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Supplementary Information for:

Chiral Recognition of Dicarboxylate Anions by Sapphyrin-Based Receptors

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Tables of positional and thermal parameters, bond lengths, angles and torsion angles, and figures for the [**1a** • H]$^+$ • $(C_6H_5CO_2)^-$ • (C_4H_8O) complex (21 pages).

Supplementary Table 1. Crystallographic Data[a] for $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Supplementary Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($Å^2$) for the non-hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Supplementary Table 3. Anisotropic thermal parameters for the non-hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Supplementary Table 4. Fractional coordinates and isotropic thermal parameters ($Å^2$) for the hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Supplementary Table 5. Bond Lengths (Å) and Angles (°) for the non-hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Supplementary Table 6. Bond Lengths (Å) and Angles (°) for the hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Supplementary Table 7. Torsion angles (°) for the non-hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Supplementary Table 8. Observed and calculated structure factor amplitudes for $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O). Values for Fo, Fc and σ(Fo) have been multiplied by 10.

Supplementary Figure 1. View of $(C_{40}H_{50}N_5)^{1+}$ showing the atom labeling scheme. Thermal ellipsoids are scaled to the 30% probability level. Hydrogen atoms are drawn to an arbitrary scale. All hydrogens bound to nitrogen were observed in a ΔF map and refined without constraints.

Supplementary Figure 2. Unit cell packing diagram for $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O). The view is approximately perpendicular to the plane through the macrocycle.

Supplementary Table 1. Crystallographic Data[a] for $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Formula	$C_{51}H_{63}N_5O_3$
fw	794.06
a, Å	13.210(1)
b, Å	13.936(1)
c, Å	14.960(2)
α, °	99.258(8)
β, °	111.011(8)
γ, °	110.480(8)
V, Å3	2275.7(4)
Z	2
F(000)	856
Crystal System	Triclinic
Space Group	$P\bar{1}$
T, °C	-85
2θ range (°)	4 - 50
Scan speed (°/min) (1.0° ω scan)	4 - 8
ρcalc, g/cc	1.16
Reflections measured	8567
Unique reflections	7725
Decay Correction	0.9934 - 1.019

Supplementary Table 1. Crystallographic Data (continued).

R_{int} (F^2)	0.069
μ, cm-1	0.72
Crystal size, mm	0.14x0.21x0.54
Transmission factor range	N/A
$R_w(F^2)$[b]	0.195
R(F)[c]	0.0821
Goodness of fit, S[d]	1.047
Parameters	549
Max $\lvert\Delta/\sigma\rvert$	<0.1
Min, max peaks ($e^-/Å^3$)	-0.36, 0.46

[a] Data were collected on a Siemens P4 diffractometer, equipped with a Nicolet LT-2 low-temperature device and using graphite monochromatized Mo Kα radiation (λ = 0.71073Å). Data were collected using ω scans with a scan range of 1° in ω. Lattice parameters were obtained from the least-squares refinement of 33 reflections with $16.6 < 2\theta < 23.9°$.

[b] $R_w = \{\Sigma w(|F_o|^2 - |F_c|^2)^2/\Sigma w(|F_o|)^4\}^{1/2}$ and where the weight, w, is defined as follows: $w = 1/\{\sigma^2(|F_o|^2) + (a*P)^2 + b*P\}$; P = [1/3*(Maximum of (0 or $|F_o|^2$) + 2/3*$|F_c|^2$]. The parameters a and b were suggested during refinement and are 0.0359 and 3.6261, respectively.

[c] The conventional R index based on F where the 3900 observed reflections have $F_o > 4(\sigma(F_o))$.

[d] $S = [\Sigma w(|F_o|^2 - |F_c|^2)^2/(n - p)]^{1/2}$, where n is the number of reflections and p is the number of refined parameters.

