LBL-13866
Preprint

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

RECEIVED
LAWRENCE
BERKELEY LABORATORY
FEB 10 1982
LIBRARY AND
DOCUMENTS SECTION

Materials & Molecular Research Division

Submitted to Acta Crystallographica, Section B

ANOMALOUS SCATTERING BY PRASEODYMIUM, SAMARIUM AND GADOLINIUM AND STRUCTURES OF ETHYLENEDIAMINE-TETRAACETATE SALTS

Lieselotte K. Templeton, David H. Templeton,
Allan Zalkin and Helena W. Ruben

January 1982

TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks. For a personal retention copy, call Tech. Info. Division, Ext. 6782

Prepared for the U.S. Department of Energy under Contract W-7405-ENG-48

LBL-13866 c.2

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

ANOMALOUS SCATTERING BY PRASEODYMIUM, SAMARIUM AND GADOLINIUM AND STRUCTURES OF ETHYLENEDIAMINETETRAACETATE SALTS

Lieselotte K. Templeton, David H. Templeton,
Allan Zalkin and Helena W. Ruben

Materials and Molecular Research Division
Lawrence Berkeley Laboratory and
Department of Chemistry
University of California
Berkeley, California 94720
USA

JANUARY 1982

ABSTRACT

$NaPr(C_{10}H_{12}N_2O_8)\cdot 8H_2O$ is orthorhombic, space group Fdd2, with a = 19.589(3), b = 35.763(5), c = 12.121(2) Å. For the isomorphous Sm salt a = 19.503(11), b = 35.596(17), c = 12.119(5) Å. For the isomosphous Gd salt a = 19.409(3), b = 35.477(4), c = 12.119(1) Å. The structures were refined to R of 0.037, 0.030, and 0.024 respectively for diffraction data measured with MoKα X-rays. Anomalous scattering terms f" derived for this wavelength are 2.87(11), 3.64(10), and 3.91(9) e/atom respectively for Pr, Sm and Gd, in good agreement with theoretical values.

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract Number W-7405-ENG-48; and the National Science Foundation under Grant No. CHE-7919532.

INTRODUCTION

To measure anomalous scattering of X-rays by rare earth elements in experiments with synchrotron radiation (Templeton, Templeton and Phizackerley, 1980; Templeton, Templeton, Phizackerley and Hodgson, 1982) we needed the crystal structure parameters for sodium praseodymium ethylenediaminetetraacetate octahydrate and the isomorphous samarium and gadolinium salts. In this paper we report determinations of these three structures using MoKα radiation. Values of the anomalous scattering terms for this wavelength, derived from these diffraction data, are also reported.

These salts and several others crystallize according to the orthorhombic space group Fdd2 (Hoard, Lee and Lind, 1965). This samarium salt was used by Koetzle and Hamilton (1975) to measure anomalous neutron scattering, and Koetzle (1978) kindly gave us the parameters determined in that work. We repeated the determination for Sm using X-rays so that the synchrotron experiments could be analyzed with atomic form factors identical (apart from anomalous scattering terms) with those used in the structure determination. Nassimbeni, Wright, van Niekerk and McCallum (1979) reported the structure of the dysprosium salt in this space group with parameters similar to those found for these other salts. We have adopted their scheme of atomic identification and choice of asymmetric unit to simplify comparison. However, all the crystals that we have tested of the dysprosium compound, and also the holmium one, are monoclinic, but with a structure very nearly the same as the orthorhombic one. A refinement of this monoclinic structure will be reported elsewhere.

EXPERIMENTAL

The compounds were made from oxides of Pr ("99.8%"), Sm ("99.9%") and Gd ("99.98%") from Research Chemical Corporation and $Na_2H_2(edta)\cdot 2H_2O$ from Aldrich Chemical Company. The oxide was dissolved in HCl and mixed with a hot solution of the edta salt. The pH was adjusted to about 5 with sodium hydroxide. Crystals were grown by slow cooling or slow evaporation. Larger crystals were grown by slow evaporation after dissolving the first crops in hot water.

Crystals were mounted on glass fibers with epoxy glue. Data were measured with a Picker FACS-I diffractometer for Pr and Sm and with an Enraf-Nonius CAD-4 instrument for Gd, all using MoKα X-rays (graphite monochromator, 0.70930 Å for $K\alpha_1$). Crystal data and other details are listed in Table I.

Faces of the types {111}, $\{11\bar{1}\}$, {131} and $\{13\bar{1}\}$ occur most frequently. Many crystals exhibit only two or three of these forms in accord with the mm2 symmetry, but which faces are present is not a reliable guide to the absolute orientation of the polar c axis. For example, the Sm crystal (Table I) exhibited only the $\{11\bar{1}\}$ and {131} faces, while the Gd crystal showed $\{13\bar{1}\}$ and three each of {111} and $\{11\bar{1}\}$. Similar variation occured among many other crystals we have examined. The absolute setting used here may be identified by the intensity inequalities $004 > 00\bar{4}$, $008 < 00\bar{8}$.

STRUCTURE ANALYSIS

The trial structures for refinement were derived directly or indirectly from Koetzle's (1978) coordinates for the Sm salt, but modified by various transformations of setting. We defined the origin by holding the lanthanide atom at a fixed z coordinate. Scattering factors, including anomalous scattering effects for all atoms except hydrogen, were taken from International Tables (1974) for Ln^{+3}, Na^{+}, $O^{-1/2}$ (edta oxygens), for neutral C, N, and O (water oxygens), and for spherical bonded hydrogen. For each rare-earth atom f'' was determined as an adjustable parameter. Only 20 of the 28 hydrogen atoms were included in the calculations; those on water molecules W2 to W5 (the ones with the largest apparent thermal motion) were omitted. For the Pr and Sm structures the hydrogen cooordinates were derived from the Sm neutron-diffraction values (Koetzle, 1978). Isotropic thermal parameters, constrained to be equal for each pair of hydrogen atoms bonded to the same carbon or oxygen atom, were refined using the Pr data. The same values were used without change in the refinement of the Sm structure. For the Gd structure the coordinates of the same 20 hydrogen atoms were adjusted in the refinement, but with restraints to hold distances close to C-H = 1.00, O-H = 0.90, H-H = 1.63 (carbon H), and H-H = 1.47 Å (water H), all ± 0.05 Å. Again the isotropic thermal parameters were constrained to be equal by pairs. All non-hydrogen atoms were assigned anisotropic thermal parameters. In the final cycles whose results are reported here only the non-hydrogen atoms were refined, but the parameters changed little from the earlier

cycles where hydrogen parameters were adjusted. Zero weight was assigned to reflections weaker than 1σ; for others $w = [\sigma(F)]^{-2}$; $\sigma(F)$ was derived from $\sigma(F^2) = [S^2 + (pF^2)^2]^{1/2}$ where S^2 is the variance due to counting statistics and p is listed in Table I. In the Gd refinement zero weight was also assigned to the four lowest-angle reflections, and a small extinction correction was applied; the latter affected no structure factor more than 1%.

Final values of R, R_w and f'' are listed in Table I. Other parameters are listed in Table II and the supplementary material.*

*Lists of hydrogen atom parameters, anisotropic thermal parameters, interatomic distances and angles, and structure factors have been deposited with the British Library Lending Division as Supplementary Publication No.

DISCUSSION

With R values in the range 0.024 to 0.037 this work achieved its primary objective of obtaining parameters which fit X-ray diffraction intensities accurately enough to be used to analyze our synchrotron radiation experiments cited above. A second result is the experimental values of f'' for these three rare-earth elements for MoKα radiation (Table I). Like our earlier results for Cs (Templeton and Templeton, 1978) and Co and Cl (Templeton, Zalkin, Ruben and Templeton, 1979) the agreement is excellent with the values calculated by Cromer and Liberman (1970, 1981) for this wavelength remote from the absorption edges. This is in contrast to huge differences observed in the immediate regions of absorption edges. In this analysis we assumed that the theoretical values for f' were correct in order to avoid difficult-to-analyze systematic errors which might result from strong coupling of f' with thermal parameters, errors in absorption corrections, and other effects correlated with diffraction angle. A test refinement of the Gd data, in which both f' and f'' as well as all the structural parameters were varied, yield f'' = 3.87(9), hardly different from the value cited above, and f' = -1.11(17), different by about 3σ from Cromer and Liberman's value.

In structure determinations of non-centric crystals, particularly polar ones, it is important to avoid inversion twinning, or else consider it explicitly in the calculations (Templeton and Templeton, 1978; Rietz, Zalkin, Templeton, Edelstein and Templeton, 1978; Rogers, 1981).

When scattering factors are being measured as in the present work it is crucial to avoid twinning. For this reason we adopted these edta crystals for this work only after much labor failed to achieve satisfactory crystals of any lanthanide tartrate salts. With optically pure salts of tartaric acid the intrinsic chirality makes inversion twinning impossible. Fortunately, inversion twinning (if it occurs at all) is rare in these edta salts, at least in well-formed crystals such as we have selected. The good agreement of measured and theoretical f'' values cited above indicates it was absent in these three crystals. Nor was any evidence of it detected in any of the several other crystals we have used in synchrotron radiation experiments.

The crystal structure itself, which has already been described by earlier authors cited above, needs little comment here. The principal differences among these isomorphous crystals are the result of the different sizes of the lanthanide ions. The neighbor distances of these ions are listed in Table III with corresponding values reported by Nassimbeni, et al. (1979) for the Dy compound. Corresponding distances for our three structures trend downward consistently with increasing atomic number, with an average decrease of 0.061 Å from Pr to Gd; the ionic radii calculated from oxide and chloride structures (Templeton and Dauben, 1954) decrease 0.075 Å in the same interval. The distances for the Dy salt do not fit this pattern. Nassimbeni, et al. (1979) do not mention anomalous scattering nor the determination of the absolute polarity of their crystal. This fact suggests that the polar dispersion

error may have occurred (Ueki, Zalkin and Templeton, 1966; Cruickshank and McDonald, 1967). If the z coordinate of Dy is changed to 0.006 (a change of about 0.07 Å) distances are calculated (Table III) which are much more consistent with our values. This change is more than one would estimate if anomalous scattering (f'' = 4.4 for Dy at MoKα) had simply been neglected, but is a reasonable amount if the refinement had been done with the correct f'' but the configuration reverse to that of the specimen. Whatever the facts, this example illustrates again the need for care with anomalous scattering effects in polar space groups.

There is nothing novel about the bond structure of the edta moiety, but the redundancy of these three determinations permits averaging of from 3 to 12 independent measurements to get accurate average values for each chemical type of bond distance and angle. These averages are shown in Fig. 1.

The large and highly anisotropic thermal parameters for some of the water molecules (not including any of those coordinated to rare-earth atoms) evidently indicate some disorder of location and partial occupancy of sites. This aspect of the structure has been under investigation by neutron diffraction at low temperature by Koetzle and Engel (1981). For our purposes the description by highly anisotropic thermal parameters seemed to be sufficient, and we have not attempted to resolve the details of this disorder.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Chemical Sciences Division of the U.S. Department of Energy under Contract Number W-7405-ENG-48; and the National Science Foundation under Grant No. CHE-7919532.

REFERENCES

Cromer, D.T. and Liberman, D. (1970). J. Chem. Phys. 53, 1891-1898.

Cromer, D.T. and Liberman, D. (1981). Acta Cryst. A37, 267-268.

Cruickshank, D.W.J. and McDonald, W.S. (1967). Acta Cryst. 23, 9-11.

Hoard, J.L., Lee, B. and Lind, M.D. (1965). J. Am. Chem. Soc. 87, 1612-1613.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham:Kynoch Press.

Koetzle, T.F. (1978). Private communication.

Koetzle, T.F. and Engel, D.W. (1981). Private communication.

Koetzle, T.F. and Hamilton, W.C. (1975). Anomalous Scattering, edited by S. Ramaseshan and S. C. Abrahams, pp. 489-502. Copenhagen: Munksgaard.

Nassimbeni, L.R., Wright, M.R.W., van Niekerk, J.C. and McCallum, P.A. (1979). Acta Cryst. B35, 1341-1345.

Rietz, R.R., Zalkin, A., Templeton, D.H., Edelstein, N.M. and Templeton, L.K. (1978). Inorg. Chem. 17, 653-658.

Rogers, D. (1981). Acta Cryst. A37, 734-741.

Templeton, D.H. and Dauben, C.H. (1954). J. Am. Chem. Soc. 76, 5237-5239.

Templeton, D.H., Zalkin, A., Ruben, H.W. and Templeton, L.K. (1979). Acta Cryst. B35, 1608-1613.

Templeton, L.K. and Templeton, D.H. (1978). Acta Cryst. A34, 368-371

Templeton, L.K., Templeton, D.H. and Phizackerley, R.P. (1980). J. Am. Chem. Soc. 102, 1185-1186.

Templeton, L.K., Templeton, D.H., Phizackerley, R.P. and Hodgson, K.O. (1982). Acta Cryst. A, in press.

Ueki, T., Zalkin, A. and Templeton, D.H. (1966). Acta Cryst. 20, 836-841.

Table I. Crystal and Diffraction Data, $NaLn(edta)\cdot 8H_2O$.

Ln	Pr	Sm	Gd
a(Å)	19.589(3)	19.503(11)	19.409(3)
b(Å)	35.763(5)	35.596(17)	35.477(4)
c(Å)	12.121(2)	12.119(5)	12.119(1)
U(Å^3)	8491.5	8413.4	8344.8
M_r	596.24	605.68	612.58
Z	16	16	16
D_x (Mg m^{-3})	1.865	1.913	1.950
μ, MoKα (mm^{-1})	2.38	2.90	3.29
faces	16	8	10
volume (mm^3)	6.32×10^{-4}	1.12×10^{-3}	4.93×10^{-4}
absorption correction	1.15 - 1.22	1.21 - 1.30	1.17 - 1.36
p	.04	.02	.025
reflections measured	4012	3991	7772
unique reflections, $F^2 > \sigma$	3449	3368	3386
max $(\sin\theta)/\lambda$	0.596	0.596	0.594
$R = \Sigma\|\Delta\|/\Sigma\|F_o\|$	0.037	0.030	0.024
$R_w = (\Sigma w\Delta^2/\Sigma wF_o^2)^{1/2}$	0.036	0.029	0.025
f'', exper.	2.87(11)	3.64(10)	3.91(9)
f'', calc.	2.82[a]	3.442[b]	3.904[b]

a. Cromer and Liberman (1981).
b. Cromer and Liberman (1970).

Table II. Atomic coordinates and equivalent isotropic thermal parameters, $B_{eq} = \frac{8}{3}\pi^2 \text{ trace } \tilde{U}$

Atom	x	y	z	B_{eq}
		$NaPr(edta)\cdot 8H_2O$		
Pr	.08342(2)	.15424(1)	0	1.670(7)
Na	.13665(18)	.13164(10)	.3162(3)	3.8(1)
O(1)	.0977(3)	.18278(14)	.1826(4)	2.7(1)
O(2)	-.0296(3)	.16991(16)	.0711(5)	3.0(1)
O(3)	.2067(3)	.16902(15)	.0279(4)	2.5(1)
O(4)	.0186(3)	.16490(14)	-.1692(4)	2.2(1)
O(5)	.1061(4)	.23178(18)	.2947(5)	5.1(2)
O(6)	-.0968(4)	.21156(21)	.1514(6)	5.9(2)
O(7)	.3122(3)	.17571(19)	-.0344(5)	4.1(2)
O(8)	.0117(3)	.17261(18)	-.3525(4)	3.2(2)
O(9)	.0015(3)	.09753(12)	-.0142(4)	2.8(1)
O(10)	.1370(3)	.10858(16)	-.1280(5)	2.8(2)
O(11)	.1353(3)	.10426(14)	.1217(4)	2.4(1)
N(1)	.0579(3)	.22827(15)	.0068(6)	2.6(1)
N(2)	.1496(3)	.19316(18)	-.1617(5)	2.1(2)
C(1)	.0792(4)	.24674(28)	-.0955(7)	2.8(2)
C(2)	.1489(4)	.23358(21)	-.1336(6)	2.9(2)
C(3)	.0983(6)	.24401(26)	.1033(8)	3.8(3)
C(4)	.1008(4)	.21770(22)	.2022(7)	3.0(2)
C(5)	-.0151(5)	.23416(22)	.0235(7)	3.8(3)
C(6)	-.0484(5)	.20290(26)	.0879(7)	3.6(2)
C(7)	.2216(4)	.18098(23)	-.1641(7)	2.7(2)
C(8)	.2494(4)	.17531(22)	-.0482(6)	2.6(2)
C(9)	.1174(4)	.18586(23)	-.2698(6)	2.7(2)
C(10)	.0422(4)	.17362(19)	-.2624(7)	2.4(2)
W(1)	.0625(3)	.03971(16)	.1031(5)	4.1(2)
W(2)	.1478(5)	.09818(23)	.5435(9)	9.4(4)
W(3)	.1153(7)	.17824(25)	.4508(7)	10.1(4)
W(4)	.0187(6)	.11154(33)	.3155(11)	11.5(4)
W(5)	.2646(8)	.21580(41)	.5645(10)	15.7(6)

Table II. (Continued)

Atom	x	y	z	B_{eq}
		$NaSm(edta)\cdot 8H_2O$		
Sm	.08333(1)	.15487(1)	0	1.397(6)
Na	.13752(16)	.13227(9)	.31437(26)	3.42(9)
O(1)	.0972(2)	.19234(12)	.1821(4)	2.3(1)
O(2)	-.0284(2)	.16881(13)	.0724(4)	2.4(1)
O(3)	.2053(2)	.16902(13)	.0302(3)	2.2(1)
O(4)	.0181(2)	.16416(13)	-.1658(4)	1.9(1)
O(5)	.1057(3)	.23154(15)	.2947(4)	3.9(2)
O(6)	-.0985(3)	.20939(17)	.1530(5)	4.9(2)
O(7)	.3114(2)	.17648(17)	-.0301(4)	3.6(2)
O(8)	.0103(3)	.17186(16)	-.3489(4)	3.0(1)
O(9)	.0028(2)	.09809(11)	-.0137(4)	2.1(1)
O(10)	.1362(3)	.10966(14)	-.1254(4)	2.5(1)
O(11)	.1335(2)	.10553(13)	.1213(4)	2.2(1)
N(1)	.0566(3)	.22792(13)	.0055(6)	2.2(1)
N(2)	.1493(3)	.19304(16)	-.1598(4)	1.8(1)
C(1)	.0783(4)	.24753(25)	-.0964(7)	2.5(2)
C(2)	.1479(4)	.23391(20)	-.1333(6)	2.5(2)
C(3)	.0953(5)	.24365(23)	.1027(7)	3.0(2)
C(4)	.0989(4)	.21696(20)	.2011(6)	2.6(2)
C(5)	-.0175(4)	.23309(20)	.0225(6)	3.2(2)
C(6)	-.0499(4)	.20187(21)	.0886(6)	2.8(2)
C(7)	.2214(3)	.18091(20)	-.1605(6)	2.2(2)
C(8)	.2488(4)	.17521(19)	-.0453(5)	2.3(2)
C(9)	.1168(3)	.18530(20)	-.2688(5)	2.1(2)
C(10)	.0428(3)	.17300(17)	-.2609(6)	1.9(2)
W(1)	.0633(3)	.04011(14)	.1034(4)	3.4(1)
W(2)	.1482(4)	.09850(19)	.5497(7)	7.6(3)
W(3)	.1182(5)	.17830(21)	.4537(5)	8.6(3)
W(4)	.0200(4)	.11310(28)	.3313(9)	10.8(4)
W(5)	.2604(6)	.21434(34)	.5609(8)	15.5(5)

Table II. (Continued)

Atom	x	y	z	B_{eq}
		$NaGd(edta)\cdot 8H_2O$		
Gd	.08251(1)	.15503(1)	0	1.420(5)
Na	.13651(14)	.13233(7)	.31280(22)	3.82(7)
O(1)	.0964(2)	.18200(10)	.1811(3)	2.3(1)
O(2)	-.0289(2)	.16839(11)	.0723(3)	2.5(1)
O(3)	.2033(2)	.16881(11)	.03138(27)	2.3(1)
O(4)	.0176(2)	.16431(10)	-.16449(29)	1.80(9)
O(5)	.1059(3)	.23117(13)	.2938(3)	4.1(1)
O(6)	-.1003(3)	.20893(15)	.1512(4)	5.4(2)
O(7)	.3109(2)	.17657(13)	-.0275(3)	3.6(1)
O(8)	.0087(2)	.17149(13)	-.3471(3)	3.1(1)
O(9)	.0034(2)	.09854(9)	-.0137(3)	2.27(9)
O(10)	.1348(2)	.11013(12)	-.1243(3)	2.5(1)
O(11)	.1317(2)	.10593(11)	.1210(3)	2.2(1)
N(1)	.0562(2)	.22775(11)	.0077(4)	2.2(1)
N(2)	.1485(2)	.19319(13)	-.1586(4)	1.8(1)
C(1)	.0769(3)	.24709(19)	-.0953(6)	2.3(2)
C(2)	.1465(3)	.23404(17)	-.1328(5)	2.7(2)
C(3)	.0942(4)	.24353(19)	.1034(6)	3.1(2)
C(4)	.0980(3)	.21683(16)	.2010(5)	2.2(1)
C(5)	-.0194(3)	.23265(16)	.0242(5)	3.1(2)
C(6)	-.0513(3)	.20128(18)	.0886(5)	2.8(2)
C(7)	.2208(3)	.18104(17)	-.1597(5)	2.5(1)
C(8)	.2477(3)	.17527(16)	-.0436(4)	2.3(1)
C(9)	.1161(3)	.18532(15)	-.2663(5)	2.4(1)
C(10)	.0413(2)	.17304(13)	-.2583(5)	2.0(1)
W(1)	.0625(2)	.03988(12)	.1024(4)	3.7(1)
W(2)	.1492(4)	.09816(18)	.5551(7)	8.2(2)
W(3)	.1187(5)	.17871(19)	.4544(5)	9.0(3)
W(4)	.0207(4)	.11274(28)	.3329(9)	12.5(4)
W(5)	.2579(6)	.21439(42)	.5607(8)	18.3(6)

Table III. Neighbor distances for rare-earth ions, Å.

Ln	59 Pr	62 Sm	64 Gd	66 Dy[a]	66 Dy[b]
Ln-O(1)	2.453(5)	2.429(4)	2.409(4)	2.464(14)	2.397
-O(2)	2.441(5)	2.401(5)	2.381(4)	2.396(15)	2.368
-O(3)	2.495(5)	2.458(4)	2.425(4)	2.420(14)	2.408
-O(4)	2.442(5)	2.400(4)	2.381(3)	2.285(15)	2.346
ave.	2.458	2.422	2.399	2.391[c]	2.380
Ln-O(9)	2.592(5)	2.565(4)	2.531(3)	2.553(12)	2.559
-O(10)	2.485(5)	2.442(5)	2.416(4)	2.351(16)	2.397
-O(11)	2.531(5)	2.490(5)	2.469(4)	2.483(14)	2.440
ave.	2.536	2.499	2.472	2.462	2.465
Ln-N(1)	2.696(5)	2.653(5)	2.632(4)	2.642(16)	2.637
-N(2)	2.731(6)	2.693(5)	2.677(4)	2.614(17)	2.665
ave.	2.714	2.673	2.655	2.628	2.651

a. Nassimbeni, Wright, van Niekerk and McCallum (1979).
b. Recalculated as described in the text.
c. Reported incorrectly as 2.319 (Footnote a).

FIGURE CAPTION

Fig. 1. Bond distances (Å) and angles (deg) in the edta moiety, averaged for the 3 to 12 chemically equivalent bonds in the Pr, Sm. and Gd salts.

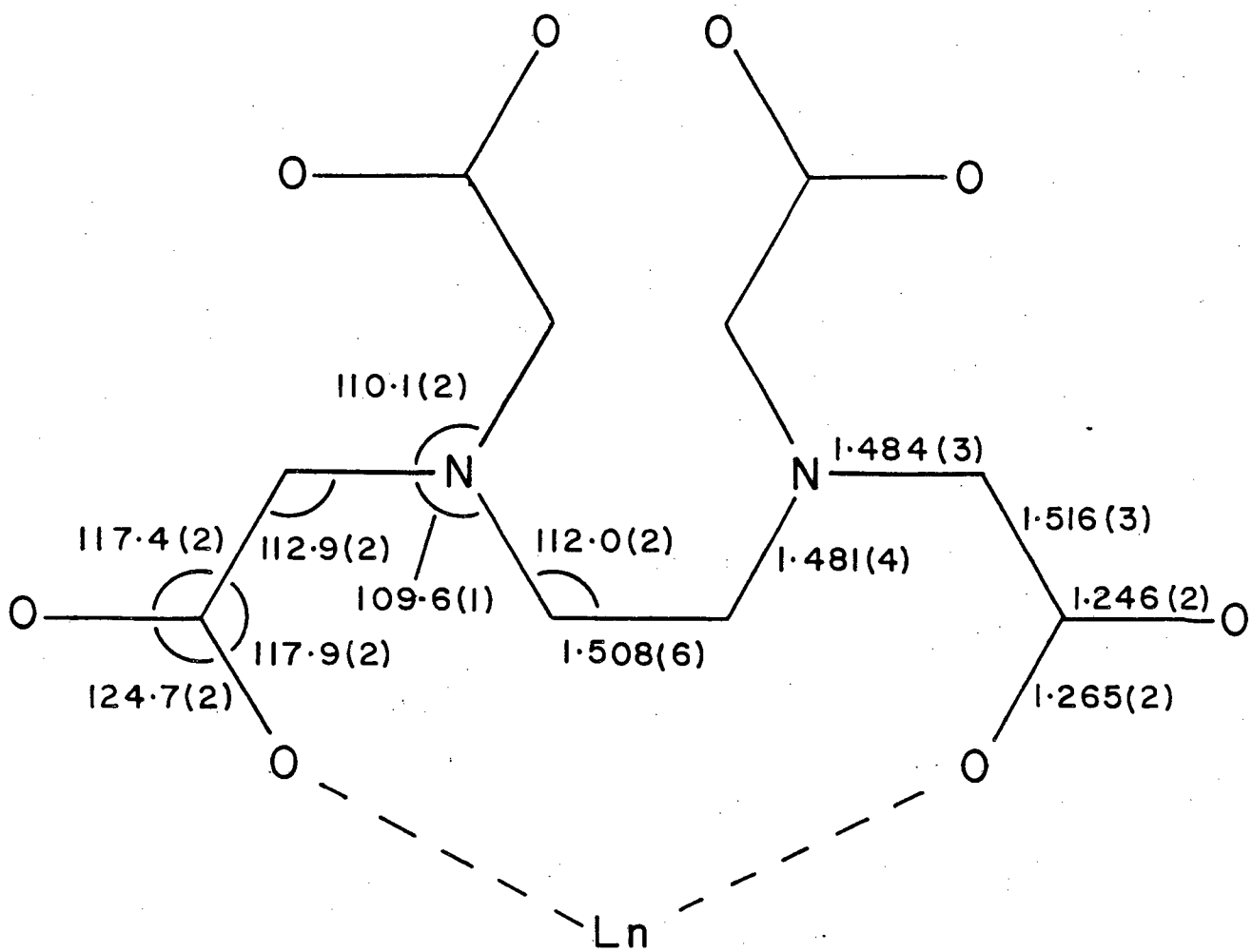
O
O
O
O
110·1(2)
N
N
1·484(3)
1·516(3)
117·4(2)
112·9(2)
112·0(2)
1·481(4)
109·6(1)
1·246(2)
O
O
117·9(2)
1·508(6)
124·7(2)
1·265(2)
O
O
Ln

Fig. 1

SUPPLEMENTARY MATERIAL FOR

ANOMALOUS SCATTERING BY PRASEODYMIUM, SAMARIUM AND GADOLINIUM AND STRUCTURES OF ETHYLENEDIAMINETETRAACETATE SALTS

Lieselotte K. Templeton, David H. Templeton
Allan Zalkin and Helena Ruben

Materials and Molecular Research Division
Lawrence Berkeley Laboratory and
Department of Chemistry
University of California
Berkeley, California 94720
USA

Bond Distances (Å)

	Pr	Sm	Gd
C(1) -N(1)	1.466(11)	1.481(10)	1.480(8)
C(1) -C(2)	1.517(12)	1.509(10)	1.499(8)
C(2) -N(2)	1.485(10)	1.490(9)	1.483(7)
C(3) -N(1)	1.521(11)	1.506(10)	1.484(8)
C(3) -C(4)	1.524(12)	1.527(11)	1.517(9)
C(4) -O(5)	1.234(9)	1.254(8)	1.244(6)
C(4) -O(1)	1.273(9)	1.254(8)	1.259(7)
C(5) -N(1)	1.480(10)	1.472(9)	1.491(7)
C(5) -C(6)	1.503(12)	1.508(10)	1.494(9)
C(6) -O(6)	1.260(10)	1.261(9)	1.246(7)
C(6) -O(2)	1.253(10)	1.264(8)	1.261(7)
C(7) -N(2)	1.477(9)	1.471(8)	1.467(7)
C(7) -C(8)	1.520(11)	1.509(9)	1.515(7)
C(8) -O(7)	1.241(9)	1.236(8)	1.243(7)
C(8) -O(3)	1.266(9)	1.267(7)	1.273(6)
C(9) -N(2)	1.478(9)	1.488(8)	1.475(7)
C(9) -C(10)	1.539(10)	1.515(8)	1.520(7)
C(10)-O(8)	1.246(9)	1.241(8)	1.249(7)
C(10)-O(4)	1.260(10)	1.289(8)	1.264(7)

Bond Angles (°)

Angle	Pr	Sm	Gd
O(1) -Ln -O(4)	138.7(2)	139.8(2)	140.1(1)
O(2) -Ln -O(3)	141.4(2)	141.4(2)	141.3(1)
O(1) -Ln -O(11)	73.9(2)	72.8(2)	72.3(1)
O(2) -Ln -O(9)	69.0(2)	68.3(2)	68.3(1)
O(4) -Ln -O(10)	78.4(2)	78.1(2)	78.0(1)
N(1) -Ln -O(9)	131.0(2)	130.8(1)	131.4(1)
N(2) -Ln -O(10)	71.7(2)	71.5(2)	71.6(2)
O(9) -Ln -O(10)	72.9(2)	72.5(2)	72.1(1)
O(9) -Ln -O(11)	74.6(2)	73.9(2)	73.4(1)
O(10)-Ln -O(11)	74.4(2)	74.7(1)	75.1(1)
N(1) -Ln -N(2)	67.0(2)	67.5(2)	67.8(2)
C(1) -N(1) -Ln	111.4(5)	112.6(5)	111.8(4)
C(3) -N(1) -Ln	106.9(5)	106.6(4)	107.5(4)
C(5) -N(1) -Ln	109.0(4)	108.6(4)	108.1(3)
C(2) -N(2) -Ln	109.1(4)	109.2(4)	109.3(3)
C(7) -N(2) -Ln	108.5(4)	108.2(4)	108.4(3)
C(9) -N(2) -Ln	110.1(4)	110.3(4)	109.6(3)
C(4) -O(1) -Ln	125.6(5)	124.4(4)	124.5(4)
C(6) -O(2) -Ln	122.7(6)	123.4(5)	123.7(4)
C(8) -O(3) -Ln	125.4(4)	125.2(4)	125.4(3)
C(10)-O(4) -Ln	126.9(5)	125.8(4)	126.5(3)
C(2) -C(1) -N(1)	111.9(7)	110.7(6)	110.9(5)

Bond Angles (°) Continued

C(1) -C(2) -N(2)	112.4(7)	113.2(6)	112.9(5)
C(4) -C(3) -N(1)	113.1(7)	113.8(6)	113.4(5)
C(3) -C(4) -O(5)	117.7(7)	117.0(6)	117.1(5)
C(3) -C(4) -O(1)	117.3(8)	117.8(6)	117.6(5)
C(6) -C(5) -N(1)	112.2(7)	113.1(6)	113.1(5)
C(5) -C(6) -O(6)	116.8(8)	118.5(7)	118.2(6)
C(5) -C(6) -O(2)	119.5(8)	117.7(6)	117.7(5)
C(8) -C(7) -N(2)	111.3(7)	111.8(6)	111.2(5)
C(7) -C(8) -O(7)	118.5(7)	118.9(6)	118.7(5)
C(7) -C(8) -O(3)	117.4(6)	117.1(6)	117.0(5)
C(10)-C(9) -N(2)	114.0(6)	113.7(6)	113.9(5)
C(9) -C(10)-O(8)	114.6(7)	116.2(6)	116.2(5)
C(9) -C(10)-O(4)	118.4(7)	119.1(6)	118.3(5)
O(1) -C(4) -O(5)	125.0(8)	125.2(7)	125.2(5)
O(2) -C(6) -O(6)	123.5(9)	123.8(7)	124.1(6)
O(3) -C(8) -O(7)	124.0(7)	124.1(6)	124.3(5)
O(4) -C(10)-O(8)	127.1(7)	124.7(6)	125.5(4)
C(1) -N(1) -C(3)	109.7(5)	109.5(5)	110.5(4)
C(1) -N(1) -C(5)	109.3(6)	109.8(6)	109.0(4)
C(2) -N(2) -C(7)	107.5(6)	107.8(5)	108.3(4)
C(2) -N(2) -C(9)	111.8(6)	110.7(5)	111.1(4)
C(3) -N(1) -C(5)	110.6(7)	109.6(6)	109.9(5)
C(7) -N(2) -C(9)	109.7(6)	110.6(5)	110.1(4)

ATOM	B11	B22	B33	B12	B13	B23
GD	1.407(8)	1.498(8)	1.355(8)	-.051(8)	-.207(8)	-.004(9)
NA	3.89(13)	3.80(13)	3.77(12)	1.06(10)	-.15(10)	-.19(10)
O(1)	2.78(18)	1.81(16)	2.18(16)	.26(13)	-.51(13)	-.17(12)
O(2)	2.15(17)	2.54(17)	2.82(17)	-.27(13)	.25(13)	-.48(14)
O(3)	2.35(16)	2.89(17)	1.75(16)	-.64(13)	-.24(12)	.43(12)
O(4)	1.47(15)	2.10(16)	1.82(15)	-.26(12)	-.23(12)	.23(12)
O(5)	7.3(3)	2.97(20)	2.12(18)	-.99(20)	-.71(18)	-.86(15)
O(6)	5.4(3)	4.86(26)	5.92(28)	1.26(21)	3.43(23)	-.47(22)
O(7)	1.15(16)	6.44(25)	3.13(23)	-.69(16)	-.49(13)	1.89(17)
O(8)	2.44(19)	4.88(24)	1.98(17)	-.80(17)	-1.10(14)	.69(16)
O(9)	2.39(15)	2.36(14)	2.05(15)	-.27(11)	-.80(13)	-.13(14)
O(10)	1.80(17)	3.11(19)	2.50(18)	.25(14)	-.85(14)	-.79(15)
O(11)	1.77(17)	2.29(18)	2.55(18)	.19(13)	-.37(13)	.11(13)
N(1)	2.49(18)	1.85(16)	2.24(18)	-.22(13)	-.31(20)	.18(18)
N(2)	1.22(19)	2.67(20)	1.51(17)	-.69(15)	-.43(14)	.38(15)
C(1)	2.69(29)	1.90(27)	2.37(26)	-.34(21)	-.65(20)	.57(20)
C(2)	2.49(27)	2.85(26)	2.82(26)	-.62(21)	-.51(20)	.97(21)
C(3)	4.5(4)	2.02(28)	2.6(3)	-.35(24)	-.54(24)	-.29(23)
C(4)	1.89(24)	2.29(24)	2.36(23)	-.20(18)	-.39(18)	-.28(19)
C(5)	3.49(29)	2.54(24)	3.4(3)	1.19(20)	.14(21)	.50(21)
C(6)	2.60(27)	3.7(3)	2.18(23)	.77(22)	-.11(21)	-.72(21)
C(7)	1.41(23)	3.83(29)	2.14(23)	-.42(20)	-.11(18)	.77(20)
C(8)	2.06(25)	2.43(23)	2.32(22)	-.16(19)	-.62(20)	.52(18)
C(9)	2.30(23)	3.29(24)	1.66(26)	-.46(18)	-.54(20)	.19(21)
C(10)	1.99(21)	1.96(19)	2.06(22)	-.20(16)	-.03(22)	.40(21)
W(1)	4.07(23)	2.67(19)	4.23(22)	.40(17)	-.01(17)	0. (16)
W(2)	9.3(5)	5.8(4)	9.4(5)	-1.2(3)	4.0(4)	-.50(29)
W(3)	17.2(7)	6.1(4)	3.60(26)	4.0(4)	-.5(3)	-.18(24)
W(4)	6.7(4)	12.4(6)	18.4(8)	1.0(4)	5.7(5)	6.7(6)
W(5)	14.9(8)	28.7(15)	11.4(7)	9.1(9)	7.5(6)	7.8(8)

	x	y	z	B
H(1)	.0858	.2760	-.0905	2.053
H(1")	.0432	.2422	-.1506	2.053
H(2)	.1583	.2486	-.1978	2.7149
H(2")	.1847	.2379	-.0735	2.7149
H(3)	.1436	.2478	.0845	4.9211
H(3")	.0729	.2684	.1266	4.9211
H(5)	-.0219	.2583	.0663	5.7663
H(5")	-.041	.2375	-.0485	5.7663
H(7)	.2534	.1999	-.1931	2.4598
H(7")	.2252	.1560	-.1922	2.4598
H(9)	.119	.2079	-.2993	2.3278
H(9")	.1360	.1654	-.3067	2.3278
H(09)	-.0109	.0920	-.0843	5.1662
H(09"	.0083	.0793	.0256	5.1662
H(C10	.1725	.0975	-.1021	2.7501
H(C10	.1132	.1005	-.174	2.7501
H(C11	.1739	.1030	.1068	4.4834
H(C11	.1112	.0827	.1196	4.4834
H(W1)	.0366	.0311	.167	4.5397
H(W1"	.0839	.0184	.0831	4.5397

