Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1998, 37(14), 3542-3547, DOI:10.1021/ic971602v

EXPERIMENTAL

DATA COLLECTION

A colorless thick-plate crystal of $EuC_{40}H_{26}O_6N_2F_9$ having approximate dimensions of 0.600 X 0.450 X 0.200 mm was mounted on a glass fiber. All measurements were made on an Enraf-Nonius CAD-4 diffractometer with graphite monochromated Mo Kα radiation.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 22 carefully centered reflections in the range $22.58 < 2\theta < 42.24°$ corresponded to a monoclinic cell with dimensions:

$a = 11.122\ (5)$Å
$b = 22.860\ (8)$Å
$c = 15.870\ (6)$Å
$\beta = 102.62\ (3)°$
$V = 3937\ (5)$Å^3

For $Z = 4$ and F.W. = 953.60, the calculated density is 1.609 g/cm^3. Based on the systematic absences of:

h0l: $h+l \neq 2n$
0k0: $k \neq 2n$

and the successful solution and refinement of the structure, the space group was determined to be:

$P2_1/n$ (#14)

The data were collected at a temperature of 24 ± 1°C using the ω scan technique to a maximum 2θ value of 50.0°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.00° with a take-off angle of 2.8°. Scans of (0.60 + 0.35 tan θ)° were made at a speed of 8.2°/min (in omega). Moving-crystal moving counter background measurements were made by scanning an additional 25% above and below the scan range. The counter aperture consisted of a variable horizontal slit with a width ranging from 2.0 to 2.5 mm and a vertical slit set to 2.0 mm. The diameter of the incident beam collimator was 0.7 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector.

DATA REDUCTION

Of the 9838 reflections which were collected, 7120 were unique (R_{int} = .033); equivalent reflections were merged. The intensities of three representative reflections which were measured after every 80 minutes of X-ray exposure time remained constant throughout data collection indicating crystal and electronic stability (no decay correction was applied).

The linear absorption coefficient for Mo Kα is 16.8 cm^{-1}. An empirical absorption correction, based on azimuthal scans of several reflections, was applied which resulted in transmission factors ranging from 0.73 to 1.00. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction was applied (coefficient = 0.10470E-07).

STRUCTURE SOLUTION AND REFINEMENT

The structure was solved by direct methods[2]. The non-hydrogen atoms were refined either anisotropically or isotropically. The final cycle of full-matrix least-squares refinement[3] was based on 4914 observed reflections ($I > 2.00\sigma(I)$) and 485 variable parameters and converged (largest parameter shift was 0.06 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma \; ||Fo| - |Fc|| \; / \; \Sigma \; |Fo| = 0.052$$

$$R_w = [(\Sigma \; w \; (|Fo| - |Fc|)^2 \; / \; \Sigma \; w \; Fo^2 \;)]^{1/2} = 0.052$$

The standard deviation of an observation of unit weight[4] was 1.70. The weighting scheme was based on counting statistics and included a factor (p = 0.03) to downweight the intense reflections. Plots of $\Sigma \; w \; (|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, $\sin \theta/\lambda$, and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.99 and -0.73 $e^-/Å^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5]. Anomalous dispersion effects were included in Fcalc[6]; the values for $\Delta f'$ and $\Delta f''$ were those of Cromer[7]. All calculations were performed using the TEXSAN[8] crystallographic software package of Molecular Structure Corporation.

3

References

(1) ORTEP:
Johnson,C.K.; ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Oak Ridge, Tennessee (1976).

(2) Structure Solution Methods:
MITHRIL
Gilmore,C.J.; MITHRIL - an integrated direct methods computer program. J. Appl. Cryst. 17, 42-46, Univ. of Glasgow, Scotland, (1984).
DIRDIF
Beurskens,P.T.; DIRDIF: Direct Methods for Difference Structures - an automatic procedure for phase extension and refinement of difference structure factors. Technical Report 1984/1 Crystallography Laboratory, Toernooiveld, 6525 Ed Nijmegen, Netherlands.

(3) Least-Squares:
Function minimized: $\Sigma\, w\, (|Fo| - |Fc|)^2$
where: $w = 4Fo^2/\sigma^2(Fo^2)$
$\sigma^2(Fo^2) = [S^2(C+R^2B) + (pFo^2)^2]/Lp^2$
S = Scan rate
C = Total Integrated Peak Count
R = Ratio of Scan Time to background counting time.
B = Total Background Count
Lp = Lorentz-polarization factor
p = p-factor

(4) Standard deviation of an observation of unit weight:

$$[\Sigma\, w(|Fo| - |Fc|)^2/(No - Nv)]^{1/2}$$

where: No = number of observations
Nv = number of variables

(5) Cromer,D.T. & Waber,J.T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers,J.A. & Hamilton,W.C.; Acta Crystallogr., 17, 781 (1964).

(7) D.T. Cromer, "International Tables for X-ray Crystallography", Vol/ IV, The Kynoch Press, Birmingham, England, Table 2.3.1 (1974).

(8) TEXSAN - TEXRAY Structure Analysis Package, Molecular Structure Corporation (1985).

4

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$EuC_{40}H_{26}O_6N_2F_9$
Formula Weight	953.60
Crystal Color, Habit	colorless, thick-plate
Crystal Dimensions (mm)	0.600 X 0.450 X 0.200
Crystal System	monoclinic
No. Reflections Used for Unit Cell Determination (2θ range)	22 (22.6 - 42.2°)
Omega Scan Peak Width at Half-height	0.00
Lattice Parameters:	a = 11.122 (5)Å b = 22.860 (8)Å c = 15.870 (6)Å β = 102.62 (3)° V = 3937 (5)Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.609 g/cm^3
F_{000}	1888
$\mu_{(MoK\alpha)}$	16.81 cm^{-1}

B. Intensity Measurements

Diffractometer	Enraf-Nonius CAD-4
Radiation	MoKα (λ = 0.71069 Å)
Temperature	24°C
Attenuator	Zr foil, (factor = 17.8)
Take-off Angle	2.8°

Detector Aperture	2.0 - 2.5 mm horizontal 2.0 mm vertical
Crystal to Detector Distance	21 cm
Scan Type	ω
Scan Rate	8.2°/min (in omega)
Scan Width	$(0.60 + 0.35 \tan\theta)°$
$2\theta_{max}$	50.0°
No. of Reflections Measured	Total: 9838 Unique: 7120 (R_{int} = .033)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.73 - 1.00) Secondary Extinction (coefficient: 0.10470E-07)

C. Structure Solution and Refinement

Structure Solution	Direct Methods
Refinement	Full-matrix least-squares
Function Minimized	Σ w $(\|Fo\| - \|Fc\|)^2$
Least-squares Weights	$4Fo^2/\sigma^2(Fo^2)$
p-factor	0.03
Anomalous Dispersion	All non-hydrogen atoms
No. Observations ($I>2.00\sigma(I)$)	4914
No. Variables	485
Reflection/Parameter Ratio	10.13
Residuals: R; R_w	0.052; 0.052
Goodness of Fit Indicator	1.70
Max Shift/Error in Final Cycle	0.06
Maximum Peak in Final Diff. Map	0.99 $e^-/Å^3$
Minimum Peak in Final Diff. Map	-0.73 $e^-/Å^3$

Positional parameters and B(eq) for [17,22] Eu(BTA)3/bipyridyl 2 4 deg

atom	x	y	z	B(eq)
EU	0.22770(3)	0.09610(2)	0.20107(2)	3.90(2)
O1A	0.1862(4)	0.0368(2)	0.3138(3)	5.3(2)
O2A	0.4074(4)	0.0445(2)	0.2649(3)	5.0(2)
O1B	0.1287(4)	0.1679(2)	0.0989(3)	4.7(2)
O2B	0.3129(5)	0.0912(2)	0.0783(3)	4.9(2)
O1C	0.3763(4)	0.1720(2)	0.2220(3)	4.8(2)
O2C	0.1662(5)	0.1666(2)	0.2881(3)	5.5(3)
N1D	-0.0041(5)	0.0698(3)	0.1659(4)	4.4(3)
N12D	0.1647(5)	-0.0029(2)	0.1268(3)	4.0(3)
C1A	0.2295(7)	-0.0085(4)	0.3545(5)	5.2(4)
C2A	0.4292(7)	0.0024(3)	0.3174(5)	5.2(4)
C3A	0.3519(8)	-0.0261(4)	0.3592(5)	5.9(4)
C4A	0.1455(8)	-0.0425(4)	0.3961(5)	5.9(4)
C5A	0.0239(9)	-0.0253(4)	0.3864(6)	6.8(5)
C6A	-0.056(1)	-0.0566(6)	0.4255(7)	9.1(7)
C7A	-0.016(1)	-0.1048(6)	0.4723(9)	10.8(8)
C8A	0.099(1)	-0.1216(7)	0.480(1)	13(1)
C9A	0.181(1)	-0.0921(5)	0.4450(8)	9.8(6)
C10A	0.566(1)	-0.0203(4)	0.3283(7)	8.7(6)
C1B	0.1607(7)	0.1973(3)	0.0410(5)	4.7(3)
C2B	0.3260(7)	0.1300(4)	0.0259(5)	4.6(4)
C3B	0.2607(8)	0.1815(4)	0.0051(5)	5.6(4)
C4B	0.0893(7)	0.2514(3)	0.0124(5)	4.9(4)
C5B	0.1094(8)	0.2861(4)	-0.0543(5)	6.3(4)

