	34.59	56.27	4.71	o	-2	7	7	21.32	18.79	9.46	o
5	7	6	808.21	809.13	42.73	o	1	2	7	414.54	384.71	20.24	o	-1	7	7	150.17	160.71	13.42	o
6	7	6	0.08	-13.29	19.34	o	2	2	7	231.21	270.44	14.74	o	0	7	7	310.97	297.55	13.09	o
7	7	6	32.56	23.46	25.49	o	3	2	7	430.88	474.40	25.55	o	1	7	7	188.02	195.01	15.03	o
8	7	6	40.09	18.73	26.97	o	4	2	7	1042.84	1090.06	52.26	o	2	7	7	79.07	95.19	11.65	o
-7	6	6	5.38	-4.22	19.08	o	5	2	7	331.25	364.47	17.47	o	3	7	7	212.05	213.03	16.83	o
10	7	6	68.07	93.13	13.90	o	6	2	7	19.18	19.18	7.10	o	4	7	7	478.92	443.34	24.75	o
11	7	6	8.48	15.99	24.39	o	7	2	7	86.10	106.84	10.62	o	5	7	7	103.58	110.02	14.83	o
-11	8	6	0.11	-8.01	25.78	o	8	2	7	128.20	135.99	13.55	o	6	7	7	36.40	41.64	11.65	o
-10	8	6	6.11	15.74	23.62	o	9	2	7	104.50	111.92	13.07	o	7	7	7	23.53	25.26	10.75	o
-9	8	6	15.55	39.00	11.71	o	10	2	7	4.38	-1.13	10.17	o	8	7	7	31.12	44.96	11.91	o
-8	8	6	21.98	16.80	11.26	o	11	2	7	0.48	14.83	18.05	o	9	7	7	0.29	-32.66	32.66	o
-7	8	6	182.04	204.44	18.47	o	12	2	7	18.84	9.81	21.01	o	10	7	7	10.72	15.64	23.45	o
-6	8	6	182.37	176.60	17.76	o	13	2	7	0.00	-33.50	33.50	o	11	7	7	2.99	-15.96	36.40	o
-5	8	6	173.12	156.36	16.28	o	14	3	7	31.99	40.13	15.00	o	-10	8	7	31.58	1.13	29.38	o
-4	8	6	67.39	79.32	13.00	o	-13	3	7	85.41	63.97	17.25	o	-9	8	7	45.10	28.45	30.67	o
-3	8	6	67.73	40.77	13.07	o	-12	3	7	5.56	12.87	24.71	o	-8	8	7	21.15	25.94	13.61	o
-2	8	6	147.88	130.49	14.26	o	-11	3	7	1.24	-5.28	25.58	o	-7	8	7	5.30	-14.22	24.71	o
-1	8	6	3.30	10.59	17.99	o	-10	3	7	187.99	177.96	15.90	o	-6	8	7	33.74	27.61	11.62	o
0	8	6	9.06	9.06	12.61	o	-9	3	7	267.76	262.27	17.47	o	-5	8	7	38.68	0.23	25.55	o
1	8	6	243.64	240.80	18.31	o	-8	3	7	302.89	251.55	17.38	o	-4	8	7	0.12	-22.53	22.53	o
2	8	6	186.81	194.46	16.32	o	-7	3	7	36.01	16.70	22.46	o	-3	8	7	236.14	257.41	17.51	o
3	8	6	58.33	77.36	13.07	o	-6	3	7	111.39	115.78	11.62	o	-2	8	7	170.91	155.65	16.25	o
4	8	6	9.33	1.09	30.47	o	-5	3	7	512.75	517.65	28.03	o	-1	8	7	0.02	-20.82	20.82	o
5	8	6	40.20	42.06	12.39	o	-4	3	7	1252.19	1103.32	55.54	o	0	8	7	10.04	-7.85	15.40	o
6	8	6	60.13	56.93	13.58	o	-3	3	7	946.01	993.11	45.07	o	1	8	7	275.07	315.33	21.77	o
7	8	6	7.04	-23.85	25.13	o	-2	3	7	1.12	-10.91	14.51	o	2	8	7	532.46	519.26	25.74	o
8	8	6	5.83	-10.04	23.07	o	-1	3	7	436.03	400.13	18.44	o	3	8	7	1.38	-2.16	13.84	o
9	8	6	18.65	22.30	23.27	o	0	3	7	429.77	393.02	13.07	o	4	8	7	394.65	399.84	23.91	o
10	8	6	26.25	-31.09	40.00	o	1	3	7	72.24	67.71	8.01	o	5	8	7	395.98	377.66	24.10	o
-10	9	6	0.02	-32.08	32.08	o	2	3	7	96.31	96.73	9.46	o	6	8	7	200.58	211.23	19.60	o
-9	9	6	56.96	80.87	15.29	o	3	3	7	828.40	739.08	33.05	o	7	8	7	23.00	41.89	11.75	o
-8	9	6	32.40	-23.43	26.17	o	4	3	7	48.30	26.84	9.17	o	8	7	7	0.79	18.70	12.58	o
-7	9	6	16.73	23.81	23.91	o	5	3	7	365.27	346.39	18.83	o	9	8	7	0.12	20.50	21.82	o
-6	9	6	19.67	38.07	11.71	o	6	3	7	336.53	339.98	18.47	o	10	8	7	16.03	56.31	13.61	o
-5	9	6	151.86	134.74	16.73	o	7	3	7	657.16	619.69	28.77	o	-9	9	7	28.66	31.41	31.76	o
-4	9	6	142.14	171.84	15.38	o	8	3	7	145.67	148.80	14.48	o	-8	9	7	0.05	2.48	20.18	o
-3	9	6	18.75	19.73	9.94	o	9	3	7	1.68	1.90	16.12	o	-7	9	7	6.41	14.74	16.41	o
-2	9	6	49.31	-0.51	26.07	o	10	3	7	5.27	14.61	21.79	o	-6	9	7	4.00	16.70	11.13	o
-1	9	6	715.36	657.76	34.53	o	11	3	7	8.81	14.38	20.40	o	-5	9	7	0.48	-24.52	24.52	o
0	9	6	40.81	12.98	18.95	o	12	3	7	76.12	99.15	14.96	o	-4	9	7	49.05	38.23	14.35	o
1	9	6	139.71	133.93	14.93	o	13	3	7	17.69	13.61	28.48	o	-3	9	7	0.03	-18.05	21.46	o
2	9	6	39.01	49.88	11.23	o	-13	4	7	2.73	9.04	12.39	o	-2	9	7	7.77	4.38	15.45	o
3	9	6	18.60	-10.75	24.07	o	-12	4	7	74.75	32.73	32.86	o	-1	9	7	8.36	-16.48	23.75	o
4	9	6	161.55	180.75	16.57	o	-11	4	7	30.50	-1.35	29.61	o	0	9	7	292.46	284.10	41.85	o
5	9	6	58.82	40.82	14.00	o	-10	4	7	14.15	-9.20	21.56	o	1	9	7	47.59	18.06	12.93	o
6	9	6	12.24	-14.03	24.07	o	-9	4	7	33.29	51.55	11.04	o	2	9	7	23.33	35.66	11.39	o
7	9	6	2.99	18.44	22.27	o	-8	4	7	141.03	127.18	15.48	o	3	9	7	283.46	278.74	20.56	o
8	9	6	13.31	-1.71	32.63	o	-7	4	7	188.51	171.52	14.90	o	4	9	7	0.18	11.46	24.62	o
9	9	6	5.71	8.69	30.28	o	-6	4	7	23.16	-9.65	19.34	o	5	9	7	22.52	15.06	25.74	o
-8	10	6	31.61	36.01	14.29	o	-5	4	7	1.41	5.50	10.78	o	6	9	7	2.77	9.81	29.70	o