ATOM	B11	B22	B33	B12	B13	B23
SM	1.403(10)	1.460(10)	1.326(10)	-.045(12)	-.187(12)	-.004(13)
NA	3.44(15)	3.11(15)	3.70(15)	.85(12)	-.10(12)	-.49(12)
O(1)	3.12(24)	1.60(20)	2.18(21)	.15(17)	-.34(17)	.06(16)
O(2)	2.03(20)	2.51(22)	2.55(21)	.20(17)	.21(17)	-.40(17)
O(3)	1.83(19)	3.05(22)	1.63(21)	-.30(17)	-.26(15)	.70(15)
O(4)	1.45(19)	2.54(22)	1.75(19)	-.33(17)	-.09(16)	.03(16)
O(5)	7.2(4)	2.48(24)	1.98(22)	-.70(24)	-.70(22)	-.88(18)
O(6)	5.1(3)	4.1(3)	5.6(3)	.89(25)	3.10(27)	-1.00(25)
O(7)	1.40(19)	6.4(3)	2.84(28)	-.63(21)	-.41(17)	1.80(21)
O(8)	2.61(23)	4.60(29)	1.88(21)	-1.00(22)	-1.05(18)	.44(20)
O(9)	2.20(18)	2.09(17)	2.11(19)	-.16(15)	-.47(17)	-.03(19)
O(10)	2.12(22)	2.71(24)	2.67(23)	.38(19)	-.72(18)	-1.17(19)
O(11)	1.77(21)	2.23(23)	2.53(23)	.37(17)	-.27(17)	.07(17)
N(1)	2.66(22)	1.86(20)	2.13(22)	-.21(17)	-.22(27)	.22(25)
N(2)	1.36(25)	2.79(27)	1.27(22)	-.54(20)	-.04(18)	.86(19)
C(1)	3.1(4)	2.8(4)	1.8(3)	.2(3)	-1.04(27)	.51(27)
C(2)	2.9(3)	2.2(3)	2.5(3)	-.85(26)	-1.04(25)	1.10(25)
C(3)	4.7(5)	1.4(3)	3.0(4)	-.6(3)	-.5(3)	-.73(28)
C(4)	3.0(4)	2.4(3)	2.3(3)	-.25(27)	-.58(25)	-.19(26)
C(5)	4.0(4)	2.6(3)	3.0(4)	1.11(27)	.41(29)	-.06(27)
C(6)	3.4(4)	3.4(4)	1.71(28)	.3(3)	-.13(28)	-.24(27)
C(7)	1.22(26)	3.3(3)	2.10(29)	-.04(25)	-.24(23)	.81(25)
C(8)	2.2(3)	2.5(3)	2.19(27)	-.63(26)	-.33(26)	.81(23)
C(9)	1.65(25)	3.7(3)	.9(3)	-.80(23)	-.14(22)	.26(24)
C(10)	1.96(25)	2.15(25)	1.67(28)	.13(21)	-.14(27)	.38(26)
W(1)	4.23(28)	2.14(22)	3.91(26)	.07(21)	-.08(21)	.28(19)
W(2)	9.1(5)	4.6(4)	9.1(5)	-.8(3)	3.9(4)	-.9(3)
W(3)	17.4(8)	5.0(4)	3.5(3)	4.0(5)	.2(4)	.06(27)
W(4)	6.9(5)	10.3(6)	15.3(7)	-.4(5)	3.8(5)	4.7(6)
W(5)	16.4(9)	20.6(11)	9.5(6)	8.6(8)	8.8(6)	7.1(7)

	x	y	z	B
H(1)	.082	.280	-.084	5.6088
H(1")	.039	.241	-.161	5.6088
H(2)	.163	.251	-.209	1.8497
H(2")	.188	.238	-.062	1.8497
H(3)	.149	.251	.081	5.3072
H(3")	.075	.270	.127	5.3072
H(5)	-.030	.259	.055	7.5213
H(5")	-.040	.233	-.057	7.5213
H(7)	.254	.201	-.207	5.081
H(7")	.224	.152	-.202	5.081
H((9)	.118	.210	-.318	5.1889
H((9"	.145	.162	-.312	5.1889
H(09)	-.014	.091	-.089	5.9598
H(09"	.020	.075	.021	5.9598
H(010	.180	.096	-.112	3.2849
H(010	.112	.093	-.174	3.2849
H(011	.185	.101	.107	8.6647
H(011	.109	.080	.117	8.6647
H(W1)	.037	.035	.179	11.6777
H(W1"	.090	.019	.077	11.6777

ATOM	B11	B22	B33	B12	B13	B23
PR	1.734(12)	1.641(12)	1.634(12)	-.023(14)	-.226(15)	-.066(15)
NA	3.81(17)	3.60(17)	3.95(17)	1.04(13)	.10(14)	-.48(13)
O(1)	3.79(28)	1.94(22)	2.41(23)	.13(19)	-.42(20)	.14(18)
O(2)	2.75(25)	3.03(25)	3.20(26)	.05(20)	.04(20)	-.97(20)
O(3)	2.24(22)	3.59(24)	1.77(24)	-.26(19)	-.36(17)	.51(17)
O(4)	2.05(23)	2.60(24)	2.10(22)	-.25(18)	.03(18)	.07(18)
O(5)	9.4(5)	3.3(3)	2.61(27)	-1.0(3)	-.2(3)	-1.23(22)
O(6)	6.1(4)	5.6(4)	6.0(4)	1.6(3)	2.9(3)	-1.0(3)
O(7)	1.93(24)	6.9(4)	3.5(3)	-.56(24)	-.68(20)	2.27(25)
O(8)	3.02(27)	4.5(3)	2.15(24)	-.71(23)	-1.34(21)	.72(22)
O(9)	2.91(22)	2.60(20)	2.95(23)	-.15(17)	-.80(21)	.04(23)
O(10)	1.56(23)	3.60(28)	3.30(27)	.39(20)	-.71(20)	-1.10(21)
O(11)	2.60(25)	2.35(25)	2.30(24)	-.00(19)	-.33(19)	.25(18)
N(1)	3.48(28)	2.23(22)	2.20(25)	-.01(20)	-.5(3)	.64(27)
N(2)	1.91(29)	3.2(3)	1.31(23)	-1.03(22)	-.22(20)	.82(21)
C(1)	3.3(4)	3.1(4)	2.0(3)	-1.2(3)	-1.1(3)	1.3(3)
C(2)	4.0(4)	2.1(3)	2.7(4)	-.8(3)	-.6(3)	.84(26)
C(3)	5.5(5)	2.1(4)	3.9(5)	-1.2(4)	-1.5(4)	.2(3)
C(4)	3.7(4)	2.4(4)	3.0(4)	-.4(3)	-.5(3)	-.09(29)
C(5)	4.6(5)	2.7(3)	4.1(5)	1.4(3)	.1(4)	.1(3)
C(6)	3.7(4)	4.2(5)	2.9(4)	.1(4)	-.1(3)	-.9(3)
C(7)	1.3(3)	3.8(4)	2.9(3)	-.25(27)	-.36(27)	.8(3)
C(8)	2.2(3)	3.0(3)	2.6(3)	-.52(29)	-.6(3)	.91(27)
C(9)	2.7(3)	4.0(4)	1.4(4)	-.71(28)	-.14(27)	.28(28)
C(10)	2.06(29)	2.29(28)	2.8(4)	.26(23)	.0(3)	.4(3)
W(1)	4.9(3)	2.62(26)	4.9(3)	.69(25)	-.13(26)	.73(23)
W(2)	10.8(7)	5.7(4)	11.8(8)	-1.1(4)	4.9(6)	-.8(4)
W(3)	20.4(10)	5.9(5)	4.0(4)	4.6(6)	.6(5)	.1(3)
W(4)	7.5(6)	10.9(7)	16.1(9)	-.9(5)	2.8(6)	2.3(7)
W(5)	17.0(11)	19.6(13)	10.5(8)	7.8(10)	8.4(8)	5.1(9)

	x	y	z	B
H(1)	.082	.280	-.084	5.6088
H(1")	.039	.241	-.161	5.6088
H(2)	.163	.251	-.209	1.8497
H(2")	.188	.238	-.062	1.8497
H(3)	.149	.251	.081	5.3072
H(3")	.075	.270	.127	5.3072
H(5)	-.030	.259	.055	7.5213
H(5")	-.040	.233	-.057	7.5213
H(7)	.254	.201	-.207	5.081
H(7")	.224	.152	-.202	5.081
H(9)	.118	.210	-.318	5.1889
H(9")	.145	.162	-.312	5.1889
H(09)	-.014	.091	-.089	5.9598
H(09"	.020	.075	.021	5.9598
H(010	.180	.096	-.112	3.2849
H(010	.112	.093	-.174	3.2849
H(011	.185	.101	.107	8.6647
H(011	.109	.080	.117	8.6647
H(W1)	.037	.035	.179	11.6777
H(W1"	.090	.019	.077	11.6777

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 5.0)
NAPR(EDTA).8H2O F(0,0,0) = 5833

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	0,		0	-4	708	16	3	2	503	12	3	3	652	14	14	-13	147	17	-5
-12	453	12	13	0	1092	23	20	6	524	13	2	5	275	9	4	-11	260	11	-9
-8	613	14	4	4	702	15	8	10	393	13	-8	7	480	11	11	-9	243	10	6
-4	798	17	-4	8	354	10	-6	H,K=	0,		28	9	314	10	9	-7	275	9	5
4	852	18	-13	12	235	11	10	-8	164	14	0	11	196	12	-8	-5	461	11	-3
8	595	14	17	H,K=	0,		14	-4	335	11	-8	13	156	22	-2	-3	318	8	-10
12	430	12	-7	-10	330	11	-7	0	95	18	-2	H,K=	1,		3	-1	86	22	-21
H,K=	0,		2	-6	402	11	-2	4	367	11	4	-13	249	11	4	1	30	55	-20*
-14	148	13	22	-2	210	8	-6	8	182	12	13	-11	396	12	6	3	338	8	2
-10	158	11	3	2	234	8	10	H,K=	0,		30	-9	379	11	-11	5	470	11	6
-6	461	12	3	6	407	10	-6	-10	213	21	-7	-7	522	12	1	7	272	9	7
-2	420	10	21	10	341	11	6	-6	249	11	-4	-5	449	10	-3	9	258	10	2
2	421	10	24	H,K=	0,		16	-2	253	10	-0	-3	479	10	14	11	267	11	-10
6	469	11	7	-12	329	12	4	2	251	10	-11	-1	908	19	-38	13	149	15	-9
10	178	11	16	-8	631	15	-7	6	280	11	19	1	921	19	-27	H,K=	1,		11
14	141	23	7	-4	757	17	1	10	201	13	-13	3	493	11	10	-13	170	14	-1
H,K=	0,		4	0	880	18	0	H,K=	0,		32	5	495	11	6	-11	114	18	-31
-12	330	15	15	4	773	17	7	-8	278	12	-11	7	530	12	-2	-9	223	10	4
-8	459	13	6	8	637	15	-7	-4	448	12	-1	9	363	10	-4	-7	238	9	4
-4	711	15	3	12	336	12	9	0	311	10	-8	11	389	12	-0	-5	249	8	-2
0	1061	22	112	H,K=	0,		18	4	444	12	9	13	231	13	-13	-3	636	14	-9
4	734	15	14	-10	0	56	-3*	8	279	14	-3	H,K=	1,		5	-1	815	17	10
8	433	11	-3	-6	191	14	-1	H,K=	0,		34	-13	115	17	-5	1	833	17	20
12	295	11	-5	-2	269	8	-1	-6	43	50	16*	-11	146	14	-3	3	644	14	-4
H,K=	0,		6	2	284	8	9	-2	52	67	-13*	-9	125	11	12	5	254	8	-7
-14	233	14	-0	6	198	9	4	2	30	53	-34*	-7	213	8	6	7	238	10	-9
-10	213	11	2	10	0	54	-10*	6	33	65	3*	-5	640	15	14	9	223	10	7
-6	812	18	-3	H,K=	0,		20	H,K=	0,		36	-3	194	10	-3	11	135	14	3
-2	650	14	-7	-12	300	13	-10	-4	402	12	-3	-1	496	11	-13	13	172	14	2
2	658	14	-4	-8	570	14	-10	0	426	12	-18	1	484	11	-10	H,K=	1,		13
6	801	18	-9	-4	358	10	-15	4	387	12	-12	3	177	15	-0	-13	234	12	2
10	233	11	-1	0	344	10	-8	H,K=	0,		38	5	646	14	22	-11	245	15	-6
14	256	12	15	4	390	10	8	-6	287	16	25	7	214	8	5	-9	328	11	-16
H,K=	0,		8	8	591	14	11	-2	169	13	-2	9	151	12	18	-7	472	11	2
-12	68	24	46	12	317	12	4	2	138	21	-25	11	181	12	9	-5	545	13	-9
-8	266	9	9	H,K=	0,		22	6	285	12	22	13	133	13	10	-3	661	15	13
-4	390	9	6	-10	305	11	-0	H,K=	0,		40	H,K=	1,		7	-1	657	14	-12
0	234	6	-3	-6	297	10	4	-4	218	12	13	-13	187	13	-15	1	625	13	-7
4	397	9	2	-2	511	12	3	0	195	12	7	-11	288	11	5	3	637	14	11
8	257	9	-7	2	504	14	-8	4	195	13	-4	-9	284	10	1	5	585	13	21
H,K=	0,		10	6	305	11	-1	H,K=	0,		42	-7	265	11	-5	7	480	12	2
-14	297	12	10	10	312	12	7	-2	325	13	16	-5	552	12	2	9	346	11	-9
-10	534	14	-15	H,K=	0,		24	2	304	12	-4	-3	746	16	-1	11	266	19	9
-6	559	13	-15	-8	239	11	-0	H,K=	1,		1	-1	453	10	3	13	244	12	5
-2	918	19	-1	-4	279	10	-6	-13	143	15	-11	1	469	10	15	H,K=	1,		15
2	911	19	6	0	197	9	5	-11	175	12	-20	3	756	16	10	-13	159	15	-7
6	552	12	-10	4	289	9	9	-9	324	11	7	5	593	13	10	-11	242	11	12
10	537	13	-20	8	237	11	-2	-7	457	13	-4	7	272	9	5	-9	300	11	3
14	286	13	-9	H,K=	0,		26	-5	277	8	-1	9	273	10	9	-7	246	10	-1
H,K=	0,		12	-10	418	13	15	-3	650	14	6	11	269	11	-6	-5	225	8	4
-12	235	15	7	-6	508	14	-3	-1	633	15	-55	13	208	14	11	-3	503	11	9
-8	354	10	-0	-2	510	12	-4	1	635	16	-47	H,K=	1,		9	-1	494	11	8

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	530	12	19	3	402	10	9	-3	177	12	-6	4	139	8	13	-10	72	22	31
3	500	12	6	5	310	12	8	-1	255	10	13	6	832	18	-3	-8	286	9	5
5	237	8	4	7	348	11	-6	1	245	17	-3	8	171	10	-3	-6	158	9	2
7	226	9	-5	9	227	13	-11	3	182	17	2	10	466	12	-2	-4	260	8	-5
9	296	11	-3	11	187	13	5	5	246	13	13	12	138	13	7	-2	341	8	9
11	219	11	-7	H,K=	1,	25		7	174	14	-8	14	208	14	-20	0	632	13	24
13	150	15	-11	-11	161	14	2	9	165	17	-8	H,K=	2,	4		2	355	9	5
H,K=	1,	17		-9	200	12	-3	H,K=	1,	35		-14	170	14	21	4	283	9	-11
-13	191	16	6	-7	303	11	1	-7	192	13	3	-12	268	17	-1	6	161	9	-7
-11	155	13	19	-5	226	10	17	-5	238	21	-4	-10	135	13	-14	8	286	10	7
-9	292	11	2	-3	219	11	11	-3	185	11	9	-8	256	10	-5	10	58	35	0
-7	271	9	5	-1	373	10	8	-1	200	13	-4	-6	320	9	-6	12	200	12	0
-5	478	12	18	1	366	10	6	1	206	11	-9	-4	837	18	3	H,K=	2,	12	
-3	317	9	1	3	215	11	-15	3	185	11	9	-2	225	7	7	-12	277	17	13
-1	395	10	-2	5	229	10	-0	5	236	12	6	0	939	19	38	-10	96	19	-19
1	399	10	3	7	271	12	-17	7	192	13	6	2	188	8	-4	-8	343	10	-11
3	334	9	21	9	212	11	11	H,K=	1,	37		4	834	17	11	-6	232	9	-7
5	455	11	8	11	172	17	14	-7	118	19	-26	6	329	9	8	-4	742	17	0
7	247	10	-3	H,K=	1,	27		-5	104	17	3	8	253	9	0	-2	161	7	7
9	273	14	-17	-11	128	16	6	-3	186	13	-10	10	129	16	-7	0	319	8	-7
11	136	13	11	-9	167	17	-5	-1	162	13	12	12	277	11	3	2	159	7	6
13	191	13	-1	-7	203	12	-8	1	153	17	-2	14	149	15	4	4	769	17	15
H,K=	1,	19		-5	178	12	-4	3	200	11	12	H,K=	2,	6		6	249	9	5
-11	231	19	17	-3	204	10	-1	5	94	23	-10	-14	95	25	-14	8	380	10	16
-9	292	12	2	-1	256	10	5	7	135	17	-9	-12	239	14	-4	10	121	15	4
-7	356	10	3	1	252	10	-2	H,K=	1,	39		-10	183	11	3	12	276	19	16
-5	358	10	-13	3	194	12	-3	-5	188	14	-10	-8	232	11	1	H,K=	2,	14	
-3	244	8	1	5	183	11	4	-3	252	13	3	-6	360	9	-5	-12	50	66	-23*
-1	478	11	5	7	203	11	-10	-1	191	12	-7	-4	12	44	-44*	-10	400	14	-4
1	474	11	-4	9	152	15	-19	1	200	13	-2	-2	527	11	2	-8	127	13	-16
3	229	8	-1	11	110	21	-12	3	249	16	-1	0	252	6	21	-6	433	11	-6
5	362	13	-15	H,K=	1,	29		5	177	15	-14	2	528	11	1	-4	300	8	-0
7	328	10	-3	-9	200	14	-1	H,K=	1,	41		4	73	29	-30	-2	775	17	16
9	297	11	7	-7	254	11	12	-3	130	18	-20	6	346	9	-6	0	0	39	-19*
11	210	12	-3	-5	356	11	-20	-1	152	15	-6	8	230	9	6	2	772	16	3
H,K=	1,	21		-3	335	10	-8	1	150	17	-14	10	189	11	8	4	293	8	0
-11	174	15	24	-1	299	10	10	3	151	15	4	12	238	11	4	6	440	12	-2
-9	216	12	-4	1	296	10	2	H,K=	2,	0		14	117	29	6	8	128	15	-12
-7	227	10	-2	3	324	11	-10	-14	191	14	-18	H,K=	2,	8		10	401	15	4
-5	242	9	2	5	382	11	8	-10	365	11	1	-14	0	70	-25*	12	115	15	28
-3	76	16	-13	7	221	18	-28	-6	456	11	-5	-12	431	12	6	H,K=	2,	16	
-1	219	8	0	9	209	13	5	-2	491	10	-31	-10	43	69	-19*	-12	80	34	-46
1	229	8	11	H,K=	1,	31		2	539	12	-25	-8	438	12	-15	-10	205	21	-20
3	59	25	-20	-9	118	17	-1	6	444	10	-9	-6	151	10	1	-8	60	30	2
5	241	9	1	-5	238	15	10	10	360	11	-3	-4	773	17	-3	-6	463	11	-6
7	195	15	-16	-3	152	25	5	14	198	19	-11	-2	519	11	8	-4	285	8	2
9	236	11	5	-1	143	13	-16	H,K=	2,	2		0	587	12	-5	-2	458	11	-0
11	167	13	20	1	154	12	-8	-14	246	12	20	2	513	11	7	0	408	11	10
H,K=	1,	23		3	131	14	-3	-12	136	14	2	4	780	17	16	2	455	11	9
-11	166	15	-15	5	252	11	23	-10	466	12	18	6	143	9	-6	4	273	8	-9
-9	223	11	-3	7	106	17	12	-8	153	15	-11	8	453	11	-4	6	480	12	20
-7	333	11	-16	9	125	16	6	-6	812	18	-19	10	83	17	18	8	77	20	29
-5	292	10	-5	H,K=	1,	33		-4	144	8	11	12	433	13	11	10	211	11	-14
-3	403	10	-7	-9	192	12	17	-2	648	14	49	14	0	66	-23*	12	124	15	4
-1	469	12	-7	-7	162	15	-16	0	380	11	-27	H,K=	2,	10		H,K=	2,	18	
1	458	11	-12	-5	239	11	1	2	618	13	45	-12	181	14	-18	-12	118	16	14

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-10	376	12	5	-4	319	10	-11	0	214	12	10	-5	765	17	14	-13	0	60	-28*
-8	80	26	32	-2	118	12	4	2	235	17	1	-3	566	12	-22	-11	90	16	33
-6	418	13	-6	0	294	9	7	4	79	23	25	-1	343	8	3	-9	73	28	-9
-4	119	10	14	2	122	11	11	6	182	17	4	1	331	8	8	-7	104	14	3
-2	869	19	6	4	330	10	-7	H,K=	2,	38		3	582	12	-8	-5	118	15	-15
0	223	8	-1	6	39	51	-11*	-6	231	13	-0	5	748	16	18	-3	313	8	16
2	875	20	-3	8	195	12	0	-4	167	12	16	7	514	13	-0	-1	239	7	-2
4	99	15	-13	10	43	54	25*	-2	246	12	-9	9	410	12	2	1	244	8	4
6	434	11	7	H,K=	2,	28		0	58	58	-13*	11	322	11	12	3	299	8	2
8	38	49	-4*	-10	81	32	9	2	263	11	9	13	220	13	-8	5	129	9	-1
10	372	12	0	-8	300	13	1	4	155	14	6	H,K=	3,	7		7	108	14	6
12	83	43	-19	-6	150	13	-7	6	219	13	-8	-13	144	17	12	9	69	25	-14
H,K=	2,	20		-4	439	12	5	H,K=	2,	40		-11	232	18	-17	11	66	28	9
-12	111	19	3	-2	200	10	-2	-4	240	19	2	-9	213	9	12	13	22	55	-4*
-10	199	11	-8	0	407	11	-8	-2	81	27	-7	-7	136	10	-4	H,K=	3,	15	
-8	286	13	-10	2	191	11	-4	0	295	15	-13	-5	341	9	-4	-13	213	14	-6
-6	264	10	9	4	409	11	-13	2	67	50	-22	-3	490	11	16	-11	201	12	-3
-4	348	10	-2	6	151	15	-4	4	247	14	8	-1	191	7	5	-9	231	13	-5
-2	476	11	1	8	293	13	4	H,K=	2,	42		1	174	13	9	-7	393	11	6
0	61	16	36	10	77	24	2	-2	47	70	-18*	3	537	12	28	-5	580	13	-1
2	463	11	-1	H,K=	2,	30		0	146	14	8	5	347	9	6	-3	660	14	5
4	351	10	11	-10	167	15	-11	2	0	59	-68*	7	168	11	12	-1	542	12	-9
6	234	10	-9	-8	112	20	-18	H,K=	3,	1		9	197	13	9	1	530	12	-2
8	300	11	1	-6	347	16	-2	-13	186	12	-2	11	232	12	-15	3	668	15	2
10	210	12	7	-4	159	13	-8	-11	394	11	4	13	126	19	-6	5	581	13	2
12	105	22	-7	-2	288	10	-6	-9	380	11	-8	H,K=	3,	9		7	376	12	5
H,K=	2,	22		0	89	19	9	-7	586	14	8	-13	206	15	6	9	262	10	16
-12	128	38	-15	2	288	10	2	-5	367	9	4	-11	200	12	-4	11	197	13	-18
-10	197	19	-3	4	165	11	13	-3	506	11	6	-9	421	11	6	13	209	13	-1
-8	149	12	6	6	355	11	6	-1	532	11	16	-7	196	13	-11	H,K=	3,	17	
-6	274	10	6	8	147	13	6	1	547	11	33	-5	284	8	-10	-13	183	15	5
-4	113	18	-23	10	168	15	-13	3	549	12	21	-3	445	10	-12	-11	199	12	6
-2	382	10	-13	H,K=	2,	32		5	354	9	3	-1	834	18	8	-9	292	10	9
0	282	9	2	-8	106	28	2	7	595	13	10	1	844	18	6	-7	270	9	2
2	406	10	12	-6	198	12	-1	9	379	11	-1	3	475	11	-3	-5	375	10	-1
4	139	13	-16	-4	207	11	-4	11	410	12	8	5	253	8	-4	-3	311	9	-19
6	260	10	-6	-2	259	10	2	13	182	13	1	7	208	9	6	-1	444	10	-9
8	120	14	-5	0	68	28	3	H,K=	3,	3		9	410	11	-3	1	444	10	-3
10	205	11	13	2	254	10	4	-13	62	67	12*	11	206	11	-5	3	333	9	18
12	154	19	13	4	189	12	-8	-11	0	56	-47*	13	215	15	17	5	376	10	-12
H,K=	2,	24		6	220	11	23	-9	62	31	-7	H,K=	3,	11		7	258	10	-6
-10	66	31	-20	8	88	23	-18	-7	354	10	-2	-13	249	13	8	9	265	11	-10
-8	453	12	-17	H,K=	2,	34		-5	245	8	9	-11	386	12	-13	11	174	16	-20
-6	158	11	9	-8	88	22	35	-3	329	8	-2	-9	207	11	-10	13	166	17	-9
-4	367	10	6	-6	260	12	-4	-1	77	14	-1	-7	474	13	-1	H,K=	3,	19	
-2	214	9	17	-4	0	78	-38*	1	65	13	0	-5	413	10	-10	-11	107	16	12
0	485	12	16	-2	375	12	6	3	348	9	-1	-3	640	14	-12	-9	115	13	12
2	188	10	-7	0	0	69	-1*	5	226	8	5	-1	593	13	-2	-7	115	14	-3
4	358	11	-10	2	380	12	-2	7	350	12	5	1	588	13	2	-5	166	9	8
6	139	14	-12	4	42	55	3*	9	79	57	0	3	689	15	8	-3	230	8	5
8	470	12	1	6	272	12	7	11	70	21	19	5	422	10	-8	-1	399	11	4
10	105	16	17	8	51	69	-2*	H,K=	3,	5		7	453	11	-12	1	397	10	-0
H,K=	2,	26		H,K=	2,	36		-13	239	13	6	9	223	11	2	3	239	9	9
-10	0	58	-17*	-6	181	13	5	-11	321	17	9	11	394	12	2	5	152	11	-8
-8	180	14	-10	-4	7	57	-48*	-9	394	11	-6	13	210	14	-27	7	90	25	-18
-6	58	38	4	-2	220	12	-7	-7	487	13	-5	H,K=	3,	13		9	128	13	5

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
11	98	19	-2	-5	79	20	-3	H,K=	4,	0		H,K=	4,	8		H,K=	4,	16	
H,K=	3,	21		-3	64	27	-8	-12	116	15	14	-12	47	53	4*	-12	119	20	14
-11	233	12	-4	-1	68	24	28	-8	314	10	-2	-10	352	11	2	-10	54	67	19*
-9	359	12	6	1	61	42	10	-4	231	7	4	-8	66	28	23	-8	316	11	2
-7	296	11	-16	3	91	17	9	0	841	17	7	-6	550	13	-18	-6	179	10	-11
-5	383	10	0	5	70	26	-8	4	184	11	4	-4	396	10	1	-4	293	9	-4
-3	421	11	1	7	0	66	-23*	8	321	10	10	-2	773	16	0	-2	219	8	-22
-1	674	16	-16	9	53	58	-8*	12	126	14	13	0	442	11	-13	0	138	15	-13
1	665	15	-5	H,K=	3,	31		H,K=	4,	2		2	782	16	-1	2	234	8	-6
3	433	11	4	-9	247	11	13	-14	61	37	-7	4	409	10	9	4	289	9	3
5	378	10	6	-7	228	12	6	-12	321	14	-6	6	534	12	-18	6	201	9	-3
7	300	11	2	-5	370	12	-5	-10	191	11	7	8	0	66	-46*	8	342	10	17
9	333	12	-19	-3	308	13	-11	-8	518	14	-14	10	352	12	6	10	83	17	46
11	232	12	1	-1	376	11	16	-6	184	8	-6	12	27	57	-13*	12	126	35	13
H,K=	3,	23		1	350	13	-3	-4	912	20	-8	H,K=	4,	10		H,K=	4,	18	
-11	0	60	-59*	3	310	10	-2	-2	293	9	15	-12	95	18	8	-12	281	16	-5
-9	17	58	-36*	5	359	11	-8	0	821	17	16	-10	356	12	13	-10	86	19	-23
-7	160	11	-1	7	228	12	-5	2	289	9	22	-8	153	10	8	-8	418	13	-2
-5	143	12	1	9	259	12	26	4	899	19	9	-6	316	10	-2	-6	47	61	24*
-3	161	15	-8	H,K=	3,	33		6	177	9	-7	-4	364	9	-0	-4	491	12	-12
-1	203	9	-6	-7	69	32	-5	8	521	12	-0	-2	542	13	0	-2	111	11	11
1	178	10	-12	-5	121	17	-11	10	182	14	1	0	192	8	2	0	493	11	-4
3	161	10	5	-3	167	13	-16	12	315	11	-7	2	531	12	6	2	108	14	5
5	160	11	10	-1	251	12	-7	14	69	41	2	4	338	9	-5	4	518	12	-4
7	153	13	-2	1	250	12	-11	H,K=	4,	4		6	297	9	0	6	54	29	25
9	44	56	-21*	3	188	11	0	-14	185	14	1	8	144	11	6	8	402	11	-10
11	48	57	-10*	5	105	22	-26	-12	124	16	0	10	337	11	4	10	110	16	5
H,K=	3,	25		7	71	30	-6	-10	302	14	-3	12	101	19	22	12	302	15	12
-11	224	11	21	H,K=	3,	35		-8	222	9	-4	H,K=	4,	12		H,K=	4,	20	
-9	163	11	-1	-7	126	33	-31	-6	452	11	-18	-12	86	24	4	-12	160	16	12
-7	313	10	3	-5	174	13	-2	-4	290	8	-0	-10	364	11	-6	-10	112	26	-8
-5	322	10	11	-3	184	20	-23	-2	471	11	-2	-8	222	10	10	-8	279	10	0
-3	371	10	-12	-1	123	15	-6	0	234	9	28	-6	465	13	-10	-6	288	10	-17
-1	371	10	-10	1	98	21	-34	2	476	12	20	-4	295	8	2	-4	119	11	-7
1	378	11	-6	3	221	11	11	4	312	8	8	-2	696	15	1	-2	312	12	-13
3	378	12	-18	5	170	14	-4	6	464	11	0	0	178	8	4	0	443	11	0
5	300	10	-5	7	159	15	-6	8	233	10	4	2	698	15	2	2	285	10	-9
7	308	11	-4	H,K=	3,	37		10	300	14	-0	4	300	9	16	4	138	12	-3
9	153	20	-8	-5	207	17	-1	12	143	17	16	6	486	12	5	6	293	10	-12
11	196	14	-5	-3	222	13	-20	14	174	15	-10	8	218	10	1	8	282	10	-1
H,K=	3,	27		-1	254	12	-18	H,K=	4,	6		10	375	11	-2	10	152	15	20
-11	160	19	-3	1	265	12	-5	-14	134	18	0	12	96	31	2	12	142	17	-9
-9	155	12	-1	3	246	11	-5	-12	179	15	-8	H,K=	4,	14		H,K=	4,	22	
-7	352	11	2	5	195	15	-13	-10	270	10	-4	-12	304	12	-18	-12	186	13	12
-5	383	11	9	H,K=	3,	39		-8	215	9	6	-10	93	17	7	-10	139	13	13
-3	362	11	1	-5	70	28	30	-6	384	10	1	-8	377	11	-17	-8	240	10	-0
-1	312	12	-10	-3	48	58	-5*	-4	237	7	-10	-6	378	10	3	-6	156	12	-26
1	299	10	-11	-1	75	27	24	-2	503	11	-6	-4	545	12	2	-4	374	10	6
3	335	11	-14	1	41	59	-12*	0	140	11	4	-2	149	8	5	-2	426	12	7
5	380	11	9	3	65	29	17	2	496	11	-5	0	724	16	-8	0	264	9	-4
7	345	11	1	5	0	56	-44*	4	248	8	-3	2	150	8	17	2	425	11	0
9	158	14	-8	H,K=	3,	41		6	385	10	-2	4	545	12	-2	4	376	11	1
11	185	13	13	-3	230	12	2	8	216	10	2	6	356	10	-13	6	198	10	14
H,K=	3,	29		-1	170	16	-24	10	267	11	-3	8	378	11	-6	8	261	10	3
-9	61	71	6*	1	185	14	-18	12	171	14	-17	10	110	15	17	10	133	14	13
-7	26	51	4*	3	219	13	-11	14	134	18	3	12	317	13	6	12	148	19	-25

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		4,	24	H,K=		4,	34	3	613	13	11	-5	151	9	-9	-7	292	10	-4
-10	325	11	4	-8	285	12	12	5	364	9	8	-3	358	9	-4	-5	338	13	4
-8	82	20	6	-6	24	53	9*	7	483	11	8	-1	385	9	2	-3	325	9	9
-6	410	11	4	-4	287	11	-11	9	368	11	-4	1	383	9	9	-1	309	9	-1
-4	0	52	-34*	-2	22	52	-14*	11	256	11	-6	3	343	9	8	1	321	10	9
-2	506	12	-5	0	424	14	-2	13	172	44	-26	5	173	8	-3	3	318	13	-2
0	310	9	3	2	0	51	-35*	H,K=		5,	5	7	286	9	10	5	331	10	6
2	512	12	1	4	291	11	-11	-13	103	22	-21	9	223	12	-12	7	293	10	-4
4	63	25	16	6	45	55	30*	-11	126	15	2	11	190	13	-16	9	302	11	4
6	408	11	4	8	258	13	-13	-9	185	10	9	13	174	13	7	11	129	16	12
8	27	71	-45*	H,K=		4,	36	-7	323	9	3	H,K=		5,	13	H,K=		5,	21
10	331	11	5	-6	90	20	11	-5	676	16	9	-13	202	14	-18	-11	48	71	-26*
H,K=		4,	26	-4	148	18	-6	-3	203	8	-4	-11	269	11	0	-9	125	15	-4
-10	123	17	-6	-2	121	16	6	-1	146	13	9	-9	373	13	4	-7	171	13	6
-8	0	55	-48*	0	205	12	-4	1	94	11	-4	-7	418	12	-3	-5	246	9	-16
-6	249	10	-2	2	136	15	18	3	189	7	2	-5	374	11	-6	-3	236	9	-10
-4	86	20	25	4	148	16	-8	5	696	15	26	-3	575	13	-4	-1	81	14	-3
-2	314	10	11	6	84	22	-5	7	308	9	-2	-1	393	9	6	1	76	17	-24
0	0	73	-14*	H,K=		4,	38	9	166	11	-11	1	396	10	-4	3	233	9	-5
2	290	10	-6	-6	104	30	-3	11	111	17	-4	3	556	12	3	5	268	10	-3
4	67	23	4	-4	278	11	5	13	100	21	-24	5	390	11	10	7	172	11	-5
6	235	11	-18	-2	82	34	-3	H,K=		5,	7	7	416	11	-6	9	120	18	-17
8	75	22	26	0	257	11	11	-13	234	12	2	9	350	11	-10	11	106	18	26
10	130	17	13	2	92	24	1	-11	206	10	33	11	268	11	-0	H,K=		5,	23
H,K=		4,	28	4	280	14	9	-9	306	10	-3	13	222	17	4	-11	193	14	-5
-10	322	12	16	6	110	19	6	-7	393	10	10	H,K=		5,	15	-9	250	11	2
-8	52	67	4*	H,K=		4,	40	-5	322	9	-5	-13	107	28	-18	-7	277	12	-4
-6	347	11	-14	-4	67	32	0	-3	667	15	-6	-11	154	14	-3	-5	252	10	-6
-4	142	12	-7	-2	288	12	14	-1	522	11	1	-9	216	10	10	-3	392	10	4
-2	471	12	-12	0	99	15	62	1	509	11	13	-7	321	10	-3	-1	400	11	-1
0	0	54	-50*	2	265	13	-11	3	665	14	12	-5	151	9	-7	1	392	10	0
2	491	12	-7	4	87	24	11	5	327	9	-8	-3	276	9	7	3	402	11	20
4	167	13	9	H,K=		5,	1	7	388	10	0	-1	371	9	19	5	286	10	4
6	353	11	-16	-13	149	15	-5	9	310	10	6	1	377	9	12	7	288	10	4
8	6	64	-38*	-11	267	11	8	11	144	14	-12	3	253	8	-3	9	260	20	12
10	287	13	-17	-9	166	12	-8	13	239	12	-5	5	179	9	-4	11	196	14	-5
H,K=		4,	30	-7	256	9	-3	H,K=		5,	9	7	322	10	4	H,K=		5,	25
-8	212	15	0	-5	423	10	-2	-13	154	19	-9	9	199	11	-6	-11	171	19	-2
-6	153	20	-1	-3	350	9	-7	-11	208	12	-6	11	155	13	2	-9	216	12	-3
-4	322	11	4	-1	555	12	-10	-9	330	11	1	13	146	14	28	-7	164	16	11
-2	256	11	8	1	574	12	11	-7	391	10	-14	H,K=		5,	17	-5	174	11	-4
0	284	11	7	3	327	8	3	-5	552	13	-2	-11	208	12	2	-3	363	10	14
2	275	10	15	5	423	10	-9	-3	370	9	-12	-9	266	10	12	-1	384	11	-12
4	322	11	0	7	258	9	-7	-1	440	10	-6	-7	257	11	-12	1	415	12	10
6	162	13	-1	9	172	11	-9	1	424	10	-7	-5	409	10	0	3	365	10	8
8	244	11	25	11	258	10	-3	3	355	9	-3	-3	410	10	-7	5	168	11	-2
H,K=		4,	32	13	167	13	15	5	558	13	13	-1	343	9	-1	7	107	16	-30
-8	87	23	-6	H,K=		5,	3	7	403	10	4	1	332	9	-1	9	216	12	1
-6	108	16	-10	-13	208	12	13	9	317	13	-14	3	425	12	8	11	176	14	8
-4	244	10	1	-11	259	20	-15	11	221	11	9	5	421	12	-0	H,K=		5,	27
-2	146	12	3	-9	370	14	-20	13	174	14	12	7	265	10	4	-9	203	12	-15
0	300	10	0	-7	450	12	-4	H,K=		5,	11	9	259	11	1	-7	219	10	11
2	149	12	7	-5	390	11	-4	-13	157	16	-8	11	208	12	-1	-5	253	10	18
4	258	10	16	-3	620	13	4	-11	178	17	-17	H,K=		5,	19	-3	212	11	-13
6	99	19	-25	-1	564	12	-8	-9	230	13	-5	-11	106	20	-7	-1	358	11	-13
8	90	22	-2	1	613	13	2	-7	272	9	-4	-9	280	11	-5	1	383	11	1