Positional parameters and B(eq) for [17,22] Eu(BTA)3/bipyridyl . 4 deg

atom	x	y	z	B(eq)
C6B	0.037(1)	0.3367(4)	-0.0793(6)	7.6(5)
C7B	-0.052(1)	0.3511(4)	-0.0380(7)	8.0(6)
C8B	-0.074(1)	0.3168(4)	0.0261(7)	9.0(6)
C9B	-0.005(1)	0.2677(4)	0.0517(6)	7.0(5)
C10B	0.4301(8)	0.1166(4)	-0.0225(6)	6.6(5)
C1C	0.3780(7)	0.2248(3)	0.2409(5)	4.8(4)
C2C	0.1903(8)	0.2199(4)	0.2955(5)	5.9(4)
C3C	0.2827(8)	0.2515(4)	0.2741(6)	6.5(5)
C4C	0.4900(7)	0.2588(3)	0.2317(5)	5.2(4)
C5C	0.510(1)	0.3166(4)	0.2587(6)	7.1(5)
C6C	0.618(1)	0.3447(4)	0.2524(7)	8.5(6)
C7C	0.703(1)	0.3157(5)	0.2174(7)	8.7(7)
C8C	0.682(1)	0.2606(5)	0.1889(8)	9.3(6)
C9C	0.5748(8)	0.2323(4)	0.1945(7)	7.9(5)
C10C	0.096(1)	0.2553(4)	0.3390(8)	9.2(6)
C2D	-0.0826(8)	0.1058(4)	0.1902(6)	6.2(4)
C3D	-0.2062(8)	0.0924(4)	0.1827(6)	6.3(4)
C4D	-0.2491(7)	0.0399(4)	0.1492(6)	6.5(5)
C5D	-0.1662(7)	0.0013(3)	0.1240(5)	5.4(4)
C6D	-0.0449(6)	0.0169(3)	0.1334(4)	4.2(3)
C7D	0.0485(6)	-0.0224(3)	0.1092(4)	3.8(3)
C8D	0.0174(7)	-0.0760(3)	0.0708(5)	5.3(4)
C9D	0.1093(8)	-0.1108(3)	0.0521(5)	5.7(4)
C10D	0.2262(8)	-0.0910(3)	0.0692(5)	5.3(4)
C11D	0.2521(7)	-0.0371(3)	0.1063(5)	4.9(4)

Positional parameters and B(eq) for [17,22] Eu(BTA)3/bipyridyl 4 deg

atom	x	y	z	B(eq)
H1	0.3820	-0.0593	0.3932	7.4
H2	-0.0053	0.0081	0.3526	8.5
H3	-0.1385	-0.0441	0.4195	11.3
H4	-0.0699	-0.1263	0.4993	13.3
H5	0.1249	-0.1561	0.5124	16.4
H6	0.2637	-0.1057	0.4536	12.0
H7	0.2845	0.2072	-0.0353	7.1
H8	0.1722	0.2759	-0.0838	7.5
H9	0.0521	0.3605	-0.1250	8.9
H10	-0.1002	0.3853	-0.0542	9.4
H11	-0.1384	0.3268	0.0541	11.3
H12	-0.0216	0.2445	0.0975	8.7
H13	0.2837	0.2927	0.2817	8.1
H14	0.4495	0.3368	0.2815	9.1
H15	0.6322	0.3838	0.2721	10.9
H16	0.7780	0.3347	0.2137	10.9
H17	0.7420	0.2409	0.1646	12.0
H18	0.5599	0.1938	0.1722	9.9
H19	-0.0534	0.1426	0.2139	7.7
H20	-0.2601	0.1195	0.2007	8.0
H21	-0.3334	0.0296	0.1430	8.2
H22	-0.1938	-0.0357	0.1003	6.6
H23	-0.0660	-0.0888	0.0575	6.5
H24	0.0904	-0.1484	0.0274	7.0
H25	0.2902	-0.1142	0.0555	6.6

4 deg Positional parameters and B(eq) for [17,22] Eu(BTA)3/bipyridyl 2

atom	x	y	z	B(eq)
H26	0.3348	-0.0234	0.1181	6.2
F11A	0.5969(8)	-0.0577(3)	0.3887(4)	8.9(1)
F12A	0.5826(7)	-0.0409(3)	0.2543(4)	8.9(1)
F13A	0.6411(8)	0.0270(2)	0.3468(5)	8.9(1)
F14A	0.641(2)	0.0117(7)	0.306(1)	8.3(3)
F15A	0.612(2)	-0.0238(8)	0.4244(8)	8.3(3)
F16A	0.567(2)	-0.0746(7)	0.309(1)	8.3(3)
F11B	0.4548(8)	0.0583(2)	-0.0241(5)	8.3(1)
F12B	0.4050(7)	0.1334(3)	-0.1047(4)	8.3(1)
F13B	0.5335(7)	0.1418(3)	0.0165(4)	8.3(1)
F14B	0.455(1)	0.1654(5)	-0.064(1)	7.9(2)
F15B	0.533(1)	0.1068(6)	0.0383(7)	7.9(2)
F16B	0.406(1)	0.0747(6)	-0.0731(9)	7.9(2)
F14C	0.122(1)	0.3068(6)	0.352(1)	8.9(2)
F15C	-0.017(1)	0.2512(6)	0.2781(7)	8.9(2)
F16C	0.075(1)	0.2264(6)	0.4058(7)	8.9(2)
F11C	-0.0086(8)	0.2316(4)	0.3269(6)	9.4(2)
F12C	0.1451(8)	0.2646(4)	0.4201(4)	9.4(2)
F13C	0.0790(9)	0.3111(4)	0.3021(5)	9.4(2)

U values for [17,22] Eu(BTA)3/bipyridyl 24 deg

ATOM	U11	U22	U33	U12	U13	U23
EU	0.0451(2)	0.0426(2)	0.0593(2)	0.0004(2)	0.0089(2)	0.0003(2)
O1A	0.060(3)	0.075(4)	0.067(3)	0.012(3)	0.016(3)	0.019(3)
O2A	0.046(3)	0.064(3)	0.076(3)	0.004(3)	0.008(3)	0.012(3)
O1B	0.055(3)	0.051(3)	0.072(3)	-0.001(2)	0.010(3)	0.007(3)
O2B	0.068(3)	0.051(3)	0.071(3)	-0.003(3)	0.025(3)	0.004(3)
O1C	0.052(3)	0.046(3)	0.081(4)	-0.002(2)	0.006(3)	-0.009(3)
O2C	0.071(4)	0.065(4)	0.075(4)	-0.003(3)	0.022(3)	-0.020(3)
N1D	0.047(4)	0.057(4)	0.063(4)	0.006(3)	0.013(3)	0.000(3)
N12D	0.044(4)	0.047(3)	0.060(4)	-0.006(3)	0.010(3)	0.000(3)
C1A	0.060(5)	0.072(5)	0.062(5)	-0.001(5)	0.004(4)	0.010(4)
C2A	0.052(5)	0.064(5)	0.074(5)	0.002(4)	-0.001(4)	0.007(4)
C3A	0.064(6)	0.076(6)	0.087(6)	0.013(5)	0.019(5)	0.032(5)
C4A	0.059(6)	0.082(6)	0.077(6)	-0.002(5)	0.002(5)	0.022(5)
C5A	0.069(6)	0.107(7)	0.086(6)	-0.006(6)	0.020(5)	0.018(6)
C6A	0.069(7)	0.17(1)	0.114(9)	-0.022(8)	0.023(6)	0.025(8)
C7A	0.09(1)	0.18(1)	0.15(1)	-0.03(1)	0.029(8)	0.06(1)
C8A	0.09(1)	0.19(1)	0.21(2)	-0.01(1)	0.02(1)	0.13(1)

U values for [17,22] Eu(BTA)3/bipyridyl 24 deg

ATOM	U11	U22	U33	U12	U13	U23
C9A	0.067(6)	0.13(1)	0.17(1)	0.015(7)	0.022(7)	0.072(9)
C10A	0.110(8)	0.090(8)	0.12(1)	-0.000(6)	0.008(7)	0.079(7)
C1B	0.052(5)	0.044(4)	0.074(5)	-0.011(4)	-0.008(4)	0.002(4)
C2B	0.045(4)	0.070(5)	0.062(5)	-0.009(4)	0.012(4)	-0.002(4)
C3B	0.063(5)	0.066(5)	0.087(6)	-0.008(5)	0.026(5)	0.011(5)
C4B	0.062(5)	0.053(5)	0.065(5)	-0.011(4)	-0.002(4)	-0.002(4)
C5B	0.079(6)	0.064(5)	0.085(6)	-0.007(5)	-0.006(5)	0.017(5)
C6B	0.13(1)	0.063(6)	0.082(7)	-0.001(6)	-0.009(6)	0.013(5)
C7B	0.13(1)	0.063(6)	0.089(8)	0.020(7)	-0.015(7)	0.001(6)
C8B	0.15(1)	0.076(7)	0.114(9)	0.049(7)	0.034(8)	0.016(6)
C9B	0.106(8)	0.069(6)	0.089(7)	0.014(6)	0.014(6)	0.008(5)
C10B	0.083(7)	0.080(6)	0.085(6)	-0.015(5)	0.013(6)	0.002(5)
C1C	0.058(5)	0.055(5)	0.063(5)	-0.006(4)	0.003(4)	-0.005(4)
C2C	0.061(6)	0.072(6)	0.087(6)	0.008(5)	0.009(5)	-0.031(5)
C3C	0.067(6)	0.057(5)	0.124(8)	-0.006(5)	0.024(6)	-0.028(5)
C4C	0.061(5)	0.056(5)	0.074(5)	-0.001(4)	0.006(4)	-0.003(4)
C5C	0.114(8)	0.066(6)	0.098(7)	-0.028(6)	0.040(6)	-0.022(5)
C6C	0.13(1)	0.086(7)	0.117(8)	-0.063(7)	0.050(7)	-0.031(6)