-7	10	6	5.48	9.81	12.20	o	-4	4	7	24.56	19.60	8.43	o	7	9	7	10.05	-20.63	22.20	o
-6	10	6	21.93	41.61	10.59	o	-3	4	7	220.17	196.56	12.52	o	8	9	7	0.18	-33.37	33.37	o
-5	10	6	2.50	-19.28	26.55	o	-2	4	7	70.06	69.70	9.33	o	9	9	7	44.88	68.16	14.74	o
-4	10	6	0.34	2.64	18.09	o	-1	4												

-13	1	8	4.86	0.35	24.20	0	9	5	8	113.09	138.95	16.06	0	5	1	9	15.03	-8.72	17.60	0
-12	1	8	38.64	25.29	31.15	0	10	5	8	1.32	-5.89	21.88	0	6	1	9	36.18	29.86	9.88	0
-11	1	8	35.14	56.28	12.68	0	11	5	8	42.49	-5.76	27.74	0	7	1	9	161.12	163.41	15.38	0
-10	1	8	1.93	-14.74	21.40	0	12	5	8	14.82	11.39	19.82	0	8	1	9	385.64	402.35	22.59	0
-9	1	8	221.19	245.11	17.67	0	-12	6	8	22.59	16.41	20.34	0	9	1	9	6.71	-11.62	20.88	0
-8	1	8	3.11	12.49	9.07	0	-11	8	8	128.25	128.66	18.86	0	10	1	9	7.08	-0.61	23.59	0
-7	1	8	208.80	240.38	15.06	0	-10	6	8	39.22	59.85	13.64	0	11	1	9	14.17	-25.71	25.71	0
-6	1	8	125.58	107.26	11.68	0	-9	6	8	0.07	-14.32	24.88	0	12	1	9	45.67	37.10	13.61	0
-5	1	8	221.97	215.38	14.32	0	-8	6	8	136.05	152.47	15.03	0	13	1	9	69.07	-8.46	37.52	0
-4	1	8	83.75	72.28	9.30	0	-7	6	8	173.78	198.49	17.47	0	-13	2	9	0.26	24.65	11.81	0
-3	1	8	60.73	55.45	9.43	0	-6	6	8	736.81	713.30	34.24	0	-12	2	9	83.56	76.14	16.44	0
-2	1	8	1525.22	1661.36	65.10	0	-5	6	8	555.77	511.50	27.58	0	-11	2	9	7.82	-18.70	26.58	0
-1	1	8	1598.32	1656.62	64.52	0	-4	6	8	56.48	53.87	11.71	0	-10	2	9	147.44	131.07	15.80	0
0	1	8	1812.50	1843.55	48.79	0	-3	6	8	258.97	224.39	16.67	0	-9	2	9	0.01	-0.74	11.58	0
1	1	8	103.48	133.61	10.10	0	-2	6	8	495.63	490.78	25.94	0	-8	2	9	109.33	116.23	13.39	0
2	1	8	21.97	13.32	16.09	0	-1	6	8	116.37	121.45	12.74	0	-7	2	9	2.05	-5.21	19.37	0
3	1	8	9.16	14.06	16.51	0	0	6	8	19.56	30.20	6.79	0	-6	2	9	1075.09	1095.89	46.11	0
4	1	8	603.21	525.27	24.39	0	1	6	8	292.73	306.93	18.12	0	-5	2	9	33.64	18.31	9.46	0
5	1	8	3.59	13.71	15.61	0	2	6	8	85.81	84.89	11.84	0	-4	2	9	286.84	303.78	15.93	0
6	1	8	8.31	-2.12	16.93	0	3	6	8	26.13	16.15	19.60	0	-3	2	9	129.04	95.86	10.72	0
7	1	8	8.37	-0.48	10.94	0	4	6	8	16.61	11.81	20.21	0	-2	2	9	288.28	35.14	8.21	0
8	1	8	18.72	1.00	21.59	0	5	6	8	4.31	6.47	15.58	0	-1	2	9	135.69	148.16	11.49	0
9	1	8	0.34	-15.29	17.83	0	6	6	8	108.92	116.62	15.29	0	0	2	9	2.35	2.57	8.97	0
10	1	8	2.15	14.83	21.79	0	7	6	8	131.92	132.97	16.35	0	1	2	9	161.25	144.65	11.84	0
11	1	8	13.64	16.67	22.37	0	8	6	8	42.57	27.45	32.60	0	2	2	9	181.94	178.21	12.58	0
12	1	8	14.61	0.01	29.35	0	9	6	8	11.29	-0.23	22.75	0	3	2	9	540.22	582.84	32.48	0
13	1	8	5.45	9.59	12.90	0	10	6	8	115.84	98.05	18.21	0	4	2	9	11.25	5.28	18.44	0
-14	2	8	26.18	8.88	25.26	0	11	6	8	9.61	-13.87	28.80	0	5	2	9	18.61	5.99	9.94	0
-13	2	8	22.00	12.23	29.16	0	-11	7	8	5.15	18.79	19.50	0	6	2	9	201.31	220.63	16.09	0
-12	2	8	0.15	-0.74	17.63	0	-10	7	8	9.32	13.71	16.44	0	7	2	9	65.76	66.10	12.07	0
-11	2	8	422.91	389.54	25.20	0	-9	7	8	12.98	-9.27	15.74	0	8	2	9	10.83	13.81	19.92	0
-10	2	8	191.06	174.16	17.47	0	-8	7	8	76.02	26.19	32.53	0	-10	3	9	8.86	9.01	21.27	0
-9	2	8	27.11	27.77	10.52	0	-7	7	8	69.12	46.79	14.35	0	10	2	9	33.16	-19.57	32.08	0
-8	2	8	188.30	209.65	15.80	0	-6	7	8	397.74	404.31	24.42	0	11	2	9	0.35	16.83	11.78	0
-7	2	8	415.55	403.05	20.79	0	-5	7	8	409.82	443.09	23.27	0	-12	2	9	9.63	-1.03	26.84	0
-6	2	8	756.18	764.21	36.40	0	-4	7	8	138.57	82.83	14.90	0	-13	3	9	40.08	12.23	25.68	0
-5	2	8	0.05	10.20	14.42	0	-3	7	8	7.95	-16.19	20.47	0	-12	3	9	0.08	9.88	26.71	0
-4	2	8	110.12	111.63	10.81	0	-2	7	8	149.13	133.29	14.29	0	-11	3	9	117.82	132.16	16.41	0
-3	2	8	2170.21	2316.19	83.51	0	-1	7	8	18.26	-11.26	16.44	0	-10	3	9	61.81	93.32	13.48	0
-2	2	8	210.90	176.86	12.32	0	0	7	8	35.40	44.54	7.85	0	-9	3	9	7.50	16.25	10.30	0
-1	2	8	902.47	927.65	48.50	0	1	7	8	18.18	-9.30	22.20	0	-8	3	9	98.60	81.42	14.67	0
0	2	8	4.38	-9.78	9.78	0	2	7	8	96.08	104.23	13.29	0	-7	3	9	19.37	14.93	23.30	0
1	2	8	2.56	15.00	15.00	0	3	7	8	97.20	114.59	13.68	0	-6	3	9	7.47	-8.85	21.30	0
2	2	8	307.81	293.74	15.90	0	4	7	8	615.55	575.76	28.45	0	-5	3	9	1095.10	1139.59	61.24	0
3	2	8	451.13	243.30	24.30	0	5	7	8	216.65	31.39	26.65	0	-4	3	9	1146.25	1078.29	59.82	0
4	2	8	0.02	-10.91	15.67	0	6	7	8	2.74	-19.73	24.04	0	-3	3	9	18.11	171.42	13.55	0