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	243	10	10	H,K=	5,	41		-6	64	20	7	-6	617	15	-3	2	44	50	-31*
5	240	11	-4	-1	126	16	6	-4	268	8	21	-4	159	9	1	4	0	51	-49*
7	215	12	5	1	116	20	-8	-2	160	8	-0	-2	603	13	-19	6	196	11	-6
9	213	13	1	H,K=	6,		0	0	459	10	8	0	0	40	-3*	8	92	23	-15
H,K=	5,	29		-10	613	15	4	2	170	9	11	2	608	14	-18	10	84	22	-14
-9	169	12	1	-6	467	13	-4	4	262	8	14	4	148	10	-10	H,K=	6,	26	
-7	230	12	-5	-2	849	19	-10	6	48	38	-0	6	619	14	1	-10	37	72	3*
-5	298	11	-15	2	914	19	11	8	75	21	-5	8	0	62	-28*	-8	410	12	0
-3	388	11	14	6	465	11	-8	10	79	18	21	10	398	13	3	-6	73	26	34
-1	345	11	-9	10	609	17	2	12	72	29	2	H,K=	6,	18		-4	559	14	-12
1	343	14	-6	H,K=	6,		2	H,K=	6,		10	-12	0	57	-46*	-2	18	59	-19*
3	389	11	13	-12	97	27	-37	-12	364	12	-2	-10	43	66	20*	0	596	14	2
5	329	11	2	-10	95	24	-1	-10	96	17	-8	-8	65	23	26	2	50	52	13*
7	243	14	5	-8	177	11	-3	-8	653	15	-2	-6	93	19	8	4	568	14	-13
9	167	13	7	-6	90	13	-1	-6	136	14	3	-4	228	9	-4	6	0	55	-39*
H,K=	5,	31		-4	424	11	-2	-4	690	17	-4	-2	98	16	14	8	411	12	-0
-9	153	15	16	-2	49	23	-5	-2	318	9	14	0	0	66	-9*	10	96	18	62
-7	149	15	25	0	662	14	15	0	1008	22	11	2	84	19	-1	H,K=	6,	28	
-5	87	43	-9	2	50	37	-5	2	307	8	3	4	226	11	-5	-10	123	24	-26
-3	155	16	-5	4	420	10	10	4	700	16	-2	6	99	19	14	-8	0	57	-27*
-1	186	12	-8	6	67	20	-23	6	138	10	5	8	34	50	-1*	-6	160	13	-9
1	199	10	-10	8	209	10	17	8	643	15	-7	10	0	53	-22*	-4	113	16	-5
3	165	12	-0	10	74	28	-22	10	104	20	0	12	41	54	-8*	-2	223	10	8
5	85	32	-19	12	138	16	4	12	366	12	0	H,K=	6,	20		0	30	69	-9*
7	105	41	-17	H,K=	6,		4	H,K=	6,		12	-12	0	60	-18*	2	221	10	4
9	127	18	-10	-12	0	60	-18*	-12	52	74	35*	-10	306	12	-13	4	117	14	-2
H,K=	5,	33		-10	276	10	0	-10	312	12	9	-8	92	17	37	6	162	11	0
-7	145	14	-14	-8	246	11	3	-8	85	18	-11	-6	397	14	-10	8	0	65	-28*
-5	195	15	9	-6	473	12	-6	-6	312	9	-6	-4	104	22	-5	10	162	13	17
-3	193	20	1	-4	82	13	-5	-4	151	8	9	-2	523	13	6	H,K=	6,	30	
-1	302	10	9	-2	662	14	-3	-2	471	11	-21	0	140	9	-3	-8	257	12	16
1	306	11	5	0	171	7	-19	0	146	8	2	2	530	12	7	-6	60	46	43
3	214	13	13	2	654	14	-2	2	446	10	-10	4	117	13	9	-4	280	10	8
5	199	11	12	4	80	13	-7	4	139	9	-3	6	403	11	-4	-2	81	20	-9
7	178	13	13	6	497	12	2	6	323	10	8	8	79	20	23	0	523	13	-16
H,K=	5,	35		8	250	10	8	8	87	18	-7	10	313	12	-9	2	79	23	-11
-7	78	35	-54	10	285	10	12	10	306	11	-2	12	48	56	30*	4	281	13	12
-5	176	13	-9	12	41	56	23*	12	47	70	31*	H,K=	6,	22		6	20	54	1*
-3	162	14	-24	H,K=	6,		6	H,K=	6,		14	-10	89	18	23	8	214	13	-22
-1	249	12	3	-12	314	13	16	-12	197	20	5	-8	378	11	-2	H,K=	6,	32	
1	251	12	-1	-10	15	84	-60*	-10	67	28	-42	-6	56	26	34	-8	13	80	-1*
3	178	14	-15	-8	557	15	-1	-8	343	10	1	-4	442	11	-6	-6	350	12	3
5	199	14	19	-6	139	13	9	-6	130	12	-15	-2	56	27	-7	-4	62	28	-14
7	143	14	10	-4	903	21	10	-4	397	10	-5	0	482	12	17	-2	366	11	-3
H,K=	5,	37		-2	37	49	1*	-2	132	9	1	2	90	13	26	0	0	66	-15*
-5	154	15	2	0	822	17	17	0	619	14	-30	4	441	11	-8	2	369	12	-7
-3	138	14	13	2	0	42	-36*	2	138	9	7	6	72	21	49	4	79	18	2
-1	127	17	0	4	901	19	19	4	413	11	4	8	384	12	-2	6	361	14	2
1	104	27	-27	6	140	9	9	6	138	19	-5	10	49	62	-17*	8	0	81	-15*
3	140	14	14	8	547	13	-7	8	348	11	4	H,K=	6,	24		H,K=	6,	34	
5	170	14	13	10	94	18	19	10	123	14	14	-10	79	28	-18	-6	64	36	23
H,K=	5,	39		12	316	13	5	12	186	14	4	-8	107	19	2	-4	32	56	-18*
-3	200	18	-10	H,K=	6,		8	H,K=	6,		16	-6	201	11	-1	-2	0	61	-21*
-1	211	11	3	-12	57	58	-12*	-12	93	21	4	-4	64	25	13	0	30	58	-12*
1	212	13	-4	-10	45	68	-9*	-10	384	12	-7	-2	100	13	22	2	0	55	-21*
3	212	13	5	-8	44	55	-38*	-8	0	52	-29*	0	40	53	18*	4	67	78	16*

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
6	50	56	8*	-1	345	8	11	-9	288	11	1	-3	243	9	7	-5	216	11	0
H,K=		6,	36	1	377	9	9	-7	415	11	-10	-1	268	9	-1	-3	145	17	18
-6	360	14	26	3	213	8	-2	-5	412	10	7	1	261	9	-5	-1	162	21	-1
-4	64	26	49	5	362	10	-5	-3	574	14	-18	3	237	9	-1	1	166	11	6
-2	294	12	6	7	254	10	-6	-1	360	9	7	5	182	11	-6	3	123	15	-10
0	94	23	3	9	248	13	-6	1	375	10	6	7	201	11	-11	5	219	11	3
2	287	12	-1	11	151	14	11	3	590	14	-9	9	196	12	2	7	100	31	-27
4	0	66	-16*	13	156	15	20	5	403	10	9	11	122	18	-7	H,K=		7,	33
6	325	13	-5	H,K=		7,	7	7	420	14	-8	H,K=		7,	23	-7	231	12	7
H,K=		6,	38	-13	200	13	2	9	289	11	2	-11	221	15	-15	-5	211	12	-7
-4	225	13	-2	-11	278	13	-10	11	194	13	-4	-9	258	12	-3	-3	169	12	-3
-2	83	16	58	-9	242	11	-3	13	164	16	-31	-7	235	13	-8	-1	240	17	-10
0	216	12	3	-7	324	10	-4	H,K=		7,	15	-5	301	10	-3	1	234	11	-10
2	0	59	-25*	-5	448	13	1	-11	122	16	6	-3	446	12	-8	3	166	13	7
4	214	13	-11	-3	352	9	2	-9	235	11	-5	-1	208	9	2	5	226	11	4
H,K=		6,	40	-1	604	13	-2	-7	61	31	-32	1	206	10	2	7	235	14	11
-2	178	14	-4	1	602	13	1	-5	248	9	-3	3	449	11	-3	H,K=		7,	35
0	82	28	18	3	346	9	-1	-3	318	11	-6	5	313	10	11	-7	165	15	6
2	183	13	11	5	445	11	-4	-1	352	9	5	7	236	11	-4	-5	189	12	12
H,K=		7,	1	7	323	10	6	1	349	9	-3	9	249	12	-1	-3	158	21	-1
-13	161	15	2	9	262	10	6	3	330	10	2	11	209	13	-19	-1	210	12	-3
-11	228	11	3	11	261	11	-28	5	271	9	16	H,K=		7,	25	1	231	12	22
-9	313	11	-1	13	225	11	30	7	103	23	-6	-9	220	12	6	3	157	12	9
-7	233	9	9	H,K=		7,	9	9	240	11	-5	-7	205	12	6	5	181	13	-8
-5	337	9	2	-13	130	25	6	11	118	17	-7	-5	228	11	-5	7	154	15	3
-3	256	8	-4	-11	133	20	-23	H,K=		7,	17	-3	295	11	-19	H,K=		7,	37
-1	334	8	-1	-9	319	11	-1	-11	134	21	-8	-1	183	11	-16	-5	107	20	-24
1	373	9	10	-7	448	12	-16	-9	230	11	-4	1	209	10	3	-3	95	22	-6
3	283	8	-2	-5	286	9	-11	-7	204	11	-2	3	307	11	-4	-1	169	12	15
5	328	9	9	-3	470	12	3	-5	238	9	-9	5	227	10	15	1	152	13	-1
7	244	9	11	-1	542	12	9	-3	296	9	16	7	214	17	8	3	84	27	-17
9	304	12	-15	1	547	13	1	-1	315	9	6	9	214	13	-10	5	140	17	5
11	237	11	12	3	485	12	11	1	311	9	3	H,K=		7,	27	H,K=		7,	39
13	166	15	5	5	292	9	3	3	271	9	-7	-9	170	16	4	-3	182	13	-0
H,K=		7,	3	7	462	12	-5	5	258	10	-7	-7	163	13	-4	-1	200	15	13
-13	186	14	-19	9	315	11	-8	7	212	10	4	-5	184	11	-2	1	186	12	5
-11	232	11	-3	11	159	14	-1	9	213	11	-15	-3	274	10	10	3	183	13	1
-9	255	10	-7	13	137	18	14	11	163	11	20	-1	200	9	20	H,K=		8,	0
-7	329	10	-7	H,K=		7,	11	H,K=		7,	19	1	208	9	20	-12	233	13	-6
-5	592	15	-7	-13	173	15	2	-11	229	11	22	3	267	10	2	-8	309	13	-18
-3	475	12	-7	-11	232	11	7	-9	219	11	-10	5	169	13	-16	-4	501	13	-4
-1	724	16	-16	-9	227	18	-8	-7	226	10	-7	7	174	13	3	0	163	8	8
1	742	16	-5	-7	153	11	6	-5	325	11	-2	9	180	12	18	4	501	12	8
3	492	11	-3	-5	202	9	-10	-3	484	13	-8	H,K=		7,	29	8	325	10	-5
5	585	13	-15	-3	327	9	3	-1	430	11	5	-9	222	13	-14	12	232	13	-15
7	346	10	3	-1	570	13	3	1	415	11	-17	-7	233	11	-3	H,K=		8,	2
9	271	10	-8	1	589	13	10	3	495	12	2	-5	287	12	-3	-12	310	12	14
11	221	11	-19	3	338	9	2	5	325	11	-4	-3	346	11	-1	-10	143	13	4
13	207	15	-4	5	200	9	-16	7	227	11	-14	-1	270	11	9	-8	371	11	-6
H,K=		7,	5	7	138	11	11	9	215	12	-15	1	257	13	-2	-6	133	18	6
-13	157	13	25	9	247	12	6	11	201	14	0	3	334	11	2	-4	803	18	-4
-11	146	19	-2	11	223	11	11	H,K=		7,	21	5	292	11	13	-2	378	9	9
-9	243	12	-1	13	166	24	1	-11	130	15	2	7	230	12	-4	0	478	11	-12
-7	271	10	5	H,K=		7,	13	-9	182	13	-10	9	222	14	-13	2	381	9	18
-5	352	11	-25	-13	207	13	11	-7	228	12	1	H,K=		7,	31	4	801	17	6
-3	198	10	-7	-11	196	12	-1	-5	182	10	2	-7	118	18	-7	6	137	11	7

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
8	377	11	-8	8	94	22	22	8	439	12	0	0	75	25	-30	3	653	14	5
10	130	17	-6	10	210	13	-13	10	24	56	-17*	2	253	13	-3	5	475	11	-8
12	305	16	0	12	104	17	13	12	265	13	-14	4	96	18	-3	7	242	10	4
H,K=		8,	4	H,K=		8,	12	H,K=		8,	20	6	366	15	-14	9	282	10	-17
-12	115	17	9	-12	60	47	-16	-10	165	13	-1	8	141	13	34	11	281	12	4
-10	358	16	7	-10	305	11	-9	-8	92	16	28	H,K=		8,	30	13	163	13	4
-8	154	17	-9	-8	112	26	-13	-6	181	11	-6	-8	249	12	-3	H,K=		9,	3
-6	312	12	-7	-6	396	11	3	-4	137	12	1	-6	194	13	2	-13	20	62	-49*
-4	405	10	-10	-4	285	9	8	-2	366	10	8	-4	282	12	-6	-11	51	55	-7*
-2	661	15	3	-2	513	13	-7	0	251	9	0	-2	164	11	2	-9	0	54	-27*
0	176	8	14	0	209	8	-1	2	360	10	4	0	263	10	16	-7	104	15	1
2	689	15	18	2	525	12	9	4	133	13	-9	2	149	22	-3	-5	236	9	-1
4	412	10	1	4	279	9	-2	6	202	11	7	4	286	11	8	-3	69	17	3
6	350	12	11	6	401	11	15	8	91	15	16	6	174	15	-12	-1	247	8	4
8	178	11	7	8	130	15	-4	10	183	21	18	8	251	12	-5	1	230	8	3
10	342	12	-3	10	320	11	2	H,K=		8,	22	H,K=		8,	32	3	92	13	16
12	143	14	29	12	56	53	-17	-10	148	15	3	-8	132	17	-26	5	223	15	-14
H,K=		8,	6	H,K=		8,	14	-8	259	11	5	-6	168	12	-3	7	69	44	-29
-12	194	12	13	-12	229	12	-11	-6	173	12	-5	-4	37	61	-65*	9	60	37	24
-10	234	11	-20	-10	73	42	1	-4	300	10	-0	-2	116	15	-2	11	81	25	21
-8	288	11	-2	-8	298	13	-5	-2	197	10	-7	0	203	11	3	13	59	60	-15*
-6	262	9	-9	-6	205	11	-15	0	288	9	3	2	131	12	23	H,K=		9,	5
-4	265	8	-12	-4	518	14	-11	2	182	11	-15	4	97	19	-4	-13	227	13	-1
-2	540	12	1	-2	199	9	-9	4	299	10	5	6	189	12	18	-11	297	11	1
0	66	15	3	0	607	13	0	6	178	11	5	8	181	14	16	-9	312	11	-6
2	558	12	15	2	218	8	10	8	267	11	7	H,K=		8,	34	-7	430	12	-11
4	257	11	-7	4	539	13	-3	10	149	13	4	-6	73	24	50	-5	557	15	-0
6	261	9	-14	6	220	10	1	H,K=		8,	24	-4	283	12	4	-3	479	13	4
8	289	10	-4	8	330	11	19	-10	320	13	11	-2	32	50	1*	-1	588	14	-2
10	239	11	-6	10	62	30	-5	-8	0	54	-13*	0	411	12	8	1	588	13	4
12	198	12	18	12	236	13	-6	-6	329	11	-5	2	0	55	-30*	3	486	12	-8
H,K=		8,	8	H,K=		8,	16	-4	95	16	-4	4	267	13	-4	5	557	13	-6
-12	89	18	25	-12	179	13	3	-2	460	12	-7	6	0	60	-23*	7	431	11	-12
-10	348	11	10	-10	25	53	-16*	0	58	27	15	H,K=		8,	36	9	300	11	-10
-8	60	27	24	-8	169	12	-23	2	472	12	-4	-4	101	19	-6	11	298	11	11
-6	536	14	-1	-6	23	52	-42*	4	105	17	4	-2	65	36	-4	13	241	15	17
-4	240	10	10	-4	292	9	-5	6	304	11	-13	0	156	11	18	H,K=		9,	7
-2	898	20	-13	-2	61	23	-9	8	42	54	20*	2	76	33	1	-13	18	63	-66*
0	79	13	-7	0	370	10	-6	10	317	13	6	4	121	15	5	-11	105	19	14
2	921	19	1	2	61	19	2	H,K=		8,	26	H,K=		8,	38	-9	214	11	-9
4	228	8	3	4	310	11	5	-10	184	14	-3	-4	225	11	24	-7	196	11	9
6	529	13	-19	6	58	33	-8	-8	87	22	-3	-2	118	16	8	-5	105	13	9
8	22	51	-18*	8	168	14	-19	-6	289	12	-2	0	228	12	-2	-3	242	8	-6
10	336	12	9	10	0	57	-42*	-4	43	63	-13*	2	110	18	3	-1	524	12	9
12	38	67	-26*	12	176	14	-3	-2	298	14	-11	4	196	14	-13	1	546	12	15
H,K=		8,	10	H,K=		8,	18	0	57	61	23*	H,K=		8,	40	3	248	8	-1
-12	107	19	22	-12	280	14	-3	2	304	10	-13	0	62	49	-27	5	90	16	-4
-10	205	12	-14	-10	68	26	31	4	7	55	-53*	H,K=		9,	1	7	175	12	-17
-8	46	55	-25*	-8	456	13	10	6	273	11	-7	-13	140	19	-20	9	226	10	7
-6	287	10	-11	-6	52	67	-32*	8	94	20	2	-11	293	11	12	11	73	64	-3
-4	100	11	12	-4	526	13	-3	10	185	15	-3	-9	291	11	1	13	106	33	11
-2	468	12	-13	-2	88	15	10	H,K=		8,	28	-7	221	9	-1	H,K=		9,	9
0	412	10	7	0	393	11	10	-8	86	28	-20	-5	485	12	-1	-11	232	11	9
2	488	12	4	2	95	12	18	-6	376	12	-6	-3	632	15	-5	-9	197	11	-1
4	101	13	-3	4	518	12	-12	-4	86	19	-24	-1	663	17	-10	-7	275	10	0
6	308	9	11	6	93	16	6	-2	252	10	-7	1	679	16	-5	-5	187	9	-17

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-3	202	8	-0	5	224	10	2	-3	291	11	-13	6	447	11	-10	10	65	30	25
-1	598	14	12	7	217	11	-13	-1	269	10	-5	10	263	12	5	12	255	12	-7
1	599	13	23	9	214	11	2	1	270	10	-0	H,K=	10,	2		H,K=	10,	10	
3	204	8	-5	11	182	14	-7	3	330	11	17	-12	0	58	-19*	-12	162	13	11
5	205	10	-21	H,K=	9,	19		5	275	14	14	-10	398	12	-13	-8	245	11	-4
7	264	10	-3	-11	151	21	9	7	298	18	18	-8	108	15	19	-6	112	12	25
9	195	14	-8	-9	145	14	-10	9	251	14	3	-6	292	10	-8	-4	227	9	-14
11	225	12	1	-7	171	13	6	H,K=	9,	29		-4	124	12	-9	-2	40	46	-27*
H,K=	9,	11		-5	119	13	-3	-9	104	17	21	-2	798	19	1	0	366	13	-11
-11	240	11	17	-3	182	10	6	-7	46	57	-9*	0	302	8	-10	2	41	50	-20*
-9	342	11	3	-1	178	10	-4	-5	110	19	12	2	819	17	-1	4	269	10	-0
-7	429	12	-6	1	155	10	-9	-3	52	59	13*	4	107	14	-10	6	100	15	12
-5	382	12	-1	3	163	13	-7	-1	0	52	-50*	6	323	10	0	8	254	11	5
-3	419	13	-9	5	110	14	2	1	39	51	-5*	8	89	20	-12	10	167	12	11
-1	529	13	4	7	165	12	-8	3	0	54	-33*	10	399	12	3	12	170	14	11
1	526	13	5	9	123	18	-27	5	112	15	19	12	42	54	26*	H,K=	10,	12	
3	433	10	1	11	146	15	7	7	38	77	-18*	H,K=	10,	4	-12	208	13	-4	
5	367	10	4	H,K=	9,	21		9	48	63	-29*	-12	175	14	-9	-10	147	16	2
7	445	12	-1	-11	243	13	-19	H,K=	9,	31		-10	139	14	-8	-8	420	12	-18
9	320	11	-17	-9	244	11	-10	-7	243	12	6	-8	310	10	5	-6	252	10	-12
11	232	11	2	-7	284	11	9	-5	205	12	-9	-6	298	9	12	-2	296	9	-10
H,K=	9,	13		-5	266	10	9	-3	246	11	7	-4	365	10	-8	0	725	16	16
-11	76	25	35	-3	466	12	7	-1	290	12	-2	-2	452	12	-1	2	310	10	5
-9	0	52	-7*	-1	328	10	1	1	285	11	-6	0	233	9	-7	6	262	10	3
-7	74	26	-15	1	336	10	13	3	232	12	-1	2	443	12	-7	8	410	12	-22
-5	75	16	33	3	468	12	5	5	218	11	6	4	379	10	-2	10	142	16	-6
-3	93	39	7	5	258	12	6	7	234	13	-3	6	292	13	2	12	212	27	2
-1	205	9	13	7	284	11	-1	H,K=	9,	33		8	325	10	11	H,K=	10,	14	
1	186	9	-8	9	253	12	-2	-7	115	18	-3	10	139	14	-1	-12	55	57	11*
3	94	15	9	11	276	12	10	-5	128	25	7	12	188	16	-1	-10	307	11	1
5	27	53	-16*	H,K=	9,	23		-3	113	17	-4	H,K=	10,	6	-8	176	12	0	
7	77	24	-14	-9	114	17	6	-1	188	16	1	-12	143	15	11	-6	361	11	-11
9	0	57	-6*	-7	108	13	27	1	169	12	-8	-10	80	27	-36	-4	70	23	4
11	34	56	-4*	-5	89	25	-5	3	63	46	-43	-8	256	12	-5	-2	496	12	-7
H,K=	9,	15		-3	135	13	-17	5	36	72	-82*	-6	225	12	13	0	132	17	9
-11	191	12	-3	-1	100	16	-16	7	131	15	9	-4	248	9	-3	2	503	14	4
-9	285	10	13	1	110	14	-8	H,K=	9,	35		-2	249	9	-6	4	81	17	23
-7	385	11	-3	3	175	10	22	-5	96	24	-18	0	414	10	-9	6	379	11	-3
-5	447	11	16	5	82	21	-1	-3	143	13	20	2	251	9	-6	8	155	15	-16
-3	457	13	-5	7	106	16	30	-1	153	20	-19	4	253	9	9	10	308	14	4
-1	409	10	-3	9	91	23	-17	1	161	23	-6	6	233	10	16	12	0	61	-47*
1	396	10	3	H,K=	9,	25		3	103	23	-20	8	286	11	13	H,K=	10,	16	
3	466	11	-3	-9	139	16	-13	5	92	28	-23	10	126	20	14	-10	178	13	15
5	433	12	2	-7	238	12	1	H,K=	9,	37		12	160	14	22	-8	111	16	-26
7	395	11	6	-5	313	11	-1	-3	261	12	19	H,K=	10,	8	-6	340	10	-8	
9	276	11	6	-3	319	11	-17	-1	211	12	0	-12	257	13	-1	-4	73	28	15
11	211	13	10	-1	227	10	11	1	205	15	-7	-10	47	54	8*	-2	314	9	9
H,K=	9,	17		1	233	15	22	3	242	13	-3	-8	456	12	4	0	225	9	-5
-11	203	11	11	3	329	11	2	H,K=	9,	39		-6	161	11	8	2	296	10	13
-9	203	12	-14	5	313	11	10	-1	0	57	-26*	-4	462	13	3	4	58	30	10
-7	219	11	2	7	236	11	-2	1	59	37	37	-2	76	20	2	6	345	13	1
-5	208	11	-17	9	143	16	-4	H,K=	10,	0		0	590	13	-15	8	130	15	-3
-3	440	11	-18	H,K=	9,	27		-10	262	12	-0	2	64	65	-10*	10	162	15	-7
-1	232	9	-10	-9	258	16	6	-6	460	11	-2	4	472	12	13	H,K=	10,	18	
1	252	9	-3	-7	300	11	22	-2	385	10	3	6	135	15	-16	-10	282	12	-2
3	455	11	-6	-5	274	11	0	2	414	11	9	8	447	13	-5	-8	49	58	-7*

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-6	422	13	-3	-8	257	13	-13	9	235	12	-5	-9	182	11	2	1	284	10	-1
-4	103	15	13	-6	48	61	-9*	11	173	14	-13	-7	231	11	-11	3	374	11	-4
-2	443	13	3	-4	332	11	9	H,K=	11,		3	-5	177	11	-12	5	375	11	9
0	115	12	-12	-2	133	12	21	-11	238	12	-5	-3	206	9	-18	7	271	17	4
2	428	11	-4	0	396	14	-11	-9	249	11	4	-1	188	9	13	9	219	12	1
4	95	17	-0	2	95	19	-14	-7	282	12	-2	1	167	13	-5	H,K=	11,		21
6	406	12	-8	4	322	11	-4	-5	430	11	-20	3	197	10	-8	-9	118	17	-5
8	76	23	21	6	68	26	25	-3	321	11	-13	5	177	11	-1	-7	166	18	-6
10	263	17	-25	8	278	12	9	-1	374	10	-9	7	244	10	-5	-5	202	13	7
H,K=	10,		20	H,K=	10,		30	1	417	10	12	9	186	11	-2	-3	219	14	8
-10	160	14	-8	-8	91	25	-24	3	318	10	-4	11	115	16	19	-1	129	18	-5
-8	147	13	-1	-6	259	11	15	5	446	11	-10	H,K=	11,		13	1	142	11	0
-6	175	13	-11	-4	82	31	9	7	286	11	2	-11	224	13	-5	3	195	11	-2
-4	298	10	2	-2	259	11	-9	9	265	11	9	-9	279	13	16	5	198	10	5
-2	302	10	6	0	228	12	-28	11	236	24	-9	-7	351	11	1	7	169	13	-9
0	169	11	-1	2	267	11	0	H,K=	11,		5	-5	218	10	-14	9	90	29	-33
2	291	10	5	4	64	35	-6	-11	102	21	9	-3	350	10	-1	H,K=	11,		23
4	290	14	-7	6	253	11	9	-9	186	12	-1	-1	444	13	-24	-9	192	21	-10
6	185	11	3	8	110	24	4	-7	80	21	23	1	470	11	4	-7	225	12	-11
8	141	15	2	H,K=	10,		32	-5	118	13	-5	3	354	10	0	-5	288	11	-12
10	161	15	-5	-6	150	14	21	-3	318	10	-8	5	227	13	-18	-3	400	11	-1
H,K=	10,		22	-4	68	32	-30	-1	314	9	1	7	342	14	6	-1	260	10	8
-10	170	14	3	-2	168	15	7	1	328	11	-7	9	258	14	-0	1	255	10	-1
-8	162	14	-9	0	162	13	10	3	299	9	-9	11	221	14	-8	3	405	11	-2
-6	344	12	3	2	169	24	8	5	124	13	2	H,K=	11,		15	5	273	12	-10
-4	200	22	-1	4	91	23	-12	7	19	55	-39*	-11	135	19	-22	7	247	12	3
-2	268	15	0	6	158	14	22	9	171	17	-4	-9	208	11	4	9	208	12	10
0	197	11	-13	H,K=	10,		34	11	89	41	13	-7	189	11	-10	H,K=	11,		25
2	257	10	2	-6	269	13	-1	H,K=	11,		7	-5	206	12	16	-9	147	16	-7
4	184	12	-27	-4	34	58	-10*	-11	202	16	4	-3	267	10	-12	-7	233	11	11
6	332	12	-7	-2	277	12	-19	-9	293	11	25	-1	114	14	-22	-5	159	13	0
8	175	12	2	0	55	79	28*	-7	219	11	-10	1	129	12	-11	-3	201	14	-20
10	155	16	-21	2	292	12	-2	-5	386	11	2	3	284	12	13	-1	258	14	3
H,K=	10,		24	4	54	56	9*	-3	314	11	-16	5	208	10	17	1	255	10	3
-10	120	15	26	6	246	13	-22	-1	248	8	5	7	203	11	-6	3	223	11	-1
-8	304	11	-1	H,K=	10,		36	1	236	9	10	9	207	12	6	5	181	13	-1
-6	0	55	-35*	-4	106	20	-3	3	336	10	-1	11	173	13	17	7	241	11	22
-4	403	12	-15	-2	162	13	8	5	377	10	-2	H,K=	11,		17	9	177	14	19
-2	57	62	26*	0	0	62	-43*	7	217	11	-3	-11	143	17	-9	H,K=	11,		27
0	485	13	-10	2	155	20	3	9	274	11	6	-9	201	16	5	-7	162	11	35
2	76	19	36	4	110	17	7	11	211	12	4	-7	299	10	4	-5	146	13	3
4	400	11	-14	H,K=	10,		38	H,K=	11,		9	-5	243	10	-1	-3	213	11	0
6	44	53	20*	-2	210	12	-1	-11	211	12	18	-3	229	10	-7	-1	249	10	6
8	299	13	-6	0	94	29	-24	-9	262	12	-18	-1	425	12	-4	1	244	11	-10
10	90	24	0	2	223	16	12	-7	317	13	5	1	430	11	2	3	198	16	-20
H,K=	10,		26	H,K=	11,		1	-5	258	10	-7	3	240	9	-3	5	152	14	-1
-8	107	24	-4	-11	199	14	2	-3	360	13	8	5	256	12	12	7	125	16	0
-6	50	53	19*	-9	212	12	-28	-1	337	10	2	7	290	14	-2	H,K=	11,		29
-4	275	12	-7	-7	245	10	8	1	345	10	1	9	192	19	5	-7	180	13	9
-2	60	28	-2	-5	341	10	6	3	328	10	-15	11	166	13	16	-5	186	16	-14
0	150	12	2	-3	299	12	-17	5	271	10	-8	H,K=	11,		19	-3	228	11	6
2	31	53	-33*	-1	365	10	-6	7	316	11	-2	-9	226	12	5	-1	259	11	-12
4	261	11	-25	1	366	9	9	9	273	11	-7	-7	274	11	9	1	280	11	4
6	55	59	26*	3	308	9	5	11	187	13	-2	-5	361	12	-5	3	230	12	7
8	113	18	-2	5	359	10	11	H,K=	11,		11	-3	378	11	-9	5	185	13	-4
H,K=	10,		28	7	236	10	0	-11	49	63	-53*	-1	296	10	11	7	211	11	37

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	11,	31		6	0	64	-57*	H,K=	12,	14		8	52	56	11*	-7	284	11	-13
-7	122	24	20	8	346	14	11	-10	152	14	-0	H,K=	12,	24		-5	259	13	-12
-5	159	13	9	10	0	58	-48*	-8	9	56	-71*	-8	90	36	19	-3	328	10	-4
-3	163	13	10	12	264	13	-2	-6	230	12	-9	-6	90	20	-4	-1	268	14	2
-1	175	12	8	H,K=	12,		6	-4	146	11	37	-4	201	12	5	1	287	10	14
1	160	13	-4	-12	86	21	45	-2	265	10	-9	-2	44	52	8*	3	318	15	5
3	161	13	11	-10	323	11	-1	0	98	17	29	0	157	11	19	5	265	10	-3
5	177	10	21	-8	72	32	3	2	282	9	1	2	67	26	31	7	262	11	-9
7	64	75	-32*	-6	540	13	-9	4	111	15	3	4	187	12	-15	9	132	17	-10
H,K=	11,	33		-4	34	48	21*	6	259	11	4	6	95	23	2	11	224	12	25
-5	186	12	16	-2	495	13	-18	8	0	59	-78*	8	61	44	-5	H,K=	13,		3
-3	190	11	14	0	0	48	-24*	10	140	16	-22	H,K=	12,	26		-11	203	14	5
-1	251	23	15	2	507	13	-5	H,K=	12,	16		-8	0	68	-49*	-9	301	14	-2
1	250	12	2	4	0	52	-14*	-10	82	31	29	-6	352	12	-6	-7	289	11	-3
3	186	22	8	6	544	13	7	-8	412	12	7	-4	83	28	11	-5	449	12	10
5	168	16	-2	8	71	27	0	-4	565	15	-8	-2	386	12	-3	-3	344	10	-2
H,K=	11,	35		10	307	12	-10	-2	184	10	-3	0	32	55	-1*	-1	338	11	-8
-3	176	13	17	12	71	33	28	0	574	14	-14	2	401	12	11	1	336	11	-1
-1	214	14	-25	H,K=	12,		8	2	187	10	-0	4	51	56	-28*	3	354	10	15
1	249	12	9	-12	67	29	11	4	589	14	14	6	356	12	-9	5	425	12	-6
3	165	14	4	-10	45	56	-23*	6	85	23	-18	8	62	33	13	7	293	11	10
H,K=	11,	37		-8	106	17	2	8	397	12	1	H,K=	12,	28		9	303	17	-6
-1	113	17	10	-6	126	15	-15	10	63	45	10	-6	74	23	53	11	202	13	-0
1	109	21	11	-4	124	14	-22	H,K=	12,	18		-4	157	16	2	H,K=	13,		5
H,K=	12,	0		-2	38	50	-15*	-10	51	57	10*	-2	25	62	-3*	-11	158	14	21
-12	348	15	9	0	102	14	20	-8	77	25	-0	0	154	13	-9	-9	119	18	-11
-8	430	12	6	2	63	25	10	-6	136	13	6	2	48	53	20*	-7	218	11	-5
-4	631	16	-21	4	135	12	-12	-4	57	43	-35	4	159	15	-1	-5	325	11	-20
0	567	14	-22	6	148	13	4	-2	56	32	23	6	59	63	39*	-3	218	10	-23
4	621	14	-1	8	118	14	16	0	0	64	-3*	H,K=	12,	30		-1	255	9	7
8	436	14	3	10	77	37	12	2	0	50	-27*	-6	207	13	-6	1	241	10	3
12	336	13	-3	12	39	61	-15*	4	109	14	15	-4	61	35	35	3	221	11	-8
H,K=	12,	2		H,K=	12,	10		6	130	36	7	-2	249	12	-15	5	341	11	-5
-12	17	61	-12*	-10	369	14	-4	8	0	60	-76*	0	0	56	-30*	7	220	11	7
-10	150	14	11	-8	58	43	-38	10	0	58	-35*	2	291	11	18	9	132	26	-3
-8	0	59	-44*	-6	413	11	2	H,K=	12,	20		4	52	65	27*	11	149	17	16
-6	233	11	-7	-4	89	16	9	-10	0	60	-50*	6	215	12	2	H,K=	13,		7
-4	131	20	-8	-2	567	13	3	-8	337	12	2	H,K=	12,	32		-11	175	13	1
-2	196	9	-7	0	144	10	18	-6	72	26	-16	-4	296	18	-15	-9	271	14	-6
0	174	9	11	2	588	14	24	-4	504	13	-9	-2	0	58	-51*	-7	227	11	-12
2	182	10	-15	4	98	14	18	-2	45	57	-55*	0	403	14	3	-5	302	10	-2
4	146	11	7	6	411	11	8	0	520	13	-8	2	68	28	16	-3	253	10	13
6	261	10	25	8	96	25	-2	2	105	18	5	4	303	12	-10	-1	349	13	-23
8	62	33	20	10	376	12	-2	4	528	13	5	H,K=	12,	34		1	376	10	-4
10	138	17	1	H,K=	12,	12		6	106	15	16	-4	0	85	-34*	3	239	10	-3
12	65	43	34	-10	41	57	14*	8	308	13	-27	-2	0	67	-15*	5	325	10	21
H,K=	12,	4		-8	239	11	-3	10	0	65	-50*	0	70	28	26	7	229	11	-8
-12	257	13	-7	-6	88	16	36	H,K=	12,	22		2	0	67	-15*	9	278	11	0
-10	0	60	-46*	-4	250	10	3	-8	34	55	-8*	4	41	62	7*	11	195	13	17
-8	327	13	-14	-2	0	53	-48*	-6	288	11	-13	H,K=	12,	36		H,K=	13,		9
-6	35	58	-24*	0	421	11	-8	-4	25	54	-21*	-2	61	38	33	-11	169	13	20
-4	559	13	-2	2	27	69	-21*	-2	328	10	-2	0	323	12	3	-9	178	12	-3
-2	193	9	-7	4	234	12	-5	0	76	21	36	2	0	63	-28*	-7	250	12	1
0	323	10	-10	6	36	55	-14*	2	332	11	11	H,K=	13,	1		-5	260	10	6
2	195	10	-4	8	245	12	6	4	0	52	-47*	-11	171	15	-22	-3	298	10	-10
4	555	13	1	10	0	58	-24*	6	294	12	-7	-9	155	15	9	-1	362	10	3

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	351	10	-7	-7	210	12	-5	H,K=	13,	31		8	170	13	2	0	108	19	2
3	323	10	8	-5	271	11	-8	-5	129	16	3	10	151	15	22	2	328	13	-20
5	252	10	-3	-3	265	14	1	-3	131	14	4	H,K=	14,		8	4	151	13	9
7	231	14	1	-1	264	11	-21	-1	208	12	-1	-10	76	23	41	6	173	20	-6
9	185	19	3	1	285	10	5	1	203	13	-11	-8	388	12	4	8	103	22	-18
11	154	27	2	3	275	11	-1	3	142	17	10	-6	27	61	5*	10	145	18	-18
H,K=	13,	11		5	266	13	-8	5	140	15	13	-4	397	11	-27	H,K=	14,	18	
-11	108	20	-16	7	216	18	-18	H,K=	13,	33		-2	64	24	16	-8	99	20	-24
-9	173	13	-3	9	233	12	16	-3	198	21	14	0	548	13	-17	-6	309	11	-5
-7	100	17	-0	H,K=	13,	21		-1	175	15	-14	2	54	56	8*	-4	43	54	17*
-5	143	13	12	-9	152	14	10	1	164	15	-21	4	403	12	-14	-2	422	12	-8
-3	85	17	42	-7	151	16	-3	3	190	13	12	6	53	43	31	0	63	43	59
-1	284	9	-6	-5	103	17	-5	H,K=	13,	35		8	408	14	19	2	442	12	14
1	281	10	-10	-3	246	13	4	-1	194	15	-11	10	0	59	-33*	4	60	69	38*
3	64	64	-9*	-1	182	16	-13	1	209	13	0	H,K=	14,		10	6	317	11	-5
5	140	14	4	1	192	11	-14	H,K=	14,		0	-10	65	42	-8	8	97	24	-27
7	82	25	-9	3	247	11	-4	-10	214	12	1	-8	166	13	3	H,K=	14,	20	
9	178	15	2	5	129	14	12	-6	410	12	-1	-6	258	10	-21	-8	133	17	-13
11	123	19	-3	7	152	14	-1	-2	377	10	6	-4	270	10	3	-6	117	16	-5
H,K=	13,	13		9	157	13	12	2	357	10	3	-2	135	13	-4	-4	235	11	1
-11	194	15	-9	H,K=	13,	23		6	427	12	13	0	241	11	4	-2	243	11	0
-9	209	13	1	-9	154	21	-17	10	237	12	16	2	124	27	-11	0	200	11	-4
-7	283	11	5	-7	184	13	-10	H,K=	14,		2	4	265	10	4	2	240	11	-2
-5	226	11	-12	-5	230	11	14	-10	272	14	1	6	277	14	3	4	256	10	18
-3	423	13	-3	-3	230	12	-8	-8	109	16	-4	8	183	12	8	6	106	32	-12
-1	327	10	-9	-1	336	11	2	-6	488	14	-6	10	50	61	-25*	8	127	16	-15
1	361	10	19	1	332	11	1	-4	33	56	-32*	H,K=	14,	12		H,K=	14,	22	
3	443	12	10	3	236	11	-5	-2	440	13	-11	-10	115	19	-9	-8	132	18	-2
5	222	11	-6	5	235	11	14	0	58	33	48	-8	333	11	7	-6	186	12	11
7	284	10	-2	7	184	14	-13	2	435	11	-7	-6	183	13	-8	-4	206	11	4
9	204	21	-9	9	191	18	14	4	63	37	-13	-4	307	10	-2	-2	244	11	5
11	184	15	-15	H,K=	13,	25		6	488	14	1	-2	208	10	7	0	173	12	9
H,K=	13,	15		-7	185	14	7	8	134	19	14	0	318	10	-6	2	244	11	5
-9	182	14	-1	-5	213	11	18	10	273	12	7	2	190	11	-18	4	185	13	-5
-7	163	12	-11	-3	193	12	-8	H,K=	14,		4	4	295	11	-10	6	168	14	-10
-5	232	11	2	-1	88	67	-5	-10	169	13	9	6	215	11	18	8	143	17	4
-3	135	20	-21	1	74	32	-20	-8	232	12	-19	8	310	12	-15	H,K=	14,	24	
-1	256	9	2	3	189	12	-7	-6	272	12	1	10	156	14	29	-8	267	17	-1
1	258	12	8	5	191	12	-1	-4	171	11	4	H,K=	14,	14		-6	79	31	29
3	147	11	2	7	191	13	1	-2	171	12	3	-10	204	13	-16	-4	318	11	4
5	246	11	6	H,K=	13,	27		0	462	12	2	-8	0	57	-50*	-2	106	17	16
7	183	12	14	-7	125	20	-41	2	160	12	-8	-6	357	11	13	0	366	12	-0
9	185	13	0	-5	143	18	-9	4	167	12	3	-4	216	11	-18	2	107	20	17
H,K=	13,	17		-3	145	13	12	6	278	15	12	-2	291	10	-6	4	336	13	13
-9	51	68	-49*	-1	176	12	-6	8	221	12	-16	0	82	22	10	6	0	62	-49*
-7	242	10	12	1	201	10	22	10	168	14	6	2	285	10	3	8	245	14	-23
-5	238	11	-24	3	125	17	-18	H,K=	14,		6	4	233	14	2	H,K=	14,	26	
-3	409	12	12	5	131	16	-20	-10	122	19	-6	6	345	11	9	-6	0	60	-28*
-1	146	17	-17	7	188	13	28	-8	148	19	-8	8	55	36	21	-4	160	14	9
1	201	10	16	H,K=	13,	29		-6	145	14	-14	10	233	13	13	-2	43	54	18*
3	382	11	-17	-5	227	12	2	-4	236	13	3	H,K=	14,	16		0	225	12	4
5	246	11	-9	-3	179	12	-10	-2	257	10	-17	-10	165	15	-6	2	0	80	-25*
7	234	11	2	-1	205	11	20	0	113	15	11	-8	110	18	-10	4	166	14	17
9	77	32	-29	1	203	15	15	2	271	10	-10	-6	193	11	11	6	36	68	11*
H,K=	13,	19		3	197	11	12	4	234	10	-17	-4	138	12	-0	H,K=	14,	28	
-9	235	12	14	5	230	12	-2	6	146	26	-15	-2	343	11	6	-6	56	61	-42*