Supplementary Table 2. Fractional coordinates and equivalent isotropic thermal parameters ($Å^2$) for the non-hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Atom	x	y	z	U
N1	0.6814(3)	0.6243(3)	0.2833(3)	0.035(2)
N2	0.8668(4)	0.8532(3)	0.3296(3)	0.037(2)
N3	0.7274(3)	0.9427(3)	0.1291(3)	0.030(2)
N4	0.4621(3)	0.7423(3)	-0.0149(3)	0.028(2)
N5	0.4707(3)	0.5624(3)	0.1079(3)	0.030(2)
C1	0.5806(5)	0.5343(4)	0.2612(3)	0.035(3)
C2	0.5911(5)	0.4970(4)	0.3483(4)	0.040(3)
C3	0.7047(5)	0.5653(4)	0.4226(4)	0.045(3)
C4	0.7592(5)	0.6440(4)	0.3807(3)	0.038(3)
C5	0.8739(5)	0.7291(4)	0.4313(4)	0.045(3)
C6	0.9267(5)	0.8189(4)	0.4051(3)	0.042(3)
C7	1.0515(5)	0.8927(4)	0.4523(3)	0.043(3)
C8	1.0659(5)	0.9712(4)	0.4074(4)	0.045(3)
C9	0.9493(5)	0.9478(4)	0.3304(3)	0.040(3)
C10	0.9337(5)	1.0161(4)	0.2730(4)	0.044(3)
C11	0.8454(4)	1.0184(4)	0.1893(3)	0.038(3)
C12	0.8681(5)	1.1034(4)	0.1460(4)	0.046(3)
C13	0.7661(4)	1.0779(4)	0.0617(4)	0.038(3)
C14	0.6754(4)	0.9770(3)	0.0507(3)	0.028(2)
C15	0.5601(4)	0.9242(3)	-0.0281(3)	0.031(2)
C16	0.4660(4)	0.8205(3)	-0.0607(3)	0.028(2)
C17	0.3614(4)	0.7712(4)	-0.1574(3)	0.028(2)
C18	0.2985(4)	0.6651(4)	-0.1678(3)	0.030(2)
C19	0.3615(4)	0.6459(3)	-0.0778(3)	0.029(2)
C20	0.3281(4)	0.5456(4)	-0.0637(3)	0.032(2)
C21	0.3749(4)	0.5067(4)	0.0137(3)	0.030(2)
C22	0.3245(4)	0.3956(3)	0.0084(3)	0.032(2)
C23	0.3884(4)	0.3884(4)	0.1009(3)	0.032(2)
C24	0.4814(4)	0.4941(4)	0.1634(3)	0.032(2)
C25	0.4919(5)	0.4131(4)	0.3599(4)	0.054(3)
C26	0.7625(6)	0.5645(5)	0.5291(4)	0.061(3)
C27	0.8451(6)	0.5082(6)	0.5417(5)	0.087(4)
C28	1.1486(5)	0.8815(5)	0.5350(4)	0.060(3)
C29	1.1838(5)	1.0589(5)	0.4258(4)	0.057(3)
C30	1.2273(6)	1.0300(6)	0.3492(5)	0.081(4)
C31	0.9868(5)	1.2063(5)	0.1916(5)	0.081(4)
C32	1.0783(7)	1.1887(7)	0.1635(7)	0.127(6)
C33	0.7500(5)	1.1372(4)	-0.0144(4)	0.046(3)
C34	0.7699(6)	1.0913(5)	-0.1025(4)	0.069(4)
C35	0.3320(4)	0.8258(4)	-0.2357(3)	0.036(3)
C36	0.3910(5)	0.8159(4)	-0.3048(4)	0.048(3)
C37	0.1857(4)	0.5817(4)	-0.2574(3)	0.046(3)
C38	0.2244(4)	0.3033(4)	-0.0859(4)	0.040(3)
C39	0.0997(5)	0.2720(6)	-0.0929(5)	0.086(4)
C40	0.3691(5)	0.2851(4)	0.1253(4)	0.042(3)

Supplementary Table 2. (continued).