U values for [17,22] Eu(BTA)3/bipyridyl 24 deg

ATOM	U11	U22	U33	U12	U13	U23
C7C	0.100(9)	0.102(9)	0.13(1)	-0.043(7)	0.034(7)	-0.007(7)
C8C	0.084(7)	0.078(7)	0.20(1)	-0.022(6)	0.056(8)	-0.028(7)
C9C	0.063(6)	0.061(6)	0.18(1)	-0.008(5)	0.027(7)	-0.014(6)
C10C	0.089(8)	0.071(7)	0.18(1)	-0.037(6)	0.023(8)	-0.029(8)
C2D	0.058(5)	0.072(6)	0.107(7)	0.001(5)	0.018(5)	-0.008(5)
C3D	0.058(5)	0.081(6)	0.106(7)	0.013(5)	0.028(5)	-0.003(6)
C4D	0.049(5)	0.087(7)	0.115(7)	-0.005(5)	0.025(5)	0.002(6)
C5D	0.047(5)	0.061(5)	0.094(6)	-0.007(4)	0.013(4)	0.008(4)
C6D	0.043(4)	0.052(4)	0.061(5)	0.001(4)	0.005(4)	0.010(4)
C7D	0.051(5)	0.043(4)	0.051(4)	-0.004(3)	0.009(4)	0.008(3)
C8D	0.059(5)	0.058(5)	0.083(6)	-0.015(4)	0.010(4)	-0.000(4)
C9D	0.074(6)	0.051(5)	0.089(6)	-0.007(4)	0.016(5)	-0.009(4)
C10D	0.070(5)	0.055(5)	0.076(5)	0.004(4)	0.017(4)	-0.003(4)
C11D	0.050(5)	0.054(5)	0.085(6)	0.000(4)	0.018(4)	-0.002(4)
H1	0.0938					
H2	0.1078					
H3	0.1433					
H4	0.1682					

U values for [17,22] Eu(BTA)3/bipyridyl 24 deg

ATOM	U11	U22	U33	U12	U13	U23
H5	0.2082					
H6	0.1520					
H7	0.0893					
H8	0.0944					
H9	0.1131					
H10	0.1186					
H11	0.1431					
H12	0.1097					
H13	0.1030					
H14	0.1158					
H15	0.1383					
H16	0.1384					
H17	0.1520					
H18	0.1257					
H19	0.0981					
H20	0.1010					
H21	0.1040					
H22	0.0838					

U values for [17,22] Eu(BTA)3/bipyridyl 24 deg

ATOM	U11	U22	U33	U12	U13	U23
H23	0.0827					
H24	0.0888					
H25	0.0832					
H26	0.0782					
F11A	0.113(2)					
F12A	0.113(2)					
F13A	0.113(2)					
F14A	0.105(4)					
F15A	0.105(4)					
F16A	0.105(4)					
F11B	0.106(2)					
F12B	0.106(2)					
F13B	0.106(2)					
F14B	0.100(3)					
F15B	0.100(3)					
F16B	0.100(3)					
F14C	0.113(3)					
F15C	0.113(3)					

U values for [17,22] Eu(BTA)3/bipyridyl 24 deg

ATOM	U11	U22	U33	U12	U13	U23
F16C	0.113(3)					
F11C	0.119(2)					
F12C	0.119(2)					
F13C	0.119(2)					

Intramolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	atom	atom	distance
EU	O1A	2.369(5)	C7A	C8A	1.31(2)
EU	O2A	2.351(5)	C8A	C9A	1.36(2)
EU	O1B	2.399(5)	C10A	F11A	1.27(1)
EU	O2B	2.349(6)	C10A	F12A	1.32(1)
EU	O1C	2.369(5)	C10A	F13A	1.36(1)
EU	O2C	2.321(5)	C10A	F14A	1.22(2)
EU	N1D	2.586(6)	C10A	F15A	1.50(2)
EU	N12D	2.577(5)	C10A	F16A	1.28(2)
O1A	C1A	1.259(9)	C1B	C3B	1.40(1)
O2A	C2A	1.264(9)	C1B	C4B	1.49(1)
O1B	C1B	1.25(1)	C2B	C3B	1.39(1)
O2B	C2B	1.25(1)	C2B	C10B	1.55(1)
O1C	C1C	1.243(9)	C4B	C5B	1.38(1)
O2C	C2C	1.25(1)	C4B	C9B	1.38(1)
N1D	C2D	1.32(1)	C5B	C6B	1.41(1)
N1D	C6D	1.353(9)	C6B	C7B	1.35(2)
N12D	C7D	1.338(9)	C7B	C8B	1.35(2)
N12D	C11D	1.34(1)	C8B	C9B	1.37(1)
C1A	C3A	1.41(1)	C10B	F11B	1.36(1)
C1A	C4A	1.48(1)	C10B	F12B	1.33(1)
C2A	C3A	1.36(1)	C10B	F13B	1.31(1)
C2A	C10A	1.58(1)	C10B	F14B	1.35(2)
C4A	C5A	1.38(1)	C10B	F15B	1.35(2)
C4A	C9A	1.38(1)	C10B	F16B	1.24(2)
C5A	C6A	1.39(2)	C1C	C3C	1.42(1)
C6A	C7A	1.35(2)	C1C	C4C	1.50(1)

Distances are in angstroms. Estimated standard deviations in the least significant figures are given in parentheses.

Intramolecular Distances Involving the Nonhydrogen Atoms (cont)

atom	atom	distance
C2C	C3C	1.36(1)
C2C	C10C	1.60(2)
C4C	C5C	1.39(1)
C4C	C9C	1.36(1)
C5C	C6C	1.38(2)
C6C	C7C	1.38(2)
C7C	C8C	1.34(2)
C8C	C9C	1.38(1)
C10C	F14C	1.22(2)
C10C	F15C	1.41(2)
C10C	F16C	1.31(2)
C10C	F11C	1.26(1)
C10C	F12C	1.30(1)
C10C	F13C	1.40(1)
C2D	C3D	1.39(1)
C3D	C4D	1.36(1)
C4D	C5D	1.40(1)
C5D	C6D	1.37(1)
C6D	C7D	1.49(1)
C7D	C8D	1.38(1)
C8D	C9D	1.38(1)
C9D	C10D	1.35(1)
C10D	C11D	1.37(1)
F11A	F15A	0.95(2)
F11A	F16A	1.30(2)
F12A	F14A	1.52(2)
F12A	F16A	1.20(2)
F13A	F14A	0.74(2)
F11B	F15B	1.61(1)
F11B	F16B	0.92(1)
F12B	F14B	1.05(1)
F12B	F16B	1.43(2)
F13B	F14B	1.49(1)
F13B	F15B	0.87(2)
F14C	F12C	1.43(2)
F14C	F13C	0.83(2)
F15C	F11C	0.88(2)
F15C	F13C	1.73(2)
F16C	F11C	1.39(1)
F16C	F12C	1.16(2)

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Hydrogen Atoms

atom	atom	distance	atom	atom	distance
C3A	H1	0.950	C5C	H14	0.949
C5A	H2	0.950	C6C	H15	0.949
C6A	H3	0.948	C7C	H16	0.950
C7A	H4	0.950	C8C	H17	0.950
C8A	H5	0.948	C9C	H18	0.949
C9A	H6	0.949	C2D	H19	0.950
C3B	H7	0.950	C3D	H20	0.949
C5B	H8	0.951	C4D	H21	0.950
C6B	H9	0.951	C5D	H22	0.950
C7B	H10	0.951	C8D	H23	0.950
C8B	H11	0.949	C9D	H24	0.950
C9B	H12	0.951	C10D	H25	0.950
C3C	H13	0.950	C11D	H26	0.950