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	314	11	16	-9	126	18	20	-7	172	15	-33	-3	70	31	-7	-4	86	21	-9
-2	44	58	-39*	-7	201	12	-0	-5	215	12	4	-1	46	53	1*	-2	419	12	-2
0	287	12	-9	-5	276	10	5	-3	219	13	11	1	96	18	49	0	19	65	-8*
2	79	80	-2*	-3	124	16	3	-1	203	12	-18	3	70	31	-6	2	424	12	3
4	298	13	-2	-1	128	15	17	1	197	11	-15	5	70	31	35	4	101	17	9
6	97	23	-2	1	98	26	-4	3	189	13	-19	H,K=	15,	31		6	440	14	-1
H,K=	14,	30		3	127	16	-0	5	211	15	-1	-3	216	12	3	8	21	57	-31*
-4	112	16	19	5	279	17	-3	7	203	13	1	-1	286	15	15	10	300	13	10
-2	199	13	-4	7	195	13	-5	9	144	14	8	1	266	13	-3	H,K=	16,	10	
0	69	26	19	9	103	30	-9	H,K=	15,	19		3	235	16	18	-8	105	19	15
2	218	13	14	H,K=	15,	9		-9	110	19	16	H,K=	16,	0		-6	165	15	-16
4	94	21	-0	-9	130	16	9	-7	122	24	-3	-8	121	32	-10	-4	151	12	22
H,K=	14,	32		-7	199	14	-20	-5	120	17	-5	-4	161	18	-5	-2	293	11	5
-2	183	15	2	-5	172	13	1	-3	153	12	-3	0	262	11	-2	0	90	19	-11
0	149	16	-15	-3	285	10	0	-1	151	15	-14	4	203	11	13	2	296	10	8
2	164	15	-14	-1	206	11	-11	1	163	12	4	8	134	16	5	4	128	16	-0
H,K=	14,	34		1	198	11	-7	3	127	16	-21	H,K=	16,	2		6	166	13	-13
0	93	20	23	3	280	11	1	5	123	15	9	-10	55	61	-17*	8	108	17	9
H,K=	15,	1		5	152	14	-7	7	125	16	-3	-8	309	13	-3	H,K=	16,	12	
-11	160	28	-10	7	222	11	-10	9	68	50	-24	-6	107	16	4	-8	111	18	5
-9	252	12	2	9	106	21	-14	H,K=	15,	21		-4	300	10	18	-6	249	12	-5
-7	248	11	-2	H,K=	15,	11		-7	269	12	-5	-2	0	57	-35*	-4	148	13	2
-5	328	13	12	-9	264	12	-7	-5	208	13	-27	0	607	15	-18	-2	286	11	7
-3	209	11	2	-7	293	12	-6	-3	283	11	-4	2	81	19	34	0	176	12	-18
-1	348	12	-14	-5	343	11	-5	-1	386	11	1	4	315	11	5	2	271	11	-3
1	336	10	-14	-3	344	10	14	1	365	12	-15	6	111	18	3	4	166	16	1
3	193	11	-13	-1	314	11	4	3	288	12	-2	8	311	12	-1	6	268	11	12
5	336	11	-7	1	305	10	2	5	211	17	-17	10	99	21	25	8	85	28	-20
7	244	11	-8	3	315	11	-12	7	253	12	-19	H,K=	16,	4		H,K=	16,	14	
9	260	11	20	5	371	11	20	H,K=	15,	23		-10	172	19	14	-8	267	13	-4
11	170	14	-2	7	303	12	-1	-7	84	25	-5	-8	118	24	-2	-6	111	18	-17
H,K=	15,	3		9	249	13	-22	-5	93	20	21	-6	303	12	-4	-4	317	11	0
-11	29	61	-11*	H,K=	15,	13		-3	142	15	-4	-4	196	11	-19	-2	164	13	-16
-9	134	14	10	-9	64	44	-10	-1	137	14	-3	-2	323	11	-9	0	319	11	3
-7	48	57	-20*	-7	43	74	29*	1	124	25	-18	0	153	16	37	2	169	20	-13
-5	159	13	14	-5	47	52	1*	3	150	13	-5	2	323	11	-6	4	300	11	-7
-3	203	11	-5	-3	43	75	-6*	5	91	18	16	4	214	15	-7	6	106	20	-11
-1	102	16	3	-1	62	27	43	7	72	31	-17	6	291	12	-12	8	267	13	-8
1	52	58	-58*	1	0	56	-18*	H,K=	15,	25		8	128	18	6	H,K=	16,	16	
3	200	25	-14	3	83	18	35	-7	195	14	-11	10	171	14	6	-8	122	35	-17
5	139	14	-4	5	54	75	9*	-5	180	13	3	H,K=	16,	6		-6	49	57	3*
7	51	68	-22*	7	28	56	14*	-3	194	10	31	-10	180	14	13	-4	234	11	-7
9	113	26	-4	9	96	18	19	-1	224	11	12	-8	116	21	-31	-2	81	19	27
11	94	22	60	H,K=	15,	15		1	199	25	-11	-6	229	13	-21	0	194	12	-5
H,K=	15,	5		-9	279	11	27	3	164	18	-1	-4	220	14	14	2	105	13	47
-9	183	21	-17	-7	263	11	3	5	173	13	-7	-2	207	13	-19	4	248	11	10
-7	316	11	0	-5	334	11	28	7	199	14	-5	0	343	11	11	6	0	57	-40*
-5	360	12	3	-3	353	11	6	H,K=	15,	27		2	224	16	-3	8	137	17	-5
-3	373	11	-15	-1	301	10	-4	-5	215	12	9	4	235	11	26	H,K=	16,	18	
-1	452	12	5	1	278	11	-15	-3	191	13	-30	6	267	11	9	-8	297	14	-6
1	445	12	8	3	338	11	-11	-1	271	11	12	8	142	15	-4	-6	64	35	32
3	373	11	-8	5	290	11	-2	1	256	11	1	10	175	15	4	-4	348	12	-15
5	380	13	6	7	277	12	13	3	220	15	-6	H,K=	16,	8		-2	45	55	11*
7	310	11	-11	9	245	17	4	5	189	13	-7	-10	250	19	-31	0	437	12	4
9	225	12	21	H,K=	15,	17		H,K=	15,	29		-8	0	58	-52*	2	0	57	-40*
H,K=	15,	7		-9	139	17	9	-5	30	69	-5*	-6	423	13	-18	4	364	12	-1

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
6	65	36	28	-9	185	14	-13	-5	203	12	2	-3	65	78	-8*	-2	0	57	-23*
8	296	13	-1	-7	256	12	1	-3	186	15	-20	-1	126	25	19	0	440	13	-5
H,K=		16,	20	-5	238	12	-10	-1	330	15	6	1	106	20	-5	2	30	57	7*
-8	140	15	20	-3	261	10	7	1	310	11	-19	3	56	60	-16*	4	429	12	5
-6	174	15	6	-1	336	12	5	3	199	12	-11	H,K=		17,	29	6	0	73	-9*
-4	186	13	-6	1	335	11	-4	5	220	11	17	-1	161	16	-9	8	277	13	-3
-2	211	14	8	3	245	11	-11	7	161	15	-10	1	171	18	6	H,K=		18,	12
0	147	14	-14	5	256	11	3	H,K=		17,	15	H,K=		18,	0	-8	34	59	2*
2	208	12	-1	7	253	12	0	-7	119	21	-14	-6	383	15	7	-6	128	21	-12
4	167	13	-22	9	190	14	-9	-5	149	14	-10	-2	474	13	-11	-4	43	74	23*
6	170	18	0	H,K=		17,	5	-3	146	13	6	2	466	13	-4	-2	322	15	10
8	153	22	33	-9	95	27	-29	-1	169	13	-8	6	402	12	27	0	48	54	29*
H,K=		16,	22	-7	150	21	16	1	166	13	-3	H,K=		18,	2	2	343	11	25
-6	163	12	15	-5	181	13	12	3	157	13	5	-8	120	16	17	4	55	58	37*
-4	175	12	6	-3	191	12	-8	5	169	13	1	-6	0	58	-43*	6	154	15	15
-2	187	12	-21	-1	208	11	1	7	134	17	4	-4	141	15	-3	8	0	60	-35*
0	211	11	-1	1	229	10	13	H,K=		17,	17	-2	68	36	31	H,K=		18,	14
2	209	18	-2	3	200	12	2	-7	166	19	6	0	187	12	0	-6	70	26	27
4	161	13	1	5	183	13	2	-5	182	11	21	2	0	56	-38*	-4	246	14	1
6	126	18	-13	7	118	20	-12	-3	211	13	3	4	148	17	8	-2	48	56	10*
H,K=		16,	24	9	136	14	23	-1	175	20	-33	6	24	65	-21*	0	151	14	-12
-6	240	17	-18	H,K=		17,	7	1	185	15	-30	8	34	67	-68*	2	0	59	-38*
-4	0	56	-16*	-9	188	14	-1	3	215	20	-3	H,K=		18,	4	4	247	12	-2
-2	290	12	10	-7	263	12	0	5	150	15	-9	-8	30	58	-5*	6	60	67	20*
0	55	47	13	-5	284	11	5	7	151	25	1	-6	305	13	4	H,K=		18,	16
2	276	12	3	-3	367	11	15	H,K=		17,	19	-4	36	58	-14*	-6	305	12	-4
4	0	57	-20*	-1	269	11	-7	-7	248	17	14	-2	300	11	-10	-4	64	34	4
6	283	12	16	1	259	11	-20	-5	239	11	30	0	79	22	-2	-2	331	11	-3
H,K=		16,	26	3	367	11	8	-3	238	12	-7	2	311	11	1	0	58	31	35
-4	66	29	36	5	264	14	-8	-1	213	11	15	4	98	35	47	2	353	13	13
-2	194	41	-20	7	241	13	-14	1	189	12	-8	6	308	11	11	4	65	33	5
0	0	66	-78*	9	218	13	27	3	240	14	-6	8	34	65	-0*	6	314	16	1
2	184	20	-18	H,K=		17,	9	5	208	16	2	H,K=		18,	6	H,K=		18,	18
4	21	55	-10*	-9	158	21	9	7	235	13	0	-8	258	12	4	-6	0	58	-20*
H,K=		16,	28	-7	107	28	-31	H,K=		17,	21	-6	36	58	-18*	-4	5	58	-19*
-4	73	24	27	-5	259	11	-1	-5	104	22	-17	-4	445	15	-17	-2	48	56	25*
-2	270	12	8	-3	310	11	1	-3	0	57	-81*	-2	33	76	-34*	0	80	28	-37
0	90	23	5	-1	271	11	-13	-1	184	11	22	0	428	12	-6	2	31	75	9*
2	257	12	-5	1	289	11	-4	1	142	38	-24	2	74	37	6	4	0	59	-27*
4	0	69	-44*	3	316	11	11	3	99	18	23	4	472	13	7	6	0	74	-19*
H,K=		16,	30	5	269	11	3	5	133	16	4	6	39	59	-13*	H,K=		18,	20
-2	0	66	-106*	7	133	17	-11	H,K=		17,	23	8	237	13	-8	-6	276	14	-2
0	166	15	-4	9	173	14	21	-5	197	13	-13	H,K=		18,	8	-4	82	23	10
2	135	15	25	H,K=		17,	11	-3	199	12	16	-8	51	56	29*	-2	253	13	-11
H,K=		17,	1	-9	144	15	15	-1	213	15	-10	-6	46	56	-7*	0	65	69	7*
-9	122	24	-24	-7	122	19	-9	1	220	12	8	-4	56	60	-14*	2	250	12	-13
-7	116	22	-10	-5	249	12	9	3	155	16	-17	-2	44	67	-20*	4	85	29	12
-5	182	13	-3	-3	216	13	15	5	205	18	-6	0	0	72	-3*	6	301	12	17
-3	232	12	7	-1	144	22	-19	H,K=		17,	25	2	87	19	27	H,K=		18,	22
-1	256	11	1	1	140	15	-7	-5	141	17	-5	4	58	77	-14*	-4	211	15	-15
1	267	11	9	3	193	15	7	-3	112	28	-6	6	15	59	-42*	-2	0	74	-27*
3	202	13	-9	5	231	11	-3	-1	199	12	4	8	91	19	64	0	339	13	6
5	168	14	-10	7	157	17	33	1	191	13	-1	H,K=		18,	10	2	0	59	-26*
7	124	18	-3	9	104	27	-31	3	125	17	11	-8	277	13	-6	4	219	14	-9
9	151	16	1	H,K=		17,	13	5	154	15	3	-6	40	53	30*	H,K=		18,	24
H,K=		17,	3	-7	181	14	17	H,K=		17,	27	-4	425	13	0	-4	54	60	21*

STRUCTURE FACTORS CONTINUED FOR
NAPR(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	98	20	0	-3	163	15	-19	4	263	14	6	-2	55	58	40*	-3	230	13	3
0	55	55	51*	-1	153	16	-31	6	91	21	55	0	286	13	-10	-1	180	15	-8
2	120	17	16	1	194	12	7	H,K=	20,		4	2	0	58	-16*	1	157	16	-33
4	48	70	17*	3	177	14	-4	-6	153	16	2	4	270	12	11	3	241	13	14
H,K=	18,		26	5	91	35	-40	-4	94	20	1	H,K=	20,		20	H,K=	21,		17
-2	33	60	-2*	7	130	17	-7	-2	200	18	8	-2	130	19	-3	-1	153	37	-5
0	292	12	23	H,K=	19,		13	0	203	12	26	0	122	19	-9	1	139	18	-12
2	33	60	-1*	-7	204	12	11	2	180	14	-12	2	154	16	20	H,K=	22,		0
H,K=	19,		1	-5	269	12	-5	4	17	81	-87*	H,K=	21,		1	-2	159	16	18
-7	143	16	-15	-3	199	15	-19	6	160	15	9	-5	174	16	34	2	134	21	-4
-5	170	14	4	-1	217	12	4	H,K=	20,		6	-3	216	12	13	H,K=	22,		2
-3	135	18	-14	1	221	12	3	-6	167	13	6	-1	204	13	3	-4	75	32	29
-1	205	11	8	3	224	12	4	-4	112	18	6	1	192	14	-10	-2	263	17	-17
1	205	12	-3	5	291	12	18	-2	151	15	-11	3	198	17	-3	0	73	30	25
3	133	17	-10	7	193	13	6	0	250	12	-10	5	155	15	21	2	281	13	3
5	147	25	-21	H,K=	19,		15	2	150	15	-11	H,K=	21,		3	4	29	63	-15*
7	169	15	9	-5	122	23	-4	4	121	19	9	-5	0	88	-30*	H,K=	22,		4
H,K=	19,		3	-3	50	61	-64*	6	176	17	16	-3	49	61	-19*	-4	203	14	-15
-7	182	15	-10	-1	147	14	15	H,K=	20,		8	-1	121	17	18	-2	127	17	1
-5	185	14	-6	1	92	33	-38	-6	274	12	1	1	99	30	-7	0	179	14	6
-3	225	13	-3	3	89	24	-12	-4	0	70	-47*	3	93	21	30	2	150	14	30
-1	231	11	10	5	139	16	4	-2	280	12	-9	5	83	32	47	4	227	13	11
1	232	11	10	H,K=	19,		17	0	0	63	-56*	H,K=	21,		5	H,K=	22,		6
3	218	12	-10	-5	194	14	-2	2	289	12	1	-5	224	13	5	-4	181	14	15
5	183	14	-9	-3	196	13	6	4	42	66	-1*	-3	221	14	-14	-2	139	16	21
7	207	15	15	-1	193	12	2	6	280	13	6	-1	214	13	-2	0	85	25	-9
H,K=	19,		5	1	179	13	-7	H,K=	20,		10	1	216	14	3	2	120	20	1
-7	149	13	38	3	181	14	-9	-6	183	18	9	3	250	12	8	4	178	14	15
-5	153	14	31	5	190	15	-3	-4	119	22	-2	5	219	18	4	H,K=	22,		8
-3	178	14	-11	H,K=	19,		19	-2	210	13	23	H,K=	21,		7	-2	46	59	15*
-1	186	24	2	-5	140	19	-8	0	54	68	28*	-5	154	16	-10	0	295	12	6
1	163	22	-20	-3	110	20	-24	2	201	12	14	-3	129	17	15	2	33	61	4*
3	196	18	10	-1	198	13	-32	4	98	28	-18	-1	86	28	-6	H,K=	22,		10
5	117	17	-0	1	208	13	-13	6	189	26	16	1	86	23	4	-2	0	65	-85*
7	101	59	-18	3	160	14	23	H,K=	20,		12	3	95	24	-15	0	129	16	42
H,K=	19,		7	5	174	17	17	-6	230	20	6	5	158	15	-0	2	106	20	26
-7	181	15	-7	H,K=	19,		21	-4	57	61	2*	H,K=	21,		9	H,K=	22,		12
-5	159	14	-4	-3	110	23	12	-2	259	12	8	-5	179	15	-1	-2	89	24	8
-3	269	12	13	-1	147	15	6	0	117	20	-13	-3	186	13	9	0	205	12	6
-1	270	13	6	1	154	16	15	2	254	12	4	-1	179	14	10	2	90	41	6
1	280	11	11	3	92	24	-12	4	33	68	-33*	1	156	19	1	H,K=	22,		14
3	264	13	2	H,K=	19,		23	6	197	15	-25	3	149	18	-23	0	11	63	-56*
5	149	15	-3	-3	160	16	-3	H,K=	20,		14	5	198	14	18	H,K=	23,		1
7	188	18	2	-1	178	15	-14	-4	264	12	12	H,K=	21,		11	-1	155	16	18
H,K=	19,		9	1	207	13	16	-2	124	18	4	-5	214	14	-3	1	151	16	11
-7	124	22	-20	3	159	17	-4	0	197	13	-13	-3	210	13	-0	H,K=	23,		3
-5	213	12	17	H,K=	20,		0	2	148	15	27	-1	229	13	17	-1	205	13	13
-3	215	12	6	-4	128	20	-14	4	249	13	3	1	218	13	6	1	201	14	6
-1	198	15	7	0	129	17	9	H,K=	20,		16	3	204	13	-2	H,K=	23,		5
1	196	13	1	4	171	13	18	-4	122	19	-4	5	207	15	-4	-1	133	22	32
3	217	12	2	H,K=	20,		2	-2	96	21	13	H,K=	21,		13	1	124	18	16
5	216	12	11	-6	34	60	-3*	0	169	14	13	-3	0	62	-36*				
7	118	20	-26	-4	235	19	-21	2	0	64	-83*	-1	54	59	43*				
H,K=	19,		11	-2	81	26	-4	4	152	14	22	1	66	33	54				
-7	135	17	1	0	299	12	-3	H,K=	20,		18	3	53	59	15*				
-5	118	20	-16	2	94	37	14	-4	268	13	7	H,K=	21,		15				

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 5.0)
NASM(EDTA).8H2O F(0,0,0) = 5894

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		0,	0	-8	420	8	7	6	565	11	-2	9	326	8	-14	-7	294	7	-10
-12	521	10	4	-4	796	10	1	10	467	10	13	11	250	10	11	-5	471	8	-6
-8	707	10	-2	0	1102	13	-3	H,K=		0,	28	13	185	12	4	-3	357	6	-4
-4	816	9	-18	4	774	10	-7	-4	402	9	-12	H,K=		1,	3	-1	109	8	-25
4	894	10	-17	8	417	8	-1	0	164	11	-12	-13	290	11	-4	1	74	9	0
8	666	9	-2	12	304	11	6	4	447	9	5	-11	433	9	-2	3	369	6	-2
12	521	12	9	H,K=		0,	14	8	240	11	7	-9	429	9	-16	5	468	7	-12
H,K=		0,	2	-10	368	9	17	H,K=		0,	30	-7	558	8	-5	7	294	7	-5
-14	143	12	-5	-6	421	9	14	-10	217	16	-6	-5	461	7	2	9	275	8	0
-10	178	14	0	-2	174	6	-8	-6	259	10	14	-3	516	6	4	11	302	10	-4
-6	516	8	2	2	186	6	3	-2	241	9	-2	-1	955	10	-34	13	210	13	19
-2	472	7	32	6	424	8	9	2	239	9	-8	1	963	10	-30	H,K=		1,	11
2	465	6	30	10	350	9	-4	6	262	9	4	3	540	7	5	-13	197	11	5
6	536	8	16	H,K=		0,	16	10	204	12	-12	5	504	8	2	-11	167	10	3
10	191	9	11	-12	395	10	2	H,K=		0,	32	7	581	8	3	-9	229	8	1
14	171	12	12	-8	675	10	-4	-8	359	10	11	9	409	8	-7	-7	257	8	-3
H,K=		0,	4	-4	847	12	-6	-4	522	12	1	11	440	10	4	-5	284	7	1
-12	357	10	-11	0	924	13	-6	0	348	11	-15	13	283	13	-10	-3	671	9	-1
-8	503	9	2	4	882	11	15	4	514	12	9	H,K=		1,	5	-1	834	10	10
-4	718	9	5	8	695	10	5	8	333	12	-6	-13	153	13	1	1	845	10	11
0	1056	11	39	12	410	12	15	H,K=		0,	34	-11	126	14	-25	3	669	10	-10
4	743	9	14	H,K=		0,	18	-6	38	46	-15*	-9	113	11	-6	5	303	8	6
8	470	8	-10	-10	0	47	-34*	-2	29	48	9*	-7	236	7	-4	7	270	8	-5
12	347	9	-1	-6	262	8	2	2	0	48	-17*	-5	668	8	19	9	225	11	1
H,K=		0,	6	-2	349	8	-9	6	19	59	-33*	-3	226	7	-7	11	143	13	-4
-14	291	13	7	2	355	8	-10	H,K=		0,	36	-1	547	7	-2	13	200	11	9
-10	246	9	9	6	260	9	-6	-4	455	10	16	1	528	6	-4	H,K=		1,	13
-6	910	11	-8	10	33	47	0*	0	456	10	2	3	201	5	-7	-13	263	11	-4
-2	722	8	-0	H,K=		0,	20	4	43*	10	11	5	659	8	9	-11	292	10	-1
2	727	8	-5	-12	358	11	7	H,K=		0,	38	7	240	7	-4	-9	362	8	-4
6	895	11	-18	-8	584	10	-9	-6	360	11	14	9	137	10	-5	-7	513	9	5
10	257	8	-0	0	373	7	-15	-2	244	11	12	11	200	9	17	-5	598	9	8
14	274	14	-17	4	381	8	-10	2	206	12	-16	13	148	13	-4	-3	703	10	3
H,K=		0,	8	8	594	10	1	6	336	12	-8	H,K=		1,	7	-1	706	9	-9
-12	84	15	34	12	369	10	15	H,K=		0,	40	-13	229	11	-10	1	658	9	-12
-8	248	8	-6	H,K=		0,	22	-4	192	12	-7	-11	313	9	5	3	690	10	17
-4	413	7	14	-10	382	10	16	0	131	17	-10	-9	319	10	-4	5	616	9	12
0	263	5	-1	-6	381	8	13	4	189	12	-4	-7	309	7	2	7	526	10	9
4	423	7	14	-2	588	11	-6	H,K=		0,	42	-5	567	9	4	9	371	9	-8
8	260	8	-0	2	615	9	14	-2	370	11	13	-3	792	9	8	11	302	10	-1
12	50	51	1*	6	395	12	4	2	344	12	-10	-1	486	6	6	13	273	11	-2
H,K=		0,	10	10	355	10	-10	H,K=		1,	1	1	486	6	4	H,K=		1,	15
-14	345	12	13	H,K=		0,	24	-11	226	9	-2	3	788	9	3	-13	200	12	2
-10	602	10	-8	-4	275	8	9	-9	349	8	-7	5	614	10	9	-11	273	12	-1
-6	628	10	-9	0	147	10	8	-7	507	9	5	7	300	7	-3	-9	327	9	-14
-2	928	11	-12	4	243	8	-18	-5	322	6	8	9	306	8	7	-7	287	8	-7
2	917	11	-4	8	198	11	-11	-3	692	8	11	11	307	9	8	-5	267	8	6
6	605	10	-15	H,K=		0,	26	-1	666	8	-58	13	240	12	7	-3	554	8	4
10	604	10	-19	-10	445	11	-7	1	656	8	-60	H,K=		1,	9	-1	540	9	5
14	353	18	10	-6	572	9	17	3	680	8	5	-13	178	12	-7	1	577	8	12
H,K=		0,	12	-2	564	9	-10	5	308	6	5	-11	294	9	0	3	563	8	13
-12	317	10	12	2	553	9	-1	7	522	8	9	-9	264	8	13	5	264	7	-8

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	269	8	-4	11	220	11	9	3	164	10	-10	14	268	17	-2	0	672	8	14
9	346	9	1	H,K=	1,	25		5	270	10	3	H,K=	2,	4		2	396	6	18
11	263	10	-8	-11	177	14	-9	7	182	12	-12	-14	190	13	9	4	318	6	-6
13	168	14	-21	-9	232	10	-5	9	187	12	-2	-12	294	10	-5	6	229	7	11
H,K=		1,	17	-7	338	9	-3	H,K=		1,	35	-10	159	10	3	8	296	8	-11
-13	220	13	16	-5	228	9	-1	-7	248	11	13	-8	310	7	-3	10	54	23	-14
-11	159	12	3	-3	244	8	1	-5	277	10	-7	-6	363	7	4	12	247	10	17
-9	316	9	-1	-1	412	11	-11	-3	214	13	3	-4	888	10	-4	H,K=		2,	12
-7	284	8	-3	1	415	9	-3	-1	238	10	-4	-2	270	5	15	-12	301	10	5
-5	504	10	16	3	283	8	10	1	238	13	-17	0	964	10	4	-10	147	15	9
-3	334	7	10	5	245	9	-8	3	201	12	-9	2	227	5	3	-8	380	8	3
-1	425	7	6	7	312	9	-6	5	274	14	5	4	881	10	3	-6	273	7	8
1	423	7	4	9	244	10	8	7	230	11	2	6	358	7	0	-4	771	10	4
3	336	7	15	11	155	15	-29	H,K=		1,	37	8	304	7	-0	-2	183	6	3
5	482	10	8	H,K=		1,	27	-7	153	13	1	10	126	12	-12	0	339	6	-20
7	278	8	11	-11	155	12	14	-5	94	21	-28	12	286	10	-21	2	188	8	7
9	329	9	12	-9	171	12	-13	-3	190	12	-4	14	168	15	-6	4	781	13	-2
11	149	11	6	-7	214	9	-6	-1	146	12	7	H,K=		2,	6	6	289	7	18
13	223	11	8	-5	199	9	13	1	155	12	9	-14	130	14	8	8	377	9	-12
H,K=		1,	19	-3	216	11	-4	3	200	11	17	-12	289	10	-5	10	143	11	5
-11	257	10	0	-1	253	9	-6	7	162	12	13	-10	210	9	6	12	296	11	5
-9	324	14	-14	1	255	8	-6	H,K=		1,	39	-8	247	8	-1	H,K=		2,	14
-7	390	8	-9	3	203	9	-9	-5	242	11	10	-6	373	7	5	-12	64	24	1
-5	423	8	5	5	195	8	10	-3	285	11	14	-4	51	19	-6	-10	450	9	-7
-3	316	7	2	7	222	9	-1	-1	224	13	10	-2	529	7	2	-8	138	10	-9
-1	532	9	4	9	164	16	-19	3	255	11	-16	0	276	5	10	-6	507	9	-4
1	537	8	2	11	137	14	-5	5	226	11	6	2	533	7	5	-4	305	7	-4
3	309	10	9	H,K=		1,	29	H,K=		1,	41	4	94	8	-11	-2	802	11	-12
5	423	8	-2	-9	234	10	2	-3	166	16	-13	6	327	7	-26	0	20	35	-14*
7	371	8	-0	-7	267	10	-11	-1	184	12	-7	8	238	8	-4	2	836	11	6
9	336	10	-1	-5	408	9	-6	1	199	13	1	10	204	10	-1	4	292	7	-9
11	236	11	-18	-3	377	8	-1	3	164	13	-8	12	294	9	9	6	504	8	-8
H,K=		1,	21	-1	323	8	1	H,K=		2,	0	14	125	13	-2	8	149	8	6
-11	185	11	19	1	326	9	-2	-14	242	12	2	H,K=		2,	8	10	455	9	6
-9	205	12	-41	3	387	9	7	-10	401	9	-11	-14	0	55	-45*	12	53	47	-30
-7	221	10	1	5	416	11	1	-6	499	8	-6	-12	492	10	4	H,K=		2,	16
-5	267	7	3	7	276	10	-11	-2	504	6	-21	-10	41	47	-13*	-12	121	13	2
-3	96	9	0	9	226	12	-12	2	545	6	-31	-8	510	8	-11	-10	243	10	-11
-1	237	9	-0	H,K=		1,	31	6	490	8	-9	-6	168	7	5	-8	77	16	1
1	233	7	2	-9	144	14	3	10	407	11	-4	-4	842	10	-2	-6	526	10	3
3	92	9	1	-7	167	11	11	14	234	12	-10	-2	540	7	1	-4	275	7	3
5	262	9	-2	-5	249	9	-1	H,K=		2,	2	0	653	8	-13	-2	507	8	5
7	201	8	7	-3	205	12	3	-14	258	12	-8	2	534	7	-1	0	479	9	18
9	258	9	-3	-1	207	10	4	-12	162	11	-1	4	825	10	-5	2	497	8	8
11	163	12	3	1	204	9	-1	-10	487	11	-1	6	163	7	-0	4	274	7	1
H,K=		1,	23	3	180	9	-2	-8	182	8	12	8	523	9	-2	6	507	9	-5
-11	210	12	-2	5	255	10	2	-6	849	12	-8	10	86	13	28	8	65	18	-4
-9	260	10	4	7	161	15	23	-4	168	6	19	12	491	10	5	10	263	10	9
-7	365	10	-9	9	151	13	11	-2	698	8	37	14	33	55	-9*	12	106	17	-8
-5	311	8	-5	H,K=		1,	33	0	411	6	-13	H,K=		2,	10	H,K=		2,	18
-3	438	9	-6	-9	198	11	9	2	683	8	52	-12	240	10	12	-12	86	24	-42
-1	503	9	-13	-7	188	16	-1	4	146	6	7	-10	34	42	-6*	-10	414	10	-14
1	503	8	-3	-5	268	10	-6	6	851	12	-15	-8	300	8	-8	-8	78	14	7
5	320	8	-0	-3	172	11	-2	8	169	8	-14	-6	200	8	-1	-6	466	8	6
7	377	11	-4	-1	230	10	-3	10	526	10	16	-4	274	7	-15	-4	144	8	28
9	264	10	-8	1	252	11	12	12	158	12	-2	-2	365	6	10	-2	912	13	4

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
0	274	7	-7	8	214	10	2	2	259	10	9	H,K=	3,	7		7	123	11	-9
2	945	13	20	H,K=	2,	28		4	200	11	16	-13	173	13	12	9	92	14	-16
4	125	12	-3	-10	105	15	16	6	247	10	28	-11	265	10	-13	11	91	13	7
6	468	9	-1	-8	339	10	-2	H,K=	2,	40		-9	222	9	-1	13	31	52	16*
8	66	16	2	-6	190	10	-2	-4	306	11	9	-7	176	7	6	H,K=	3,	15	
10	437	10	8	-4	431	9	1	-2	86	15	10	-5	387	7	3	-13	270	11	17
12	113	18	-10	-2	249	9	3	0	352	11	-13	-3	496	7	19	-11	236	13	17
H,K=	2,	20		0	448	10	-8	2	31	71	-45*	-1	240	5	4	-9	261	9	20
-12	141	12	-11	2	237	9	-0	4	297	12	-2	1	200	5	-9	-7	419	8	-4
-10	229	10	-0	4	407	9	-5	H,K=	2,	42		3	532	8	10	-5	624	10	-3
-8	374	9	9	6	182	10	-7	0	155	16	-2	5	375	8	-6	-3	687	9	2
-6	273	8	-1	8	326	10	-4	H,K=	3,	1		7	196	7	4	-1	577	8	-3
-4	424	8	15	10	98	17	6	-13	230	11	14	9	211	9	2	1	541	8	-14
-2	486	9	0	H,K=	2,	30		-11	448	9	10	11	287	9	10	3	700	10	2
0	47	61	-30*	-10	217	16	-8	-9	421	8	-8	13	165	13	5	5	635	11	8
2	477	8	3	-8	122	12	2	-7	632	9	2	H,K=	3,	9		7	408	9	-0
4	407	8	11	-6	421	9	-3	-5	406	6	9	-13	231	11	1	9	243	9	-6
6	245	9	-15	-4	158	11	-1	-3	516	6	8	-11	228	11	2	11	237	14	5
8	370	9	-1	-2	368	9	8	-1	588	7	25	-9	448	9	-8	H,K=	3,	17	
10	225	10	1	0	0	50	-60*	1	584	7	23	-7	237	7	7	-13	225	14	1
12	140	14	-16	2	342	9	-8	3	560	6	16	-5	305	7	-6	-11	252	10	12
H,K=	2,	22		4	145	12	1	5	378	7	-2	-3	443	6	1	-9	344	9	10
-12	170	13	-12	6	423	12	-2	7	641	9	3	-1	847	10	11	-7	311	9	-11
-10	214	11	9	8	139	12	5	9	411	9	-9	1	847	10	-3	-5	432	9	-14
-8	189	10	6	10	201	14	-27	11	449	10	-7	3	464	7	-4	-3	396	7	-2
-6	262	8	-1	H,K=	2,	32		13	214	13	9	5	265	6	2	-1	505	9	-4
-4	160	7	4	-8	91	14	4	H,K=	3,	3		7	217	8	1	1	493	8	-8
-2	385	7	0	-6	237	10	8	-13	36	52	-15*	9	443	9	-9	3	372	11	-4
0	344	8	-2	-4	176	12	-9	-11	0	73	-59*	11	230	9	-3	5	450	8	-10
4	167	9	-11	-2	274	9	-24	-9	77	15	11	13	225	12	-3	7	311	8	-5
6	270	9	10	0	0	51	-32*	-7	380	7	-2	H,K=	3,	11		9	315	11	-12
8	137	14	-21	2	301	9	14	-5	266	6	2	-13	280	10	0	11	239	10	-4
10	200	10	5	4	166	11	-2	-3	346	6	2	-11	456	10	1	13	229	14	8
12	177	11	-2	6	253	10	17	-1	85	16	-2	-9	260	9	7	H,K=	3,	19	
H,K=	2,	24		8	69	26	-14	1	67	9	-1	-7	537	8	0	-11	103	11	29
-10	52	52	-33*	H,K=	2,	34		3	372	6	6	-5	452	7	-13	-9	92	15	-2
-8	552	11	-8	-8	0	56	-60*	5	254	6	9	-3	677	10	-5	-7	108	13	-2
-6	141	11	-0	-4	0	49	-19*	7	377	7	8	-1	647	8	-9	-3	224	8	11
-4	408	8	6	-2	415	9	-0	9	63	20	-13	1	646	8	0	-1	373	7	9
-2	178	8	-8	0	47	53	-5*	11	78	14	14	3	712	9	-6	1	360	7	-6
0	542	11	18	2	433	10	-0	13	71	21	9	5	463	7	-11	3	230	7	12
2	187	10	3	4	0	56	-14*	H,K=	3,	5		7	522	9	-5	5	181	15	6
4	413	8	5	6	308	10	4	-13	285	10	8	9	261	9	7	7	105	12	10
6	160	9	17	H,K=	2,	36		-11	371	9	11	11	453	10	5	9	129	10	11
8	550	10	-9	-6	206	11	11	-9	457	8	9	13	252	14	-22	11	79	22	-1
10	93	16	6	-4	95	16	-17	-7	524	8	-1	H,K=	3,	13		H,K=	3,	21	
H,K=	2,	26		-2	237	9	7	-5	803	10	1	-13	41	51	19*	-11	290	10	9
-10	89	17	30	0	266	12	-6	-3	597	7	-15	-11	92	11	8	-9	419	10	6
-8	196	11	-10	2	238	17	-0	-1	394	5	13	-9	112	11	8	-7	365	11	6
-6	65	22	-22	4	103	14	-9	1	369	5	5	-7	137	8	10	-5	450	9	20
-4	352	11	-2	6	185	11	-8	3	590	8	-22	-5	149	8	9	-3	475	9	2
-2	164	14	9	H,K=	2,	38		5	790	11	13	-3	262	6	-7	-1	728	10	-17
0	327	8	-1	-6	199	13	-25	7	546	8	-6	-1	228	6	4	1	713	10	-4
2	156	9	11	-4	183	12	-5	9	460	10	-2	1	230	6	11	3	472	9	-6
4	373	9	8	-2	256	10	6	11	348	9	-11	3	270	6	4	5	423	9	3
6	96	11	16	0	78	24	-29	13	274	11	2	5	134	8	3	7	352	8	10