Atom	x	y	z	U
O1A	0.5965(3)	0.7987(2)	0.2000(2)	0.033(2)
C2A	0.5458(4)	0.8516(4)	0.2311(3)	0.031(2)
O3A	0.5197(3)	0.9183(3)	0.1947(3)	0.050(2)
C4A	0.5135(4)	0.8273(4)	0.3147(3)	0.033(2)
C5A	0.4600(5)	0.8816(5)	0.3524(4)	0.052(3)
C6A	0.4268(6)	0.8568(5)	0.4271(5)	0.072(4)
C7A	0.4473(6)	0.7781(5)	0.4643(4)	0.063(4)
C8A	0.5020(5)	0.7251(5)	0.4285(4)	0.055(3)
C9A	0.5350(5)	0.7495(4)	0.3537(3)	0.041(3)
O1B	0.0846(9)	0.4730(7)	0.1846(8)	0.197(6)
C2B	0.0780(13)	0.5701(13)	0.1986(11)	0.210(8)
C3B	0.1509(12)	0.6354(10)	0.1544(10)	0.187(7)
C4B	0.2084(11)	0.5781(11)	0.1311(10)	0.168(7)
C5B	0.1987(14)	0.5042(12)	0.1893(11)	0.204(8)

For anisotropic atoms, the U value is U_{eq}, calculated as $U_{eq} = 1/3\ \Sigma_i\Sigma_j\ U_{ij}\ a_i^*\ a_j^*\ A_{ij}$ where A_{ij} is the dot product of the i^{th} and j^{th} direct space unit cell vectors.