Distances are in angstroms. Estimated standard deviations in the least significant figures are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
O1A	EU	O2A	71.1(2)	O2C	EU	N12D	142.7(2)
O1A	EU	O1B	140.0(2)	N1D	EU	N12D	62.5(2)
O1A	EU	O2B	141.3(2)	EU	O1A	C1A	137.9(5)
O1A	EU	O1C	123.9(2)	EU	O2A	C2A	133.6(5)
O1A	EU	O2C	79.4(2)	EU	O1B	C1B	134.6(5)
O1A	EU	N1D	71.3(2)	EU	O2B	C2B	130.3(5)
O1A	EU	N12D	76.4(2)	EU	O1C	C1C	135.9(5)
O2A	EU	O1B	148.8(2)	EU	O2C	C2C	130.5(6)
O2A	EU	O2B	82.8(2)	EU	N1D	C2D	119.0(5)
O2A	EU	O1C	78.8(2)	EU	N1D	C6D	121.7(5)
O2A	EU	O2C	115.2(2)	C2D	N1D	C6D	118.8(6)
O2A	EU	N1D	133.6(2)	EU	N12D	C7D	122.9(4)
O2A	EU	N12D	83.0(2)	EU	N12D	C11D	118.9(4)
O1B	EU	O2B	71.4(2)	C7D	N12D	C11D	118.2(6)
O1B	EU	O1C	78.3(2)	O1A	C1A	C3A	121.3(8)
O1B	EU	O2C	77.0(2)	O1A	C1A	C4A	117.0(7)
O1B	EU	N1D	74.0(2)	C3A	C1A	C4A	121.7(7)
O1B	EU	N12D	104.6(2)	O2A	C2A	C3A	129.5(7)
O2B	EU	O1C	75.8(2)	O2A	C2A	C10A	111.3(7)
O2B	EU	O2C	138.7(2)	C3A	C2A	C10A	119.1(7)
O2B	EU	N1D	111.9(2)	C1A	C3A	C2A	123.0(7)
O2B	EU	N12D	72.4(2)	C1A	C4A	C5A	119.9(8)
O1C	EU	O2C	72.3(2)	C1A	C4A	C9A	123.4(8)
O1C	EU	N1D	146.4(2)	C5A	C4A	C9A	116.7(9)
O1C	EU	N12D	145.0(2)	C4A	C5A	C6A	120.6(9)
O2C	EU	N1D	83.1(2)	C5A	C6A	C7A	120(1)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle
C6A	C7A	C8A	120(1)
C7A	C8A	C9A	123(1)
C4A	C9A	C8A	120(1)
C2A	C10A	F11A	113.5(9)
C2A	C10A	F12A	109.9(8)
C2A	C10A	F13A	107.1(8)
C2A	C10A	F14A	118(1)
C2A	C10A	F15A	104(1)
C2A	C10A	F16A	111(1)
F11A	C10A	F12A	111.3(9)
F11A	C10A	F13A	108.6(8)
F11A	C10A	F14A	122(1)
F11A	C10A	F15A	39.1(8)
F11A	C10A	F16A	61.2(9)
F12A	C10A	F13A	106.0(9)
F12A	C10A	F14A	73(1)
F12A	C10A	F15A	144(1)
F12A	C10A	F16A	55(1)
F13A	C10A	F14A	32.8(9)
F13A	C10A	F15A	76.5(9)
F13A	C10A	F16A	142(1)
F14A	C10A	F15A	103(1)
F14A	C10A	F16A	118(2)
F15A	C10A	F16A	100(1)
O1B	C1B	C3B	122.5(7)
O1B	C1B	C4B	116.9(7)
C3B	C1B	C4B	120.5(7)
O2B	C2B	C3B	129.2(8)
O2B	C2B	C10B	113.5(7)
C3B	C2B	C10B	117.3(7)
C1B	C3B	C2B	122.8(8)
C1B	C4B	C5B	123.2(8)
C1B	C4B	C9B	119.5(8)
C5B	C4B	C9B	117.2(7)
C4B	C5B	C6B	120.6(9)
C5B	C6B	C7B	119.8(9)
C6B	C7B	C8B	120(1)
C7B	C8B	C9B	121(1)
C4B	C9B	C8B	121.2(9)
C2B	C10B	F11B	112.1(8)
C2B	C10B	F12B	114.2(7)
C2B	C10B	F13B	110.5(8)
C2B	C10B	F14B	109.3(9)
C2B	C10B	F15B	106.8(9)
C2B	C10B	F16B	113(1)
F11B	C10B	F12B	105.3(8)
F11B	C10B	F13B	106.2(8)
F11B	C10B	F14B	137(1)
F11B	C10B	F15B	73.0(8)
F11B	C10B	F16B	41.2(7)
F12B	C10B	F13B	108.1(8)
F12B	C10B	F14B	46.0(7)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
F12B	C10B	F15B	136(1)	C2C	C10C	F11C	112.9(9)
F12B	C10B	F16B	67.6(8)	C2C	C10C	F12C	109.8(8)
F13B	C10B	F14B	67.7(8)	C2C	C10C	F13C	108.9(9)
F13B	C10B	F15B	38.2(7)	F14C	C10C	F15C	109(1)
F13B	C10B	F16B	133(1)	F14C	C10C	F16C	115(1)
F14B	C10B	F15B	105(1)	F14C	C10C	F11C	128(1)
F14B	C10B	F16B	111(1)	F14C	C10C	F12C	69(1)
F15B	C10B	F16B	111(1)	F14C	C10C	F13C	36.3(8)
O1C	C1C	C3C	122.3(7)	F15C	C10C	F16C	103(1)
O1C	C1C	C4C	116.6(7)	F15C	C10C	F11C	38.1(7)
C3C	C1C	C4C	121.0(7)	F15C	C10C	F12C	144(1)
O2C	C2C	C3C	130.9(9)	F15C	C10C	F13C	75.7(8)
O2C	C2C	C10C	112.8(8)	F16C	C10C	F11C	65.6(9)
C3C	C2C	C10C	116.3(8)	F16C	C10C	F12C	52.6(8)
C1C	C3C	C2C	122.0(8)	F16C	C10C	F13C	140(1)
C1C	C4C	C5C	122.8(8)	F11C	C10C	F12C	113(1)
C1C	C4C	C9C	118.8(7)	F11C	C10C	F13C	107.0(9)
C5C	C4C	C9C	118.5(8)	F12C	C10C	F13C	104.6(9)
C4C	C5C	C6C	120.1(9)	N1D	C2D	C3D	122.9(8)
C5C	C6C	C7C	119.6(9)	C2D	C3D	C4D	119.1(9)
C6C	C7C	C8C	120(1)	C3D	C4D	C5D	118.2(8)
C7C	C8C	C9C	120(1)	C4D	C5D	C6D	120.1(7)
C4C	C9C	C8C	120.9(9)	N1D	C6D	C5D	120.9(7)
C2C	C10C	F14C	114(1)	N1D	C6D	C7D	116.3(6)
C2C	C10C	F15C	104.0(9)	C5D	C6D	C7D	122.8(6)
C2C	C10C	F16C	110(1)	N12D	C7D	C6D	116.2(6)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (cont)

atom	atom	atom	angle	atom	atom	atom	angle
N12D	C7D	C8D	121.8(7)	C10B	F13B	F14B	57.4(7)
C6D	C7D	C8D	122.0(7)	C10B	F13B	F15B	73(1)
C7D	C8D	C9D	118.8(7)	F14B	F13B	F15B	129(1)
C8D	C9D	C10D	119.5(7)	C10B	F14B	F12B	65.8(8)
C9D	C10D	C11D	119.5(8)	C10B	F14B	F13B	54.9(7)
N12D	C11D	C10D	122.2(7)	F12B	F14B	F13B	114(1)
C10A	F11A	F15A	83(1)	C10B	F15B	F11B	54.0(6)
C10A	F11A	F16A	59.6(9)	C10B	F15B	F13B	69(1)
F15A	F11A	F16A	143(1)	F11B	F15B	F13B	116(1)
C10A	F12A	F14A	50.4(9)	C10B	F16B	F11B	76(1)
C10A	F12A	F16A	61(1)	C10B	F16B	F12B	59.1(7)
F14A	F12A	F16A	104(1)	F11B	F16B	F12B	129(1)
C10A	F13A	F14A	63(2)	C10C	F14C	F12C	58.2(9)
C10A	F14A	F12A	56.3(9)	C10C	F14C	F13C	84(1)
C10A	F14A	F13A	84(2)	F12C	F14C	F13C	140(1)
F12A	F14A	F13A	140(2)	C10C	F15C	F11C	62(1)
C10A	F15A	F11A	57.5(8)	C10C	F15C	F13C	51.8(7)
C10A	F16A	F11A	59.2(9)	F11C	F15C	F13C	106(1)
C10A	F16A	F12A	64(1)	C10C	F16C	F11C	55.4(7)
F11A	F16A	F12A	118(1)	C10C	F16C	F12C	63.3(9)
C10B	F11B	F15B	53.1(6)	F11C	F16C	F12C	114(1)
C10B	F11B	F16B	62.3(9)	C10C	F11C	F15C	80(1)
F15B	F11B	F16B	112(1)	C10C	F11C	F16C	59.0(9)
C10B	F12B	F14B	68.2(9)	F15C	F11C	F16C	139(1)
C10B	F12B	F16B	53.3(7)	C10C	F12C	F14C	52.7(7)
F14B	F12B	F16B	118(1)	C10C	F12C	F16C	64.2(8)

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Nonhydrogen Atoms (co

atom	atom	atom	angle	atom	atom	atom	angle
F14C	F12C	F16C	111.0(9)				
C10C	F13C	F14C	60(1)				
C10C	F13C	F15C	52.4(6)				
F14C	F13C	F15C	108(1)				

Angles are in degrees. Estimated standard deviations in the significant figure are given in parentheses.

Intramolecular Bond Angles Involving the Hydrogen Atoms

atom	atom	atom	angle	atom	atom	atom	angle
C1A	C3A	H1	118.44	C4C	C5C	H14	119.93
C2A	C3A	H1	118.51	C6C	C5C	H14	119.93
C4A	C5A	H2	119.75	C5C	C6C	H15	120.28
C6A	C5A	H2	119.67	C7C	C6C	H15	120.17
C5A	C6A	H3	120.05	C6C	C7C	H16	119.83
C7A	C6A	H3	119.95	C8C	C7C	H16	119.79
C6A	C7A	H4	120.23	C7C	C8C	H17	119.84
C8A	C7A	H4	120.20	C9C	C8C	H17	119.76
C7A	C8A	H5	118.49	C4C	C9C	H18	119.54
C9A	C8A	H5	118.52	C8C	C9C	H18	119.53
C4A	C9A	H6	119.91	N1D	C2D	H19	118.56
C8A	C9A	H6	119.91	C3D	C2D	H19	118.52
C1B	C3B	H7	118.56	C2D	C3D	H20	120.49
C2B	C3B	H7	118.59	C4D	C3D	H20	120.39
C4B	C5B	H8	119.67	C3D	C4D	H21	121.00
C6B	C5B	H8	119.75	C5D	C4D	H21	120.76
C5B	C6B	H9	120.03	C4D	C5D	H22	119.99
C7B	C6B	H9	120.12	C6D	C5D	H22	119.95
C6B	C7B	H10	119.97	C7D	C8D	H23	120.60
C8B	C7B	H10	120.09	C9D	C8D	H23	120.63
C7B	C8B	H11	119.39	C8D	C9D	H24	120.23
C9B	C8B	H11	119.44	C10D	C9D	H24	120.28
C4B	C9B	H12	119.42	C9D	C10D	H25	120.28
C8B	C9B	H12	119.34	C11D	C10D	H25	120.24
C1C	C3C	H13	118.99	N12D	C11D	H26	118.90
C2C	C3C	H13	119.00	C10D	C11D	H26	118.91

Angles are in degrees. Estimated standard deviations in the least significant figure are given in parentheses.