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
9	423	9	12	3	308	9	-11	8	607	9	1	4	382	5	12	2	335	7	-5
11	270	13	-2	5	424	9	13	10	204	9	1	8	178	6	-8	4	132	10	-10
H,K=		3,	23	7	230	11	-22	12	374	13	-8	10	375	7	-1	6	377	8	-2
-11	94	19	4	9	263	11	12	14	88	24	8	12	109	9	-7	8	284	9	-8
-9	82	20	-8	H,K=		3,	33	H,K=		4,	4	H,K=		4,	12	10	175	11	-1
-7	198	9	-3	-7	137	16	11	-14	218	15	-1	-12	85	15	-14	12	188	15	14
-5	188	8	-2	-5	187	10	6	-12	116	14	-18	-6	487	8	-1	H,K=		4,	22
-3	210	8	-4	-3	239	11	-8	-10	337	10	-18	12	122	14	10	-12	171	17	-4
-1	223	8	-7	-1	322	9	1	-8	244	8	4	H,K=		4,	14	-10	180	10	8
1	191	8	-8	1	308	10	-18	-6	537	9	3	-12	362	12	-12	-8	241	9	12
3	209	8	13	3	246	10	-6	-4	340	6	5	-10	87	16	-1	-6	208	9	-6
5	208	8	5	5	194	11	12	-2	516	7	11	-8	467	9	-3	-4	361	9	9
7	209	10	18	7	131	15	4	0	245	5	22	-6	405	8	4	-2	463	10	-4
9	99	14	1	H,K=		3,	35	2	490	6	6	-4	611	10	1	0	238	12	-20
11	93	16	3	-7	137	15	-5	4	351	7	-0	-2	135	8	-5	2	474	9	-1
H,K=		3,	25	-5	177	12	7	6	541	8	13	0	813	11	3	4	370	8	8
-11	225	12	8	-3	191	12	0	8	253	8	5	2	130	7	6	6	217	9	-2
-9	183	10	6	-1	118	13	11	10	351	9	3	6	390	8	-3	8	240	10	-11
-7	314	10	-17	1	88	22	-21	14	222	19	5	8	458	9	0	10	175	10	10
-5	324	8	10	3	186	10	-7	H,K=		4,	6	10	98	14	4	12	174	13	2
-3	355	8	-23	5	188	10	20	-14	167	12	3	12	372	10	1	H,K=		4,	24
-1	395	8	11	H,K=		3,	37	-12	197	11	-13	H,K=		4,	16	-10	366	10	-1
1	372	8	-11	-5	264	10	19	-10	330	9	12	-12	116	16	-17	-8	71	18	19
3	400	8	6	-3	299	10	19	-8	227	8	-7	-10	32	44	22*	-6	458	10	-9
5	303	9	-1	-1	318	10	4	-6	431	7	-6	-8	325	9	-6	-4	61	17	13
7	332	9	-1	1	310	10	-2	-4	241	7	4	-6	183	8	-3	-2	552	13	-13
9	179	12	7	3	286	10	-6	-2	543	7	-1	-4	344	8	14	0	293	7	3
11	207	13	-6	5	239	11	-8	0	153	5	6	-2	215	6	0	2	551	10	-12
H,K=		3,	27	H,K=		3,	39	2	532	7	-1	0	156	6	-1	4	0	44	-59*
-9	177	13	-11	-5	66	25	2	4	237	6	-3	2	205	6	-8	6	468	9	6
-7	439	9	20	-1	84	27	-15	8	239	8	1	4	319	7	8	8	67	20	20
-5	437	9	7	1	122	13	15	10	304	9	-13	6	195	8	-4	10	370	10	-6
-3	408	9	-4	3	90	15	16	14	164	12	2	8	354	9	8	H,K=		4,	26
-1	378	9	2	H,K=		3,	41	H,K=		4,	8	10	0	46	-21*	-10	164	11	9
1	366	8	6	-3	245	12	13	-12	56	29	9	12	120	17	-23	-8	114	12	14
3	396	9	1	-1	214	13	9	-10	394	9	-15	H,K=		4,	18	-6	267	10	0
5	427	9	-2	1	201	13	-5	-8	52	18	7	-12	314	11	-6	-4	41	44	14*
7	421	10	11	3	235	13	1	-6	611	9	-16	-10	120	11	-15	-2	336	9	6
9	191	13	-7	H,K=		4,	0	-4	415	7	12	-8	457	9	-16	0	46	25	11
H,K=		3,	29	-12	92	20	-11	-2	827	9	1	-6	0	44	-12*	2	329	9	8
-9	51	36	8	-4	254	6	5	0	421	6	-7	-4	535	9	-6	4	0	63	-43*
-7	0	55	-18*	0	888	10	19	2	856	10	18	-2	121	8	-6	6	262	11	-6
-5	47	29	6	4	204	6	8	4	417	7	10	0	550	8	7	8	98	16	-1
-3	103	12	2	8	350	8	16	6	587	10	-24	2	134	8	3	10	139	15	3
-1	0	42	-23*	12	124	14	13	8	0	45	-48*	4	558	9	-4	H,K=		4,	28
1	40	48	13*	H,K=		4,	2	10	404	9	1	6	0	42	-25*	-10	351	12	17
3	102	15	-2	-14	108	14	27	12	61	29	16	8	457	9	-8	-8	82	16	2
7	39	46	18*	-12	392	10	4	H,K=		4,	10	10	117	13	-13	-6	375	9	-7
9	59	28	13	-8	618	9	-2	-12	127	14	-0	12	340	11	12	-4	183	10	-9
H,K=		3,	31	-6	213	7	-6	-10	387	9	-0	H,K=		4,	20	-2	493	9	-7
-9	254	12	2	-4	987	11	9	-8	198	8	6	-12	180	14	9	0	45	38	-14
-7	240	11	3	-2	294	6	18	-6	370	7	6	-10	159	12	-4	2	515	10	-2
-5	402	9	-16	0	867	10	13	-4	395	7	-3	-8	284	11	-3	4	201	12	-2
-3	325	9	-3	2	277	5	16	-2	585	8	1	-6	368	8	-7	6	397	9	6
-1	375	11	-21	4	948	12	6	0	217	6	-2	-2	365	9	-15	8	90	16	14
1	382	9	-1	6	197	7	-12	2	557	7	-5	0	450	8	-0	10	345	10	14

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		4,	30	3	339	6	-8	-3	433	7	1	-7	287	9	-9	1	456	8	4
-8	280	12	6	5	480	9	2	-1	454	6	-13	-5	406	8	-10	3	417	8	15
-6	146	12	-6	7	282	7	-6	1	434	6	-13	-3	451	8	13	5	199	9	-13
-4	391	13	8	9	205	8	-18	3	415	7	10	-1	365	8	0	7	192	10	6
-2	266	9	8	11	280	10	-12	5	633	11	9	1	368	7	14	9	253	10	-0
0	337	10	-10	13	199	12	17	7	436	11	-5	3	449	9	9	11	196	17	-9
2	267	9	-4	H,K=		5,	3	9	382	9	3	5	424	10	-4	H,K=		5,	27
4	387	9	1	-13	212	14	-10	11	270	9	5	7	285	8	1	-9	251	10	6
6	169	14	5	-11	325	10	-9	13	194	12	-8	9	275	12	-17	-7	226	11	6
8	291	10	5	-9	430	9	3	H,K=		5,	11	11	234	11	-1	-5	229	9	13
H,K=		4,	32	-7	492	8	-11	-13	185	13	-5	H,K=		5,	19	-3	235	9	-16
-8	132	13	15	-5	451	7	6	-11	216	10	-7	-11	115	17	-29	-1	362	8	-1
-6	72	38	-11	-3	670	8	1	-9	271	9	7	-9	306	9	-18	1	379	8	-1
-4	279	9	-10	-1	607	7	-2	-7	287	8	-10	-7	336	8	12	3	264	8	4
-2	127	11	12	1	665	8	9	-5	134	9	-9	-5	366	8	-3	5	225	10	-3
0	297	10	-14	3	658	9	7	-3	367	6	-6	-3	351	7	-1	7	210	11	-12
2	105	19	-11	5	399	7	-2	-1	417	6	4	-1	361	9	-2	9	231	10	-9
4	285	10	-2	7	532	8	2	1	399	7	-3	1	357	7	-11	H,K=		5,	29
6	89	16	-2	9	398	9	-7	3	330	9	-8	3	358	8	-1	-9	204	11	17
H,K=		4,	34	11	305	9	-15	5	154	8	-7	5	362	8	6	-7	276	9	4
-8	318	11	10	13	239	11	14	7	301	9	5	7	337	9	11	-5	351	9	1
-6	50	35	36	H,K=		5,	5	9	263	9	2	9	345	10	4	-3	423	10	5
-4	322	10	-9	-11	150	11	3	11	226	10	-12	11	136	13	-10	-1	387	9	-10
0	474	10	-9	-9	179	9	-16	13	169	14	-23	H,K=		5,	21	1	390	9	3
2	52	29	29	-7	358	8	1	H,K=		5,	13	-11	79	20	-6	3	413	10	-6
4	319	10	-18	-5	738	9	12	-13	247	12	-13	-9	139	12	-8	5	366	9	-2
8	312	11	9	-3	266	6	5	-11	308	10	-0	-7	173	10	-7	7	265	13	-9
H,K=		4,	36	-1	149	6	9	-9	407	9	-14	-5	289	8	-5	9	163	13	-17
-6	126	14	-3	1	82	15	-9	-7	458	9	-1	-3	270	8	9	H,K=		5,	31
-4	168	12	-8	3	252	6	14	-5	434	9	10	-1	109	9	-1	-9	154	18	-15
-2	191	10	10	5	732	10	3	-3	631	10	-9	1	123	8	-11	-7	149	13	2
0	224	13	4	7	359	9	13	-1	405	7	0	3	246	8	-9	-5	131	12	19
2	198	14	11	9	205	9	6	1	425	7	-0	5	317	8	11	-3	199	9	-2
4	163	12	-12	11	151	10	17	3	611	8	2	7	182	10	-12	-1	194	9	2
6	135	13	-5	13	142	13	-3	7	458	8	0	9	150	11	-9	1	208	11	-7
H,K=		4,	38	H,K=		5,	7	9	403	9	-6	11	58	44	-32	3	204	11	-2
-4	259	11	-10	-13	262	13	3	11	329	9	19	H,K=		5,	23	5	122	14	2
-2	109	20	-9	-11	209	9	12	13	267	10	10	-11	219	11	13	7	151	15	5
0	244	10	-1	-9	348	8	5	H,K=		5,	15	-9	274	10	-6	9	176	15	7
2	143	15	15	-7	436	8	6	-13	141	35	-4	-7	308	9	5	H,K=		5,	33
4	275	11	7	-5	348	7	-7	-11	195	14	3	-5	248	8	-5	-7	195	13	19
H,K=		4,	40	-3	728	9	3	-9	250	9	2	-3	422	8	3	-5	210	11	10
-4	0	59	-58*	-1	553	7	-7	-7	373	8	5	-1	419	8	-1	-3	199	10	1
-2	334	11	3	1	523	7	-6	-5	163	8	4	1	414	8	0	-1	337	11	14
0	46	52	38*	3	695	9	-5	-3	283	9	2	3	424	9	10	1	335	11	3
2	335	13	4	5	358	8	-6	-1	399	7	14	5	291	9	11	3	205	11	-7
4	66	29	-2	7	436	8	-1	1	410	7	7	7	300	11	-6	5	174	12	-26
H,K=		5,	1	9	345	8	7	3	281	8	16	9	288	10	7	7	190	11	11
-13	178	13	-8	11	189	10	16	5	191	8	2	11	195	17	-20	H,K=		5,	35
-11	292	10	-6	13	275	11	-2	7	361	8	1	H,K=		5,	25	-7	142	17	-12
-9	207	9	-1	H,K=		5,	9	9	239	9	-8	-11	190	18	-20	-5	237	11	11
-7	279	8	-1	-13	204	12	3	11	191	10	4	-9	263	10	8	-3	231	10	7
-5	466	7	-4	-11	272	9	3	13	140	16	-9	-7	201	10	-6	-1	269	10	-8
-3	384	6	-1	-9	376	9	-8	H,K=		5,	17	-5	226	13	2	1	295	10	8
-1	599	7	-5	-7	446	8	-3	-11	231	10	2	-3	411	9	20	3	242	10	7
1	605	7	1	-5	640	9	5	-9	296	10	9	-1	438	8	-2	5	210	12	-9

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
7	154	12	-1	-4	979	13	3	-2	142	7	11	0	550	10	5	2	5	48	-20*
H,K=		5,	37	-2	29	37	-16*	0	622	9	-13	2	37	47	-27*	4	49	27	11
-5	165	13	4	0	853	9	4	2	134	7	3	4	554	9	14	6	53	40	5
-3	135	14	0	2	58	21	13	4	419	8	1	6	29	48	-3*	H,K=		6,	36
-1	136	15	-18	4	947	13	-16	6	143	8	2	8	450	10	-3	-6	367	11	3
1	164	12	3	6	135	9	28	8	337	9	-5	10	81	15	5	-4	48	32	30
3	128	15	-8	8	613	10	-11	10	104	16	-6	H,K=		6,	24	-2	292	10	-5
5	160	13	-7	10	63	24	-14	12	203	13	2	-10	78	20	12	0	90	16	4
H,K=		5,	39	12	371	11	7	H,K=		6,	16	-8	110	25	-7	2	296	10	-6
-3	225	13	-7	H,K=		6,	8	-12	88	21	-18	-6	180	10	10	4	35	44	17*
-1	229	10	11	-12	81	19	-2	-10	464	11	1	-4	42	45	-24*	6	361	11	1
1	234	11	5	-10	67	16	21	-8	41	43	-4*	-2	55	18	18	H,K=		6,	38
3	234	11	8	-8	87	12	6	-6	696	10	4	0	0	45	-17*	-4	274	12	-18
H,K=		5,	41	-6	42	32	-12	-4	173	7	9	2	0	43	-24*	-2	0	55	-22*
-1	128	18	-18	-4	248	6	0	-2	659	11	-29	4	56	37	-8	0	273	10	-14
1	150	14	8	-2	148	6	7	0	42	43	35*	6	151	10	-19	2	0	65	-22*
H,K=		6,	0	0	437	6	18	2	674	12	-14	H,K=		6,	26	4	291	11	4
-10	692	10	5	2	149	6	9	4	164	8	-1	-10	0	62	-40*	H,K=		6,	40
-6	508	8	-21	4	248	6	0	6	703	11	16	-8	435	10	-17	-2	183	10	25
-2	903	10	1	6	74	11	28	8	73	15	28	-6	61	61	24*	0	0	57	-76*
2	973	12	15	8	85	15	6	10	456	11	-14	-4	626	10	-5	2	131	16	-13
6	525	8	-1	10	38	49	-11*	12	102	18	-4	0	624	9	-9	H,K=		7,	1
10	681	11	-5	12	83	19	-1	H,K=		6,	18	2	42	44	5*	-13	183	10	8
H,K=		6,	2	H,K=		6,	10	-12	87	17	21	4	632	10	-12	-11	258	10	-3
-12	137	13	-22	-12	425	10	4	-10	0	48	-27*	6	44	47	8*	-9	332	9	-7
-10	122	14	5	-8	720	10	2	-8	67	21	-9	8	443	10	-12	-7	228	8	-15
-8	191	8	1	-6	117	9	-4	-6	120	11	3	10	25	47	-16*	-5	369	7	15
-6	122	8	-4	-4	754	10	2	-4	296	8	-7	H,K=		6,	28	-3	257	7	1
-4	461	7	5	-2	322	6	16	-2	88	10	5	-10	199	13	-16	-1	365	6	7
-2	46	33	2	0	1017	13	-3	0	37	30	-10	-8	48	50	6*	1	395	6	7
0	694	8	15	2	313	6	8	2	90	9	7	-6	234	10	-2	3	295	6	8
2	43	51	-1*	4	757	10	-5	4	287	7	-13	-2	294	9	-0	5	343	7	10
4	445	8	9	6	119	10	-2	6	123	11	7	0	0	48	-29*	7	249	8	-2
6	125	8	0	8	713	12	4	8	65	18	-9	2	303	8	6	9	345	8	0
8	209	8	5	10	82	18	-24	10	41	48	16*	4	137	10	12	11	257	10	-5
10	118	11	-1	12	404	10	-15	12	84	18	15	6	224	10	1	13	177	13	-3
12	149	13	-5	H,K=		6,	12	H,K=		6,	20	8	53	38	9	H,K=		7,	3
H,K=		6,	4	-12	55	29	46	-12	22	63	-0*	10	224	8	13	-13	246	14	2
-12	15	52	-5*	-10	370	9	6	-10	336	10	-18	H,K=		6,	30	-11	257	11	-9
-10	299	9	-5	-8	108	12	4	-8	56	27	-4	-8	238	8	2	-9	281	12	2
-8	243	9	-8	-6	368	8	-15	-6	435	8	6	-6	0	42	-3*	-7	362	8	3
-6	511	8	-9	-4	154	14	3	-4	112	11	-11	-4	259	9	-16	-5	644	9	-0
-4	95	8	7	-2	562	9	-6	-2	546	9	2	0	529	14	-3	-3	515	7	-1
-2	693	8	-3	0	177	6	9	0	146	8	-8	2	82	17	-4	-1	760	9	-16
0	191	7	0	2	514	8	-8	2	553	9	1	4	264	13	-8	1	789	9	1
2	675	9	-9	4	164	7	12	4	129	9	7	6	47	49	43*	3	522	8	-11
4	85	9	-3	6	370	9	-9	6	442	9	11	H,K=		6,	32	5	634	10	-9
6	552	9	15	8	102	12	-0	8	81	16	20	2	435	9	-12	7	366	8	-2
8	251	10	1	10	362	9	-8	10	362	10	4	4	84	15	-12	9	302	10	1
10	299	9	-6	12	22	54	15*	12	0	54	-21*	6	409	10	-14	11	268	13	-4
12	0	55	-21*	H,K=		6,	14	H,K=		6,	22	8	0	52	-35*	13	230	11	-22
H,K=		6,	6	-12	220	12	6	-10	99	14	23	H,K=		6,	34	H,K=		7,	5
-12	368	10	17	-10	126	10	17	-8	452	10	8	-6	44	51	-2*	-13	151	15	-6
-10	77	31	0	-8	328	9	-10	-6	37	42	5*	-4	10	57	-35*	-11	193	10	5
-8	630	10	0	-6	163	7	22	-4	529	9	-12	-2	51	34	27	-9	282	8	10
-6	125	8	10	-4	407	7	-4	-2	58	18	-5	0	0	52	-5*	-7	280	8	-4

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-5	416	8	2	-11	224	10	-5	-3	252	9	12	-5	233	13	-8	12	358	13	9
-3	202	7	-6	-9	328	9	-7	-1	285	8	-12	-3	135	14	-18	H,K=	8,		4
-1	338	6	-3	-7	454	9	-6	1	269	8	-21	-1	196	11	-4	-10	398	11	-4
1	383	6	-0	-5	457	11	3	3	254	8	10	1	201	10	6	-8	178	13	-9
3	219	6	3	-3	619	9	-17	5	231	9	11	3	153	14	-9	-6	362	7	6
5	386	7	-16	-1	392	8	5	7	246	10	-5	5	244	10	0	-4	445	8	-10
7	273	10	-4	1	408	8	2	9	215	14	-0	7	160	15	4	-2	719	9	15
9	283	9	-2	3	648	11	1	11	135	15	-15	H,K=	7,	33	0	174	6	18	
11	176	12	1	5	438	10	8	H,K=	7,	23		-7	239	14	-7	2	721	10	-2
13	170	12	8	7	453	11	-13	-11	263	12	-11	-5	235	11	5	4	441	8	-9
H,K=	7,		7	9	324	11	-9	-9	286	10	-6	-3	205	11	0	6	397	8	15
-13	245	10	9	11	215	11	-11	-7	260	10	-16	-1	265	10	-1	8	204	9	3
-11	312	10	-16	13	196	14	-23	-5	339	9	0	1	244	12	-16	H,K=	8,		6
-9	276	9	7	H,K=	7,	15		-3	477	10	-15	3	199	9	9	-12	229	10	25
-7	375	8	4	-11	142	12	11	-1	235	8	9	5	221	11	-13	-10	286	10	-12
-5	483	8	-7	-9	250	9	-16	1	221	8	2	7	279	10	30	-8	297	8	-8
-3	384	7	1	-7	124	10	2	3	471	9	-17	H,K=	7,	35		-6	290	8	-16
-1	610	8	-16	-5	271	11	-14	5	328	9	-7	-5	189	12	-11	-4	298	7	-5
1	614	8	-6	-3	368	7	-3	7	267	10	-1	-3	162	13	-15	-2	581	8	3
3	379	7	-2	-1	372	7	-6	9	298	10	12	-1	242	11	-20	0	37	29	-15
5	488	8	-2	1	388	9	3	11	274	12	9	1	270	9	12	2	588	8	4
7	353	8	-2	3	373	7	-2	H,K=	7,	25		3	168	11	2	4	278	7	-7
9	292	9	5	5	293	7	3	-9	252	11	-8	5	217	11	0	6	297	8	-15
11	315	10	-15	9	258	11	-16	-7	236	10	3	H,K=	7,	37		8	303	8	-7
13	228	11	-3	11	141	12	-2	-5	271	9	14	-5	152	14	7	12	218	11	15
H,K=	7,		9	H,K=	7,	17		-3	367	12	2	-3	106	25	-13	H,K=	8,		8
-13	148	13	0	-11	177	10	12	-1	245	10	-1	-1	181	10	24	-12	59	26	-7
-11	194	11	3	-9	254	13	-6	1	265	9	8	1	157	12	4	-10	389	9	-6
-9	366	9	5	-7	233	8	5	3	347	9	-16	3	132	13	17	-8	13	48	-19*
-7	506	9	-1	-5	256	8	-11	5	232	9	2	5	135	14	-16	-6	570	9	-15
-5	356	8	-0	-3	286	8	-2	7	232	10	-10	H,K=	7,	39		-4	234	7	-4
-3	507	8	0	-1	322	8	0	9	272	10	1	-3	193	12	-0	-2	979	13	-10
-1	605	9	7	1	323	7	1	H,K=	7,	27		-1	239	11	20	0	111	7	13
1	621	9	8	3	288	8	3	-9	189	11	1	1	213	11	3	4	241	7	8
3	513	9	-2	5	294	8	7	-7	181	11	1	3	206	16	13	6	587	11	-14
5	340	7	-6	7	233	9	4	-5	180	10	-15	H,K=	8,		0	8	0	48	-35*
7	516	10	3	9	248	10	-5	-3	271	11	-1	-12	277	10	-2	10	378	9	0
9	362	9	-3	11	163	12	-3	-1	188	9	4	-8	363	9	-5	12	43	62	-23*
11	193	10	1	H,K=	7,	19		1	196	11	6	-4	562	8	3	H,K=	8,		10
13	121	30	-25	-11	224	12	-17	3	270	9	-1	0	142	6	9	-12	121	16	10
H,K=	7,		11	-9	278	10	7	5	198	10	2	4	549	9	2	-10	257	9	7
-13	175	17	-29	-7	281	9	9	7	177	10	-8	8	357	8	-12	-8	111	12	4
-11	252	11	-3	-5	367	9	-8	9	183	12	-2	12	286	11	-4	-6	335	8	14
-9	252	10	-12	-3	538	10	-8	H,K=	7,	29		H,K=	8,		2	-4	101	10	-1
-5	234	7	-12	-1	460	9	2	-9	294	11	19	-12	332	10	-5	-2	531	9	1
-3	370	7	14	1	470	8	2	-7	270	10	1	-10	170	10	-1	0	461	7	4
-1	578	9	6	3	540	9	-6	-5	310	11	-11	-8	418	9	-11	2	531	8	-6
1	589	8	1	5	378	10	-1	-3	407	9	-7	-6	155	8	16	4	128	8	5
3	372	8	3	7	268	9	-18	-1	277	9	-0	-4	854	11	-2	8	88	26	-18
5	245	9	-4	9	282	10	8	1	289	8	13	-2	401	8	12	10	261	11	5
7	131	12	15	11	257	11	23	3	397	9	2	0	520	8	-19	12	113	20	-3
9	278	9	1	H,K=	7,	21		5	312	9	8	2	400	7	17	H,K=	8,		12
11	244	10	7	-11	171	11	20	7	289	10	20	4	839	12	-5	-12	96	18	0
13	178	27	-20	-9	224	10	9	9	274	11	1	6	150	9	6	-10	339	9	-7
H,K=	7,		13	-7	279	9	8	H,K=	7,	31		8	415	10	-22	-8	173	11	4
-13	211	12	-10	-5	219	8	13	-7	138	23	-13	10	165	11	-3	-6	425	8	2

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-4	307	7	-5	2	432	8	8	2	165	10	17	1	236	7	6	3	477	9	-5
-2	563	9	-2	4	146	9	5	4	324	9	-16	3	52	33	0	5	404	12	-9
0	229	8	-25	6	248	12	2	6	189	10	-1	5	252	7	8	7	505	9	9
2	566	9	6	8	86	17	7	8	290	12	-26	7	98	19	-7	9	375	9	-8
4	332	7	14	10	245	10	19	H,K=	8,	32		9	37	45	-8*	11	284	11	1
6	401	11	-14	H,K=	8,	22		-8	170	15	-22	11	63	23	8	H,K=	9,	13	
8	160	11	-23	-10	176	13	-5	-6	170	17	13	13	100	16	24	-11	60	25	17
10	356	10	3	-8	270	9	3	-2	87	16	2	H,K=	9,	5		-9	8	42	-2*
12	57	57	-30*	-6	214	9	0	0	254	10	9	-13	283	11	8	-7	83	17	-25
H,K=	8,	14		-4	303	8	4	2	76	17	4	-11	354	9	3	-5	76	14	0
-12	263	12	-10	-2	234	10	-5	4	134	13	7	-9	341	11	-17	-3	111	10	-2
-10	84	14	5	0	271	8	5	6	156	13	-1	-7	485	9	-5	-1	244	8	7
-8	360	9	5	2	223	8	-5	8	205	16	3	-5	616	10	-2	1	249	7	7
-6	219	8	-5	4	283	8	-8	H,K=	8,	34		-3	516	8	-2	3	108	9	-5
-4	563	12	-9	6	205	9	-3	-6	0	54	-4*	-1	636	9	-6	5	87	16	9
-2	225	7	9	8	276	10	3	-4	314	11	-3	1	625	10	-5	7	111	13	-1
2	220	7	6	10	164	14	-17	-2	67	22	6	3	553	8	12	9	58	22	46
4	587	11	-3	H,K=	8,	24		0	448	10	5	5	624	11	-1	11	0	54	-35*
6	235	8	12	-10	372	11	1	2	23	52	-38*	7	492	8	0	H,K=	9,	15	
8	363	9	-3	-8	0	48	-16*	4	325	12	21	9	343	9	-6	-11	204	12	-6
10	71	23	0	-6	392	9	10	6	0	55	-8*	11	346	10	7	-9	310	9	14
12	288	10	11	-4	55	61	-15*	H,K=	8,	36		13	283	12	14	-7	415	9	-7
H,K=	8,	16		-2	536	9	1	-4	101	14	3	H,K=	9,	7		-5	466	8	-7
-12	186	13	-10	0	90	13	11	-2	125	14	-3	-11	122	15	-9	-3	484	8	4
-10	22	49	-6*	2	549	10	2	0	183	11	28	-9	228	9	-30	-1	433	9	-15
-8	225	12	-14	4	61	22	-9	2	110	33	-27	-7	201	9	-6	1	419	8	-9
-6	48	23	8	6	359	9	2	4	82	44	-28	-5	132	9	-8	5	482	8	8
-4	331	10	-5	8	0	48	-23*	H,K=	8,	38		-3	302	7	-4	7	417	11	-7
-2	95	8	12	10	388	10	13	-4	202	13	13	-1	577	9	14	9	302	9	7
0	404	8	-4	H,K=	8,	26		-2	136	15	-11	3	301	8	-6	11	225	11	6
2	45	45	-25*	-10	208	12	-8	0	234	11	2	5	118	10	-17	H,K=	9,	17	
4	347	8	3	-8	90	21	-27	2	143	12	1	7	207	10	-8	-9	265	10	9
6	39	45	-10*	-6	318	9	-6	4	213	14	16	9	242	9	-13	-7	263	9	1
8	237	9	4	-4	110	12	3	H,K=	9,	1		11	132	11	19	-5	258	9	-5
10	27	47	2*	-2	313	11	-28	-13	180	15	-7	13	141	13	24	-3	495	10	-7
H,K=	8,	18		0	68	23	-3	-11	329	10	2	H,K=	9,	9		-1	299	9	-7
-12	303	11	-17	2	336	9	-16	-9	316	9	-4	-11	239	11	-12	1	312	8	-10
-10	74	19	11	4	121	12	3	-7	256	8	9	-9	215	10	-8	3	503	9	-4
-8	498	10	-0	6	313	12	5	-5	527	9	-2	-7	287	9	-2	5	275	8	14
-6	109	12	-7	8	133	13	13	-3	678	9	6	-5	190	7	-8	7	286	9	8
-4	587	9	15	10	214	13	-1	-1	730	9	2	-3	207	7	-3	9	252	10	2
-2	103	12	6	H,K=	8,	28		1	742	10	1	-1	621	10	12	11	240	10	10
0	445	9	19	-8	122	16	-15	3	697	10	10	1	617	9	20	H,K=	9,	19	
2	104	10	10	-6	408	10	2	5	520	10	-6	3	212	8	-8	-11	160	8	14
4	572	10	-0	-4	140	11	-4	7	264	8	-5	5	220	8	-5	-9	158	12	-3
6	126	13	6	-2	269	9	-6	9	337	9	6	7	279	8	1	-5	91	16	-18
8	491	10	1	0	172	14	15	11	329	10	7	9	236	9	6	-3	166	8	6
10	76	20	6	2	270	9	-1	13	186	12	1	11	254	10	1	-1	200	8	12
12	303	11	-13	4	134	11	3	H,K=	9,	3		H,K=	9,	11		1	165	8	-2
H,K=	8,	20		6	397	13	-9	-13	84	20	16	-11	286	10	8	3	145	10	-9
-10	223	12	-5	H,K=	8,	30		-11	62	23	8	-9	389	9	4	H,K=	9,	21	
-8	84	16	11	-8	307	11	0	-9	42	46	9*	-7	479	10	-3	-11	294	11	-0
-6	231	9	-5	-6	177	13	-21	-7	121	10	11	-5	428	8	-7	-9	297	12	2
-4	137	9	3	-4	351	9	-0	-5	241	8	-1	-3	488	8	12	-7	314	9	3
-2	423	9	-5	-2	160	10	-0	-3	32	38	-9*	-1	583	11	-1	-5	288	8	-4
0	265	7	-8	0	325	11	11	-1	259	6	10	1	576	10	-3	-3	502	9	-6

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-1	360	9	-5	5	229	10	-7	-12	169	13	4	-10	379	10	10	8	200	11	1
1	363	10	1	7	261	13	-7	-10	145	10	17	-8	170	10	-8	10	177	12	8
3	506	11	-8	H,K=	9,	33		-8	288	9	6	-6	403	9	-19	H,K=	10,	24	
5	296	9	9	-7	168	13	7	-6	237	8	16	-4	75	16	5	-10	115	15	24
7	317	9	-7	-5	174	12	14	-4	281	7	-0	-2	583	10	4	-8	358	10	4
9	303	10	7	-1	255	13	9	-2	263	6	-9	0	110	9	6	-6	54	28	-4
11	302	8	2	1	231	10	-3	0	481	9	4	2	587	11	11	-4	490	10	-5
H,K=	9,	23		3	139	10	0	2	268	7	-3	4	57	19	1	-2	0	44	-11*
-9	148	12	-5	7	168	14	1	4	272	7	0	6	413	10	-22	0	528	11	-16
-7	121	12	4	H,K=	9,	35		6	237	9	10	8	163	11	-10	2	0	64	-22*
-5	132	10	-1	-5	65	41	-28	8	288	9	-9	10	363	12	-5	4	494	11	2
-3	205	11	-1	-3	117	22	11	10	111	13	-9	12	57	30	7	6	52	27	5
-1	159	10	-3	-1	154	11	3	H,K=	10,	8		H,K=	10,	16		8	362	10	9
1	169	8	5	1	136	15	-8	-12	309	11	3	-10	201	12	3	10	90	18	2
3	217	9	10	3	77	23	-27	-10	0	46	-37*	-8	129	11	-8	H,K=	10,	26	
5	126	12	5	5	93	21	4	-8	513	9	0	-6	380	9	-11	-8	129	14	7
7	122	15	12	H,K=	9,	37		-6	159	9	-8	-4	81	10	19	-6	0	47	-21*
9	143	12	-4	-3	277	11	-7	-4	519	8	-2	-2	327	11	-5	-4	319	10	-1
H,K=	9,	25		-1	256	11	5	-2	66	12	-7	0	190	7	-10	-2	109	12	-11
-9	158	12	6	3	294	11	9	0	663	10	-14	2	324	7	19	0	150	12	1
-7	263	10	7	H,K=	9,	39		2	76	10	4	4	45	46	-4*	2	121	10	-4
-5	306	9	-20	-1	0	55	-31*	4	536	11	13	6	380	9	-4	4	322	9	-5
-3	342	9	-3	1	0	48	-24*	6	160	9	-5	8	137	11	3	8	123	18	-7
-1	224	9	7	H,K=	10,	0		8	520	9	5	10	197	11	-8	H,K=	10,	28	
1	201	9	-7	-10	270	14	-21	10	0	47	-38*	H,K=	10,	18		-8	290	14	3
3	328	11	-6	-6	534	9	6	12	303	11	-6	-10	329	10	8	-6	84	18	2
5	299	9	-15	-2	409	7	7	H,K=	10,	10		-8	70	17	19	-4	354	10	-7
7	264	11	6	6	518	11	-4	-12	184	13	9	-6	453	9	-9	-2	132	13	-8
9	148	11	3	10	283	10	-3	-10	216	13	10	-4	103	12	-6	0	414	9	-2
H,K=	9,	27		H,K=	10,	2		-8	263	10	-1	-2	501	10	8	2	122	21	-12
-9	299	11	-1	-12	0	51	-25*	-6	124	9	10	0	165	8	1	4	351	10	-10
-7	355	10	19	-10	477	10	5	-4	253	7	-10	2	492	9	10	6	88	18	24
-5	328	9	-0	-8	90	13	-1	-2	112	10	2	4	141	9	21	8	291	10	2
-3	373	11	6	-6	346	8	4	0	388	7	4	6	453	9	2	H,K=	10,	30	
-1	314	10	-9	-4	146	8	3	2	98	10	-6	10	314	13	-9	-8	97	18	-15
1	319	9	-2	-2	840	11	4	4	301	9	1	H,K=	10,	20		-6	310	11	5
3	388	9	10	0	334	6	3	6	120	9	4	-10	191	12	7	-4	83	19	2
5	306	10	-4	2	870	12	4	8	262	9	-1	-8	196	11	7	-2	334	9	-5
7	342	10	3	4	130	8	5	10	196	11	0	-6	212	11	-1	0	224	10	-14
9	300	11	4	6	365	8	2	12	199	11	12	-4	373	10	-11	2	344	9	7
H,K=	9,	29		8	134	10	27	H,K=	10,	12		-2	302	8	-5	4	104	12	28
-7	46	49	8*	10	437	12	-18	-12	264	10	16	0	228	12	-11	6	320	10	15
-5	90	15	7	12	44	53	20*	-10	199	11	20	2	298	10	3	8	100	17	1
-3	29	48	-13*	H,K=	10,	4		-8	467	9	-11	4	377	11	-8	H,K=	10,	32	
-1	0	56	-47*	-12	199	12	-19	-6	297	8	6	6	199	10	-7	-6	132	15	-15
1	61	18	18	-10	166	9	6	-4	460	8	-5	8	189	11	9	-4	83	16	11
3	59	20	21	-6	323	9	0	-2	340	7	0	10	169	14	-15	-2	217	10	22
5	110	13	30	-4	418	7	1	0	758	13	2	H,K=	10,	22		0	105	16	-11
7	17	60	-21*	-2	496	7	3	2	331	8	-8	-8	195	12	-3	2	200	12	5
H,K=	9,	31		0	291	6	-7	4	460	9	1	-6	328	9	-12	4	67	23	-11
-7	273	12	6	4	415	9	-11	6	292	8	6	-4	222	9	-8	6	162	13	6
-5	248	9	8	6	325	8	-4	8	464	11	-6	-2	264	8	-5	H,K=	10,	34	
-3	261	10	-9	8	358	9	2	10	187	11	5	0	237	9	-13	-4	81	19	17
-1	317	9	5	10	158	9	7	12	228	17	-20	2	249	9	-3	-2	338	10	9
1	317	9	6	12	232	11	10	H,K=	10,	14		4	247	9	4	0	0	51	-12*
3	274	10	11	H,K=	10,	6		-12	0	51	-45*	6	334	10	-4	2	323	10	-6