5	2	8	169.51	175.28	12.29	0	7	7	8	28.35	42.12	13.45	0	-2	3	9	51.44	41.87	9.98	0
6	2	8	488.67	500.33	25.10	0	8	7	8	39.39	17.12	23.33	0	-1	3	9	824.02	832.17	36.33	0
7	2	8	214.50	183.52	14.74	0	9	7	8	92.84	122.54	15.96	0	0	3	9	1080.32	1123.88	40.82	0
8	2	8	0.00	-11.33	21.40	0	10	7	8	9.09	25.71	10.59	0	1	3	9	259.01	278.87	15.96	0
9	2	8	11.61	12.36	14.74	0	-10	8	8	115.58	117.78	19.86	0	2	3	9	324.14	292.32	16.86	0
10	2	8	366.96	348.38	24.07	0	-9	8	8	2.12	10.20	14.29	0	3	3	9	270.57	282.54	16.03	0
11	2	8	136.34	149.54	18.28	0	-8	8	8	1.47	-5.25	20.69	0	4	3	9	119.25	105.78	11.78	0
12	2	8	0.98	-19.05	19.05	0	-7	8	8	116.78	173.71	16.57	0	5	3	9	3.00	-21.11	21.11	0
13	2	8	30.55	-39.45	44.54	0	-6	8	8	0.91	-25.62	25.62	0	6	3	9	71.25	45.41	11.84	0
-13	3	8	18.63	-30.60	30.60	0	-5	8	8	15.68	19.92	11.04	0	7	3	9	135.10	171.45	15.48	0
-12	3	8	11.71	-32.57	32.57	0	-4	8	8	89.75	90.62	13.68	0	8	3	9	58.83	66.07	13.10	0
-11	3	8	1.54	3.73	14.71	0	-3	8	8	18.81	16.28	10.04	0	9	3	9	14.96	17.63	12.00	0
-10	3	8	242.79	236.36	19.73	0	-2	8	8	6.67	10.81	21.62	0	10	3	9	2.22	-25.45	26.32	0
-9	3	8	209.17	164.92	17.67	0	-1	8	8	42.58	59.98	11.65	0	11	3	9	50.75	54.29	13.45	0
-8	3	8	84.49	95.22	12.81	0	0	8	8	56.53	54.11	20.97	0	12	3	9	129.72	164.28	18.92	0
-7	3	8	366.04	343.13	20.05	0	1	8	8	60.89	4.51	30.54	0	-12	4	9	1.92	17.22	21.91	0
-6	3	8	26.62	17.83	20.14	0	2	8	8	324.87	308.03	22.20	0	-11	4	9	86.95	-43.83	43.83	0
-5	3	8	526.56	517.36	25.49	0	3	8	8	142.52	129.72	16.52	0	-10	4	9	42.81	57.89	12.45	0
-4	3	8	246.05	246.72	14.90	0	4	8	8	160.48	160.48	16.95	0	-9	4	9	12.02	0.07	0.07	0
-3	3	8	87.42	84.31	10.10	0	5	8	8	122.82	112.05	16.41	0	-8	4	9	2.88	6.47	10.68	0
-2	3	8	189.05	189.60	12.16	0	6	8	8	44.96	-0.45	28.93	0	-7	4	9	39.37	10.04	18.83	0
-1	3	8	253.39	277.04	14.26	0	7	8	8	39.25	49.27	14.22	0	-6	4	9	607.41	586.48	28.96	0
0	3	8	33.16	64.26	5.66	0	8	8	8	1.10	-27.77	27.77	0	-5	4	9	11.37	10.30	13.19	0
1	3	8	267.89	261.46	15.03	0	9	8	8	0.25	-23.85	31.70	0	-4	4	9	187.91	201.54	14.48	0
2	3	8	0.10	7.56	13.90	0	-9	8	8	76.18	119.16	17.18	0	-3	4	9	368.75	336.67	19.24	0
3	3	8	0.13	7.92	14.55	0	-8	8	8	22.31	14.74	31.99	0	-2	4	9	283.35	268.35	16.93	0
4	3	8	1072.30	1061.68	57.12	0	-7	9	8	1.74	1.48	22.08	0	-1	4	9	59.51	51.71	10.56	0
5																				

8	6	9	3.12	-30.70	30.70	o	12	1	10	0.34	21.40	29.41	o	-2	7	10	15.69	26.81	9.94	o
9	6	9	0.30	-24.88	24.88	o	-13	2	10	77.56	68.35	17.60	o	-1	7	10	3.81	-0.35	21.30	o
10	6	9	61.00	12.49	34.50	o	-12	2	10	134.99	166.69	18.50	o	0	7	10	83.25	90.66	9.73	o
11	6	9	17.14	-29.28	33.05	o	-11	2	10	0.68	-9.27	27.26	o	1	7	10	0.01	6.73	19.11	o
-10	7	9	0.04	-29.12	29.12	o	-10	2	10	1.35	29.70	10.07	o	2	7	10	201.02	219.02	19.40	o
-9	7	9	62.10	57.29	14.03	o	-9	2	10	26.92	52.36	12.16	o	3	7	10	20.89	-29.35	29.35	o
-8	7	9	79.14	67.51	14.96	o	-8	2	10	87.19	107.48	13.42	o	4	7	10	405.39	421.01	25.33	o
-7	7	9	0.14	14.13	16.77	o	-7	2	10	57.14	71.18	12.45	o	5	7	10	54.23	41.13	15.19	o
-6	7	9	59.50	58.57	14.29	o	-6	2	10	15.21	26.36	9.11	o	6	7	10	212.06	231.37	18.73	o
-5	7	9	0.41	-7.59	17.06	o	-5	2	10	6.35	-2.54	18.50	o	7	7	10	66.34	0.06	34.21	o
-4	7	9	64.77	67.67	10.56	o	-4	2	10	70.76	83.70	11.78	o	8	7	10	0.68	-8.27	26.10	o
-3	7	9	0.02	13.26	21.34	o	-3	2	10	111.29	102.69	11.07	o	9	7	10	20.95	12.36	22.04	o
-2	7	9	70.78	79.65	12.01	o	-2	2	10	166.11	177.60	13.39	o	-9	8	10	9.42	-27.16	28.87	o
-1	7	9	62.81	70.35	11.26	o	-1	2	10	16.24	4.34	11.01	o	-8	8	10	36.64	29.48	15.45	o
0	7	9	109.67	115.80	9.49	o	0	2	10	15.30	29.83	5.67	o	-7	8	10	99.67	76.65	16.89	o
1	7	9	44.54	9.62	25.97	o	1	2	10	496.85	464.26	24.01	o	-6	8	10	142.29	119.13	17.44	o
2	7	9	137.83	134.29	13.97	o	2	2	10	384.31	402.64	21.56	o	-5	8	10	7.68	18.21	21.72	o
3	7	9	0.04	-2.35	19.47	o	3	2	10	195.22	191.12	13.81	o	-4	8	10	0.95	20.11	22.91	o
4	7	9	681.01	624.81	33.43	o	4	2	10	472.29	469.86	24.88	o	-3	8	10	12.15	9.81	27.61	o
5	7	9	0.05	-14.48	25.74	o	5	2	10	475.04	472.98	25.62	o	-2	8	10	17.57	9.85	15.61	o
6	7	9	0.58	-3.09	22.17	o	6	2	10	445.33	447.98	23.23	o	-1	8	10	6.89	20.66	9.46	o
7	7	9	40.14	-5.05	21.72	o	7	2	10	18.27	20.34	22.65	o	0	8	10	109.70	113.62	10.80	o