Torsion or Conformation Angles

(1)	(2)	(3)	(4)	angle
EU	O1A	C1A	C3A	23(1)
EU	O1A	C1A	C4A	-156.6(5)
EU	O2A	C2A	C3A	-4(1)
EU	O2A	C2A	C10A	172.2(5)
EU	O1B	C1B	C3B	19(1)
EU	O1B	C1B	C4B	-159.2(5)
EU	O2B	C2B	C3B	-25(1)
EU	O2B	C2B	C10B	156.5(5)
EU	O1C	C1C	C3C	14(1)
EU	O1C	C1C	C4C	-169.5(5)
EU	O2C	C2C	C3C	-20(1)
EU	O2C	C2C	C10C	161.5(5)
EU	N1D	C2D	C3D	-172.8(7)
EU	N1D	C6D	C5D	172.8(5)
EU	N1D	C6D	C7D	-7.1(8)
EU	N12D	C7D	C6D	1.2(8)
EU	N12D	C7D	C8D	-178.8(5)
EU	N12D	C11D	C10D	178.0(6)
O1A	EU	O2A	C2A	11.7(6)
O1A	EU	O1B	C1B	179.6(6)
O1A	EU	O2B	C2B	-179.8(5)
O1A	EU	O1C	C1C	-86.7(7)
O1A	EU	O2C	C2C	155.4(6)
O1A	EU	N1D	C2D	92.8(6)
O1A	EU	N1D	C6D	-78.6(5)
O1A	EU	N12D	C7D	72.6(5)
O1A	EU	N12D	C11D	-106.0(5)
O1A	C1A	C3A	C2A	-3(1)
O1A	C1A	C4A	C5A	3(1)
O1A	C1A	C4A	C9A	-178.0(9)
O2A	EU	O1A	C1A	-22.4(7)
O2A	EU	O1B	C1B	6.5(8)
O2A	EU	O2B	C2B	-132.7(6)
O2A	EU	O1C	C1C	-144.6(7)
O2A	EU	O2C	C2C	92.3(6)
O2A	EU	N1D	C2D	130.2(6)
O2A	EU	N1D	C6D	-41.2(6)
O2A	EU	N12D	C7D	144.7(5)
O2A	EU	N12D	C11D	-33.8(5)
O2A	C2A	C3A	C1A	-5(1)
O2A	C2A	C10A	F11A	171.5(7)
O2A	C2A	C10A	F12A	-63(1)
O2A	C2A	C10A	F13A	52(1)
O2A	C2A	C10A	F14A	18(1)
O2A	C2A	C10A	F15A	131(1)
O2A	C2A	C10A	F16A	-122(1)
O1B	EU	O1A	C1A	161.4(6)
O1B	EU	O2A	C2A	-173.0(6)
O1B	EU	O2B	C2B	29.7(5)
O1B	EU	O1C	C1C	56.7(6)
O1B	EU	O2C	C2C	-57.3(6)
O1B	EU	N1D	C2D	-66.7(6)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle
O1B	EU	N1D	C6D	121.9(5)
O1B	EU	N12D	C7D	-66.1(5)
O1B	EU	N12D	C11D	115.3(5)
O1B	C1B	C3B	C2B	5(1)
O1B	C1B	C4B	C5B	-176.0(7)
O1B	C1B	C4B	C9B	2(1)
O2B	EU	O1A	C1A	27.8(8)
O2B	EU	O2A	C2A	-139.3(7)
O2B	EU	O1B	C1B	-29.0(6)
O2B	EU	O1C	C1C	130.2(7)
O2B	EU	O2C	C2C	-16.7(7)
O2B	EU	N1D	C2D	-128.5(6)
O2B	EU	N1D	C6D	60.2(5)
O2B	EU	N12D	C7D	-130.7(5)
O2B	EU	N12D	C11D	50.8(5)
O2B	C2B	C3B	C1B	-2(1)
O2B	C2B	C10B	F11B	23.1(9)
O2B	C2B	C10B	F12B	142.8(7)
O2B	C2B	C10B	F13B	-95.1(8)
O2B	C2B	C10B	F14B	-167.8(8)
O2B	C2B	C10B	F15B	-55(1)
O2B	C2B	C10B	F16B	68(1)
O1C	EU	O1A	C1A	-83.8(7)
O1C	EU	O2A	C2A	143.8(7)
O1C	EU	O1B	C1B	49.8(6)
O1C	EU	O2B	C2B	-52.5(5)
O1C	EU	O2C	C2C	24.4(6)
O1C	EU	N1D	C2D	-31.0(7)
O1C	EU	N1D	C6D	157.6(5)
O1C	EU	N12D	C7D	-156.5(4)
O1C	EU	N12D	C11D	25.0(6)
O1C	C1C	C3C	C2C	7(1)
O1C	C1C	C4C	C5C	-173.4(7)
O1C	C1C	C4C	C9C	7(1)
O2C	EU	O1A	C1A	-143.9(7)
O2C	EU	O2A	C2A	79.7(7)
O2C	EU	O1B	C1B	124.1(6)
O2C	EU	O2B	C2B	-12.2(7)
O2C	EU	O1C	C1C	-23.3(6)
O2C	EU	N1D	C2D	11.7(6)
O2C	EU	N1D	C6D	-159.7(5)
O2C	EU	N12D	C7D	21.6(6)
O2C	EU	N12D	C11D	-156.9(5)
O2C	C2C	C3C	C1C	-4(1)
O2C	C2C	C10C	F14C	176(1)
O2C	C2C	C10C	F15C	-66(1)
O2C	C2C	C10C	F16C	44(1)
O2C	C2C	C10C	F11C	-27(1)
O2C	C2C	C10C	F12C	100.5(9)
O2C	C2C	C10C	F13C	-145.5(7)
N1D	EU	O1A	C1A	129.9(7)
N1D	EU	O2A	C2A	-25.7(7)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
N1D	EU	O1B	C1B	-149.4(7)	C2A	C10A	F11A	F16A	102(1)
N1D	EU	O2B	C2B	93.0(6)	C2A	C10A	F12A	F14A	115(1)
N1D	EU	O1C	C1C	21.7(8)	C2A	C10A	F12A	F16A	-102(1)
N1D	EU	O2C	C2C	-132.4(6)	C2A	C10A	F13A	F14A	-116(2)
N1D	EU	N12D	C7D	-3.3(5)	C2A	C10A	F14A	F12A	-104(1)
N1D	EU	N12D	C11D	178.2(6)	C2A	C10A	F14A	F13A	77(2)
N1D	C2D	C3D	C4D	0(1)	C2A	C10A	F15A	F11A	111(1)
N1D	C6D	C5D	C4D	-1(1)	C2A	C10A	F16A	F11A	-106(1)
N1D	C6D	C7D	N12D	3.9(9)	C2A	C10A	F16A	F12A	100(1)
N1D	C6D	C7D	C8D	-176.2(7)	C3A	C1A	C4A	C5A	-176.8(8)
N12D	EU	O1A	C1A	64.7(7)	C3A	C1A	C4A	C9A	3(1)
N12D	EU	O2A	C2A	-66.2(7)	C3A	C2A	C10A	F11A	-12(1)
N12D	EU	O1B	C1B	-94.3(6)	C3A	C2A	C10A	F12A	113.4(9)
N12D	EU	O2B	C2B	142.5(6)	C3A	C2A	C10A	F13A	-131.8(8)
N12D	EU	O1C	C1C	155.5(6)	C3A	C2A	C10A	F14A	-165(1)
N12D	EU	O2C	C2C	-154.5(6)	C3A	C2A	C10A	F15A	-52(1)
N12D	EU	N1D	C2D	176.8(6)	C3A	C2A	C10A	F16A	55(1)
N12D	EU	N1D	C6D	5.5(5)	C4A	C5A	C6A	C7A	-1(2)
N12D	C7D	C6D	C5D	-176.1(7)	C4A	C9A	C8A	C7A	-1(2)
N12D	C7D	C8D	C9D	2(1)	C5A	C4A	C9A	C8A	0(2)
N12D	C11D	C10D	C9D	0(1)	C5A	C6A	C7A	C8A	0(2)
C1A	C3A	C2A	C10A	178.9(8)	C6A	C5A	C4A	C9A	1(1)
C1A	C4A	C5A	C6A	-179.6(9)	C6A	C7A	C8A	C9A	1(2)
C1A	C4A	C9A	C8A	-179(1)	C10A	F11A	F16A	F12A	27(1)
C2A	C3A	C1A	C4A	176.1(8)	C10A	F12A	F14A	F13A	2(3)
C2A	C10A	F11A	F15A	-83(1)	C10A	F12A	F16A	F11A	-26(1)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle
C10A	F13A	F14A	F12A	-2(2)
C10A	F14A	F12A	F16A	-32(1)
C10A	F15A	F11A	F16A	6(2)
C10A	F16A	F11A	F15A	-7(3)
C10A	F16A	F12A	F14A	28(1)
C1B	C3B	C2B	C10B	176.8(7)
C1B	C4B	C5B	C6B	179.2(7)
C1B	C4B	C9B	C8B	-178.9(8)
C2B	C3B	C1B	C4B	-176.4(7)
C2B	C10B	F11B	F15B	-102(1)
C2B	C10B	F11B	F16B	100(1)
C2B	C10B	F12B	F14B	94(1)
C2B	C10B	F12B	F16B	-106(1)
C2B	C10B	F13B	F14B	-103(1)
C2B	C10B	F13B	F15B	91(1)
C2B	C10B	F14B	F12B	-105(1)
C2B	C10B	F14B	F13B	104.9(8)
C2B	C10B	F15B	F11B	108.6(8)
C2B	C10B	F15B	F13B	-102(1)
C2B	C10B	F16B	F11B	-98(1)
C2B	C10B	F16B	F12B	107.8(9)
C3B	C1B	C4B	C5B	5(1)
C3B	C1B	C4B	C9B	-176.6(7)
C3B	C2B	C10B	F11B	-155.9(7)
C3B	C2B	C10B	F12B	-36(1)
C3B	C2B	C10B	F13B	85.8(9)
C3B	C2B	C10B	F14B	13(1)
C3B	C2B	C10B	F15B	126.0(9)
C3B	C2B	C10B	F16B	-111(1)
C4B	C5B	C6B	C7B	0(1)
C4B	C9B	C8B	C7B	-1(1)
C5B	C4B	C9B	C8B	-1(1)
C5B	C6B	C7B	C8B	-1(1)
C6B	C5B	C4B	C9B	1(1)
C6B	C7B	C8B	C9B	1(2)
C10B	F11B	F15B	F13B	-32(1)
C10B	F11B	F16B	F12B	28(1)
C10B	F12B	F14B	F13B	27(1)
C10B	F12B	F16B	F11B	-33(2)
C10B	F13B	F14B	F12B	-30(1)
C10B	F13B	F15B	F11B	27(1)
C10B	F14B	F12B	F16B	-19(1)
C10B	F14B	F13B	F15B	18(2)
C10B	F15B	F11B	F16B	21(1)
C10B	F15B	F13B	F14B	-16(2)
C10B	F16B	F11B	F15B	-19(1)
C10B	F16B	F12B	F14B	22(1)
C1C	C3C	C2C	C10C	175.3(8)
C1C	C4C	C5C	C6C	176.9(8)
C1C	C4C	C9C	C8C	-176.4(9)
C2C	C3C	C1C	C4C	-169.6(7)
C2C	C10C	F14C	F12C	-103(1)