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
4	81	16	19	3	381	8	-3	H,K=	11,	17		-5	166	11	9	8	44	56	8*
H,K=	10,	36		5	422	9	-1	-11	171	13	-10	-3	236	12	4	10	177	12	11
-4	149	15	-17	7	242	9	-4	-9	230	10	-0	-1	256	10	-6	12	0	54	-28*
-2	151	16	-4	9	322	10	10	-7	319	9	-4	1	259	10	-17	H,K=	12,		4
0	89	19	-9	11	235	12	3	-5	276	9	5	3	230	9	-9	-12	318	11	4
2	151	14	-3	H,K=	11,		9	-3	250	8	10	H,K=	11,	29		-10	41	48	-6*
4	176	12	19	-11	242	11	10	1	456	11	-9	-7	209	10	18	-8	392	9	0
H,K=	10,	38		-9	341	10	4	3	244	9	-6	-5	238	10	7	-4	629	11	6
0	130	17	-32	-7	351	9	2	5	277	10	9	-3	262	10	2	-2	212	8	1
H,K=	11,		1	-5	282	8	-8	7	311	9	-6	-1	281	10	-6	0	357	10	-10
-11	229	11	-3	-3	395	8	-10	9	202	12	-19	1	280	10	-12	2	205	8	-6
-9	259	9	-9	-1	377	7	-2	11	152	15	-25	3	272	9	12	4	603	11	-10
-7	274	10	7	1	397	7	4	H,K=	11,	19		5	222	12	7	6	67	19	-11
-5	379	8	16	3	385	8	-11	-9	274	10	13	7	206	12	8	8	390	9	6
-3	348	8	-8	5	302	9	-4	-7	324	9	8	H,K=	11,	31		10	0	52	-49*
-1	412	7	4	7	351	11	-4	-5	395	9	-12	-7	133	21	-4	12	307	12	-8
1	395	9	2	9	326	11	-12	-3	434	9	1	-5	175	12	0	H,K=	12,		6
3	340	7	1	11	235	13	9	-1	345	12	6	-3	197	10	13	-10	385	11	-5
5	370	8	-9	H,K=	11,		11	1	332	10	-7	-1	285	10	1	-8	102	14	8
7	271	9	6	-11	136	16	4	3	410	12	-9	3	155	13	-25	-6	631	10	-4
9	257	12	-11	-9	202	12	1	5	403	9	-6	5	181	13	1	-4	8	40	-9*
11	227	11	10	-7	248	9	4	7	324	11	3	7	128	17	-2	-2	567	11	-10
H,K=	11,		3	-5	202	9	-8	9	262	10	8	H,K=	11,	33		0	30	32	25*
-11	283	10	10	-3	258	8	-0	H,K=	11,	21		-5	179	16	-12	2	571	10	-7
-9	267	9	-5	-1	195	8	-2	-9	122	16	-13	-3	197	11	5	4	0	41	-15*
-7	303	9	-8	3	242	8	4	-5	213	9	-9	-1	252	11	1	6	604	9	-17
-5	502	9	0	5	192	12	-3	-3	228	9	1	1	274	10	4	8	76	19	-20
-3	378	7	-9	7	252	11	-1	-1	134	10	-9	3	194	13	-4	10	373	10	-9
-1	433	8	3	9	216	10	6	1	141	10	-9	5	176	13	-13	12	64	38	13
1	465	9	8	11	117	15	-3	3	179	12	-30	H,K=	11,	35		H,K=	12,		8
3	365	7	-11	H,K=	11,		13	5	221	9	0	-3	202	12	9	-12	41	52	-20*
5	499	9	-11	-11	270	11	3	7	188	13	-11	-1	281	12	4	-10	114	15	19
7	307	8	-4	-9	300	10	0	9	141	12	6	1	271	10	-6	-8	84	21	-7
9	295	9	7	-7	409	9	13	H,K=	11,	23		3	187	12	-9	-6	151	14	-3
11	288	10	11	-5	261	8	2	-9	219	11	-4	H,K=	11,	37		-4	130	10	-10
H,K=	11,		5	-3	377	14	-8	-7	283	10	10	-1	105	17	-6	-2	59	16	4
-11	137	14	24	-1	485	8	-6	-5	331	9	-2	1	126	15	21	0	70	12	13
-9	220	9	5	1	483	9	-9	-3	439	9	4	H,K=	12,		0	2	27	43	-29*
-7	80	18	3	3	385	8	-3	-1	270	10	2	-12	396	11	-7	4	144	8	1
-5	154	10	8	5	265	8	-10	1	275	8	-2	-8	485	9	16	6	162	12	5
-3	353	7	-8	7	367	9	-7	3	422	9	-24	-4	704	10	-9	8	92	15	4
-1	336	7	1	9	281	11	-13	5	303	9	-6	0	647	9	-16	10	40	60	-51*
1	366	7	3	11	272	12	0	7	287	10	7	4	673	12	-5	12	73	28	14
3	329	7	-9	H,K=	11,		15	9	205	12	-13	8	460	10	-16	H,K=	12,		10
5	124	10	-20	-11	196	12	7	H,K=	11,	25		12	417	10	14	-10	426	10	-2
7	77	16	0	-9	233	10	-6	-9	159	18	-22	H,K=	12,		2	-8	105	13	-5
9	205	10	5	-7	221	12	4	-7	248	10	-15	-12	0	59	-24*	-6	458	9	-0
11	112	15	22	-5	215	9	9	-5	187	10	10	-10	180	11	10	-4	63	15	-11
H,K=	11,		7	-3	326	9	4	-3	250	10	-10	-8	0	46	-39*	-2	625	11	4
-11	230	12	7	-1	165	8	-11	-1	282	9	-8	-6	260	9	-8	2	626	10	5
-9	303	10	-8	1	165	9	-20	1	294	9	7	-4	162	8	20	4	86	9	13
-7	261	9	1	3	309	9	-5	3	244	9	-20	-2	215	9	-4	6	454	9	-2
-5	440	9	11	5	199	11	-5	7	256	11	-3	0	174	7	6	8	99	14	-11
-3	369	11	-7	7	227	10	-2	9	190	13	0	2	216	7	0	10	428	14	-7
-1	277	7	3	9	211	11	-25	H,K=	11,	27		4	141	13	-1	H,K=	12,		12
1	237	7	-16	11	185	13	-6	-7	142	12	7	6	272	8	7	-10	59	28	22

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-8	306	9	-4	-6	376	11	-0	-7	329	9	-6	7	264	13	-5	-1	309	8	-10
-4	297	8	3	-4	50	53	1*	-5	311	8	8	9	203	10	-12	1	309	9	3
-2	27	48	-15*	-2	390	9	-17	-3	364	8	1	11	199	12	13	3	300	9	-8
0	508	10	15	0	14	46	-17*	-1	303	6	11	H,K=	13,	11		5	332	9	-4
2	53	19	11	2	397	9	3	3	334	10	-5	-11	138	15	4	7	273	10	8
4	282	8	-2	4	61	18	12	5	294	8	-3	-9	199	11	8	9	271	10	18
8	293	10	-14	6	370	10	-6	7	285	9	-17	-7	146	10	13	H,K=	13,	21	
10	66	23	32	8	43	49	1*	9	163	12	-14	-5	131	11	-8	-9	151	14	-12
H,K=	12,	14		H,K=	12,	24		11	220	14	-2	-3	0	46	-22*	-7	169	11	-0
-10	159	12	8	-6	94	33	-7	H,K=	13,	3		-1	317	8	4	-5	129	18	4
-8	64	24	-9	-4	190	9	11	-11	218	12	-16	1	320	8	5	-3	278	9	7
-6	238	9	3	-2	0	48	-34*	-9	356	10	-1	3	55	19	-4	-1	206	16	7
-4	124	9	11	2	15	46	-20*	-7	344	8	13	5	164	8	13	1	220	9	8
-2	260	8	-15	4	175	10	-11	-5	479	9	-9	7	122	11	4	3	280	9	1
0	90	10	11	6	91	20	-10	-3	403	8	3	9	200	11	8	5	107	18	-31
2	273	8	-9	8	62	25	20	1	358	8	-7	11	126	14	-12	7	134	15	-31
4	98	13	-14	H,K=	12,	26		3	384	8	-4	H,K=	13,	13		9	178	13	12
6	271	10	14	-6	392	10	-9	5	469	10	-8	-11	235	11	-6	H,K=	13,	23	
8	40	50	-30*	-4	57	27	-14	7	316	9	-3	-9	242	11	3	-9	207	11	4
10	177	11	10	-2	442	9	10	9	362	11	0	-7	302	9	-6	-7	213	10	-2
H,K=	12,	16		0	0	46	-28*	11	239	11	1	-5	268	10	-11	-5	245	10	8
-10	68	30	8	2	433	10	0	H,K=	13,	5		-3	472	12	15	-3	249	10	-5
-8	480	10	5	4	65	22	-5	-11	142	15	-15	-1	366	8	-7	-1	377	9	10
-6	120	13	-5	6	414	10	6	-9	154	12	1	1	375	9	-1	1	353	9	-8
-4	642	10	1	8	8	62	-55*	-7	255	10	-8	3	467	9	0	3	254	10	-4
-2	220	8	16	H,K=	12,	28		-5	373	8	-14	5	259	9	-8	5	238	11	-6
0	651	10	-13	-6	70	21	44	-3	258	7	-3	7	307	10	-13	7	223	10	4
2	209	8	5	-4	224	12	16	-1	296	7	10	9	234	10	-13	9	224	11	14
4	639	11	-4	-2	71	18	30	1	261	8	-12	11	239	14	5	H,K=	13,	25	
6	129	12	4	0	225	13	1	3	249	8	3	H,K=	13,	15		-7	232	11	15
8	464	10	3	2	63	26	23	5	388	9	-1	-9	230	11	16	-5	232	11	8
10	81	23	20	4	241	15	27	7	250	9	2	-7	210	10	4	-3	215	10	-12
H,K=	12,	18		6	0	59	-24*	9	165	11	6	-5	267	9	-3	-1	126	12	-2
-10	83	16	11	H,K=	12,	30		11	163	12	14	-3	187	9	-5	1	121	15	-4
-8	87	16	-1	-6	195	13	-9	H,K=	13,	7		-1	276	8	-13	3	213	12	-9
-6	189	10	4	-4	49	50	5*	-11	206	12	2	1	291	8	9	5	209	11	-11
-4	99	13	19	-2	270	10	12	-9	320	10	8	3	179	9	2	7	218	12	-15
-2	102	10	23	0	29	50	-13*	-7	262	10	-26	5	272	9	-10	H,K=	13,	27	
0	54	19	39	2	278	10	9	-5	315	10	-18	7	198	10	-1	-7	179	13	1
2	83	17	11	6	221	13	14	-3	285	8	14	9	206	11	-11	-5	160	10	1
4	45	49	-37*	H,K=	12,	32		-1	408	8	0	H,K=	13,	17		-3	139	11	-1
8	76	27	-11	-4	370	10	5	1	417	18	-1	-9	109	18	-6	-1	191	10	3
10	78	23	11	-2	17	52	-42*	3	285	8	11	-7	261	10	-2	1	194	10	11
H,K=	12,	20		0	469	10	-7	5	327	8	-5	-5	287	11	-9	3	160	10	9
-10	37	54	-16*	2	34	49	-26*	9	323	10	8	-3	420	10	-10	5	147	12	-7
-8	384	10	6	4	376	11	7	11	204	15	-5	-1	158	9	-4	7	165	14	-8
-6	100	16	-2	H,K=	12,	34		H,K=	13,	9		1	185	9	-4	H,K=	13,	29	
-4	543	10	-4	-4	27	53	-5*	-11	207	10	25	3	425	9	-6	-5	258	12	-4
-2	133	9	8	-2	0	49	-42*	-9	223	13	7	5	284	9	-3	-3	226	10	14
2	118	11	-8	2	48	55	9*	-7	284	10	-7	7	266	9	-3	-1	227	10	9
4	549	11	-9	4	48	58	15*	-5	289	9	-2	9	124	13	4	1	219	10	-1
6	84	26	-20	H,K=	12,	36		-3	363	8	11	H,K=	13,	19		3	192	12	-15
8	386	10	9	0	346	12	-13	-1	402	10	-2	-9	252	12	-6	5	280	10	6
10	58	27	6	H,K=	13,	1		1	400	8	-1	-7	262	10	10	H,K=	13,	31	
H,K=	12,	22		-11	209	13	-4	3	355	9	-4	-5	332	9	-9	-5	148	14	-1
-8	0	53	-43*	-9	181	12	-4	5	292	8	1	-3	295	9	-0	-3	137	19	-4

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-1	231	11	-14	-4	454	12	-22	-6	366	11	12	4	62	22	-30	3	308	10	5
1	238	12	-8	-2	43	26	7	-4	70	25	15	H,K=	14,	32		5	148	11	-10
3	133	25	-15	0	604	10	-9	-2	471	11	-8	-2	204	9	-13	9	133	16	0
5	168	12	18	2	44	56	10*	0	60	16	41	0	154	10	6	H,K=	15,	11	
H,K=	13,	33		4	458	9	-7	2	482	10	8	2	211	9	-2	-9	308	11	-7
-3	215	10	16	6	19	46	-14*	4	53	26	5	H,K=	15,	1		-7	365	9	17
-1	217	11	8	8	434	10	-19	6	385	9	21	-11	199	13	11	-5	402	11	7
1	214	12	9	H,K=	14,	10		8	133	15	-14	-9	384	10	11	-3	359	10	-1
3	195	12	4	-10	91	20	-14	H,K=	14,	20		-7	291	10	2	-1	364	9	1
H,K=	13,	35		-8	181	13	-11	-8	195	12	3	-5	352	9	9	1	349	10	-4
-1	254	15	-4	-6	309	9	-9	-6	117	15	-23	-3	239	8	9	3	368	9	12
1	272	12	10	-4	270	9	-9	-4	297	9	11	-1	393	8	-10	5	410	11	11
H,K=	14,	0		-2	185	9	-1	0	253	11	5	1	383	8	-6	7	346	12	-7
-10	242	11	-5	0	289	12	8	2	262	9	-7	3	237	8	9	9	316	10	-1
2	391	8	3	2	173	9	-8	4	286	11	-4	5	376	9	-1	H,K=	15,	13	
6	460	9	23	4	255	11	-17	6	150	11	16	7	280	9	-11	-9	93	20	1
H,K=	14,	2		6	319	9	7	8	187	16	0	9	293	12	15	-7	0	47	-9*
-10	316	14	-2	8	203	11	-3	H,K=	14,	22		H,K=	15,	3		-5	100	12	38
-8	129	17	8	10	110	14	7	-8	197	11	19	-9	143	11	2	-3	51	22	27
-6	565	10	-4	H,K=	14,	12		-6	163	12	-10	-7	107	16	24	-1	47	27	27
-4	62	24	8	-10	121	17	-17	-4	245	12	0	-5	173	10	-8	1	0	47	-13*
-2	512	8	4	-8	368	10	15	-2	261	10	11	-3	231	8	-2	3	30	46	9*
0	0	39	-12*	-6	222	10	-4	0	194	12	-6	-1	95	11	10	5	79	14	16
2	498	8	5	-4	329	9	6	2	243	13	-10	1	99	12	-2	7	40	52	34*
4	96	10	27	-2	236	8	8	4	228	10	-2	3	247	9	7	9	80	46	-18
6	563	14	0	0	342	8	-9	6	172	12	-5	5	188	9	8	H,K=	15,	15	
8	139	12	11	2	220	9	-15	8	162	15	-21	7	95	14	5	-9	310	10	18
10	315	10	6	4	309	9	-8	H,K=	14,	24		9	130	13	-3	-7	298	10	2
H,K=	14,	4		6	235	9	-1	-8	313	11	-4	H,K=	15,	5		-5	350	10	6
-10	202	11	15	8	356	11	4	-6	40	48	-0*	-9	211	11	-15	-3	370	9	-5
-8	289	10	-9	10	139	15	-3	-4	351	10	-11	-7	371	9	8	-1	333	8	-2
-6	312	9	2	H,K=	14,	14		-2	83	16	-3	-5	388	9	7	1	306	9	-11
-4	186	11	-12	-10	264	11	-0	0	428	13	7	-3	445	9	-2	3	371	13	-7
-2	173	9	-15	-8	63	22	0	2	68	23	-17	-1	503	9	2	5	329	10	4
0	512	9	10	-6	412	10	1	4	364	10	-14	1	480	10	-7	7	309	10	9
2	183	8	-8	-4	255	9	8	6	79	15	38	3	430	9	-8	9	271	16	-9
4	196	8	4	-2	338	11	-4	8	332	11	18	5	411	9	9	H,K=	15,	17	
6	290	9	-12	0	70	19	6	H,K=	14,	26		7	380	9	9	5	273	10	13
8	273	11	-6	2	325	12	-1	-6	71	16	34	9	219	11	-13	7	244	10	-7
10	202	11	12	4	253	11	2	-4	154	13	-10	H,K=	15,	7		9	192	12	23
H,K=	14,	6		6	414	12	14	-2	62	22	0	-9	117	13	-14	H,K=	15,	19	
-10	130	14	-8	8	81	13	37	0	235	12	-12	-7	242	11	-1	-7	142	9	5
-8	185	10	6	10	264	12	-0	2	57	30	-5	-5	293	9	-4	-5	132	8	12
-6	182	9	-1	H,K=	14,	16		4	161	12	3	-3	160	9	28	-3	145	8	-6
-4	228	13	-21	-10	192	12	-12	6	58	33	31	1	140	10	10	3	144	12	-1
-2	296	8	7	-8	127	12	6	H,K=	14,	28		3	146	10	10	5	97	17	-10
0	145	10	-8	-6	228	9	13	-4	314	10	-4	5	300	10	-12	7	134	14	-7
2	297	8	1	-4	123	12	3	0	324	10	6	7	248	9	9	H,K=	15,	21	
4	256	9	-17	-2	362	9	-12	2	108	16	-5	9	144	14	5	-7	333	10	16
6	179	10	-7	0	123	10	12	4	331	10	12	H,K=	15,	9		-5	266	10	-7
8	195	11	-0	2	367	9	-20	6	129	22	-9	-9	109	17	-29	-3	355	12	12
10	123	16	-18	4	124	12	-3	H,K=	14,	30		-7	220	10	-14	-1	435	16	-2
H,K=	14,	8		6	208	10	-5	-4	76	24	-13	-5	183	9	12	1	433	10	4
-10	63	22	18	8	112	19	-11	-2	291	10	34	-3	296	9	-12	3	354	9	9
-8	453	10	9	H,K=	14,	18		0	38	54	-14*	-1	229	10	-9	5	271	12	4
-6	46	32	12	-8	153	11	9	2	247	8	-9	1	193	9	-28	7	312	7	-1

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	15,	23		-2	243	9	-8	4	268	10	-5	-1	304	9	14	5	262	10	-5
-7	102	23	-22	0	349	9	-9	8	167	12	8	3	244	9	4	7	139	12	-5
-5	133	18	22	2	247	9	-6	H,K=	16,	18		5	218	9	5	9	152	14	-3
-3	195	11	16	4	250	10	5	-8	353	11	0	7	161	11	17	H,K=	17,	13	
-1	176	16	-8	6	269	10	-6	-6	57	26	21	9	180	14	-0	-7	191	12	-2
1	169	11	-19	8	171	11	8	-4	430	10	3	H,K=	17,	3		-5	233	11	7
3	204	9	10	10	207	12	14	-2	27	47	-8*	-9	231	12	-6	-3	241	9	-3
5	126	13	11	H,K=	16,	8		0	490	10	1	-7	280	10	-9	-1	374	9	1
7	145	13	20	-10	355	11	23	2	73	16	29	-5	297	10	4	1	353	10	-27
H,K=	15,	25		-8	72	21	20	4	417	18	-11	-3	305	8	13	3	264	10	15
-7	250	11	35	-6	510	11	-3	6	41	54	-5*	-1	372	9	3	5	233	10	2
-5	195	11	3	-4	59	33	-28	8	341	10	-7	1	381	9	-0	7	203	10	4
-1	214	11	-12	-2	491	11	14	H,K=	16,	20		3	295	9	2	H,K=	17,	15	
3	182	12	15	0	0	43	-18*	-6	230	10	2	5	303	10	4	-7	140	15	-19
5	176	13	-19	2	480	9	6	-4	225	18	10	7	270	11	-16	-5	194	10	5
7	211	13	-3	4	71	19	-13	-2	261	10	3	9	225	12	-13	-3	151	12	-7
H,K=	15,	27		6	520	10	6	0	159	14	-16	H,K=	17,	5		-1	216	10	6
5	237	16	-1	8	70	16	18	2	255	10	-9	-9	139	15	-13	1	199	10	-2
H,K=	15,	31		10	348	12	4	4	214	10	4	-7	159	16	-16	3	176	10	1
-3	258	8	21	H,K=	16,	10		6	220	11	-10	-5	215	12	16	7	164	13	10
-1	316	8	5	-8	132	12	19	H,K=	16,	22		-3	218	10	-14	H,K=	17,	17	
H,K=	16,	0		-6	206	11	4	-6	181	11	9	-1	238	9	1	-7	199	12	15
-8	116	16	-18	-4	172	10	-3	-4	189	10	15	1	253	9	3	-5	188	11	6
-4	184	10	3	-2	321	9	-3	-2	237	12	-6	3	249	9	16	-3	240	10	8
0	291	8	8	0	124	10	3	0	214	10	1	5	240	9	24	-1	220	10	-6
4	217	9	6	2	320	10	-5	2	241	11	-6	7	179	17	10	1	228	11	-6
8	143	13	12	4	172	15	-4	4	151	13	-14	9	141	15	3	3	230	11	-14
H,K=	16,	2		6	195	11	0	6	152	13	-9	H,K=	17,	7		7	138	16	-34
-10	88	20	1	8	115	17	-13	H,K=	16,	24		-9	208	16	-14	H,K=	17,	19	
-8	350	10	-6	H,K=	16,	12		-6	294	11	-9	-7	298	10	-4	-7	260	11	4
-6	137	10	19	-8	126	23	-2	-4	25	54	17*	-5	306	9	-12	-5	245	11	-8
-4	339	9	11	-6	288	10	9	-2	349	10	6	-3	394	10	-5	-3	280	10	-2
-2	39	34	1	-4	156	11	-5	0	0	48	-21*	-1	297	11	-12	-1	235	10	11
0	664	11	-22	-2	309	9	11	2	339	10	4	1	301	8	-12	1	229	9	8
2	80	14	25	0	204	9	-9	4	62	21	45	3	412	9	2	3	284	10	-6
4	353	9	-9	2	302	11	12	6	311	13	-2	5	286	10	-21	7	248	12	-9
6	126	12	1	4	179	10	-16	H,K=	16,	26		7	308	10	14	H,K=	17,	21	
8	363	10	5	6	277	10	-4	-4	0	50	-62*	9	244	14	20	-5	153	13	10
10	77	28	-10	8	129	15	4	-2	220	12	-23	H,K=	17,	9		-3	116	14	6
H,K=	16,	4		H,K=	16,	14		0	133	14	3	-9	171	12	-3	-1	209	9	24
-10	217	11	28	-8	325	11	-0	2	213	12	-14	-7	177	10	9	1	182	14	-10
-8	154	10	25	-6	179	10	31	4	53	34	-11	-5	275	10	-17	3	100	17	-2
-6	347	10	-14	-4	377	9	-0	H,K=	16,	28		-3	333	11	-10	5	170	14	18
-4	239	9	10	-2	195	11	11	-2	276	12	-3	-1	312	9	-17	H,K=	17,	23	
-2	350	12	-16	0	370	12	-2	0	108	24	-18	1	341	10	0	-5	230	11	-9
0	117	11	-4	2	193	10	6	2	293	10	14	3	334	9	-3	-3	198	12	-9
2	359	8	-4	4	365	10	0	4	39	58	-31*	5	308	9	5	-1	249	10	-9
4	246	9	8	6	140	11	6	H,K=	16,	30		7	178	18	3	1	245	12	1
6	358	9	0	8	327	11	-1	-2	85	37	-22	9	183	12	4	3	189	11	-7
8	139	13	6	H,K=	16,	16		0	225	13	-1	H,K=	17,	11		5	260	11	18
10	188	14	-9	-8	151	15	-5	2	120	18	9	-9	139	15	-10	H,K=	17,	25	
H,K=	16,	6		-6	53	27	4	H,K=	17,	1		-7	144	13	-10	-3	172	13	16
-10	182	13	-7	-4	261	11	-15	-9	173	13	-0	-5	283	9	11	-1	226	13	-10
-8	161	11	-1	-2	0	43	-32*	-7	130	16	-15	-3	218	12	-15	1	219	12	-13
-6	252	12	-13	0	221	10	-6	-5	231	10	8	-1	199	10	7	3	163	13	12
-4	238	10	-4	2	0	48	-37*	-3	267	10	10	3	219	10	0	H,K=	17,	27	

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-3	82	21	11	H,K=	18,	14		H,K=	19,	3		-3	100	17	-29	-2	343	10	-4
-1	94	26	-21	-6	51	70	-1*	-7	243	11	16	1	186	10	25	0	58	34	-8
1	123	13	9	-4	267	10	8	-5	255	10	26	3	117	12	11	2	340	10	-3
3	93	18	25	-2	0	50	-41*	-3	263	10	2	5	153	13	1	4	0	50	-47*
H,K=	18,		0	0	168	12	-4	-1	272	10	7	H,K=	19,		17	6	313	11	-10
-6	450	10	13	2	0	54	-42*	1	284	10	21	-5	232	11	0	H,K=	20,		10
-2	550	10	-13	4	261	9	-1	3	276	10	15	-3	228	10	4	-6	189	13	-18
2	529	9	-18	6	32	60	-16*	5	238	12	7	-1	208	11	7	-4	135	13	-9
6	436	14	-2	H,K=	18,	16		7	260	11	35	1	184	11	-9	-2	229	11	8
H,K=	18,		2	-6	346	11	-11	H,K=	19,		5	3	237	12	13	0	36	44	20*
-8	120	16	-5	-4	80	21	11	-7	114	16	-12	5	238	11	11	2	221	11	0
-6	46	63	-5*	-2	394	10	3	-5	137	13	-3	H,K=	19,		19	4	122	15	-18
-4	161	10	-7	0	0	47	-18*	-3	222	10	10	-5	166	12	-6	6	234	11	26
-2	0	49	-28*	2	400	10	-0	-1	217	9	6	-3	164	20	-3	H,K=	20,		12
0	224	10	2	4	0	51	-68*	1	193	10	-17	-1	282	10	3	-6	265	11	9
2	0	49	-29*	6	366	11	-1	3	209	10	1	1	258	10	-9	-4	67	27	-6
4	172	11	6	H,K=	18,	18		5	163	12	30	3	149	18	-23	-2	281	11	1
6	51	53	1*	-6	0	51	-26*	7	134	14	-2	5	194	11	12	0	158	12	-2
8	145	11	21	-4	104	9	41	H,K=	19,		7	H,K=	19,		21	2	284	10	7
H,K=	18,		4	-2	21	52	-14*	-7	227	12	2	-1	116	16	-31	4	84	20	-3
-8	0	54	-41*	0	165	11	8	-5	208	10	5	1	132	17	-12	6	259	13	4
-6	345	10	-1	2	32	47	-2*	-3	293	9	4	3	129	13	9	H,K=	20,		14
-4	34	51	-7*	4	85	15	20	-1	311	10	2	H,K=	19,		23	-4	300	11	-9
-2	357	9	5	6	34	71	11*	1	306	10	-8	-1	214	12	-9	-2	133	14	1
0	97	11	4	H,K=	18,	20		3	302	10	5	1	229	11	7	0	249	10	1
2	347	9	-6	-6	309	11	-1	5	194	12	9	H,K=	20,		0	2	157	11	24
4	44	49	1*	-4	89	20	6	7	241	10	18	-4	166	14	10	4	283	12	-18
6	341	10	2	-2	297	10	10	H,K=	19,		9	0	157	11	21	H,K=	20,		16
H,K=	18,		6	0	30	54	-42*	-7	177	13	-2	4	179	16	8	-4	155	13	6
-8	312	10	5	2	268	12	-16	-5	231	11	3	H,K=	20,		2	-2	112	12	41
-6	77	18	12	4	97	19	12	-3	218	11	-22	-6	37	61	-0*	0	204	11	9
-4	548	10	13	6	315	11	-2	-1	228	10	-7	-4	302	10	3	2	86	18	16
-2	59	35	-4	H,K=	18,	22		1	242	10	3	-2	79	21	-25	4	172	12	15
0	507	11	0	-4	286	10	5	3	245	11	-2	0	335	10	-6	H,K=	20,		18
2	66	17	2	-2	0	54	-32*	5	232	12	-9	2	65	33	-33	-4	318	11	5
4	541	10	2	0	418	10	8	7	181	16	-0	4	278	10	-24	-2	39	55	6*
6	57	58	-6*	2	20	47	-11*	H,K=	19,		11	6	0	53	-37*	0	329	11	2
8	285	12	-11	4	289	12	5	-7	159	20	7	H,K=	20,		4	2	52	53	18*
H,K=	18,		8	H,K=	18,	24		-5	124	16	-27	-6	183	11	-3	4	306	11	-3
-8	5	50	-25*	-4	29	58	2*	-3	190	12	-9	-4	114	13	17	H,K=	20,		20
-6	60	17	25	-2	91	14	20	-1	201	10	-14	-2	232	10	-5	-2	170	13	-6
-4	54	31	-17	2	65	35	-15	1	205	11	-13	0	219	10	8	0	171	15	12
-2	70	20	-6	4	0	52	-24*	3	193	11	-5	2	225	12	-14	2	170	15	-10
0	0	51	-4*	H,K=	18,	26		5	142	13	-5	4	111	16	-1	H,K=	21,		1
2	71	11	-2	-2	59	25	25	7	145	15	-12	6	197	11	13	-5	194	11	22
4	46	51	-28*	0	307	11	-10	H,K=	19,		13	H,K=	20,		6	-3	223	11	-13
6	73	15	33	2	0	53	-34*	-7	219	11	-8	-6	214	12	25	-1	210	12	-27
8	0	43	-35*	H,K=	19,		1	-5	320	10	8	-4	113	13	-14	1	221	11	-20
H,K=	18,		10	-7	181	13	3	-3	271	11	12	-2	200	11	1	3	220	13	-16
-8	347	9	1	-5	180	11	-8	-1	260	10	8	0	254	10	-19	5	178	11	17
-6	0	53	-16*	-3	170	16	-3	1	261	10	4	2	214	10	18	H,K=	21,		3
H,K=	18,		12	-1	249	9	22	3	265	16	4	4	137	12	3	-3	95	19	15
2	380	9	-13	1	229	10	-14	5	301	15	-13	6	200	11	11	-1	113	14	-2
4	0	48	-14*	3	167	11	3	7	216	12	-6	H,K=	20,		8	1	117	13	-1
6	191	13	4	5	208	10	15	H,K=	19,		15	-6	328	11	4	3	73	25	-3
8	43	50	0*	7	193	12	11	-5	138	14	-2	-4	51	59	1*	5	60	31	23

STRUCTURE FACTORS CONTINUED FOR
NASM(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		21,	5	H,K=		22,	8												
-5	274	11	16	-2	45	49	17*												
-3	276	10	5	0	353	10	17												
-1	254	10	1	2	83	15	56												
1	249	10	-2	H,K=		22,	10												
3	283	10	3	-2	127	13	11												
5	244	11	-8	0	94	18	-12												
H,K=		21,	7	2	90	27	-17												
-5	190	11	-13	H,K=		22,	12												
-3	151	12	-0	-2	103	18	3												
-1	106	16	-11	0	209	16	-7												
1	108	15	3	2	94	15	-10												
3	140	14	-2	H,K=		23,	1												
5	203	10	9	-1	180	13	23												
H,K=		21,	9	1	187	11	25												
-5	220	11	17	H,K=		23,	3												
-3	186	12	-11	-1	223	11	3												
-1	203	11	3	1	227	11	4												
1	189	11	6	H,K=		23,	5												
3	192	11	2	-1	126	14	2												
5	171	14	-31	1	150	12	16												
H,K=		21,	11																
-1	234	11	-11																
1	246	11	1																
H,K=		21,	13																
-3	0	56	-31*																
-1	54	61	32*																
3	45	50	9*																
H,K=		21,	15																
-3	260	10	0																
-1	217	11	9																
1	217	10	4																
3	266	11	3																
H,K=		21,	17																
-1	187	13	-3																
1	174	13	-8																
H,K=		22,	0																
-2	165	11	2																
2	162	12	1																
H,K=		22,	2																
-4	0	57	-54*																
-2	345	11	16																
0	71	20	11																
2	325	10	-3																
4	41	53	-8*																
H,K=		22,	4																
-4	251	11	-15																
-2	139	15	-3																
0	197	11	-5																
2	131	14	-5																
4	276	12	13																
H,K=		22,	6																
-4	182	12	-6																
-2	156	10	23																
0	94	17	-15																
4	199	11	16																

OBSERVED STRUCTURE FACTORS, STANDARD DEVIATIONS, AND DIFFERENCES (ALL X 5.0)
NAGD(EDTA).8H2O F(0,0,0) = 5933

FOB AND FCA ARE THE OBSERVED AND CALCULATED STRUCTURE FACTORS.
SG = ESTIMATED STANDARD DEVIATION OF FOB. DEL = /FOB/ - /FCA/.
* INDICATES ZERO WEIGHTED DATA.

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=		0,	0	-8	434	9	2	8	234	11	-13	3	577	9	10	-11	303	7	3
12	544	9	12	-12	341	10	12	4	445	9	-12	11	011	13	-20	-13	189	8	-12
8	720	12	13	H,K=		0,	14	-0	229	9	8	-1	986	13	-42	H,K=		1,	11
4	923	13	-9	10	368	9	3	-4	431	10	6	-3	553	9	11	13	191	9	-2
-4	842	13	-9	6	425	9	4	-8	250	10	12	-5	477	8	7	11	150	8	-9
-8	759	13	13	2	182	6	-3	H,K=		0,	30	-7	582	10	-7	9	226	6	-2
-12	548	9	15	-2	198	9	17	10	230	11	8	-9	468	8	5	7	275	6	-1
H,K=		0,	2	-6	407	8	-6	6	248	10	-6	-11	435	8	6	5	322	6	-2
14	138	13	-16	-10	354	10	-4	2	239	10	-9	-13	302	9	-1	3	674	11	-6
10	189	9	1	H,K=		0,	16	-2	247	12	0	H,K=		1,	5	1	822	12	-1
6	548	11	4	12	403	12	-7	-6	252	11	11	13	177	9	17	-1	822	13	10
2	484	10	31	8	694	14	-4	-10	238	12	10	11	180	7	8	-3	659	11	-13
-2	486	10	27	4	924	20	12	H,K=		0,	32	9	151	7	1	-5	312	6	1
-6	522	11	-14	-0	949	17	-10	8	351	16	-9	7	260	6	2	-7	263	6	1
-10	179	10	-7	-4	871	17	-26	4	509	10	-10	5	655	11	-1	-9	225	6	-5
-14	159	16	14	-8	674	14	-15	-0	372	10	-16	3	194	5	-13	-11	170	9	-2
H,K=		0,	4	-12	423	11	13	-4	541	11	8	1	553	9	5	-13	199	8	6
12	352	10	-7	H,K=		0,	18	-8	371	12	4	-1	579	9	13	H,K=		1,	13
8	504	10	1	6	284	8	-6	H,K=		0,	36	-3	233	6	-1	13	283	8	6
4	754	14	-8	2	386	7	10	4	435	11	-4	-5	670	11	17	11	328	8	12
-0	1100	0	45*	-2	362	8	-6	-0	431	11	4	-7	258	6	4	9	395	7	8
-4	757	14	10	-6	274	8	-8	-4	453	11	2	-9	130	7	-0	7	533	9	5
-8	524	10	1	-10	46	50	-13*	H,K=		0,	38	-11	148	7	9	5	617	10	2
-12	370	11	-12	H,K=		0,	20	6	366	11	19	-13	163	8	1	3	706	11	4
H,K=		0,	6	12	360	11	3	2	264	10	14	H,K=		1,	7	1	676	11	7
14	322	11	19	8	576	12	-7	-2	256	14	1	13	244	9	-3	-1	718	12	2
10	283	9	9	4	385	8	-1	-6	349	11	1	11	293	7	-10	-3	741	12	13
6	947	18	-31	-0	401	8	-7	H,K=		0,	40	9	326	7	4	-5	603	10	3
2	775	13	4	-4	373	8	2	4	183	12	1	7	331	6	5	-7	521	9	4
-2	766	13	5	-8	574	11	-13	-0	152	15	18	5	634	11	11	-9	369	8	-7
-6	974	17	-7	-12	339	14	-19	-4	186	13	-2	3	806	12	1	-11	310	9	4
-10	272	8	8	H,K=		0,	22	H,K=		1,	1	1	515	8	6	-13	286	8	17
-14	296	11	-1	10	386	10	-1	13	202	8	13	-1	522	9	15	H,K=		1,	15
H,K=		0,	8	6	428	9	7	11	260	7	8	-3	796	12	-8	13	190	8	3
8	252	8	7	2	636	12	2	9	337	7	-12	-5	592	10	14	11	270	7	-12
4	398	8	1	-2	628	12	0	7	530	9	-1	-7	329	6	-2	9	348	7	1
-0	269	8	12	-6	407	9	4	5	338	6	11	-9	347	7	1	7	288	7	7
-4	390	8	1	-10	384	10	-0	3	707	11	16	-11	304	7	-7	5	293	6	5
-8	250	8	11	H,K=		0,	24	1	694	0	-50*	-13	258	8	6	3	572	9	7
H,K=		0,	10	8	193	12	-8	-1	699	0	-52*	H,K=		1,	9	1	605	10	-3
10	617	12	-8	4	247	8	8	-3	710	11	11	13	206	9	0	-1	574	10	-3
6	648	13	-8	-0	103	16	-17	-5	336	6	1	11	314	8	2	-3	570	10	7
2	957	15	-11	-4	247	8	4	-7	524	9	5	9	287	6	5	-5	278	6	3
-2	976	17	-12	-8	188	10	-13	-9	362	7	-3	7	297	6	-8	-7	296	6	-5
-6	660	13	-10	H,K=		0,	26	-11	225	7	-14	5	488	9	3	-9	343	7	1
-10	611	12	-1	10	460	11	0	-13	195	8	10	3	382	6	-6	-11	279	9	-4
H,K=		0,	12	6	588	12	9	H,K=		1,	3	1	92	8	5	-13	197	8	1
12	320	11	-4	2	593	12	1	13	299	8	-3	-1	131	5	-14	H,K=		1,	17
8	429	9	-5	-2	604	12	-5	11	431	8	-2	-3	370	6	-4	13	213	8	1
4	803	16	4	-6	575	11	7	9	435	7	2	-5	483	8	-0	11	157	8	-2
-0	1147	18	-14	-10	453	11	-3	7	612	10	7	-7	311	6	-1	9	329	7	7
-4	807	15	-5	H,K=		0,	28	5	525	9	11	-9	253	7	-8	7	266	6	-5