8	7	9	50.62	41.77	14.55	o	8	2	10	311.31	294.64	20.18	o	1	8	10	7.84	25.94	10.78	o
9	7	9	34.13	45.21	13.81	o	9	2	10	3.36	3.80	26.61	o	2	8	10	10.91	-25.74	31.73	o
10	7	9	9.18	28.06	32.53	o	10	2	10	157.57	163.09	19.86	o	3	8	10	0.73	-28.54	28.54	o
-8	8	9	13.13	13.13	16.54	o	11	2	10	2.00	20.40	21.50	o	4	8	10	41.59	-22.71	20.43	o
-8	8	9	25.67	26.68	29.64	o	12	2	10	16.17	23.36	14.26	o	5	8	10	45.69	40.13	15.58	o
-7	8	9	147.38	115.98	18.18	o	-12	3	10	0.44	10.46	16.96	o	6	8	10	24.04	6.31	26.32	o
-6	8	9	217.60	249.81	19.44	o	-11	3	10	9.80	-30.99	30.99	o	7	8	10	29.84	13.45	14.77	o
-5	8	9	18.71	30.12	11.97	o	-10	3	10	0.04	-6.40	22.78	o	8	8	10	0.54	19.08	28.00	o
-4	8	9	27.82	-9.07	30.54	o	-9	3	10	20.49	25.58	12.13	o	-7	9	10	21.48	55.45	12.26	o
-3	8	9	1.68	12.20	22.01	o	-8	3	10	15.57	11.71	13.71	o	-6	9	10	116.37	90.52	20.43	o
-2	8	9	9.05	-20.02	24.94	o	-7	3	10	79.29	84.31	12.13	o	-5	9	10	1.02	-35.53	35.53	o
-1	8	9	33.79	38.58	12.42	o	-6	3	10	80.86	64.62	12.94	o	-4	9	10	1.82	11.94	22.59	o
0	8	9	26.62	15.24	12.84	o	-5	3	10	79.59	98.02	11.62	o	-3	9	10	12.71	-42.32	42.32	o
1	8	9	215.52	202.19	21.27	o	-4	3	10	51.41	25.74	27.26	o	-2	9	10	123.26	78.36	18.70	o
2	8	9	11.51	-5.63	20.72	o	-3	3	10	12.38	6.24	18.12	o	-1	9	10	2.81	-17.18	23.20	o
3	8	9	61.02	27.90	34.92	o	-2	3	10	0.16	-15.74	18.86	o	0	9	10	30.62	-27.98	50.20	o
4	8	9	197.14	206.43	19.86	o	-1	3	10	123.18	142.36	12.39	o	1	9	10	2.06	28.83	28.83	o
5	8	9	5.73	19.95	23.04	o	0	3	10	0.76	2.32	10.31	o	2	9	10	11.98	-9.11	32.08	o
6	8	9	44.40	68.45	14.26	o	1	3	10	180.94	189.64	14.38	o	3	9	10	87.39	115.27	16.03	o
7	8	9	0.04	4.99	22.17	o	2	3	10	19.92	-3.89	20.66	o	4	9	10	49.76	29.25	35.72	o
8	8	9	1.16	2.38	27.51	o	3	3	10	73.48	66.74	11.36	o	5	9	10	0.76	28.09	14.00	o
9	8	9	9.71	24.17	37.62	o	4	3	10	435.84	416.54	21.34	o	6	9	10	10.44	-1.64	28.22	o
-2	9	9	25.58	42.90	112.61	o	5	3	10	139.51	114.85	13.19	o	-8	9	10	98.38	11.99	28.38	o
-7	9	9	34.97	10.01	27.84	o	6	3	10	0.10	-0.58	15.38	o	-4	10	10	0.14	-6.47	29.73	o
-6	9	9	33.50	41.51	14.58	o	7	3	10	8.16	11.55	10.04	o	-3	10	10	0.50	22.40	27.19	o
-5	9	9	7.72	-2.86	22.94	o	8	3	10	17.60	-12.23	26.90	o	-2	10	10	7.32	22.40	32.15	o
-4	9	9	4.39	-13.52	23.23	o	9	3	10	7.35	8.53	24.91	o	-1	10	10	0.15	-27.87	27.87	o
-3	9	9	15.28	-16.09	27.29	o	10	3	10	30.88	-9.33	27.48	o	0	10	10	16.89	-10.00	37.23	o
-2	9	9	10.95	1.38	26.32	o	11	3	10	14.34	18.31	19.37	o	1	10	10	12.13	31.77	14.18	o
-1	9	9	11.84	5.89	29.09	o	12	3	10	0.21	16.73	25.90	o	2	10	10	0.00	12.32	30.22	o
0	9	9	1.44	-0.52	15.83	o	-12	4	10	50.19	54.22	15.74	o	3	10	10	5.98	3.73	26.23	o
1	9	9	15.33	-29.12	29.12	o	-11	4	10	0.08	13.97	16.41	o	4	10	10	22.96	66.81	14.93	o
2	9	9	13.18	26.87	28.19	o	-10	4	10	10.32	-34.27	34.27	o	-12	1	11	2.89	-15.12	30.54	o
3	9	9	0.27	11.97	26.39	o	-9	4	10	68.78	72.86	13.64	o	-11	1	11	20.38	-31.83	33.27	o
4	9	9	43.33	33.40	15.93	o	-8	4	10	115.08	114.91	14.64	o	-10	1	11	88.27	96.93	16.22	o
5	9	9	4.77	11.52	18.70	o	-7	4	10	5.90	-5.82	19.98	o	-9	1	11	133.02	110.22	17.63	o
6	9	9	21.31	59.92	13.35	o	-6	4	10	13.89	-17.18	22.01	o	-8	1	11	45.60	42.70	11.10	o
7	9	9	13.07	11.33	26.84	o	-5	4	10	3.22	6.95	12.61	o	-7	1	11	10.22	11.36	19.69	o
-6	10	9	42.46	13.64	35.04	o	-4	4	10	23.92	24.94	9.62	o	-6	1	11	285.87	293.87	19.76	o
-5	10	9	0.05	25.23	12.13	o	-3	4	10	18.60	11.75	10.59	o	-5	1	11	141.32	164.18	14.03	o
-4	10	9	45.40	31.21	14.90	o	-2	4	10	1223.05	1211.80	65.58	o	-4	1	11	56.53	51.04	10.27	o
-3	10	9	2.30	9.40	12.36	o	-1	4	10	306.95	345.55	48.57	o	-3	1	11	4.64	-8.63	28.38	o
-2	10	9	101.85	151.25	17.28	o	0	4	10	295.99	255.23	25.23	o	-2	1	11	2067.62	2206.32	89.94	o
-1	10	9	34.95	15.61	28.38	o	1	4	10	409.82	458.98	24.23	o	-1	1	11	113.44	123.15	11.71	o
0	10	9	2.60	-11.00	14.55	o	2	4	10	1101.28	1123.85	47.85	o	0	1	11	6.17	12.12	7.37	o
1	10	9	21.53	30.89	14.51	o	3	4	10	100.21	105.58	12.71	o	1	1	11	132.01	135.28	13.77	o
2	10	9	29.40	4.09	29.80	o	4	4	10	1.72	24.17	8.95	o	2	1	11	150.88	149.73	13.29	o
3	10	9	30.62	13.52	32.63	o	5	4	10	394.57	387.90	21.91	o	3	1	11	890.84	842.25	40.84	o
4	10	9	13.92	-32.89	32.89	o	6	4	10	33.16	6.05	12.32	o	4	1	11	40.16	50.49	10.23	o
5	10	9	34.94	46.37	18.05	o	7	4	10	1.41	-12.29	26.36	o	5	1	11	44.77	63.17	10.36	o