The sign is positive if when looking from atom 2 to atom 3 a clock wise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle
C2C	C10C	F14C	F13C	90(1)
C2C	C10C	F15C	F11C	109(1)
C2C	C10C	F15C	F13C	-106(1)
C2C	C10C	F16C	F11C	-106.8(9)
C2C	C10C	F16C	F12C	100(1)
C2C	C10C	F11C	F15C	-84(1)
C2C	C10C	F11C	F16C	103(1)
C2C	C10C	F12C	F14C	109(1)
C2C	C10C	F12C	F16C	-101(1)
C2C	C10C	F13C	F14C	-105(2)
C2C	C10C	F13C	F15C	100(1)
C3C	C1C	C4C	C5C	3(1)
C3C	C1C	C4C	C9C	-175.8(8)
C3C	C2C	C10C	F14C	-3(1)
C3C	C2C	C10C	F15C	115(1)
C3C	C2C	C10C	F16C	-135(1)
C3C	C2C	C10C	F11C	154.0(9)
C3C	C2C	C10C	F12C	-79(1)
C3C	C2C	C10C	F13C	35(1)
C4C	C5C	C6C	C7C	2(1)
C4C	C9C	C8C	C7C	-2(2)
C5C	C4C	C9C	C8C	5(1)
C5C	C6C	C7C	C8C	0(2)
C6C	C5C	C4C	C9C	-4(1)
C6C	C7C	C8C	C9C	0(2)
C10C	F14C	F12C	F16C	-28(1)
C10C	F14C	F13C	F15C	21(1)
C10C	F15C	F11C	F16C	8(2)
C10C	F15C	F13C	F14C	-23(2)
C10C	F16C	F11C	F15C	-9(2)
C10C	F16C	F12C	F14C	25(1)
C10C	F11C	F15C	F13C	-28(1
C10C	F11C	F16C	F12C	26(1
C10C	F12C	F14C	F13C	20(2
C10C	F12C	F16C	F11C	-24(1
C10C	F13C	F14C	F12C	-17(2
C10C	F13C	F15C	F11C	32(1
C2D	N1D	C6D	C5D	1(1
C2D	N1D	C6D	C7D	-178.5(7
C2D	C3D	C4D	C5D	0(1
C3D	C2D	N1D	C6D	-1(1
C3D	C4D	C5D	C6D	0(1
C4D	C5D	C6D	C7D	179.0(
C5D	C6D	C7D	C8D	4(
C6D	C7D	N12D	C11D	179.7(
C6D	C7D	C8D	C9D	-178.4(
C7D	N12D	C11D	C10D	-1(
C7D	C8D	C9D	C10D	-2(
C8D	C7D	N12D	C11D	0(
C8D	C9D	C10D	C11D	1(
F11A	C10A	F12A	F14A	-119(
F11A	C10A	F12A	F16A	25(

The sign is positive if when looking from atom 2 to atom 3 a clo
wise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle
F11A	C10A	F13A	F14A	121(2)
F11A	C10A	F14A	F12A	105(1)
F11A	C10A	F14A	F13A	-73(2)
F11A	C10A	F16A	F12A	-154(1)
F11A	F15A	C10A	F12A	-46(2)
F11A	F15A	C10A	F13A	-145(1)
F11A	F15A	C10A	F14A	-125(2)
F11A	F15A	C10A	F16A	-4(2)
F11A	F16A	C10A	F12A	154(1)
F11A	F16A	C10A	F13A	84(2)
F11A	F16A	C10A	F14A	114(1)
F11A	F16A	C10A	F15A	3(1)
F11A	F16A	F12A	F14A	2(2)
F12A	C10A	F11A	F15A	153(1)
F12A	C10A	F11A	F16A	-23(1)
F12A	C10A	F13A	F14A	2(2)
F12A	C10A	F14A	F13A	-178(2)
F12A	F14A	C10A	F13A	178(2)
F12A	F14A	C10A	F15A	142(1)
F12A	F14A	C10A	F16A	33(1)
F12A	F16A	C10A	F13A	-70(2)
F12A	F16A	C10A	F14A	-40(1)
F12A	F16A	C10A	F15A	-151(1)
F12A	F16A	F11A	F15A	20(4)
F13A	C10A	F11A	F15A	36(2)
F13A	C10A	F11A	F16A	-139(1)
F13A	C10A	F12A	F14A	-0.9(9)
F13A	C10A	F12A	F16A	143(1)
F13A	F14A	C10A	F15A	-36(2)
F13A	F14A	C10A	F16A	-145(2)
F13A	F14A	F12A	F16A	-30(3)
F14A	C10A	F11A	F15A	70(2)
F14A	C10A	F11A	F16A	-106(2)
F14A	C10A	F12A	F16A	144(1)
F14A	F12A	C10A	F15A	-90(2)
F14A	F12A	C10A	F16A	-144(1)
F14A	F13A	C10A	F15A	144(2)
F14A	F13A	C10A	F16A	54(2)
F15A	C10A	F11A	F16A	-176(2)
F15A	C10A	F12A	F16A	54(2)
F15A	F11A	C10A	F16A	176(2)
F11B	C10B	F12B	F14B	-143(1)
F11B	C10B	F12B	F16B	17.1(9)
F11B	C10B	F13B	F14B	135(1)
F11B	C10B	F13B	F15B	-30(1)
F11B	C10B	F14B	F12B	60(2)
F11B	C10B	F14B	F13B	-90(1)
F11B	C10B	F15B	F13B	149(1)
F11B	C10B	F16B	F12B	-155(1)
F11B	F15B	C10B	F12B	-95(1)
F11B	F15B	C10B	F13B	-149(1)
F11B	F15B	C10B	F14B	-136(1)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle
F11B	F15B	C10B	F16B	-15(1)
F11B	F15B	F13B	F14B	12(2)
F11B	F16B	C10B	F12B	155(1)
F11B	F16B	C10B	F13B	60(2)
F11B	F16B	C10B	F14B	139(1)
F11B	F16B	C10B	F15B	23(2)
F11B	F16B	F12B	F14B	-11(3)
F12B	C10B	F11B	F15B	134(1)
F12B	C10B	F11B	F16B	-24(1)
F12B	C10B	F13B	F14B	22.4(9)
F12B	C10B	F13B	F15B	-143(1)
F12B	C10B	F14B	F13B	-150(1)
F12B	C10B	F15B	F13B	55(2)
F12B	F14B	C10B	F13B	150(1)
F12B	F14B	C10B	F15B	141(1)
F12B	F14B	C10B	F16B	20(1)
F12B	F14B	F13B	F15B	-12(3)
F12B	F16B	C10B	F13B	-94(1)
F12B	F16B	C10B	F14B	-16(1)
F12B	F16B	C10B	F15B	-132(1)
F12B	F16B	F11B	F15B	10(2)
F13B	C10B	F11B	F15B	19.1(8)
F13B	C10B	F11B	F16B	-139(1)
F13B	C10B	F12B	F14B	-29(1)
F13B	C10B	F12B	F16B	130(1)
F13B	F14B	C10B	F15B	-9.2(9)
F13B	F14B	C10B	F16B	-130(1)
F13B	F14B	F12B	F16B	8(2)
F13B	F15B	C10B	F14B	14(1)
F13B	F15B	C10B	F16B	134(1)
F13B	F15B	F11B	F16B	-11(2)
F14B	C10B	F11B	F15B	94(2)
F14B	C10B	F11B	F16B	-64(2)
F14B	C10B	F12B	F16B	160(1)
F14B	C10B	F13B	F15B	-166(1)
F14B	F12B	C10B	F15B	-61(2)
F14B	F12B	C10B	F16B	-160(1)
F14B	F13B	C10B	F15B	166(1)
F14B	F13B	C10B	F16B	98(2)
F15B	C10B	F11B	F16B	-158(2)
F15B	C10B	F12B	F16B	98(2)
F15B	F11B	C10B	F16B	158(2)
F15B	F13B	C10B	F16B	-67(2)
F14C	C10C	F15C	F11C	-129(2)
F14C	C10C	F15C	F13C	15(1)
F14C	C10C	F16C	F11C	122(1)
F14C	C10C	F16C	F12C	-31(1)
F14C	C10C	F11C	F15C	70(2)
F14C	C10C	F11C	F16C	-104(2)
F14C	C10C	F12C	F16C	150(1)
F14C	C10C	F13C	F15C	-155(2)
F14C	F12C	C10C	F15C	-93(2)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Torsion or Conformation Angles (cont)

(1)	(2)	(3)	(4)	angle
F14C	F12C	C10C	F16C	-150(1)
F14C	F12C	C10C	F11C	-124(1)
F14C	F12C	C10C	F13C	-7.7(9)
F14C	F12C	F16C	F11C	1(2)
F14C	F13C	C10C	F15C	155(2)
F14C	F13C	C10C	F16C	61(2)
F14C	F13C	C10C	F11C	133(2)
F14C	F13C	C10C	F12C	12(2)
F14C	F13C	F15C	F11C	9(2)
F15C	C10C	F14C	F12C	141(1)
F15C	C10C	F14C	F13C	-26(2)
F15C	C10C	F16C	F11C	3.9(9)
F15C	C10C	F16C	F12C	-149(1)
F15C	C10C	F11C	F16C	-174(1)
F15C	C10C	F12C	F16C	57(2)
F15C	F11C	C10C	F16C	174(1)
F15C	F11C	C10C	F12C	151(1)
F15C	F11C	C10C	F13C	36(1)
F15C	F11C	F16C	F12C	17(3)
F15C	F13C	C10C	F16C	-94(2)
F15C	F13C	C10C	F11C	-22.1(9)
F15C	F13C	C10C	F12C	-142(1)
F15C	F13C	F14C	F12C	4(3)
F16C	C10C	F14C	F12C	26(1)
F16C	C10C	F14C	F13C	-142(2)
F16C	C10C	F15C	F11C	-6(1)
F16C	C10C	F15C	F13C	139(1)
F16C	F11C	C10C	F12C	-23(1)
F16C	F11C	C10C	F13C	-138(1)
F16C	F11C	F15C	F13C	-21(2)
F16C	F12C	C10C	F11C	27(1)
F16C	F12C	C10C	F13C	143(1)
F16C	F12C	F14C	F13C	-9(3)
F11C	C10C	F14C	F12C	104(2)
F11C	C10C	F14C	F13C	-64(2)
F11C	C10C	F15C	F13C	144(1)
F11C	C10C	F16C	F12C	-153(1)
F11C	F15C	C10C	F12C	-49(2)
F11C	F15C	C10C	F13C	-144(1)
F11C	F16C	C10C	F12C	153(1)
F11C	F16C	C10C	F13C	88(2)
F12C	C10C	F14C	F13C	-167(2)
F12C	C10C	F15C	F13C	95(2)
F12C	F14C	C10C	F13C	167(2)
F12C	F16C	C10C	F13C	-66(2)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