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
5	495	9	9	-1	433	7	-5	-3	246	7	18	-2	289	5	11	2	193	6	6
3	347	6	11	-3	245	6	-8	-5	282	8	-2	-4	926	14	4	-0	367	6	-13
1	431	7	3	-5	247	7	5	-7	245	9	6	-6	385	7	-1	-2	184	5	-3
-1	428	7	-0	-7	342	8	-2	H,K=	1,	37		-8	329	6	1	-4	776	13	-12
-3	352	6	15	-9	252	7	6	5	137	12	3	-10	165	8	-7	-6	291	6	8
-5	512	9	12	-11	203	8	5	3	195	8	14	-12	296	8	-13	-8	391	7	2
-7	290	6	-3	H,K=	1,	27		1	156	11	15	-14	202	8	17	-10	129	9	-18
-9	319	7	-1	11	145	10	-1	-1	157	11	22	H,K=	2,	6		-12	294	9	-5
-11	171	7	-2	9	175	11	-11	-3	198	9	4	14	147	9	16	H,K=	2,	14	
-13	197	8	-4	7	229	7	7	-5	103	28	-29	12	312	8	8	12	62	36	-13
H,K=	1,	19		5	188	7	9	H,K=	1,	39		10	205	7	-17	10	463	8	1
11	257	8	-8	3	211	7	-4	5	231	8	-0	8	264	6	1	8	136	8	-11
9	351	7	-5	1	263	6	-3	3	293	8	8	6	353	6	-3	6	533	9	-0
7	390	8	2	-1	260	7	-4	1	236	9	7	4	107	6	-6	4	310	6	0
5	447	8	-6	-3	225	8	2	-1	219	9	-3	2	533	9	-4	2	866	14	6
3	346	6	-1	-5	186	7	3	-3	283	8	2	-0	316	5	22	-2	841	14	-1
1	554	9	4	-7	220	9	2	-5	224	9	-19	-2	534	9	-0	-4	316	6	0
-1	533	9	-8	-9	182	9	-5	H,K=	1,	41		-4	74	18	-4	-6	532	9	-1
-3	366	6	6	-11	155	15	10	3	171	12	-4	-6	369	6	-3	-8	148	6	-3
-5	441	7	-4	H,K=	1,	29		1	180	10	-25	-8	271	6	3	-10	473	8	6
-7	412	7	-3	9	245	8	-8	-1	199	9	2	-10	214	7	-6	-12	23	51	-33*
-9	360	8	3	7	294	7	-11	-3	181	9	0	-12	306	8	-5	H,K=	2,	16	
-11	270	8	1	5	432	8	0	H,K=	2,	0		-14	126	10	-0	12	99	14	-7
H,K=	1,	21		3	387	7	-5	14	253	8	5	H,K=	2,	8		10	266	7	-4
11	171	8	16	1	343	7	8	10	402	7	-3	12	492	9	-1	8	54	54	-20*
9	256	8	0	-1	332	8	5	6	509	8	-1	10	63	18	4	6	531	9	1
7	187	7	-3	-3	383	8	-7	2	576	10	-24	8	546	9	-1	4	268	6	-3
5	275	6	-4	-5	437	8	7	-2	525	9	-22	6	156	5	0	2	522	9	2
3	111	7	6	-7	303	8	7	-6	518	9	3	4	881	14	10	-0	487	8	17
1	253	5	14	-9	241	8	-4	-10	411	8	2	2	529	9	-5	-2	555	9	24
-1	246	6	-1	H,K=	1,	31		-14	244	8	-0	-0	687	10	-1	-4	275	6	4
-3	110	7	3	9	144	14	8	H,K=	2,	2		-2	528	9	-9	-6	540	9	-0
-5	278	7	2	7	155	9	4	14	279	8	4	-4	875	14	-11	-8	88	12	7
-7	215	6	-1	5	244	7	-1	12	156	10	-3	-6	148	6	-8	-10	262	8	-8
-9	233	7	-5	3	201	8	0	10	521	9	-0	-8	536	9	-6	-12	110	11	-2
-11	164	10	2	1	213	7	-2	8	193	6	6	-12	506	9	11	H,K=	2,	18	
H,K=	1,	23		-1	207	8	-5	6	863	14	4	-14	53	53	11*	12	146	17	16
11	218	8	-4	-3	219	7	-1	4	155	5	1	H,K=	2,	10		10	448	8	5
9	280	7	-1	-5	257	8	16	2	703	10	45	12	248	8	2	8	73	16	0
7	379	8	-8	-7	159	9	-11	-0	423	0	-17*	10	74	16	9	6	496	8	-1
5	310	7	-17	-9	140	11	-6	-2	732	11	42	8	324	6	3	4	141	7	1
3	430	7	4	H,K=	1,	33		-4	167	5	3	6	238	5	-3	2	943	15	6
1	524	9	-3	7	215	9	15	-6	827	14	-24	4	323	6	-7	-0	300	5	8
-1	530	9	-6	5	278	8	6	-8	172	7	-2	2	389	7	4	-2	928	15	9
-3	449	8	5	3	167	8	-18	-10	507	9	4	-0	701	11	19	-4	130	6	2
-5	331	7	9	1	237	8	-1	-12	158	11	-3	-2	363	6	1	-6	409	8	-2
-7	383	7	2	-1	238	7	6	-14	261	9	-10	-4	292	5	-2	-10	445	8	5
-9	270	8	3	-3	185	8	5	H,K=	2,	4		-6	231	5	7	-12	129	9	-6
-11	226	10	1	-5	271	8	-8	14	192	10	14	-8	326	6	3	H,K=	2,	20	
H,K=	1,	25		-7	193	9	-0	12	318	8	-1	-12	250	7	7	12	151	10	-10
11	191	9	-5	H,K=	1,	35		10	152	7	-3	H,K=	2,	12		10	240	8	9
9	249	8	2	7	233	11	1	8	320	6	0	12	287	8	-8	8	372	8	-2
7	328	7	7	5	274	8	4	6	380	6	-4	10	145	7	-2	6	267	6	-2
5	269	7	3	3	226	8	0	4	892	14	-15	8	396	7	-6	4	415	8	0
3	285	6	3	1	271	8	4	2	247	4	3	6	297	6	9	2	490	8	-1
1	430	7	-2	-1	260	10	3	-0	1018	14	23	4	811	13	6	-0	123	6	-10

STRUCTURE FACTORS CONTINUED FOR
NAGO(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-2	505	9	1	10	237	10	-0	-3	504	8	1	3	469	8	-1	9	346	7	3
-4	442	7	13	8	119	11	-14	-5	428	7	7	1	888	13	15	7	329	7	-6
-6	287	6	2	6	439	8	3	-7	665	11	10	-1	864	13	4	5	476	8	-7
-8	370	8	-0	4	156	7	5	-9	440	8	-4	-3	447	7	6	3	400	7	3
-10	240	7	4	2	371	7	-6	-11	433	8	-12	-5	302	6	-1	1	528	9	-3
-12	176	8	18	-0	45	41	-12	-13	234	8	4	-7	248	6	-4	-1	532	9	-7
H,K=		2,	22	-2	386	7	-1	H,K=		3,	3	-9	448	8	-2	-3	415	7	-4
12	196	9	11	-4	164	8	-2	13	99	12	49	-11	242	7	2	-5	468	8	-2
10	191	8	-1	-6	425	9	-11	11	49	44	-13	-13	238	8	6	-7	341	7	0
8	183	9	1	-8	108	11	-9	9	79	9	9	H,K=		3,	11	-9	353	7	4
6	261	6	6	-10	248	8	12	7	362	6	-2	13	272	8	-7	-11	257	9	-4
4	191	6	2	H,K=		2,	32	5	265	5	6	11	456	8	3	-13	218	9	-13
2	386	7	4	6	241	8	-4	3	392	6	11	9	277	6	0	H,K=		3,	19
-0	363	6	-8	4	129	9	-23	1	42	48	-28*	7	538	9	-8	11	62	19	-18
-2	385	7	-0	2	297	7	-3	-1	99	11	8	5	492	8	-10	9	98	11	-5
-4	167	7	-4	-0	61	20	20	-3	362	7	3	3	745	12	1	7	94	11	-1
-6	260	6	1	-2	319	7	8	-5	273	6	-6	1	659	11	-13	5	191	6	11
-8	210	7	4	-4	167	8	-1	-7	379	6	2	-1	674	11	-8	3	244	5	10
-10	209	8	7	-6	259	8	11	-9	73	13	9	-3	704	11	-4	1	340	6	-2
-12	182	14	-8	-8	86	18	5	-11	55	16	-3	-5	482	8	-10	-1	336	6	-5
H,K=		2,	24	H,K=		2,	34	H,K=		3,	5	-7	548	9	-6	-3	233	6	3
10	81	12	-4	8	59	20	1	13	285	8	-4	-9	283	7	7	-5	176	6	1
8	571	9	4	6	316	9	2	11	377	8	2	-11	460	8	3	-7	110	17	1
6	141	7	6	2	428	8	-4	9	476	8	-6	-13	286	8	3	-9	70	18	-7
4	432	7	5	-0	97	13	26	7	569	10	-8	H,K=		3,	13	-11	77	17	2
2	171	7	-6	-2	407	8	-9	5	806	13	10	13	57	31	33	H,K=		3,	21
-0	564	9	12	-6	302	8	-9	3	625	10	-17	9	96	10	-12	11	288	8	0
-2	178	6	-0	H,K=		2,	36	1	402	7	12	7	132	7	-2	9	428	8	-3
-4	426	7	5	6	175	9	-20	-1	429	7	22	5	128	6	-8	7	356	7	-3
-6	142	9	8	4	122	11	-3	-3	618	10	-25	3	259	5	9	5	433	7	-2
-8	560	9	-7	2	246	8	8	-5	813	14	-10	1	202	5	5	3	511	8	6
-10	60	31	-24	-0	293	8	5	-7	546	9	-2	-1	206	5	1	1	731	13	-1
H,K=		2,	26	-2	229	9	-2	-9	452	8	-14	-3	248	5	-2	-1	755	12	-6
8	233	8	4	-4	131	11	4	-11	375	8	-1	-5	145	6	0	-3	504	9	4
6	74	31	-14	-6	207	9	12	-13	298	8	3	-7	130	7	1	-5	447	8	2
4	382	7	7	H,K=		2,	38	H,K=		3,	7	-9	104	10	1	-7	371	7	-7
2	170	7	1	6	213	9	2	13	165	12	-11	-11	92	14	16	-9	433	8	2
-0	333	7	-3	4	197	8	4	11	280	7	-1	-13	0	47	-29*	-11	291	8	-6
-2	190	6	9	2	240	8	2	9	217	7	4	H,K=		3,	15	H,K=		3,	23
-4	364	7	-1	-0	107	15	-19	7	191	5	-4	13	237	8	-4	9	126	9	10
-6	95	14	2	-2	255	8	18	5	399	7	-9	11	247	7	4	7	210	7	3
-8	231	7	6	-4	196	9	0	3	518	9	-3	9	257	7	-1	5	211	9	-1
-10	93	12	17	-6	200	9	-16	1	215	4	-1	7	431	8	-1	3	202	6	-4
H,K=		2,	28	H,K=		2,	40	-1	244	6	1	5	641	11	-2	1	196	6	9
10	94	15	-9	4	315	8	3	-3	480	8	9	3	713	12	3	-1	211	6	-10
8	348	8	7	-0	368	9	6	-5	405	7	-6	1	557	9	-6	-3	227	6	-0
6	191	8	-11	-4	301	9	-9	-7	170	5	-1	-1	579	10	-9	-5	207	6	7
4	405	8	-8	H,K=		3,	1	-9	236	6	8	-3	695	12	-3	-7	219	7	4
2	251	6	-1	13	221	9	[illegible]	-11	280	7	-0	-5	642	11	-1	-9	110	9	-1
-0	449	8	-7	11	463	8	-1	-13	181	8	4	-7	453	8	9	-11	124	10	20
-2	260	7	0	9	443	7	10	H,K=		3,	9	-9	257	7	6	H,K=		3,	25
-4	428	8	-1	7	661	11	-3	13	240	8	10	-11	226	8	-7	11	215	8	1
-6	204	8	0	5	404	7	2	11	253	7	7	-13	251	8	-4	9	179	8	-3
-8	357	8	8	3	558	9	17	9	442	8	-5	H,K=		3,	17	7	328	8	-6
-10	120	12	22	1	630	9	29	7	232	7	-4	13	231	8	2	5	297	7	-1
H,K=		2,	30	-1	632	9	30	5	243	5	-11	11	272	9	7	3	394	7	-1

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
1	390	7	1	3	295	9	-5	10	325	7	11	8	489	8	-8	6	224	6	-3
-1	396	8	6	1	318	8	-2	8	244	6	-6	6	388	7	10	4	374	7	7
-3	378	7	-1	-1	311	9	-10	6	440	7	1	4	643	11	-3	2	477	8	3
-5	305	7	-2	-3	291	8	2	4	251	5	-0	2	128	6	-2	-0	262	6	-1
-7	332	7	2	-5	263	8	3	2	534	9	-7	-0	832	13	-11	-2	473	8	8
-9	180	8	-8	H,K=	3,	39		-0	180	5	3	-2	158	5	13	-4	362	7	4
-11	228	9	9	3	91	18	12	-2	552	9	3	-4	648	11	3	-6	213	7	-9
H,K=	3,	27		1	117	12	0	-4	246	5	-1	-6	391	7	7	-8	238	7	7
9	203	8	-4	-1	107	11	-3	-6	447	7	10	-8	491	8	-19	-10	182	8	4
7	417	8	-0	-3	89	20	1	-8	250	6	3	-10	70	71	-16*	-12	167	9	-6
5	436	8	-3	H,K=	3,	41		-10	309	7	-6	-12	389	10	2	H,K=	4,	24	
3	427	7	-0	1	209	9	1	-12	217	8	8	H,K=	4,	16	10	383	8	-10	
1	382	7	7	-1	209	8	3	-14	163	9	-1	12	132	11	-11	8	0	51	-45*
-1	392	7	3	H,K=	4,	0		H,K=	4,	8		8	341	7	12	6	467	8	-14
-3	447	8	2	12	112	15	1	12	55	34	11	6	188	6	4	4	66	20	-8
-5	445	8	8	8	343	6	3	10	433	8	-6	4	333	6	2	2	594	10	-5
-7	424	8	-2	4	184	5	-1	8	54	18	13	2	193	5	-10	-0	279	6	3
-9	208	8	9	-0	879	12	0	6	624	10	-17	-0	152	5	1	-2	605	10	2
H,K=	3,	29		-4	242	5	5	4	402	7	2	-2	207	5	2	-4	50	23	-15
9	65	24	14	-8	350	7	12	2	896	14	12	-4	346	6	4	-6	480	8	-6
5	0	48	-23*	-12	58	40	-42	-0	399	7	-19	-6	171	6	-1	-10	391	8	8
3	95	9	0	H,K=	4,	2		-2	870	13	1	-8	314	7	-3	H,K=	4,	26	
1	49	58	15*	14	97	17	15	-4	396	7	-0	-10	41	45	27*	10	154	9	19
-3	99	12	4	12	419	8	10	-6	646	11	-12	-12	137	10	3	8	119	11	6
-9	61	23	11	10	199	8	-8	-10	449	8	2	H,K=	4,	18		6	269	7	2
H,K=	3,	31		8	632	10	-14	H,K=	4,	10		12	327	10	-5	2	318	6	0
9	268	8	13	6	197	5	-11	12	144	9	8	10	110	13	-30	-0	73	12	25
7	258	8	-7	4	963	14	-15	10	377	7	-0	8	478	8	-7	-2	328	7	-1
5	403	8	-2	2	265	5	10	8	203	6	-5	6	53	23	22	-4	27	42	1*
3	322	7	-6	-0	917	13	14	6	360	6	2	4	580	10	-14	-6	278	7	11
1	392	7	-6	-2	292	5	20	4	385	6	-1	2	135	5	4	-8	88	12	-27
-1	410	8	1	-4	1019	15	3	2	567	10	2	-0	587	10	5	-10	161	9	6
-3	329	7	-6	-6	219	5	1	-0	209	4	-4	-2	126	6	-1	H,K=	4,	28	
-5	412	8	1	-8	659	11	0	-2	582	10	-9	-4	558	9	-16	10	319	8	-9
-7	243	8	-7	-10	201	7	-3	-4	425	7	10	-6	18	42	1*	8	89	13	-2
-9	249	9	-9	-12	411	8	-2	-6	376	6	-4	-8	483	8	-10	6	404	8	5
H,K=	3,	33		-14	111	13	28	-8	224	6	12	-10	138	8	-7	4	200	7	-5
7	147	9	-4	H,K=	4,	4		-10	381	7	-6	-12	329	9	3	2	522	9	-10
5	192	8	-7	14	230	9	4	-12	152	9	6	H,K=	4,	20		-0	62	21	-2
3	259	7	-6	12	119	9	-9	H,K=	4,	12		12	183	8	7	-2	510	8	-4
1	320	7	-22	10	371	7	-3	12	129	9	6	10	201	7	0	-4	180	8	-16
-1	333	7	-3	8	244	6	-3	10	416	8	2	8	284	7	-2	-6	388	8	-3
-3	253	8	-9	6	563	9	-6	8	250	6	6	6	395	8	-8	-8	80	14	-13
-5	207	8	9	4	338	6	1	6	505	9	-6	4	104	9	-31	-10	322	8	-8
-7	159	8	9	2	511	9	3	4	340	6	3	2	352	6	-1	H,K=	4,	30	
H,K=	3,	35		-0	249	6	14	2	725	13	-0	-0	444	7	5	8	312	9	8
7	133	11	-9	-2	552	9	23	-0	176	5	3	-2	387	7	-8	6	175	8	12
5	167	9	8	-4	320	5	1	-2	727	12	3	-4	131	8	12	4	411	8	-3
3	192	7	4	-6	557	9	-18	-4	354	6	5	-6	394	7	-7	2	258	7	4
1	99	11	-12	-8	237	6	-2	-6	514	8	10	-8	284	7	1	-0	366	7	-4
-1	111	10	2	-10	393	7	11	-8	235	6	-5	-10	200	8	12	-2	248	7	7
-3	180	8	-5	-12	135	12	8	-10	396	8	-10	-12	164	10	-8	-4	398	8	-11
-5	165	8	4	-14	212	9	-17	-12	120	18	10	H,K=	4,	22		-6	134	13	-16
-7	132	10	-2	H,K=	4,	6		H,K=	4,	14		12	163	9	-6	-8	298	9	5
H,K=	3,	37		14	176	8	14	12	379	9	-6	10	177	8	3	H,K=	4,	32	
5	260	8	-0	12	224	7	14	10	76	12	-14	8	252	7	-2	8	139	9	17

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
6	73	20	-6	-3	691	11	9	5	165	5	-2	7	348	7	9	-3	270	6	0
4	297	7	5	-5	457	7	-2	3	355	6	-2	5	370	7	8	-5	229	7	0
2	116	8	8	-7	499	9	-9	1	416	7	-6	3	370	7	3	-7	229	7	-2
-0	311	7	5	-9	445	8	1	-1	440	7	4	1	379	6	-2	-9	232	8	-16
-2	117	11	10	-11	346	7	5	-3	391	7	-4	-1	373	6	-3	H,K=	5,	29	
-4	295	9	-0	-13	238	8	-1	-5	154	5	3	-3	356	6	-6	9	185	11	-3
-6	60	18	-10	H,K=	5,	5		-7	317	6	3	-5	387	7	11	7	277	7	-3
-8	134	12	9	13	137	12	-20	-9	287	7	1	-7	334	7	-6	5	374	8	1
H,K=	4,	34		11	155	7	6	-11	219	9	-16	-9	332	7	3	3	422	8	-2
8	305	9	-8	9	216	6	-5	-13	171	17	-26	-11	181	10	28	1	383	7	-4
6	32	49	17*	7	364	6	5	H,K=	5,	13		H,K=	5,	21		-1	408	7	11
4	354	8	1	5	764	12	12	13	254	8	-7	11	83	18	-19	-3	414	8	-8
-0	500	9	-6	3	271	5	-3	11	325	8	4	9	165	8	-10	-5	348	7	-8
-4	329	10	-19	1	59	11	-24	9	412	8	-8	7	198	7	-13	-7	278	8	-1
-8	327	8	12	-1	135	7	-2	7	455	8	-4	5	326	6	1	-9	194	9	-0
H,K=	4,	36		-3	295	5	-1	5	448	8	1	3	273	6	2	H,K=	5,	31	
6	157	13	-1	-5	755	12	6	3	611	10	3	1	143	6	-3	9	171	10	-1
4	167	9	-8	-7	383	7	11	1	437	7	-2	-1	116	7	-10	7	143	10	-18
2	207	7	-2	-9	220	6	1	-1	421	7	3	-3	280	6	-0	5	128	10	-9
-0	215	8	6	-11	170	7	6	-3	642	11	4	-5	307	7	-6	3	219	7	-6
-2	204	9	-1	-13	113	13	-43	-5	459	8	5	-7	199	7	0	1	228	7	-3
-4	174	9	0	H,K=	5,	7		-7	461	8	-0	-9	153	8	-9	-1	205	8	-2
-6	146	16	-1	13	275	8	4	-9	437	8	5	-11	119	15	20	-3	211	8	-8
H,K=	4,	38		11	184	7	1	-11	309	8	-10	H,K=	5,	23		-5	126	9	-4
4	284	9	15	9	347	7	-3	-13	273	8	9	11	206	9	-6	-7	169	9	9
2	140	11	6	7	453	8	-3	H,K=	5,	15		9	278	8	-12	-9	167	10	-2
-0	241	9	-1	5	378	6	-3	13	152	13	-5	7	307	7	-7	H,K=	5,	33	
-2	122	13	-0	3	701	11	-11	11	212	8	4	5	274	6	-5	7	190	10	6
-4	262	8	-6	1	534	9	-10	9	264	8	1	3	413	7	2	5	196	8	-14
H,K=	4,	40		-1	576	9	-1	7	386	7	9	1	433	7	2	3	218	8	-3
2	347	8	1	-3	742	12	1	5	206	6	3	-1	447	8	10	1	331	8	-0
-2	346	9	2	-5	362	6	-12	3	294	6	3	-3	411	7	-4	-1	325	7	0
H,K=	5,	1		-7	442	8	-7	1	433	8	0	-5	267	6	13	-3	217	8	8
13	179	9	-13	-9	351	7	-3	-1	416	7	2	-7	316	8	4	-5	224	8	14
11	295	7	-8	-11	203	7	-2	-3	315	6	9	-9	283	9	-4	-7	189	8	11
9	234	6	1	-13	241	8	-13	-5	167	6	-8	-11	211	8	8	H,K=	5,	35	
7	294	6	-9	H,K=	5,	9		-7	386	7	1	H,K=	5,	25		7	156	9	-4
5	500	9	2	13	219	14	-3	-9	269	7	5	11	201	9	-7	5	229	8	-2
3	353	6	1	11	271	7	-3	-11	225	7	14	9	273	7	5	3	254	8	1
1	624	10	-0	9	391	7	-1	-13	163	13	9	7	206	7	-1	1	282	9	-3
-1	618	10	-7	7	453	8	1	H,K=	5,	17		5	224	7	-9	-1	286	7	10
-3	402	7	10	5	672	11	15	11	236	8	6	3	415	8	9	-3	237	8	-4
-5	484	8	-7	3	422	7	1	9	291	7	-11	1	458	8	4	-5	227	12	-11
-7	296	6	3	1	450	8	-5	7	303	7	4	-1	443	7	2	-7	158	11	0
-9	228	6	-1	-1	467	8	-10	5	438	8	5	-3	407	7	12	H,K=	5,	37	
-11	306	7	-0	-3	452	8	4	3	449	8	4	-5	246	8	-0	5	169	9	-7
-13	208	8	13	-5	659	11	-9	1	366	6	0	-7	222	8	-5	3	159	15	15
H,K=	5,	3		-7	456	8	-2	-1	376	6	1	-9	261	9	-6	1	166	10	-3
13	234	8	-7	-9	387	7	-2	-3	457	7	15	-11	216	9	4	-1	177	8	15
11	319	8	-7	-11	280	7	1	-5	417	8	-4	H,K=	5,	27		-3	148	12	5
9	417	7	-3	-13	215	8	-6	-7	299	7	-13	9	245	8	1	-5	174	9	3
7	535	9	-3	H,K=	5,	11		-9	302	7	4	7	236	8	4	H,K=	5,	39	
5	410	7	-3	13	207	10	9	-11	224	10	-1	5	235	7	-6	3	210	9	-13
3	666	11	1	11	242	7	-9	H,K=	5,	19		3	271	7	-9	1	247	8	10
1	680	11	-3	9	290	7	9	11	146	9	-7	1	362	7	-10	-1	226	8	0
-1	633	10	-1	7	323	6	9	9	354	8	6	-1	355	7	0	-3	239	8	11

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FCB	SG	DEL	L	FOB	SG	DEL
H,K=		5,	41	-2	149	5	17	12	71	23	-3	6	237	7	-8	13	252	8	-8
1	143	11	-13	-4	241	5	9	10	0	54	-35*	4	106	9	-1	11	292	9	-1
-1	156	11	-5	-8	99	8	2	8	96	17	6	2	321	7	-5	9	322	7	-2
H,K=		6,	0	H,K=		6,	10	6	121	8	1	-2	323	7	-0	7	381	7	-6
10	701	11	-4	12	440	8	7	4	313	6	-5	-4	102	9	-2	5	669	11	-3
6	565	9	-8	10	99	14	1	-0	55	10	-8	-6	250	8	-9	3	558	10	-3
2	985	14	0	8	711	12	-12	-2	53	18	1	-8	35	44	-7*	1	809	12	-1
-2	938	14	10	6	124	6	7	-4	314	6	-6	-10	218	9	-10	-1	794	13	-0
-6	562	10	-18	4	801	13	-5	-6	122	7	-2	H,K=		6,	30	-3	542	9	-1
-10	702	11	-4	2	313	5	-3	-8	81	11	-11	8	222	8	-3	-5	671	12	-5
H,K=		6,	2	-0	1042	16	-6	-10	61	26	22	4	264	9	-8	-7	379	7	-1
12	160	8	-2	-2	324	5	6	-12	74	16	4	2	90	13	-5	-9	293	6	-7
10	119	9	3	-4	793	13	-5	H,K=		6,	20	-0	516	9	-6	-11	285	7	-3
8	216	6	-1	-6	121	6	4	12	0	72	-21*	-2	91	10	-4	-13	251	8	-0
6	145	5	3	-8	727	12	-4	10	363	8	1	-4	277	8	1	H,K=		7,	5
4	450	8	6	-10	97	15	0	8	66	35	12	-8	225	10	-6	13	166	8	13
2	29	38	13*	-12	432	9	-2	6	449	8	3	H,K=		6,	32	11	187	10	4
-0	716	11	12	H,K=		6,	12	4	144	6	7	8	64	22	36	9	271	7	-8
-4	462	8	-1	12	55	25	33	2	581	10	7	6	452	9	12	7	280	6	1
-6	132	6	-10	10	382	8	-4	-0	145	6	-9	2	465	8	-3	5	372	21	-1
-8	213	6	9	8	113	8	-1	-2	587	10	21	-2	458	8	-5	3	199	5	-2
-10	102	14	-10	6	389	7	-10	-4	134	8	-3	-4	79	19	-8	1	382	6	-7
-12	154	9	-9	4	144	5	8	-6	450	8	7	-6	422	8	-2	-1	348	6	1
H,K=		6,	4	2	542	10	-3	-8	59	20	8	H,K=		6,	34	-3	193	5	-1
12	0	41	-22*	-0	188	5	5	-10	369	8	11	4	102	10	49	-5	390	25	5
10	304	8	-14	-2	587	10	-3	H,K=		6,	22	2	0	63	-30*	-7	282	6	-1
8	245	6	-2	-4	133	6	-6	10	63	33	-13	-6	0	53	-37*	-9	280	7	12
6	573	9	-2	-6	396	7	-10	8	479	8	3	H,K=		6,	36	-11	209	8	12
4	91	9	-0	-8	102	9	-15	6	64	15	34	6	372	9	7	-13	151	10	2
2	700	11	1	-10	390	8	8	4	567	10	-1	2	311	8	-1	H,K=		7,	7
-0	163	5	-6	H,K=		6,	14	2	52	25	-3	-0	97	39	27	13	244	8	5
-2	718	12	6	12	216	8	12	-0	583	10	9	-2	300	8	-7	11	338	8	-3
-4	93	6	5	10	128	11	24	-2	44	29	-13	-6	378	9	9	9	305	7	2
-6	541	10	-16	8	341	7	-8	-4	566	9	-2	H,K=		6,	38	7	375	7	1
-8	252	6	6	6	155	8	2	-8	466	8	-2	4	306	8	2	5	504	8	-5
-10	318	7	0	4	431	7	6	H,K=		6,	24	-0	293	8	-14	3	424	7	1
-12	0	49	-20*	2	120	7	-3	10	59	24	9	-4	305	9	-2	1	622	10	-1
H,K=		6,	6	-0	617	10	-7	8	97	17	1	H,K=		6,	40	-1	603	10	-24
12	383	8	1	-2	123	6	-3	6	155	9	-3	2	125	16	-6	-3	425	7	2
10	69	13	-1	-4	415	7	-4	4	95	9	18	-2	148	9	5	-5	512	9	1
8	643	11	5	-6	165	6	11	2	41	42	17*	H,K=		7,	1	-7	390	7	-2
6	87	12	-18	-8	333	7	-6	-4	83	10	3	13	190	9	6	-9	290	7	5
4	997	15	8	-10	86	12	-15	-6	160	7	3	11	263	8	1	-11	336	8	-4
2	68	10	16	-12	209	8	-7	-8	110	12	16	9	335	7	-7	-13	235	9	-10
-0	877	13	-3	H,K=		6,	16	H,K=		6,	26	7	251	6	2	H,K=		7,	9
-2	74	10	21	12	103	10	3	8	459	9	-10	5	357	6	11	13	152	11	-6
-4	1000	15	-1	10	492	9	-3	6	0	46	-40*	3	292	5	-1	11	211	8	5
-6	98	7	-5	6	704	12	-9	4	659	11	6	1	396	7	1	9	369	8	-1
-8	646	11	1	4	161	7	-5	-0	644	11	-11	-1	374	6	9	7	517	9	-9
-12	367	9	-5	2	714	12	-8	-2	61	21	33	-3	262	5	3	5	367	6	2
H,K=		6,	8	-2	712	12	-10	-4	638	11	-3	-5	371	6	3	3	527	9	-3
12	87	26	6	-4	164	6	-2	-6	41	29	1	-7	239	6	-4	1	653	11	6
8	97	8	2	-6	696	12	-19	-8	474	9	8	-9	339	7	3	-1	646	11	13
4	240	5	4	-10	485	9	-4	-10	30	50	-10*	-11	271	7	8	-3	534	9	14
2	134	6	3	-12	85	14	-15	H,K=		6,	28	-13	190	8	12	-5	369	6	-7
-0	461	7	16	H,K=		6,	18	10	223	10	-1	H,K=		7,	3	-7	516	9	-3

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-9	371	7	3	-11	172	8	4	1	182	6	-6	8	390	7	-6	-6	602	11	9
-11	204	10	-5	H,K=		7,	19	-1	184	6	-1	4	615	10	9	-8	13	45	-14*
-13	142	11	-18	11	235	9	-10	-3	261	7	-0	-0	101	6	2	-10	409	8	5
H,K=		7,	11	9	280	7	-5	-5	192	7	3	-4	630	11	13	-12	77	12	10
13	194	9	6	7	302	7	-8	-7	171	10	-8	-8	386	7	-8	H,K=		8,	10
11	228	9	-8	5	406	8	-1	-9	175	9	-7	-12	296	8	-7	12	126	13	10
9	260	7	-9	3	569	9	-2	H,K=		7,	29	H,K=		8,	2	10	280	7	-3
7	139	7	3	1	494	8	8	9	280	8	-1	12	356	8	5	8	124	8	3
5	244	6	1	-1	480	9	3	7	283	8	0	10	176	7	-7	6	355	7	1
3	376	6	6	-3	569	10	-3	5	313	9	-0	8	429	8	-12	4	112	8	-6
1	578	10	2	-5	393	7	-7	3	412	8	2	6	162	6	-1	2	562	10	-12
-1	564	10	4	-7	285	7	-11	1	295	7	-5	4	829	14	-14	-0	444	7	-4
-3	363	6	6	-9	283	8	2	-1	296	7	-5	2	422	7	12	-2	564	10	-6
-5	243	6	3	-11	263	8	12	-3	413	8	-16	-0	577	10	9	-4	103	7	0
-7	165	6	-0	H,K=		7,	21	-5	336	8	7	-2	428	7	12	-6	360	7	5
-9	261	7	6	11	137	10	-7	-7	278	8	-5	-4	842	14	-14	-8	122	8	3
-11	241	7	-10	9	213	7	2	-9	281	10	-2	-6	162	7	6	-10	282	7	3
-13	188	9	-4	7	246	7	-4	H,K=		7,	31	-8	435	8	2	-12	119	9	7
H,K=		7,	13	5	225	7	-4	7	165	9	3	-10	189	9	5	H,K=		8,	12
11	237	8	-6	3	240	6	8	5	223	8	-13	-12	349	8	8	12	118	12	22
9	355	7	-1	1	282	6	3	3	172	7	2	H,K=		8,	4	10	351	8	-1
7	483	8	1	-1	283	6	-3	1	200	7	-0	12	151	9	-2	8	210	7	-6
5	481	9	6	-3	230	6	2	-1	206	7	3	10	403	8	9	6	416	7	4
3	674	11	-2	-5	223	6	8	-3	148	9	-10	8	215	6	-4	4	344	7	1
1	448	8	1	-7	257	9	-9	-5	248	7	15	6	396	7	6	2	577	10	5
-1	435	7	4	-9	203	7	-8	-7	157	12	0	4	489	8	2	-0	294	5	-3
-3	661	11	-4	-11	142	10	-0	H,K=		7,	33	2	734	12	10	-2	567	9	-7
-5	488	8	-3	H,K=		7,	23	7	259	8	6	-0	138	5	6	-4	335	6	-2
-7	470	8	-5	11	267	9	-12	5	243	8	-1	-2	698	12	-3	-6	417	7	-3
-9	352	7	-4	9	276	8	-11	3	180	8	-20	-4	492	8	-1	-8	200	7	-2
-11	243	8	-1	7	284	7	-3	1	249	7	-10	-6	368	7	1	-10	351	8	4
H,K=		7,	15	5	338	7	-3	-1	271	7	5	-8	209	6	1	-12	122	10	17
11	133	10	-15	3	502	8	2	-3	217	7	3	-10	405	8	1	H,K=		8,	14
9	270	8	2	1	246	6	-2	-5	238	8	-2	-12	152	9	10	12	277	8	3
7	157	7	-2	-1	254	6	1	-7	257	8	7	H,K=		8,	6	10	57	32	-15
5	295	7	2	-3	497	8	-4	H,K=		7,	35	12	208	9	8	8	367	7	-10
3	374	6	-3	-5	335	7	-10	5	226	8	6	10	322	7	1	6	226	6	-6
1	391	7	-3	-7	301	7	5	3	169	9	-10	8	308	7	-3	4	592	10	-7
-1	385	7	-1	-9	291	8	-9	1	288	7	15	6	334	7	-6	2	227	6	6
-3	370	6	-6	-11	278	9	-8	-1	263	8	-15	4	278	6	-0	-0	711	12	-4
-5	293	6	7	H,K=		7,	25	-3	191	11	1	2	658	11	17	-2	225	6	2
-7	147	7	9	9	286	8	5	-5	203	8	1	-0	44	16	-18	-4	576	10	-5
-9	249	7	-10	7	256	7	-1	H,K=		7,	37	-2	635	11	1	-6	231	6	-2
-11	137	27	-0	5	246	7	10	5	160	9	12	-4	294	5	-1	-8	365	7	-0
H,K=		7,	17	3	377	7	-5	3	119	12	10	-6	331	6	-4	-10	79	13	-4
11	170	8	4	1	268	6	-6	1	163	9	14	-8	315	7	8	-12	259	9	-13
9	265	7	1	-1	271	6	6	-1	154	8	1	-10	322	7	-8	H,K=		8,	16
7	243	7	-3	-3	378	7	-7	-3	114	11	2	-12	190	9	-11	12	211	8	-4
5	283	6	-7	-5	260	7	-1	-5	131	10	-13	H,K=		8,	8	8	262	8	-3
3	294	6	-0	-7	245	8	-1	H,K=		7,	39	10	399	8	11	4	394	7	1
1	327	6	-2	-9	263	8	-7	3	192	9	-2	6	603	10	-4	-0	438	8	-1
-1	332	6	1	H,K=		7,	27	1	224	8	8	4	251	5	8	-2	80	16	-4
-3	300	6	5	9	185	9	9	-1	234	8	8	2	991	16	-12	-4	387	7	2
-5	271	7	2	7	188	9	5	-3	188	9	-4	-0	93	9	-7	-8	257	7	-11
-7	247	6	2	5	193	7	-1	H,K=		8,	0	-2	977	15	-16	-12	198	9	-12
-9	266	8	-4	3	259	6	-4	12	320	8	6	-4	249	5	1	H,K=		8,	18

STRUCTURE FACTCRS CONTINUED FCR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FCB	SG	DEL	L	FOB	SG	DEL
12	297	9	-14	-4	112	9	0	1	763	12	-2	3	246	5	-3	-5	283	7	-3
10	91	15	17	-6	355	8	9	-1	760	12	9	1	634	11	11	-7	272	8	5
8	488	9	-2	-8	107	15	-8	-3	698	12	5	-1	651	11	15	-9	262	8	-11
6	140	7	5	-10	250	8	18	-5	542	9	-5	-3	240	5	1	-11	253	8	12
4	573	10	-8	H,K=		8,	28	-7	270	6	11	-5	179	6	-11	H,K=		9,	19
2	127	7	9	8	134	14	-20	-9	320	7	-10	-7	279	7	-4	11	131	10	-3
-0	440	7	0	6	395	8	-4	-11	332	8	-11	-9	221	7	-11	9	150	9	1
-2	125	6	6	4	148	7	-5	-13	193	8	4	-11	250	8	3	7	177	7	9
-4	588	10	6	2	265	7	-5	H,K=		9,	3	H,K=		9,	11	5	83	11	7
-6	124	7	-6	-0	176	8	2	13	72	15	-7	11	295	8	2	3	150	7	-6
-8	493	9	-3	-2	271	7	-3	11	51	33	-6	9	395	8	0	1	152	7	3
-10	23	54	-43*	-4	156	8	-10	9	0	48	-60*	7	504	9	-5	-1	174	6	-0
-12	327	8	13	-6	408	8	6	7	114	7	-4	5	427	7	-4	-3	167	8	4
H,K=		8,	20	-8	143	11	-11	5	249	5	4	3	499	8	-6	-5	93	9	-3
10	240	8	4	H,K=		8,	30	3	67	11	9	1	614	10	7	-7	175	7	7
8	87	18	-19	8	311	8	-8	1	203	23	8	-1	623	10	10	-9	149	9	-7
6	258	7	-1	6	203	8	1	-1	224	5	6	-3	494	8	-5	-11	132	10	-5
4	170	7	1	4	351	8	-3	-3	92	9	33	-5	451	8	-0	H,K=		9,	21
2	434	7	-0	2	163	7	9	-5	242	6	-1	-7	499	8	4	11	299	9	-4
-0	288	6	-6	-0	333	7	10	-7	118	9	-3	-9	397	8	1	9	308	8	-1
-2	433	8	-4	-2	170	7	3	-11	54	18	-7	-11	284	9	-4	7	334	7	1
-4	162	6	-4	-4	358	8	-4	-13	30	59	-43*	H,K=		9,	13	5	297	7	2
-6	251	7	2	-6	216	8	7	H,K=		9,	5	11	29	52	-8*	3	527	9	10
-8	89	13	-11	-8	328	8	17	13	291	8	11	9	21	47	-19*	1	394	7	5
-10	243	8	5	H,K=		8,	32	11	354	8	1	7	116	8	6	-1	388	7	-2
H,K=		8,	22	6	129	11	-13	9	351	7	-13	5	111	7	7	-3	517	9	6
10	212	8	17	4	154	8	7	7	496	8	-6	3	122	6	-5	-5	310	7	8
8	286	8	9	2	78	19	19	5	660	11	1	1	266	5	1	-7	325	7	3
6	222	7	-4	-0	281	8	-0	3	560	10	-1	-1	260	5	-1	-9	312	8	3
4	277	6	-9	-2	44	58	-28*	1	662	11	-6	-3	122	6	-3	-11	294	9	-3
2	264	7	2	-4	154	9	-0	-1	679	11	-4	-5	111	10	9	H,K=		9,	23
-0	252	6	-4	-6	149	12	7	-3	546	10	8	-7	104	11	0	9	153	11	1
-2	266	6	-8	H,K=		8,	34	-5	648	11	-3	-9	0	47	-35*	7	114	10	0
-4	294	7	2	6	0	48	-16*	-7	500	8	-1	-11	0	51	-46*	5	132	8	-6
-6	237	6	4	4	319	8	10	-9	368	7	-6	H,K=		9,	15	3	231	6	1
-8	261	7	-7	2	91	13	21	-11	371	8	5	11	237	9	8	1	179	6	-1
-10	191	10	-5	-0	453	8	11	-13	276	9	-8	9	306	9	7	-1	183	6	8
H,K=		8,	24	-2	87	11	18	H,K=		9,	7	7	435	8	-12	-3	233	6	3
10	370	8	-1	-4	333	9	11	13	120	11	6	5	472	8	-10	-5	141	9	-9
6	359	7	3	H,K=		8,	36	11	123	9	4	3	487	8	-10	-7	112	12	-8
4	58	22	-7	4	132	12	9	9	261	8	-7	1	428	8	-4	-9	152	11	3
2	569	9	9	2	161	9	14	7	237	7	-2	-1	449	8	-2	H,K=		9,	25
-0	86	12	14	-0	180	8	5	5	169	6	8	-3	485	8	-3	9	145	9	-0
-2	546	9	-5	-2	147	8	8	3	324	6	-3	-5	466	8	-14	7	262	7	-1
-4	52	17	-12	-4	132	14	22	1	606	10	16	-7	438	8	-7	5	310	8	2
-6	382	8	2	H,K=		8,	38	-1	565	9	-4	-9	306	7	4	3	328	7	-2
-8	40	47	26*	2	150	11	-4	-3	327	6	-2	-11	214	9	-5	1	216	6	-2
-10	374	9	6	-0	211	8	-9	-5	166	6	-3	H,K=		9,	17	-1	234	6	5
H,K=		8,	26	-2	155	9	-4	-7	240	6	12	11	239	8	0	-3	333	7	-8
10	227	9	-4	H,K=		9,	1	-9	269	7	-1	9	268	7	2	-5	313	7	-6
8	106	11	-13	13	175	10	-13	-13	99	12	-2	7	278	7	-5	-7	275	8	12
6	318	8	-10	11	346	8	6	H,K=		9,	9	5	289	7	4	-9	148	9	-5
4	130	8	6	9	333	7	-8	11	247	8	0	3	510	8	1	H,K=		9,	27
2	365	8	-1	7	287	7	4	9	243	7	7	1	350	6	-9	9	304	9	2
-0	100	9	19	5	530	9	-14	7	271	6	-2	-1	334	6	-9	7	357	8	11
-2	349	7	-5	3	710	12	1	5	210	6	-9	-3	503	8	1	5	324	8	-5