-3	11	9	3.60	36.46	12.87	o	8	4	10	155.11	152.73	17.22	o	6	1	11	7.11	-0.77		

-8	4	11	9.85	-25.58	25.58	5	0	12	92.19	96.19	13.81	6	6	12	6.40	17.67	24.78	o
-7	4	11	0.06	-25.71	25.71	6	0	12	63.19	75.56	13.61	7	6	12	33.88	25.62	31.79	o
-6	4	11	1.59	1.87	16.99	7	0	12	9.26	12.90	16.96	8	6	12	0.79	-25.87	28.58	o
-5	4	11	16.59	5.86	19.31	8	0	12	23.84	28.77	12.39	8	7	12	7.80	-5.53	28.29	o
-4	4	11	131.79	145.00	13.23	9	0	12	89.63	101.50	16.60	9	7	12	82.72	53.87	16.25	o
-3	4	11	52.68	15.61	18.54	10	9	12	27.03	37.04	15.54	9	7	12	140.16	161.99	18.57	o
-2	4	11	80.55	51.97	13.07	11	0	12	68.61	89.98	15.54	9	7	12	21.91	53.06	11.94	o
-1	4	11	246.46	247.95	17.18	11	1	12	1.29	-3.54	24.91	9	7	12	6.11	-5.86	27.29	o
0	4	11	115.66	86.77	42.33	10	1	12	26.81	26.87	27.10	9	7	12	11.69	9.91	28.96	o
1	4	11	0.44	2.57	9.88	9	1	12	1.41	-2.51	21.59	9	7	12	3.23	-30.64	30.64	o
2	4	11	14.36	13.32	10.14	8	1	12	43.84	40.03	12.65	9	7	12	67.31	63.94	14.67	o
3	4	11	117.27	106.55	13.26	7	1	12	63.35	20.14	34.01	9	7	12	0.83	8.59	22.00	o
4	4	11	122.04	127.08	14.16	6	1	12	95.84	92.39	13.93	9	7	12	10.95	-18.76	30.89	o
5	4	11	8.25	-2.70	14.32	5	1	12	48.20	-4.31	26.81	2	7	12	4.41	8.59	25.90	o
6	4	11	14.83	12.58	20.24	4	1	12	50.06	69.70	11.10	3	7	12	130.86	112.21	19.50	o
7	4	11	23.31	7.72	25.55	3	1	12	322.91	279.77	18.37	4	7	12	0.13	-30.80	30.80	o
8	4	11	0.04	8.40	16.57	2	1	12	538.38	540.95	27.48	5	7	12	2.34	16.96	27.13	o
9	4	11	0.00	-23.75	27.39	1	1	12	557.55	515.97	25.42	6	7	12	0.77	3.77	18.15	o
10	4	11	36.99	-2.57	29.12	0	1	12	96.43	96.24	8.68	7	7	12	5.60	-38.42	38.42	o
-11	5	11	0.97	11.55	20.08	1	1	12	1.47	10.39	17.35	6	8	12	1.72	-33.18	33.47	o
-10	5	11	11.56	34.05	13.71	2	1	12	25.55	36.65	9.88	5	8	12	0.21	-32.82	32.82	o
-9	5	11	2.78	10.91	24.10	3	1	12	118.79	115.17	13.81	4	8	12	8.60	-11.52	12.58	o
-8	5	11	0.44	-11.62	16.15	4	1	12	39.66	4.67	25.26	3	8	12	0.00	3.89	24.20	o
-7	5	11	28.91	18.70	23.49	5	1	12	9.11	-0.80	21.88	2	8	12	31.75	55.93	13.13	o
-6	5	11	353.56	342.48	21.66	6	1	12	7.29	-13.84	19.50	1	8	12	20.02	19.70	20.82	o
-5	5	11	0.32	-13.03	23.33	7	1	12	17.33	30.96	12.13	2	8	12	12.87	-20.80	20.80	o
-4	5	11	7.06	-22.40	22.40	8	1	12	0.62	22.27	24.88	1	8	12	69.69	53.52	16.54	o
-3	5	11	23.23	27.16	10.01	9	1	12	0.00	15.35	22.40	2	8	12	89.63	124.15	16.83	o
-2	5	11	158.36	165.63	16.67	10	1	12	0.06	-5.41	15.00	3	8	12	46.28	12.23	33.79	o
-1	5	11	11.70	6.47	22.04	11	2	12	15.86	21.43	14.29	4	8	12	90.03	88.66	18.99	o
0	5	11	1.49	-16.19	31.05	10	2	12	2.30	-37.52	37.52	5	8	12	7.12	2.45	28.25	o
1	5	11	44.87	18.09	24.91	9	2	12	77.54	94.67	15.83	6	8	12	4.29	-12.13	31.95	o
2	5	11	7.46	14.29	18.37	8	2	12	43.30	0.45	26.81	7	8	12	0.56	2.48	21.53	o
3	5	11	0.80	12.61	15.96	7	2	12	65.86	42.35	14.45	8	9	12	0.36	-12.65	26.97	o
4	5	11	3.53	7.53	23.07	6	2	12	24.35	-30.22	30.22	9	9	12	58.46	68.19	15.80	o
5	5	11	71.79	85.31	13.68	5	2	12	22.25	-31.09	31.09	0	9	12	1.35	1.19	13.72	o
6	5	11	21.23	45.31	11.81	4	2	12	193.93	196.14	16.03	1	9	12	16.62	-8.88	21.27	o
7	5	11	44.20	19.44	29.12	3	2	12	53.97	154.35	11.04	2	9	12	0.01	24.01	31.57	o
8	5	11	6.95	-1.46	16.25	2	2	12	184.22	186.49	15.77	2	9	12	211.80	238.23	24.13	o
9	5	11	33.24	-39.55	39.55	1	2	12	246.91	244.57	16.32	1	13	0.96	38.20	12.87	o	
10	5	11	1.69	-6.69	23.65	0	2	12	177.51	152.25	11.27	1	13	89.85	15.80	o		
-10	6	11	1.96	3.54	26.68	1	2	12	165.00	168.85	14.55	9	1	13	13.32	7.43	29.19	o
-9	6	11	0.92	14.61	18.99	2	2	12	35.47	26.16	11.65	8	1	13	0.95	7.27	22.53	o
-8	6	11	141.56	160.16	17.73	3	2	12	45.82	26.71	26.81	7	1	13	190.70	211.49	19.92	o
-7	6	11	19.40	22.92	25.10	4	2	12	59.66	58.66	12.80	6	1	13	14.80	14.80	20.02	o
-6	6	11	162.03	172.20	18.21	5	2	12	46.10	52.78	10.23	5	1	13	9.99	-16.70	24.49	o
-5	6	11	379.53	366.79	23.68	6	2	12	12.35	-28.96	29.16	4	1	13	7.93	12.55	22.94	o
-4	6	11	22.27	7.30	24.17	7	2	12	1.80	5.66	14.83	3	1	13	108.18	139.21	13.93	o
-3	6	11	58.75	107.19	12.26	8	2	12	1.36	-12.94	27.67	2	1	13	139.48	102.07	14.22	o
-2	6	11	67.56	53.13	14.16	9	2	12	62.02	38.84	15.64	3	1	13	77.18	81.48	12.42	o
-1	6	11	13.45	-1.06	22.30	10	2	12	40.50	31.54	15.22	0	1	13	4.71	17.32	13.60	o