Intermolecular Distances Involving the Nonhydrogen Atoms

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
O1B	C9D	3.418(9)	3	C4D	F11B	3.50(1)	3
O1B	C8D	3.520(9)	3	C5D	F16B	3.14(2)	3
O1C	C6B	3.28(1)	4	C5D	F11B	3.53(1)	3
N1D	C9D	3.53(1)	3	C6D	C8D	3.59(1)	3
C3A	F15A	3.56(2)	65603	C6D	C9D	3.59(1)	3
C5A	C6A	3.48(2)	55603	C7D	C7D	3.55(1)	3
C6A	C6A	3.54(2)	55603	C7D	C8D	3.59(1)	3
C6A	C6C	3.56(2)	54502	C9D	F14C	3.58(2)	54502
C7A	F16C	3.53(2)	55603	C10D	F14C	2.99(1)	54502
C5B	C4C	3.52(1)	45404	C10D	F13B	3.45(1)	65503
C6B	C1C	3.32(1)	45404	C10D	F13C	3.46(1)	54502
C7B	F11A	3.27(1)	2	C10D	F15B	3.49(2)	65503
C7B	F15A	3.52(2)	2	C10D	F12C	3.59(1)	54502
C8B	F11A	3.21(1)	2	F12A	F16B	3.01(2)	65503
C6C	F12B	3.53(1)	4	F12A	F12B	3.20(1)	65503
C7C	F15C	3.39(2)	65501	F16A	F13C	3.36(2)	54502
C7C	F12B	3.40(1)	4	F16A	F12B	3.58(2)	65503
C8C	F15C	3.34(2)	65501	F11B	F11B	2.89(1)	65503
C10C	F14B	3.03(2)	45504	F12B	F13C	2.97(1)	55404
C10C	F12B	3.55(1)	45504	F12B	F14C	2.98(2)	55404
C3D	F15B	3.29(1)	45501	F12B	F15C	3.45(2)	55404
C3D	F14A	3.40(2)	45501	F12B	F11C	3.48(1)	55404
C4D	F14A	3.07(2)	45501	F12B	F12C	3.50(1)	55404
C4D	F15B	3.07(2)	45501	F13B	F12C	3.05(1)	55404
C4D	F16B	3.23(2)	3	F13B	F14C	3.21(2)	55404
C4D	F12A	3.33(1)	45501	F13B	F16C	3.57(2)	55404

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intermolecular Distances Involving the Nonhydrogen Atoms (cont)

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
F14B	F14C	2.60(2)	55404				
F14B	F12C	2.71(2)	55404				
F14B	F13C	2.83(2)	55404				
F14B	F16C	2.90(2)	55404				
F14B	F11C	3.00(2)	55404				
F14B	F15C	3.22(2)	55404				

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

(*)footnote

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one digit numbers and one two digit number: TA(1st digit) + TB(2nd digit) + TC(3rd digit) + SN(4th and 5th digit). TA, TB, & TC are the crystal lattice translation digits along cell edges a, b, and c. A translation digit of 5 indicates the origin unit cell. If TA=4, this indicates a translation of one unit cell length along the a axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus (+/-)4 lattice translations from the origin (TA=5,TB=5,TC=5) can be represented.

The SN or symmetry operator number refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of the symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell (TA=5,TB=5,TC=5) and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always ADC=55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of that atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (i.e.cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	+X	,	+Y	,	+Z	(2)	1/2-X	,1/2+Y	,1/2-Z
(3)	-X	,	-Y	,	-Z	(4)	1/2+X	,1/2-Y	,1/2+Z

Intermolecular Distances Involving the Hydrogen Atoms

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
O1A	H10	3.321	4	C2B	H22	3.088	3
O2A	H9	3.021	4	C3B	H23	3.038	3
O2A	H10	3.307	4	C4B	H24	3.063	3
O1B	H24	2.832	3	C5B	H6	3.111	2
O1B	H23	3.026	3	C5B	H5	3.173	2
O2B	H23	3.098	3	C6B	H6	2.947	2
O2B	H22	3.123	3	C7B	H1	3.341	2
O1C	H9	2.863	4	C7B	H6	3.346	2
O2C	H10	3.404	4	C9B	H24	3.065	3
N1D	H24	3.505	3	C10B	H22	3.230	3
N12D	H23	3.570	3	C10B	H25	3.266	65503
C1A	H10	3.524	4	C1C	H9	3.206	4
C2A	H10	3.338	4	C4C	H8	3.273	4
C2A	H9	3.462	4	C4C	H9	3.521	4
C3A	H10	3.494	4	C5C	H8	3.465	4
C4A	H3	3.548	55603	C5C	H23	3.575	2
C5A	H15	3.427	54502	C6C	H23	3.535	2
C5A	H3	3.452	55603	C6C	H22	3.575	2
C6A	H15	3.354	54502	C7C	H11	3.447	65501
C7A	H2	3.518	55603	C8C	H20	3.284	65501
C8A	H8	3.585	54502	C8C	H11	3.565	65501
C10A	H3	3.335	65501	C9C	H20	3.154	65501
C10A	H21	3.557	65501	C9C	H8	3.454	4
C1B	H24	2.983	3	C10C	H25	3.519	2
C1B	H23	2.998	3	C2D	H24	3.572	3
C2B	H23	3.055	3	C3D	H17	3.445	45501

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intermolecular Distances Involving the Hydrogen Atoms (cont)

atom	atom	distance	ADC(*)	atom	atom	distance	ADC(*)
C3D	H18	3.462	45501	H6	H8	3.385	54502
C5D	H15	3.130	54502	H6	F13A	3.596	65603
C8D	H14	3.037	54502	H9	F13A	2.826	45404
C8D	H15	3.412	54502	H9	F14A	3.346	45404
C9D	H14	3.097	54502	H9	H18	3.468	45404
C9D	H13	3.445	54502	H10	F11A	2.924	2
C10D	H13	3.578	54502	H10	F15A	2.948	2
H1	H10	3.363	54502	H11	F11A	2.797	2
H1	F15A	3.450	65603	H11	H16	2.889	45501
H2	H4	3.558	55603	H11	F16A	3.115	2
H2	H15	3.573	54502	H11	H17	3.118	45501
H3	F15A	2.834	45501	H11	F15A	3.439	2
H3	F11A	2.893	45501	H11	F12C	3.529	45404
H3	F13A	2.957	45501	H12	H24	2.944	3
H3	F14A	2.997	45501	H12	H17	3.046	45501
H3	F16A	3.433	45501	H13	H24	3.331	2
H3	H15	3.473	54502	H13	H25	3.579	2
H3	F12A	3.598	45501	H14	H23	3.108	2
H4	F16C	2.748	55603	H14	H24	3.178	2
H4	H11	3.346	44502	H15	H22	2.710	2
H4	F12C	3.579	55603	H15	H23	3.020	2
H5	H8	2.771	54502	H15	F12B	3.254	4
H5	F16C	3.239	55603	H15	F16B	3.597	4
H5	H7	3.279	54502	H16	F16A	2.768	65502
H5	F11C	3.548	55603	H16	F15C	2.979	65501
H6	H9	3.124	54502	H16	F12B	3.010	4

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intermolecular Distances Involving the Hydrogen Atoms (cont)

atom	atom	distance	ADC(*)
H16	F12A	3.225	65502
H16	F13C	3.379	65501
H16	F11A	3.408	65502
H16	F11C	3.544	65501
H17	H20	2.834	65501
H17	F15C	2.895	65501
H17	H19	3.172	65501
H17	F11C	3.355	65501
H18	H20	2.589	65501
H20	F15B	3.069	45501
H20	F14A	3.298	45501
H20	F13B	3.338	45501
H20	F13A	3.489	45501
H21	F15B	2.646	45501
H21	F16B	2.677	3
H21	F14A	2.691	45501
H21	F12A	2.705	45501
H21	F11B	2.881	3
H21	F11B	3.207	45501
H21	F13A	3.309	45501
H21	F13B	3.391	45501
H22	F16B	2.471	3
H22	F11B	2.936	3
H22	F12B	3.252	3
H24	F12C	3.496	54502
H24	F14C	3.502	54502
H25	F14C	2.398	54502
H25	F13B	2.555	65503
H25	F15B	2.715	65503
H25	F12C	2.867	54502
H25	F13C	2.950	54502
H25	F14B	3.046	65503
H25	F11B	3.248	65503
H25	F12B	3.338	65503
H25	F16B	3.449	65503
H26	F11B	3.140	65503
H26	F16B	3.329	65503

Contacts out to 3.60 angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table of Least-Squares Planes

---------- Plane number 1 ----------

Atoms Defining Plane	Distance	esd
EU	0.0000	
O1A	0.0000	
O2A	0.0000	

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

---------- Plane number 2 ----------

Atoms Defining Plane	Distance	esd
O1A	0.0552	0.0048
O2A	-0.0579	0.0048
C1A	-0.0001	0.0076
C2A	0.0350	0.0077
C3A	0.0208	0.0080
C4A	-0.1010	0.0081
C10A	0.0840	0.0099