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
3	400	9	-5	-2	887	15	-1	-10	225	7	8	-2	306	7	12	6	142	10	-3
1	332	7	-7	-4	151	6	-8	-12	153	10	-9	-4	407	7	-6	4	51	25	-11
-1	346	7	6	-6	384	8	-10	H,K=	10,	12		-6	194	8	-2	2	186	9	6
-3	400	7	8	-8	69	17	-14	12	259	9	-2	-8	212	7	-6	-0	95	17	-24
-5	333	8	-13	-10	494	9	3	10	164	9	-6	-10	171	9	4	-2	188	9	8
-7	351	10	7	-12	0	64	-31*	8	479	8	-15	H,K=	10,	22		-6	139	9	1
-9	304	8	-2	H,K=	10,		4	6	286	6	11	10	190	8	13	H,K=	10,		34
H,K=	9,	29		12	218	9	-10	4	482	8	-0	8	184	8	-8	4	17	52	-40*
7	0	50	-42*	10	131	9	-7	2	322	6	-4	6	319	8	-8	2	341	8	-5
5	82	28	-2	8	381	7	-4	-0	784	13	-5	4	226	7	-6	-2	353	8	5
3	40	44	4*	6	335	7	5	-2	319	6	-6	2	249	8	-9	-4	34	53	-25*
1	70	16	11	4	451	7	-2	-4	472	8	-16	-0	237	6	-3	H,K=	10,		36
-5	84	22	1	2	466	8	-6	-6	292	7	13	-2	274	7	-2	4	172	8	0
-7	48	47	3	-0	345	6	-2	-8	501	8	-2	-4	218	8	0	2	152	9	13
H,K=	9,	31		-2	479	8	5	-10	175	14	7	-6	321	7	-8	-0	136	9	5
7	275	8	1	-4	448	8	1	-12	254	10	-8	-8	177	9	-13	-2	146	14	5
5	245	7	-9	-6	333	6	9	H,K=	10,	14		-10	166	9	-0	-4	182	10	1
3	268	8	-1	-8	368	8	1	10	396	8	-2	H,K=	10,	24		H,K=	11,		1
1	307	7	-11	-10	148	13	3	8	156	7	2	10	86	13	-2	11	224	8	0
-1	322	7	4	-12	237	9	12	6	458	8	-4	8	383	9	4	9	287	7	1
-3	286	8	10	H,K=	10,		6	2	632	10	4	6	77	15	21	7	281	6	9
-5	248	8	-12	12	178	8	8	-0	99	7	8	4	526	9	-8	5	402	7	0
-7	282	8	7	10	130	8	4	-2	632	10	3	-0	557	10	-11	3	360	6	-3
H,K=	9,	33		8	291	7	10	-4	45	46	-11*	-2	0	59	-2*	1	419	7	2
5	169	11	7	6	241	5	5	-6	445	8	-4	-4	539	9	3	-1	430	7	-2
3	158	8	5	4	263	5	11	-8	154	9	-7	-6	64	22	-0	-3	378	7	-3
1	231	7	-7	2	284	6	-6	-10	390	8	-9	-8	390	9	10	-5	388	7	2
-1	253	8	3	-0	472	8	-2	H,K=	10,	16		-10	68	27	-24	-7	278	7	5
-3	169	9	3	-2	290	6	-0	10	191	8	-4	H,K=	10,	26		-9	273	7	-10
-5	157	9	-14	-4	267	6	5	8	141	8	0	8	119	11	-6	-11	243	8	4
H,K=	9,	35		-6	236	6	7	6	360	7	3	4	306	7	4	H,K=	11,		3
5	115	16	26	-8	267	7	1	2	298	6	4	2	145	7	0	11	279	8	-4
3	116	14	25	-10	129	9	-7	-0	195	6	0	-0	169	10	39	9	280	8	-1
1	135	8	-1	-12	153	10	-12	-2	324	6	2	-2	139	8	0	7	300	7	-10
-1	136	9	-7	H,K=	10,		8	-4	64	11	-2	-4	304	8	8	5	514	9	-4
-3	97	15	3	12	340	8	10	-6	350	7	-11	-6	44	49	17*	3	368	6	-12
-5	107	16	15	8	549	9	2	-8	132	9	-12	-8	131	12	13	1	455	8	0
H,K=	9,	37		6	175	6	6	-10	192	8	3	H,K=	10,	28		-1	422	7	-4
3	299	8	11	4	563	9	-4	H,K=	10,	18		8	296	8	3	-3	379	7	-10
1	253	8	-9	-0	725	12	-5	10	340	9	-5	6	54	60	-8*	-5	506	8	-4
-1	245	9	-14	-4	562	9	-1	6	471	8	-7	4	373	8	-14	-7	312	7	2
-3	296	8	10	-6	166	6	-5	4	110	8	6	2	136	10	1	-9	261	7	-3
H,K=	10,		0	-8	552	9	5	2	520	9	7	-0	427	8	7	-11	285	8	7
10	263	7	1	-12	320	9	-8	-0	179	6	-8	-2	141	9	1	H,K=	11,		5
6	513	9	-8	H,K=	10,		10	-2	525	9	-1	-4	388	8	2	11	128	13	15
2	404	7	8	12	166	9	-9	-4	111	8	17	-6	83	19	2	9	209	7	-7
-2	365	21	1	10	212	10	6	-6	484	8	-5	-8	300	8	6	7	116	12	12
-6	541	9	16	8	249	8	8	-8	49	19	3	H,K=	10,	30		5	195	7	5
-10	269	7	3	6	133	9	-5	-10	342	9	-2	6	337	8	11	3	355	6	-14
H,K=	10,		2	4	284	6	4	H,K=	10,	20		4	67	16	-9	1	388	7	-1
10	470	8	-7	2	125	6	-5	10	184	8	16	2	361	8	-5	-1	353	7	-6
8	93	10	-7	-0	342	20	-10	8	227	7	16	-0	217	8	4	-3	389	6	-5
6	417	7	2	-2	140	22	4	6	180	9	-8	-2	363	8	-2	-5	184	6	-7
4	131	6	-1	-4	256	6	13	4	402	7	-13	-4	100	15	19	-7	119	8	7
2	911	15	-10	-6	118	9	-16	2	293	7	9	-6	331	8	5	-9	238	8	7
-0	305	5	-7	-8	240	7	-3	-0	264	7	-1	H,K=	10,	32		-11	141	10	8

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	11,		7	5	231	6	10	9	202	9	3	12	0	68	-18*	-10	431	8	-2
11	236	8	10	3	309	6	-10	7	270	9	-2	10	183	8	-1	H,K=	12,		12
9	326	7	7	1	215	6	4	5	239	7	15	6	268	6	-3	8	320	8	-8
7	264	6	4	-1	204	6	-3	3	287	7	-3	4	132	7	3	6	76	40	4
5	425	7	-4	-3	322	7	-5	1	291	7	4	2	222	5	-4	4	291	6	-5
3	384	7	-5	-5	227	6	3	-1	295	7	5	-0	184	5	-4	-0	534	9	-11
1	256	6	2	-7	227	7	-12	-3	286	8	0	-2	218	6	-8	-2	38	22	-12
-1	275	6	-1	-9	247	8	-12	-5	199	8	4	-4	122	6	1	-4	297	6	-8
-3	374	7	-7	-11	212	10	8	-7	273	8	-2	-6	267	6	-7	-6	77	14	7
-5	428	7	-6	H,K=	11,		17	-9	207	8	16	-8	66	20	2	-8	322	7	-8
-7	265	6	-9	11	182	9	7	H,K=	11,		27	-10	190	8	2	-10	53	44	4
-9	325	7	8	9	231	10	-9	7	163	9	9	H,K=	12,		4	H,K=	12,		14
-11	215	8	-2	7	307	8	-5	5	192	7	3	12	327	9	1	10	171	8	-0
H,K=	11,		9	5	285	7	-1	3	243	9	-8	10	0	46	-25*	8	87	11	2
11	229	8	0	3	271	6	-4	1	290	7	1	8	403	7	2	6	244	7	-5
9	332	8	-13	1	478	8	6	-1	274	7	-2	6	117	7	2	4	128	8	2
7	369	8	5	-1	472	8	4	-3	247	7	4	4	634	11	-4	2	281	6	-6
5	319	6	-4	-3	250	7	-11	-5	173	10	-6	2	219	6	-11	-2	277	6	-3
3	407	7	-10	-5	290	6	2	-7	155	10	-3	-0	389	6	-1	-4	129	8	-1
1	419	7	-0	-7	321	7	2	H,K=	11,		29	-2	229	6	-6	-6	222	7	-5
-1	405	7	-2	-9	254	8	5	7	217	8	20	-4	637	11	-11	-8	90	10	5
-3	424	7	-1	-11	170	10	-9	5	204	8	-14	-6	107	8	-11	-10	154	9	-3
-5	313	6	6	H,K=	11,		19	3	256	7	6	-8	410	8	3	H,K=	12,		16
-7	354	7	-2	9	268	8	6	1	293	8	5	-12	324	8	-1	10	38	57	-27*
-9	335	7	-8	7	338	8	16	-1	284	8	1	H,K=	12,		6	8	484	9	-2
-11	239	8	6	5	405	7	-3	-3	247	8	-2	10	390	8	-3	6	120	9	2
H,K=	11,		11	3	422	7	3	-5	244	8	9	8	84	16	-0	4	649	11	-7
11	156	9	8	1	350	7	6	-7	193	9	2	6	643	10	-13	2	192	7	-3
9	233	7	5	-1	344	7	0	H,K=	11,		31	2	601	11	-5	-0	690	12	-6
7	269	7	-1	-3	433	7	-2	5	198	8	4	-2	602	10	-2	-2	196	6	1
5	198	6	-9	-5	397	8	-5	3	185	8	-10	-6	655	11	-13	-4	652	11	-2
3	273	6	-0	-7	317	7	0	1	222	8	6	-8	50	24	-31	-6	123	8	5
1	243	6	2	-9	264	8	-5	-1	233	7	13	-10	407	8	6	-8	499	9	-0
-1	235	6	0	H,K=	11,		21	-3	203	8	3	-12	0	50	-33*	-10	82	20	17
-3	294	6	0	9	151	10	3	-5	197	8	9	H,K=	12,		8	H,K=	12,		18
-5	218	8	-5	7	205	8	-16	H,K=	11,		33	10	187	12	-12	10	79	22	-1
-7	261	6	-1	5	245	7	-9	5	200	9	8	8	82	11	-3	8	98	15	8
-9	219	7	-3	3	235	6	3	3	207	8	8	6	136	7	14	6	196	7	-1
-11	155	9	-5	1	169	8	-10	1	256	8	-1	4	144	6	6	4	37	42	-3*
H,K=	11,		13	-1	177	7	5	-1	243	8	4	-0	53	15	21	2	81	10	-6
11	273	9	-1	-3	243	7	-5	-3	181	9	-13	-2	26	43	-19*	-0	0	44	-22*
9	312	8	10	-5	256	7	-0	-5	188	9	-4	-4	120	8	-16	-2	98	11	6
7	372	8	4	-7	219	7	7	H,K=	11,		35	-6	126	14	2	-4	0	45	-43*
5	277	7	-3	-9	144	10	-4	3	202	8	7	-8	87	11	-0	-6	207	7	0
3	400	7	-0	H,K=	11,		23	1	276	8	-11	-10	115	13	-11	-8	96	13	10
1	498	8	3	9	221	11	1	-1	291	9	5	H,K=	12,		10	-10	88	20	2
-1	488	9	-6	7	276	8	1	-3	189	8	-3	10	442	9	1	H,K=	12,		20
-3	392	7	-4	5	310	7	3	H,K=	12,		0	8	86	10	-15	10	58	22	3
-5	262	7	-1	3	438	8	-3	12	417	9	-9	6	483	8	-0	8	385	8	-2
-7	401	8	10	1	271	7	-11	8	489	8	3	4	70	14	-6	6	83	13	-4
-9	307	8	-2	-1	280	7	6	4	695	12	-25	2	633	11	-15	4	566	9	-2
-11	268	9	-2	-3	424	8	-5	-0	675	11	-8	-0	118	7	2	2	121	8	-5
H,K=	11,		15	-5	332	7	0	-4	769	12	12	-2	628	12	-20	-0	561	10	-8
11	201	9	-4	-7	285	7	16	-8	473	8	-6	-4	83	8	6	-2	115	8	-6
9	264	7	9	-9	222	9	-2	-12	430	9	3	-6	482	8	-5	-4	564	9	8
7	258	7	6	H,K=	11,		25	H,K=	12,		2	-8	107	11	5	-6	58	36	-28

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-8	381	8	-4	-5	305	6	10	H,K=	13,	11		-7	273	8	1	1	219	11	8
-10	74	14	15	-7	342	7	-2	11	116	15	-12	-9	279	8	5	-1	209	8	-4
H,K=	12,	22		-9	185	9	3	9	185	11	-5	H,K=	13,	21		-3	191	9	-13
6	390	8	-11	-11	210	8	-9	7	133	7	12	9	162	10	11	H,K=	14,		0
4	24	38	-3*	H,K=	13,		3	5	143	7	8	7	146	10	-11	10	285	8	1
2	423	8	-0	11	247	8	-18	3	13	42	-39*	5	126	10	1	6	474	8	0
-0	0	48	-53*	9	380	8	0	1	304	6	8	3	275	7	7	2	419	8	-10
-2	433	8	-3	7	352	7	3	-1	296	6	-0	1	181	8	-6	-2	456	8	3
-6	408	8	6	5	495	9	-12	-5	138	7	15	-1	166	8	-7	-6	475	8	6
H,K=	12,	24		3	419	7	-2	-7	118	11	-20	-3	260	7	0	-10	277	8	1
6	128	9	17	1	398	7	9	-9	196	8	8	-5	106	15	-8	H,K=	14,		2
4	180	8	4	-1	408	7	2	-11	133	9	10	-7	156	11	-7	10	325	8	17
2	81	12	45	-3	438	7	4	H,K=	13,	13		-9	165	9	19	8	126	9	-11
-0	90	13	9	-5	525	9	7	11	265	8	20	H,K=	13,	23		6	563	9	7
-4	174	8	5	-7	359	7	-4	9	264	7	-6	7	237	8	10	4	92	11	28
-6	101	11	-5	-9	376	8	-2	7	334	8	-8	5	263	7	8	2	498	8	4
-8	63	17	25	-11	269	8	5	5	274	7	-10	3	274	7	-9	-0	52	38	17
H,K=	12,	26		H,K=	13,		5	3	483	8	5	1	366	8	-8	-2	511	9	4
6	412	8	2	11	138	10	-1	1	408	7	1	-1	371	8	-9	-4	51	19	3
2	456	8	9	9	136	9	-5	-1	401	7	-4	-3	270	7	-8	-6	566	9	4
-2	434	8	-12	7	250	7	12	-3	477	8	11	-5	236	8	-9	-8	131	9	0
-4	0	54	-74*	5	365	7	5	-5	286	7	-13	-7	220	8	-1	-10	333	8	15
-6	410	8	5	3	231	6	1	-7	329	8	0	H,K=	13,	25		H,K=	14,		4
-8	0	48	-51*	1	272	6	1	-9	260	8	-1	7	232	8	-2	10	220	8	7
H,K=	12,	28		-1	289	6	7	-11	244	8	-6	5	226	8	-5	8	287	7	3
6	0	51	-42*	-3	251	6	7	H,K=	13,	15		3	225	7	-2	6	329	7	-0
4	230	9	4	-5	359	7	3	9	220	8	1	1	146	8	3	4	201	6	3
2	47	25	-18	-7	258	7	7	7	192	7	-6	-1	163	8	8	2	222	7	-10
-0	237	7	-6	-9	134	9	-3	5	291	7	2	-3	232	9	-1	-0	508	9	-8
-4	223	8	5	-11	157	9	12	3	198	7	2	-5	247	8	10	-2	230	6	3
-6	78	15	33	H,K=	13,		7	1	271	6	1	-7	231	8	13	-4	206	6	-2
H,K=	12,	30		11	225	8	3	-1	281	6	2	H,K=	13,	27		-6	337	7	-0
6	205	8	1	9	342	8	17	-3	214	6	-3	7	148	10	-1	-8	314	7	9
2	267	8	-0	7	302	7	-14	-5	272	7	-5	5	132	9	-20	-10	199	8	-12
-2	251	7	-5	5	353	7	3	-7	191	7	-17	3	143	8	-7	H,K=	14,		6
-4	0	69	-65*	3	312	6	8	-9	221	8	2	1	169	9	-3	10	132	9	2
-6	198	8	-1	1	445	8	-4	H,K=	13,	17		-1	185	8	9	8	230	7	7
H,K=	12,	32		-1	434	7	-3	9	124	10	4	-3	139	10	1	6	190	7	2
4	370	8	-8	-3	302	6	3	7	277	8	-1	-5	155	9	-3	4	285	6	-10
-0	491	9	-1	-5	353	7	2	5	284	7	-3	-7	172	9	17	2	301	7	6
-2	0	67	-58*	-7	316	7	-4	3	436	8	-2	H,K=	13,	29		-0	205	6	-1
-4	368	8	-6	-9	319	8	-3	1	198	6	-4	5	286	8	0	-2	298	6	8
H,K=	12,	34		-11	213	8	-5	-1	170	6	-8	3	238	8	10	-4	269	6	-3
4	0	57	-37*	H,K=	13,		9	-3	437	8	-1	1	233	8	-8	-6	182	7	-3
2	69	23	16	11	188	9	-11	-5	299	7	4	-1	229	8	-9	-8	193	8	-15
-0	0	48	-25*	9	224	8	-6	-7	266	7	-3	-3	233	8	3	-10	136	10	10
-2	60	19	3	7	290	7	7	-9	90	16	-21	-5	262	9	-11	H,K=	14,		8
H,K=	13,		1	5	314	7	3	H,K=	13,	19		H,K=	13,	31		8	473	8	11
11	238	8	10	3	380	7	6	9	278	8	10	5	149	9	3	6	60	16	19
9	184	7	10	1	424	7	-0	7	287	8	3	3	138	9	-5	4	462	8	-2
7	303	8	-9	-1	426	7	-2	5	361	7	0	1	238	8	-2	2	0	42	-36*
5	289	6	2	-3	366	7	-2	3	344	7	7	-1	230	8	-10	-0	617	10	11
3	347	6	-4	-5	318	7	8	1	312	7	-10	-3	154	14	20	-4	467	8	-7
1	324	6	-1	-7	302	7	-4	-1	336	7	0	-5	161	9	15	-6	65	15	22
-1	314	6	-1	-9	230	8	-3	-3	316	7	-9	H,K=	13,	33		-8	458	8	5
-3	372	7	-3	-11	200	8	5	-5	359	7	-5	3	205	10	9	-10	0	70	-48*

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
H,K=	14,	10		8	189	8	8	-5	350	7	-2	-9	335	8	6	5	175	9	-22
10	113	10	6	6	146	8	-15	-7	305	7	5	H,K=	15,	13		3	187	9	7
8	244	7	-2	4	297	7	4	-9	302	8	2	9	91	19	3	1	221	8	-2
6	308	7	-1	2	286	7	-12	H,K=	15,		3	5	60	25	-11	-1	215	8	-9
4	303	7	-1	-0	249	7	2	9	142	9	2	-1	27	59	-18*	-3	178	8	4
2	187	6	0	-2	288	7	-13	7	103	13	-10	-5	66	18	-5	-5	185	9	-10
-0	344	7	0	-4	295	7	7	5	211	7	-3	H,K=	15,	15		H,K=	15,		27
-2	195	7	2	-6	162	8	-2	3	263	6	5	9	287	8	-10	5	258	8	10
-4	305	7	-8	-8	194	8	7	1	64	16	3	7	302	8	0	3	286	8	3
-6	314	7	-1	H,K=	14,		22	-3	261	7	5	5	347	7	3	1	300	8	-5
-8	225	7	-6	8	209	8	-3	-5	204	7	-6	3	387	7	0	-1	301	8	-9
-10	115	11	6	6	157	11	-2	-7	111	13	4	1	326	7	-6	-3	263	8	-12
H,K=	14,		12	4	252	8	-13	-9	141	10	-5	-1	335	7	-11	-5	259	8	-2
10	183	8	16	2	260	7	13	H,K=	15,		5	-3	385	7	0	H,K=	15,		29
8	350	8	5	-0	249	7	-6	9	240	9	5	-5	376	8	15	3	90	14	41
6	268	7	0	-2	257	7	12	7	357	8	-18	-7	301	8	2	H,K=	15,		31
4	300	7	1	-4	274	7	-5	5	403	8	-0	-9	315	8	6	1	313	8	4
2	243	6	-9	-6	158	8	-0	3	460	8	11	H,K=	15,	17		-1	322	8	12
-0	338	7	-1	-8	205	9	-0	1	497	8	-5	9	182	8	7	H,K=	16,		0
-2	239	7	-7	H,K=	14,		24	-1	513	9	-5	7	237	9	-12	8	94	16	-6
-4	318	7	11	4	385	8	6	-3	469	8	10	5	274	8	4	4	174	9	-13
-6	262	7	5	2	83	11	3	-5	382	7	-2	3	266	7	5	-0	202	57	-19
-8	343	8	-2	-0	417	8	17	-7	380	8	14	1	269	7	2	-4	178	9	14
-10	157	11	-5	-2	64	26	-17	-9	227	8	-2	-1	285	7	6	H,K=	16,		2
H,K=	14,		14	-4	370	8	8	H,K=	15,		7	-3	264	7	4	10	80	20	2
10	272	8	5	H,K=	14,		26	9	156	9	11	-5	261	8	-10	8	380	8	-1
8	79	16	16	4	193	8	-6	7	256	7	-4	-7	259	8	8	6	93	13	-17
6	404	8	3	2	64	47	-11	5	310	7	-2	-9	166	8	-1	4	403	8	8
4	270	7	-2	-0	281	8	-11	3	145	7	15	H,K=	15,	19		2	36	37	-10*
2	328	7	0	-2	94	12	17	1	143	7	1	7	148	8	7	-0	705	12	-7
-0	92	13	2	-4	192	11	-10	-1	149	6	2	5	123	13	3	-4	377	9	14
-2	358	7	10	H,K=	14,		28	-3	132	7	2	3	127	9	-13	-6	99	9	-4
-4	273	6	-2	6	144	9	-11	-5	293	7	-5	1	178	7	-2	-8	386	10	5
-6	417	8	4	4	317	8	3	-7	243	8	-18	-1	199	7	13	-10	70	28	-8
-8	93	11	17	2	125	10	-4	-9	153	8	16	-3	139	8	-7	H,K=	16,		4
-10	273	9	3	-0	300	8	4	H,K=	15,		9	-5	128	9	-4	10	224	8	5
H,K=	14,		16	-2	129	12	-2	9	134	9	-1	-7	143	9	5	8	100	13	-14
10	218	9	3	-4	316	8	4	7	242	7	-5	H,K=	15,	21		6	372	8	-9
8	125	9	6	-6	139	10	-12	5	170	7	10	7	322	8	0	4	199	6	-13
6	248	7	-13	H,K=	14,		30	3	310	7	-7	5	285	7	3	2	389	7	6
4	100	9	-12	4	82	26	-22	1	196	6	-19	3	362	8	-6	-0	80	18	-2
2	418	7	-0	2	269	8	12	-1	235	6	0	1	448	8	9	-2	392	7	5
-0	116	9	6	-2	260	8	3	-3	321	7	-2	-1	443	8	-3	-4	205	11	1
-2	407	7	1	-4	96	24	-4	-5	176	7	6	-3	358	8	-8	-6	394	9	13
-4	117	8	12	H,K=	14,		32	-7	223	8	-5	-5	292	8	3	-8	109	10	-2
-6	265	8	-0	2	243	8	-1	-9	138	9	1	-7	328	8	2	-10	235	10	25
-8	111	9	-5	-0	139	15	-5	H,K=	15,		11	H,K=	15,	23		H,K=	16,		6
-10	212	8	-11	-2	247	8	-1	9	323	8	-6	7	141	9	5	10	152	10	-20
H,K=	14,		18	H,K=	15,		1	7	370	8	2	5	143	9	5	8	169	8	-6
8	160	8	10	9	294	8	11	5	415	8	4	3	200	9	12	6	207	33	-27
6	379	8	12	7	299	7	-2	3	363	7	-4	1	213	7	13	4	277	7	4
2	471	8	6	5	385	7	-1	1	369	7	-3	-1	196	8	0	2	189	7	-19
-2	480	8	8	3	227	8	-7	-1	390	7	9	-3	180	8	9	-0	339	8	-10
-6	369	8	11	1	406	7	5	-3	365	7	-6	-5	145	10	11	-2	184	28	-24
-8	144	12	-3	-1	421	7	5	-5	417	8	9	-7	143	9	7	-4	285	9	15
H,K=	14,		20	-3	244	7	8	-7	373	8	9	H,K=	15,	25		-6	215	10	-8

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL	L	FOB	SG	DEL
-8	166	12	-7	-2	0	43	-27*	-3	274	9	-4	7	159	9	-5	8	123	12	-10
-10	195	10	27	-4	481	8	17	-5	287	11	-8	5	218	8	-2	6	80	14	16
H,K=	16,		8	-6	55	32	17	-7	282	10	-2	3	209	8	14	4	181	9	2
10	378	8	6	-8	375	8	1	-9	234	10	9	1	205	10	-12	2	75	12	41
6	545	9	3	H,K=	16,		20	H,K=	17,		5	-1	226	10	-1	-0	247	10	2
4	65	19	-14	6	241	9	-11	9	185	8	18	-3	181	10	4	-2	43	48	9*
2	529	9	14	4	182	9	-10	7	232	7	22	-5	235	10	26	-4	195	9	14
-2	522	9	5	2	285	8	-6	5	248	7	3	-7	177	13	8	-6	93	16	19
-4	92	15	11	-0	131	11	-15	3	278	7	10	H,K=	17,		17	-8	131	19	-6
-6	552	11	12	-2	285	7	2	1	299	24	9	7	194	8	4	H,K=	18,		4
-8	37	50	-6*	-4	199	7	5	-1	284	9	9	5	189	8	-4	8	44	66	-6*
-10	361	11	3	-6	242	8	-8	-3	274	9	10	3	260	7	2	6	326	8	-16
H,K=	16,		10	H,K=	16,		22	-5	217	11	-12	1	238	9	-8	2	361	8	-8
8	138	9	11	6	157	9	5	-7	223	15	7	-1	238	10	-1	-2	365	9	-4
6	142	9	-24	4	185	8	12	-9	180	12	-1	-3	250	10	3	-4	63	13	48
4	182	7	-5	2	221	8	-4	H,K=	17,		7	-5	200	11	6	-6	360	10	12
2	277	6	-22	-0	229	8	-6	9	223	8	-6	-7	193	12	-11	H,K=	18,		6
-0	146	7	-0	-2	217	8	-5	7	266	8	-22	H,K=	17,		19	8	302	9	-14
-2	276	29	-20	-4	186	9	3	5	305	8	-14	7	236	8	-11	6	56	36	-23
-4	177	12	-8	-6	173	11	10	3	401	8	-10	5	249	8	-7	4	548	9	-15
-6	187	11	11	H,K=	16,		24	1	306	7	-11	3	279	31	-12	-0	539	11	11
-8	117	14	5	6	344	8	2	-1	320	9	8	1	215	10	1	-2	0	46	-57*
H,K=	16,		12	4	47	60	35*	-3	419	9	20	-1	229	10	15	-4	562	11	3
8	102	12	-13	2	370	9	5	-5	330	10	-0	-3	295	10	12	-6	89	24	9
6	306	8	4	-2	390	8	16	-7	299	10	2	-5	279	10	19	-8	347	10	21
4	158	7	-20	-6	338	8	5	-9	230	11	7	-7	259	11	15	H,K=	18,		8
2	340	7	18	H,K=	16,		26	H,K=	17,		9	H,K=	17,		21	8	83	20	77
-0	190	6	-4	2	218	8	6	9	181	12	-3	5	182	9	8	4	112	14	54
-2	346	7	17	-0	150	8	-3	7	191	8	4	3	147	12	15	2	79	16	13
-4	164	11	13	-2	240	8	14	5	283	8	-8	1	203	11	-6	-2	54	26	-14
-6	315	8	13	-4	70	16	1	3	327	7	-3	-1	197	11	-6	-4	0	51	-49*
-8	133	12	14	H,K=	16,		28	1	337	9	-0	-3	139	12	1	-6	0	49	-23*
H,K=	16,		14	4	95	18	34	-1	316	10	-7	-5	155	18	-11	H,K=	18,		10
8	343	8	-6	2	285	8	-6	-3	334	10	-3	H,K=	17,		23	8	342	8	-11
6	120	11	-3	-0	121	26	1	-5	298	10	15	5	226	8	-14	6	46	49	13*
4	386	9	-11	-2	297	8	4	-7	190	10	9	3	207	9	6	4	459	9	-24
2	184	7	3	H,K=	16,		30	-9	174	13	-7	1	253	10	11	-0	560	11	22
-0	417	8	11	-0	259	8	5	H,K=	17,		11	-1	258	10	-1	-4	497	10	17
-2	170	7	-8	H,K=	17,		1	7	153	10	-1	-3	212	11	-2	-8	358	13	2
-4	416	8	8	9	190	8	-0	5	288	8	-2	-5	244	17	10	H,K=	18,		12
-6	144	8	10	7	182	7	15	3	246	8	7	H,K=	17,		25	6	202	8	-0
-8	346	8	-0	5	220	7	0	1	211	9	6	3	162	9	2	4	92	19	44
H,K=	16,		16	3	266	7	0	-1	229	9	6	1	228	11	-9	2	392	9	-19
8	112	11	-20	1	337	7	13	-3	244	10	-10	-1	237	11	-2	-2	418	10	17
6	28	53	-18*	-1	322	8	4	-5	300	10	6	-3	162	15	-6	-6	183	12	-21
4	237	8	-8	-3	302	9	19	-7	172	12	10	H,K=	17,		27	H,K=	18,		14
-0	193	7	-13	-5	248	10	17	H,K=	17,		13	3	62	43	-18	6	117	9	35
-4	249	7	1	-7	169	18	-5	7	179	8	-13	1	144	12	21	4	239	7	-10
-6	54	56	-1*	-9	181	13	-2	5	214	45	-4	-1	124	16	-1	2	38	48	8*
-8	113	16	-16	H,K=	17,		3	3	233	7	-9	-3	86	16	3	-0	161	10	-7
H,K=	16,		18	9	209	45	-17	1	385	9	0	H,K=	18,		0	-2	0	49	-39*
8	366	8	-4	7	272	8	-10	-1	370	9	-4	6	440	26	-19	-4	272	10	27
6	32	48	-16*	5	293	33	-7	-3	244	10	6	2	537	9	-31	-6	108	15	20
4	473	8	8	3	253	7	-25	-5	224	11	12	-2	593	12	5	H,K=	18,		16
2	70	15	34	1	353	7	-16	-7	183	11	-5	-6	457	12	5	6	358	37	-20
-0	509	9	-6	-1	359	9	3	H,K=	17,		15	H,K=	18,		2	4	43	51	-34*

STRUCTURE FACTORS CONTINUED FOR
NAGD(EDTA).8H2O

L	FOB	SG	DEL
2	397	8	-23
-2	410	10	-1
-4	55	70	-21*
-6	380	11	10
H,K=	18,	18	
6	89	22	35
4	85	17	3
2	89	14	28
-0	168	12	-2
-2	74	16	17
H,K=	18,	20	
2	280	10	-5
-0	92	19	-15
-2	286	12	-4
-4	29	42	-40*
H,K=	18,	22	
4	296	8	-2
2	57	18	13
-0	405	12	-4
-4	297	11	3
H,K=	18,	24	
-0	60	22	3
H,K=	18,	26	
-0	345	11	16
H,K=	19,	1	
7	170	10	-14
5	195	8	-2
3	164	8	1
1	222	7	-17
-1	215	9	-8
-3	180	11	12
-5	186	10	-5
-7	190	12	10
H,K=	19,	3	
7	263	8	8
5	258	8	7
3	278	8	-11
1	312	7	13
-1	318	10	15
-3	291	10	0
-5	245	10	-4
-7	258	10	4
H,K=	19,	5	
7	124	9	3
5	117	13	1
3	187	33	-8
1	170	8	-18
-1	187	10	-4
-3	211	10	14
-5	124	14	2
H,K=	19,	7	
7	235	8	-0
5	190	12	3
3	307	7	-4
1	340	11	3
-1	339	10	6

L	FOB	SG	DEL
-3	299	10	-3
-5	199	13	-7
-7	237	11	1
H,K=	19,	9	
7	201	8	0
5	253	8	-12
3	251	8	-10
1	251	10	-5
-1	272	9	23
-3	268	10	14
-5	275	10	22
-7	209	11	10
H,K=	19,	11	
7	133	9	-7
5	111	10	-7
3	169	8	-14
1	209	11	7
-1	200	12	-1
-3	180	11	-1
-5	116	10	-7
-7	145	17	9
H,K=	19,	13	
5	340	8	6
3	287	8	-2
1	307	10	19
-1	292	10	8
-3	269	10	-18
-5	341	10	9
H,K=	19,	15	
5	123	13	-15
3	88	20	2
1	183	15	12
-1	198	10	16
-3	101	10	4
-5	133	21	4
H,K=	19,	17	
5	232	8	-6
3	221	8	-3
1	180	8	-0
-1	184	12	-4
-3	232	10	6
-5	266	10	25
H,K=	19,	19	
3	190	9	-10
1	300	10	12
-1	294	11	-6
-3	189	11	-4
H,K=	19,	21	
3	76	15	-33
1	125	12	7
-1	124	13	5
-3	117	15	16
H,K=	19,	23	
1	216	14	-25
-1	234	12	-8
H,K=	20,	0	

L	FOB	SG	DEL
4	219	8	8
-0	204	9	17
-4	204	10	9
H,K=	20,	2	
6	87	23	39
4	265	8	-30
2	133	12	13
-0	361	10	23
-2	107	15	-20
-4	291	10	-3
H,K=	20,	4	
6	181	8	1
4	131	11	-6
2	220	32	-14
-0	253	10	-5
-2	228	15	-0
-4	111	17	-10
-6	191	11	10
H,K=	20,	6	
6	238	8	14
4	140	8	6
2	234	7	3
-0	255	10	11
-2	221	11	-15
-4	140	12	13
-6	235	11	13
H,K=	20,	8	
6	281	33	-32
4	0	51	-40*
2	310	30	-30
-0	89	12	-6
-2	326	11	-18
-4	0	59	-43*
-6	315	11	0
H,K=	20,	10	
6	255	8	12
4	133	10	-15
2	284	7	23
-2	273	11	11
-4	145	12	-8
-6	243	11	1
H,K=	20,	12	
4	108	13	-10
2	247	8	-19
-0	191	8	3
-2	278	10	7
-4	127	12	20
H,K=	20,	14	
4	288	37	-10
2	175	10	25
-0	227	10	-14
-2	169	11	19
-4	328	10	23
H,K=	20,	16	
4	209	9	8
-0	249	10	13

L	FOB	SG	DEL
-2	41	44	-21*
-4	197	11	5
H,K=	20,	18	
2	48	51	-1*
-0	303	11	-1
-2	27	58	-22*
H,K=	20,	20	
2	195	11	14
-0	195	12	-2
-2	184	11	7
H,K=	21,	1	
5	167	8	0
3	246	8	4
1	249	10	-1
-1	254	12	9
-3	262	10	22
-5	192	11	14
H,K=	21,	3	
5	77	21	16
3	129	21	36
1	129	9	8
-1	113	14	-8
-5	65	24	8
H,K=	21,	5	
5	240	9	-19
3	271	8	-22
1	268	10	11
-1	266	10	9
-3	263	10	-19
-5	269	11	3
H,K=	21,	7	
5	208	8	-2
3	129	10	-19
1	129	12	5
-1	147	10	10
-3	146	14	-12
-5	231	11	14
H,K=	21,	9	
5	202	8	-10
3	176	8	-16
1	184	11	-11
-1	206	11	-5
-3	206	11	4
-5	206	11	-7
H,K=	21,	11	
3	248	8	-15
1	243	11	-9
-1	259	10	7
-3	271	11	4
H,K=	21,	13	
3	45	51	35*
1	73	17	25
-1	83	12	37
-3	57	57	37*
H,K=	21,	15	
3	278	11	7

L	FOB	SG	DEL
1	203	12	-16
-1	216	11	2
-3	275	11	9
H,K=	21,	17	
1	189	11	0
-1	189	12	-8
H,K=	22,	0	
2	140	12	16
-2	91	13	-33
H,K=	22,	2	
2	353	10	1
-2	374	10	21
-4	81	18	35
H,K=	22,	4	
4	305	12	19
2	128	12	11
-0	222	11	4
-2	112	12	-11
-4	298	11	9
H,K=	22,	6	
2	149	16	7
-0	89	19	-5
-2	160	15	18
H,K=	22,	8	
2	0	61	-26*
-0	369	11	9
H,K=	22,	10	
2	113	16	-1
-0	0	49	-76*
-2	117	16	-4
H,K=	22,	12	
-0	229	9	3

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.

TECHNICAL INFORMATION DEPARTMENT
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720