0	6	11	12.46	9.78	11.69	11	3	12	38.99	42.93	17.15	1	1	13	31.08	15.67	20.79	o
1	6	11	2.22	9.40	19.08	10	3	12	0.59	12.10	23.30	2	1	13	86.37	69.54	14.87	o
2	6	11	25.27	-4.63	23.88	9	3	12	0.38	-30.31	30.31	3	1	13	59.00	62.04	13.03	o
3	6	11	234.54	235.91	18.95	8	3	12	71.69	20.88	31.25	4	1	13	1.74	0.97	24.30	o
4	6	11	335.22	356.81	23.43	7	3	12	16.73	-3.93	28.22	5	1	13	27.76	2.22	32.12	o
5	6	11	27.69	14.61	24.94	6	3	12	125.44	86.63	16.96	6	1	13	73.20	106.74	13.97	o
6	6	11	46.11	46.11	15.58	5	3	12	5.40	-5.25	24.33	7	1	13	86.86	95.00	15.58	o
7	6	11	13.27	9.46	19.69	4	3	12	94.22	88.85	13.97	8	1	13	23.04	13.07	26.19	o
8	6	11	2.28	34.30	11.20	3	3	12	3.33	-24.04	24.52	9	1	13	0.61	-29.61	29.61	o
9	6	11	174.82	153.59	22.62	2	3	12	23.73	34.43	10.62	10	1	13	6.95	17.86	30.12	o
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-7	7	11	61.96	-77.88	14.74	1	3	12	61.59	67.29	12.20	8	2	13	0.42	8.37	21.08	o
-6	7	11	131.20	147.58	17.47	2	3	12	52.86	62.30	11.91	7	2	13	81.74	56.51	20.09	o
-5	7	11	8.98	17.83	21.24	3	3	12	248.71	242.09	17.67	6	2	13	50.67	66.93	12.90	o
-4	7	11	0.00	17.41	20.53	4	3	12	107.16	96.96	15.19	5	2	13	50.72	48.01	13.32	o
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0	7	11	3.00	-11.99	21.83	8	3	12	1.86	9.30	11.80	1	2	13	28.71	30.38	11.30	o
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2	7	11	7.60	26.36	10.14	10	3	12	2.64	1.19	23.85	1	2	13	24.22	-0.16	24.84	o
3	7	11	13.77	-30.70	30.70	10	4	12	16.34	33.92	14.83	2	2	13	33.22	31.09	11.20	o
4	7	11	79.18	81.87	15.77	9	4	12	35.38	14.51	29.93	3	2	13	14.14	11.30	10.52	o
5	7	11	86.29	89.36	15.03	8	4	12	134.46	132.55	17.25	4	2	13	56.03	28.93	12.58	o
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-8	8	11	2.51															

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2	5	13	42.25	76.11	13.61	o	7	3	14	22.78	47.63	13.42	o	-5	5	15	3.92	20.24	13.03	o
3	5	13	140.24	146.55	16.83	o	8	3	14	10.88	-19.02	21.37	o	-4	5	15	57.35	49.62	16.73	o
5	5	13	19.24	19.24	24.91	o	-8	4	14	3.94	3.31	19.86	o	-3	5	15	128.70	148.86	19.34	o
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7	5	13	32.09	27.16	30.60	o	-5	4	14	129.82	168.33	16.12	o	0	5	15	9.94	12.63	12.19	o
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-4	6	13	33.85	12.65	15.83	o	1	4	14	91.58	84.83	16.32	o	-4	6	15	23.28	34.95	13.93	o
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-6	7	13	6.03	15.03	26.93	o	-2	5	14	27.38	21.37	21.82	o	-4	0	16	37.71	25.10	30.67	o
-5	7	13	3.53	-10.84	24.13	o	-1	5	14	6.01	3.02	23.88	o	-3	0	16	42.99	56.67	12.78	o
-4	7	13	1.28	-25.45	25.45	o	0	5	14	3.19	9.02	22.04	o	-2	0	16	37.89	-5.70	32.18	o
-3	7	13	17.89	22.43	23.39	o	1	5	14	6.05	21.88	12.65	o	-1	0	16	31.31	22.11	27.74	o
-2	7	13	6.96	-16.38	27.55	o	2	5	14	4.12	-10.46	23.59	o	0	16	16	125.28	134.55	13.77	o
-1	7	13	19.52	0.06	34.05	o	3	5	14	98.08	86.18	16.89	o	1	0	16	6.24	-31.95	31.95	o
0	7	13	3.59	-17.65	17.65	o	4	5	14	156.59	-18.44	45.79	o	2	0	16	134.84	146.68	18.37	o
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6	7	13	16.03	-17.35	27.84	o	-4	6	14	36.93	22.01	15.41	o	-3	1	16	5.75	3.67	25.81	o
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-2	8	13	2.55	-8.72	26.74	o	0	6	14	23.52	11.74	26.73	o	-2	1	16	124.63	128.59	16.35	o
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1	8	13	16.49	11.01	31.67	o	3	6	14	223.98	242.57	21.66	o	1	1	16	0.18	-29.38	29.38	o
2	8	13	29.85	41.16	15.00	o	4	6	14	67.64	11.36	36.11	o	2	1	16	15.92	12.04	27.96	o
3	8	13	71.13	103.49	15.48	o	5	6	14	61.78	96.31	16.70	o	3	1	16	4.41	-28.06	28.06	o
4	8	13	1.48	24.52	26.39	o	-5	7	14	7.46	19.44	15.35	o	4	1	16	0.21	15.90	23.91	o
-1	0	14	5.84	14.58	20.37	o	-4	7	14	7.98	11.33	26.87	o	5	1	16	3.24	9.01	18.15	o
-2	0	14	142.35	164.86	19.02	o	-3	7	14	9.77	22.04	12.23	o	6	1	16	0.00	-30.41	30.41	o
-3	0	14	83.25	101.37	16.57	o	-2	7	14	0.37	11.23	25.97	o	-7	2	16	12.14	25.10	15.86	o
-4	0	14	19.26	-35.72	35.72	o	-1	7	14	14.26	12.42	20.95	o	-6	2	16	4.99	8.75	14.51	o
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-6	0	14	23.08	7.69	25.49	o	1	7	14	25.61	14.64	31.79	o	-4	2	16	45.36	24.10	32.82	o
-7	0	14	58.57	94.93	14.06	o	2	7	14	0.17	-35.37	35.37	o	-3	2	16	56.87	53.87	13.81	o