Mean deviation from plane is 0.0506 angstroms
Chi-squared: 533.1

Dihedral angles between least-squares planes

plane	plane	angle
2	1	167.30

---------- Plane number 3 ----------

Atoms Defining Plane	Distance	esd
C4A	0.0029	0.0081
C5A	-0.0058	0.0089
C6A	0.0065	0.0120
C7A	0.0032	0.0137
C8A	-0.0108	0.0148
C9A	0.0026	0.0121

Mean deviation from plane is 0.0053 angstroms
Chi-squared: 1.5

Dihedral angles between least-squares planes

plane	plane	angle
3	1	165.09
3	2	4.26

Table of Least-Squares Planes (continued)

---------- Plane number 4 ----------

Atoms Defining Plane	Distance	esd
EU	0.0000	
O1B	0.0000	
O2B	0.0000	

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

Dihedral angles between least-squares planes

plane	plane	angle
4	1	148.44
4	2	35.97
4	3	40.21

---------- Plane number 5 ----------

Atoms Defining Plane	Distance	esd
O1B	0.0167	0.0044
O2B	-0.0199	0.0044
C1B	-0.0016	0.0070
C2B	0.0155	0.0071
C3B	0.0464	0.0076
C4B	-0.0464	0.0072
C10B	-0.0021	0.0085

Mean deviation from plane is 0.0212 angstroms
Chi-squared: 118.1

Dihedral angles between least-squares planes

plane	plane	angle
5	1	154.20
5	2	21.67
5	3	25.51
5	4	21.07

Table of Least-Squares Planes (continued)

---------- Plane number 6 ----------

Atoms Defining Plane	Distance	esd
C4B	0.0056	0.0072
C5B	-0.0054	0.0079
C6B	-0.0007	0.0096
C7B	0.0087	0.0103
C8B	-0.0062	0.0102
C9B	-0.0026	0.0086

Mean deviation from plane is 0.0049 angstroms
Chi-squared: 2.2

Dihedral angles between least-squares planes

plane	plane	angle
6	1	154.98
6	2	22.98
6	3	27.06
6	4	17.22
6	5	3.94

---------- Plane number 7 ----------

Atoms Defining Plane	Distance	esd
EU	0.0000	
O1C	0.0000	
O2C	0.0000	

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

Dihedral angles between least-squares planes

plane	plane	angle
7	1	77.05
7	2	115.16
7	3	115.60
7	4	103.30
7	5	121.00
7	6	117.40

Table of Least-Squares Planes (continued)

---------- Plane number 8 ----------

Atoms Defining Plane	Distance	esd
O1C	-0.0303	0.0046
O2C	0.0435	0.0047
C1C	-0.0365	0.0068
C2C	-0.0277	0.0080
C3C	-0.1033	0.0085
C4C	0.1097	0.0073
C10C	0.0003	0.0109

Mean deviation from plane is 0.0502 angstroms
Chi-squared: 546.3

Dihedral angles between least-squares planes

plane	plane	angle
8	1	118.64
8	2	49.17
8	3	48.86
8	4	63.82
8	5	44.58
8	6	48.36
8	7	164.31

---------- Plane number 9 ----------

Atoms Defining Plane	Distance	esd
C4C	0.0169	0.0074
C5C	-0.0153	0.0087
C6C	-0.0001	0.0097
C7C	0.0122	0.0109
C8C	0.0008	0.0113
C9C	-0.0223	0.0101

Mean deviation from plane is 0.0113 angstroms
Chi-squared: 14.4

Dihedral angles between least-squares planes

plane	plane	angle
9	1	111.79
9	2	55.71
9	3	54.87
9	4	72.32
9	5	52.90
9	6	56.72
9	7	169.54
9	8	8.51

Table of Least-Squares Planes (continued)

---------- Plane number 10 ----------

Atoms Defining Plane	Distance	esd
EU	0.0000	
N1D	0.0000	
N12D	0.0000	

Mean deviation from plane is 0.0000 angstroms
Chi-squared: 0.0

Dihedral angles between least-squares planes

plane	plane	angle
10	1	76.11
10	2	116.33
10	3	118.75
10	4	90.76
10	5	111.60
10	6	107.67
10	7	25.79
10	8	151.57
10	9	158.85

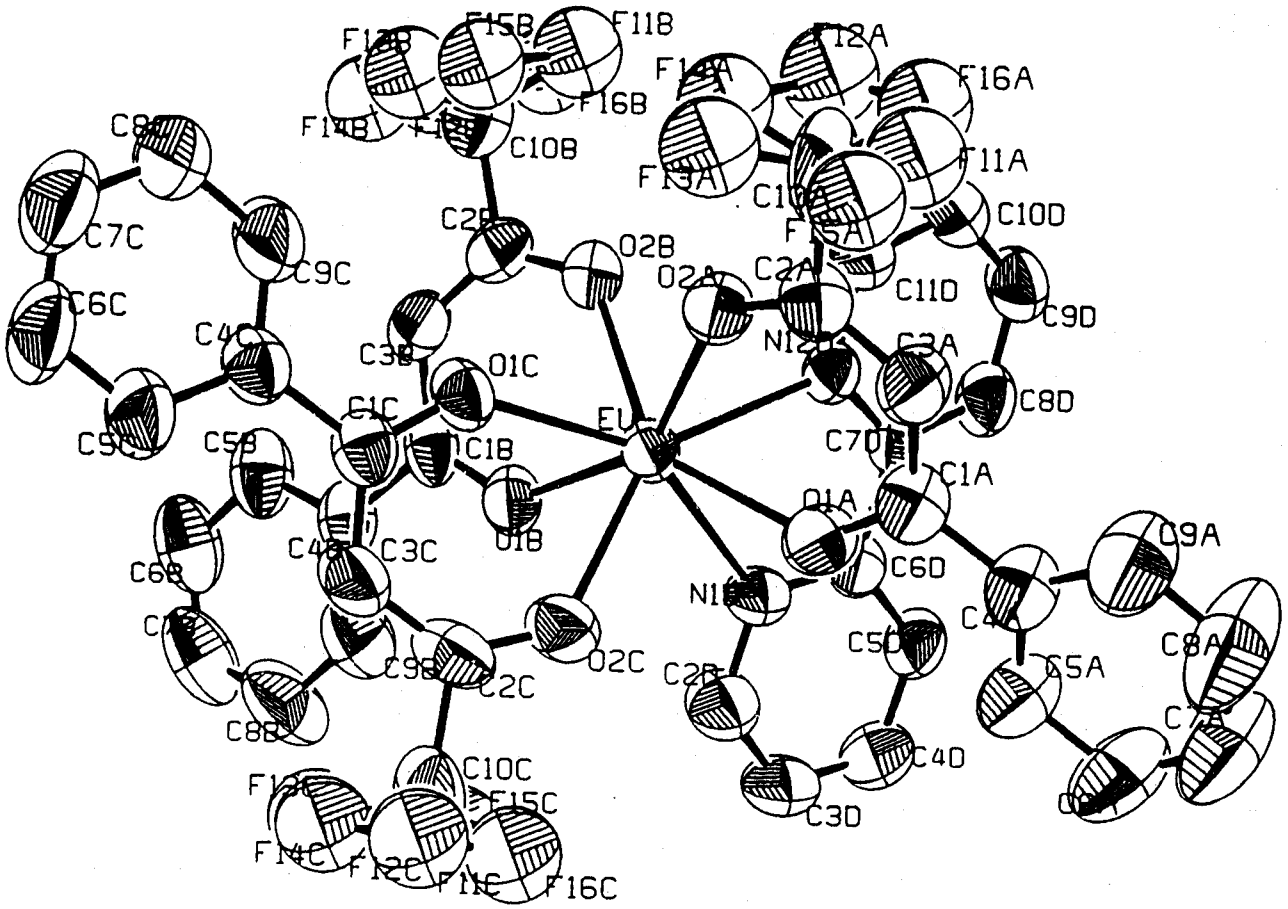
---------- Plane number 11 ----------

Atoms Defining Plane	Distance	esd
N1D	-0.0472	0.0058
C2D	-0.0167	0.0090
C3D	0.0312	0.0092
C4D	0.0541	0.0095
C5D	0.0329	0.0081
C6D	-0.0081	0.0069
C7D	-0.0113	0.0064
C8D	-0.0520	0.0079
C9D	-0.0182	0.0082
C10D	0.0110	0.0077
C11D	0.0328	0.0077
N12D	0.0282	0.0054

Mean deviation from plane is 0.0286 angstroms
Chi-squared: 230.1

Dihedral angles between least-squares planes

plane	plane	angle
11	1	106.54
11	2	60.87
11	3	58.70
11	4	85.18
11	5	64.45
11	6	68.39
11	7	157.66
11	8	23.99
11	9	16.82
11	10	175.55


F15B
F11B
F16B
C10B
C2B
O2B
C7C
C9C
C6C
C4C
C3B
O1C
C1C
C1B
O1B
C3C
C2C
O2C
C10C
F15C
F16C
F12A
F16A
F11A
C10D
C11D
C9D
C3A
C8D
C7D
C1A
O1A
C6D
C5D
C4D
C3D
C9A
C8A
C5A
C2A
O2A

Positions of triplet and singlet states relative to Eu(III) energy levels for both the fluorinated and nonfluorinated complexes.

Acceptor Eu(III) states		Donor triplet and singlet states (cm^{-1})			
		Fluorinated complex		Nonfluorinated complex	
name	(cm^{-1})	triplet	singlet	triplet	singlet
			35,852		34,215
			33,282		33,860
			33,268		33,329
				30,850	
				30,477	
				29,935	
		29,913			
		28,288			
		27,598			
$^5D_4$	27,586	27,222			
$^5G_6$	26,752				
$^5G_4$	26,735				
$^5G_2$	26,392				
				25,634	
$^5L_6$	25,325			25,260	
		25,167		25,060	
		23,938			
$^5D_2$	21,483				
$^5D_1$	19,027				
$^5D_0$	17,293				