-8	0	14	0.36	-18.70	22.46	o	3	7	14	20.87	24.68	14.64	o	-2	2	16	99.34	93.93	15.51	o
-9	0	14	75.17	67.67	14.06	o	4	7	14	35.94	-9.65	34.08	o	-1	2	16	265.60	259.18	22.17	o
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0	0	14	0.03	-4.05	9.97	o	0	8	14	4.17	27.30	11.35	o	1	2	16	0.58	15.51	28.19	o
1	0	14	0.81	8.91	21.01	o	-8	1	15	10.56	7.40	31.99	o	2	2	16	46.77	42.99	14.55	o
2	0	14	20.22	-6.11	15.12	o	-7	1	15	195.62	243.47	20.24	o	3	2	16	46.77	55.06	16.60	o
3	0	14	462.05	419.43	25.71	o	-6	1	15	17.54	63.52	14.55	o	4	2	16	29.23	-29.70	34.14	o
4	0	14	29.66	29.96	29.96	o	-5	1	15	5.60	12.87	25.26	o	-3	2	16	0.01	-1.10	14.26	o
5	0	14	15.30	-14.09	29.48	o	-4	1	15	13.62	-9.24	31.70	o	-6	3	16	1.38	-8.04	25.97	o
6	0	14	0.81	-29.57	29.57	o	-3	1	15	305.37	261.17	21.56	o	-5	3	16	18.54	11.17	20.82	o
7	0	14	124.99	123.31	17.89	o	-2	1	15	80.30	66.74	14.96	o	-4	3	16	0.80	-4.70	26.65	o
8	0	14	2.63	20.85	22.40	o	-1	1	15	23.27	36.78	12.84	o	-3	3	16	7.46	-38.23	38.23	o
9	0	14	32.86	53.80	12.61	o	0	1	15	33.37	17.28	12.15	o	-2	3	16	9.71	-14.96	25.00	o
-1	1	14	3.57	27.03	28.74	o	1	1	15	68.53	4.02	31.12	o	-1	3	16	2.72	16.25	17.76	o
-2	1	14	0.18	15.93	30.18	o	2	1	15	138.20	146.68	16.83	o	0	3	16	11.79	-6.33	18.77	o
-3	1	14	0.03	14.38	24.84	o	3	1	15	128.68	122.83	16.67	o	1	3	16	5.83	22.27	12.39	o
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Table S(3)
Crystallographic Information File for 5-methoxy isomer of C₁₈H₁₈N₂O₃S

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#####
data_[C18H18N2O3S]- 5-methoxy isomer
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# EXPERIMENTAL DATA

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  ? ? ?   ? ? ?   ? ? ?

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'H' 'H' 0.0000 0.0000
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'N' 'N' 0.0061 0.0033
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'S' 'S' 0.1246 0.1234
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Refinement of F^2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F^2, conventional R-factors R are based
on F, with F set to zero for negative F^2. The threshold expression of
F^2 > 2sigma(F^2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

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S8 S 0.79286(5) 0.10146(3) 0.35284(7) 0.02729(15) Uani 1 1 d . . .
O5 O 0.27223(13) 0.21353(7) 0.5225(2) 0.0344(4) Uani 1 1 d . . .
O8B O 0.73459(14) 0.02800(7) 0.3277(2) 0.0373(4) Uani 1 1 d . . .
O8A O 0.87730(14) 0.12071(8) 0.2650(2) 0.0352(4) Uani 1 1 d . . .
N1 N 0.61975(15) 0.30267(8) 0.3632(2) 0.0264(4) Uani 1 1 d . . .
N8 N 0.68158(15) 0.16475(8) 0.2998(2) 0.0286(4) Uani 1 1 d . . .
H8 H 0.7162 0.2114 0.2825 0.0483(16) Uiso 1 1 d . . .
C2 C 0.58679(19) 0.37347(10) 0.3800(3) 0.0270(5) Uani 1 1 d . . .
C2' C 0.6704(2) 0.43432(11) 0.3518(3) 0.0370(6) Uani 1 1 d . . .
H2A H 0.7406 0.4114 0.3239 0.072(2) Uiso 1 1 calc R . .
H2B H 0.7049 0.4647 0.4527 0.072(2) Uiso 1 1 calc R . .
H2C H 0.6205 0.4668 0.2602 0.072(2) Uiso 1 1 calc R . .
C3 C 0.4782(2) 0.39082(10) 0.4227(3) 0.0319(5) Uani 1 1 d . . .
H3 H 0.4551 0.4421 0.4291 0.0483(16) Uiso 1 1 calc R . .
C4 C 0.40594(19) 0.33452(10) 0.4551(3) 0.0302(5) Uani 1 1 d . . .
H4 H 0.3339 0.3464 0.4861 0.0483(16) Uiso 1 1 calc R . .
C4A C 0.44009(18) 0.25805(10) 0.4419(3) 0.0259(5) Uani 1 1 d . . .
C5' C 0.1968(2) 0.15316(11) 0.5500(3) 0.0348(5) Uani 1 1 d . . .
H5A H 0.1286 0.1739 0.5854 0.072(2) Uiso 1 1 calc R . .
H5B H 0.2505 0.1196 0.6363 0.072(2) Uiso 1 1 calc R . .
H5C H 0.1595 0.1246 0.4470 0.072(2) Uiso 1 1 calc R . .
C5 C 0.37139(18) 0.19552(11) 0.4718(3) 0.0281(5) Uani 1 1 d . . .
C6 C 0.40811(19) 0.12336(10) 0.4493(3) 0.0308(5) Uani 1 1 d . . .
H6 H 0.3633 0.0814 0.4716 0.0483(16) Uiso 1 1 calc R . .
C7 C 0.51149(19) 0.11133(10) 0.3938(3) 0.0304(5) Uani 1 1 d . . .
H7 H 0.5337 0.0611 0.3751 0.0483(16) Uiso 1 1 calc R . .
C8A C 0.54642(18) 0.24583(10) 0.3917(3) 0.0244(4) Uani 1 1 d . . .
C8 C 0.58107(18) 0.17049(10) 0.3658(3) 0.0264(5) Uani 1 1 d . . .
C81 C 0.87575(18) 0.11209(10) 0.5660(3) 0.0262(5) Uani 1 1 d . . .
C82 C 0.88740(19) 0.18262(10) 0.6428(3) 0.0278(5) Uani 1 1 d . . .
H82 H 0.8449 0.2254 0.5823 0.0483(16) Uiso 1 1 calc R . .
C83 C 0.96121(19) 0.18940(10) 0.8072(3) 0.0288(5) Uani 1 1 d . . .
H83 H 0.9686 0.2374 0.8594 0.0483(16) Uiso 1 1 calc R . .
C84' C 1.1017(2) 0.13482(12) 1.0800(3) 0.0366(6) Uani 1 1 d . . .
H12 H 1.1662 0.1744 1.0951 0.072(2) Uiso 1 1 calc R . .
H13 H 1.1437 0.0866 1.1213 0.072(2) Uiso 1 1 calc R . .
H14 H 1.0450 0.1483 1.1417 0.072(2) Uiso 1 1 calc R . .
C84 C 1.02557(19) 0.12754(11) 0.8993(3) 0.0289(5) Uani 1 1 d . . .
C85 C 1.0136(2) 0.05808(10) 0.8189(3) 0.0314(5) Uani 1 1 d . . .
H85 H 1.0579 0.0155 0.8783 0.0483(16) Uiso 1 1 calc R . .
C86 C 0.93892(19) 0.04973(10) 0.6553(3) 0.0305(5) Uani 1 1 d . . .
H86 H 0.9305 0.0016 0.6036 0.0483(16) Uiso 1 1 calc R . .
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O5 0.0299(8) 0.0304(7) 0.0488(11) 0.0005(7) 0.0210(7) -0.0027(6)
O8B 0.0365(8) 0.0258(7) 0.0479(11) -0.0086(7) 0.0119(7) -0.0033(6)
O8A 0.0369(8) 0.0373(7) 0.0370(10) -0.0050(7) 0.0198(7) 0.0019(7)
N1 0.0269(9) 0.0257(8) 0.0252(10) 0.0008(7) 0.0071(7) 0.0005(7)
N8 0.0278(9) 0.0260(8) 0.0328(11) 0.0016(7) 0.0114(8) 0.0027(7)
C2 0.0284(10) 0.0260(9) 0.0253(12) 0.0017(8) 0.0073(9) -0.0015(8)
C2' 0.0388(12) 0.0281(10) 0.0468(15) 0.0006(10) 0.0179(11) -0.0045(9)
C3 0.0345(11) 0.0235(9) 0.0374(13) -0.0023(9) 0.0116(10) -0.0003(8)
C4 0.0271(10) 0.0295(9) 0.0341(13) -0.0024(9) 0.0106(9) 0.0023(8)
C4A 0.0233(10) 0.0275(9) 0.0253(11) -0.0006(8) 0.0059(8) -0.0005(8)
C5' 0.0296(11) 0.0370(10) 0.0399(14) 0.0018(10) 0.0144(10) -0.0059(9)
C5 0.0227(10) 0.0325(10) 0.0275(12) -0.0014(9) 0.0063(8) -0.0004(8)
C6 0.0280(11) 0.0248(9) 0.0397(14) 0.0010(9) 0.0115(9) -0.0046(8)
C7 0.0307(11) 0.0216(9) 0.0374(13) -0.0028(9) 0.0096(9) -0.0008(8)
C8A 0.0227(10) 0.0262(9) 0.0225(11) 0.0023(8) 0.0055(8) 0.0011(7)
C8 0.0228(9) 0.0292(9) 0.0266(11) -0.0013(8) 0.0076(8) 0.0016(8)
C81 0.0241(9) 0.0288(9) 0.0292(12) -0.0014(8) 0.0137(8) 0.0001(8)
C82 0.0301(10) 0.0208(8) 0.0338(12) 0.0004(8) 0.0123(9) 0.0024(8)
C83 0.0301(10) 0.0260(9) 0.0344(13) -0.0041(9) 0.0161(9) -0.0023(8)
C84' 0.0381(12) 0.0424(11) 0.0305(13) 0.0001(10) 0.0131(10) -0.0037(10)
C84 0.0291(10) 0.0317(9) 0.0304(13) 0.0012(9) 0.0159(9) -0.0022(8)
C85 0.0358(11) 0.0243(9) 0.0367(14) 0.0060(8) 0.0155(10) 0.0034(8)
C86 0.0366(11) 0.0208(8) 0.0368(13) -0.0010(9) 0.0159(10) 0.0024(8)

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_geom_special_details

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All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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loop_

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O5 C5 1.355(3) . ?
O5 C5' 1.427(2) . ?
N1 C2 1.327(2) . ?
N1 C8A 1.369(3) . ?
N8 C8 1.419(3) . ?
C2 C3 1.412(3) . ?
C2 C2' 1.496(3) . ?
C3 C4 1.367(3) . ?
C4 C4A 1.420(3) . ?
C4A C8A 1.407(3) . ?
C4A C5 1.417(3) . ?
C5 C6 1.374(3) . ?
C6 C7 1.403(3) . ?
C7 C8 1.371(3) . ?
C8A C8 1.426(3) . ?
C81 C86 1.391(2) . ?
C81 C82 1.396(3) . ?
C82 C83 1.376(3) . ?
C83 C84 1.398(3) . ?
C84' C84 1.500(3) . ?
C84 C85 1.393(3) . ?
C85 C86 1.376(3) . ?

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loop_

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O8A S8 O8B 118.76(10) . . ?
O8A S8 N8 105.41(9) . . ?

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O8B S8 N8 108.56(9) . . ?
O8A S8 C81 108.15(10) . . ?
O8B S8 C81 107.83(10) . . ?
N8 S8 C81 107.67(10) . . ?
C5 O5 C5' 117.81(16) . . ?
C2 N1 C8A 118.07(19) . . ?
C8 N8 S8 124.85(15) . . ?
N1 C2 C3 121.8(2) . . ?
N1 C2 C2' 116.8(2) . . ?
C3 C2 C2' 121.40(18) . . ?
C4 C3 C2 120.64(18) . . ?
C3 C4 C4A 119.1(2) . . ?
C8A C4A C5 119.83(18) . . ?
C8A C4A C4 116.55(19) . . ?
C5 C4A C4 123.6(2) . . ?
O5 C5 C6 125.2(2) . . ?
O5 C5 C4A 115.05(17) . . ?
C6 C5 C4A 119.7(2) . . ?
C5 C6 C7 120.4(2) . . ?
C8 C7 C6 121.40(18) . . ?
N1 C8A C4A 123.83(17) . . ?
N1 C8A C8 116.7(2) . . ?
C4A C8A C8 119.44(19) . . ?
C7 C8 N8 125.75(19) . . ?
C7 C8 C8A 119.2(2) . . ?
N8 C8 C8A 114.88(18) . . ?
C86 C81 C82 119.99(19) . . ?
C86 C81 S8 118.60(15) . . ?
C82 C81 S8 121.21(15) . . ?
C83 C82 C81 119.25(17) . . ?
C82 C83 C84 121.74(18) . . ?
C85 C84 C83 117.76(19) . . ?
C85 C84 C84' 120.86(18) . . ?
C83 C84 C84' 121.35(19) . . ?
C86 C85 C84 121.52(18) . . ?
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