Supplementary Table 3. Anisotropic thermal parameters for the non-hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Atom	U11	U22	U33	U12	U13	U23
N1	0.045(3)	0.037(2)	0.026(2)	0.023(2)	0.013(2)	0.014(2)
N2	0.034(3)	0.044(3)	0.028(2)	0.020(2)	0.008(2)	0.012(2)
N3	0.034(2)	0.029(2)	0.031(2)	0.014(2)	0.016(2)	0.015(2)
N4	0.033(2)	0.032(2)	0.021(2)	0.015(2)	0.011(2)	0.013(2)
N5	0.037(2)	0.028(2)	0.028(2)	0.016(2)	0.014(2)	0.012(2)
C1	0.048(3)	0.037(3)	0.037(3)	0.029(3)	0.024(3)	0.021(2)
C2	0.052(3)	0.044(3)	0.037(3)	0.028(3)	0.024(3)	0.021(3)
C3	0.061(4)	0.051(3)	0.035(3)	0.034(3)	0.022(3)	0.024(3)
C4	0.048(3)	0.041(3)	0.032(3)	0.026(3)	0.017(3)	0.015(2)
C5	0.052(4)	0.053(3)	0.029(3)	0.032(3)	0.009(3)	0.017(3)
C6	0.048(3)	0.049(3)	0.027(3)	0.026(3)	0.012(3)	0.013(2)
C7	0.043(3)	0.052(3)	0.026(3)	0.025(3)	0.005(2)	0.008(3)
C8	0.036(3)	0.054(3)	0.036(3)	0.019(3)	0.008(2)	0.011(3)
C9	0.042(3)	0.048(3)	0.029(3)	0.021(3)	0.013(2)	0.011(2)
C10	0.036(3)	0.046(3)	0.042(3)	0.014(3)	0.014(3)	0.016(3)
C11	0.037(3)	0.042(3)	0.037(3)	0.017(3)	0.017(3)	0.019(2)
C12	0.039(3)	0.041(3)	0.055(3)	0.012(3)	0.020(3)	0.024(3)
C13	0.041(3)	0.038(3)	0.041(3)	0.019(3)	0.022(3)	0.020(2)
C14	0.035(3)	0.031(3)	0.027(2)	0.019(2)	0.016(2)	0.013(2)
C15	0.043(3)	0.032(3)	0.029(3)	0.024(2)	0.019(2)	0.016(2)
C16	0.037(3)	0.030(3)	0.028(3)	0.021(2)	0.018(2)	0.014(2)
C17	0.037(3)	0.036(3)	0.024(2)	0.023(2)	0.016(2)	0.014(2)
C18	0.031(3)	0.039(3)	0.028(3)	0.021(2)	0.014(2)	0.014(2)
C19	0.030(3)	0.029(3)	0.028(3)	0.013(2)	0.014(2)	0.011(2)
C20	0.030(3)	0.033(3)	0.027(3)	0.011(2)	0.011(2)	0.009(2)
C21	0.037(3)	0.033(3)	0.029(3)	0.018(2)	0.018(2)	0.014(2)
C22	0.037(3)	0.029(3)	0.036(3)	0.016(2)	0.020(2)	0.013(2)
C23	0.040(3)	0.032(3)	0.039(3)	0.020(2)	0.026(2)	0.019(2)
C24	0.042(3)	0.035(3)	0.034(3)	0.023(2)	0.022(2)	0.021(2)
C25	0.072(4)	0.058(4)	0.048(3)	0.032(3)	0.036(3)	0.030(3)
C26	0.076(4)	0.073(4)	0.039(3)	0.036(4)	0.021(3)	0.031(3)
C27	0.094(5)	0.109(6)	0.055(4)	0.055(5)	0.012(4)	0.048(4)
C28	0.050(4)	0.074(4)	0.045(3)	0.031(3)	0.006(3)	0.022(3)
C29	0.039(3)	0.072(4)	0.048(3)	0.021(3)	0.009(3)	0.019(3)
C30	0.055(4)	0.101(6)	0.095(5)	0.036(4)	0.040(4)	0.035(4)
C31	0.047(4)	0.080(5)	0.095(5)	0.010(4)	0.015(4)	0.055(4)
C32	0.059(5)	0.178(9)	0.154(8)	0.038(6)	0.053(5)	0.102(7)
C33	0.045(3)	0.044(3)	0.053(3)	0.017(3)	0.022(3)	0.031(3)
C34	0.078(5)	0.094(5)	0.074(4)	0.047(4)	0.054(4)	0.056(4)
C35	0.046(3)	0.045(3)	0.031(3)	0.029(3)	0.017(2)	0.022(2)
C36	0.070(4)	0.060(4)	0.040(3)	0.043(3)	0.033(3)	0.029(3)
C37	0.042(3)	0.051(3)	0.039(3)	0.020(3)	0.009(3)	0.020(3)
C38	0.052(3)	0.032(3)	0.044(3)	0.020(3)	0.027(3)	0.017(2)
C39	0.045(4)	0.095(5)	0.073(5)	0.006(4)	0.016(4)	-0.004(4)
C40	0.052(3)	0.037(3)	0.047(3)	0.024(3)	0.025(3)	0.022(2)

Supplementary Table 3. (continued).

Atom	U11	U22	U33	U12	U13	U23
O1A	0.040(2)	0.035(2)	0.030(2)	0.018(2)	0.019(2)	0.0150(15)
C2A	0.033(3)	0.030(3)	0.026(2)	0.012(2)	0.011(2)	0.011(2)
O3A	0.071(3)	0.053(2)	0.056(2)	0.042(2)	0.038(2)	0.036(2)
C4A	0.037(3)	0.031(3)	0.031(3)	0.016(2)	0.015(2)	0.012(2)
C5A	0.069(4)	0.063(4)	0.053(3)	0.045(3)	0.038(3)	0.029(3)
C6A	0.106(6)	0.096(5)	0.072(4)	0.070(5)	0.070(4)	0.044(4)
C7A	0.088(5)	0.081(5)	0.057(4)	0.047(4)	0.052(4)	0.040(4)
C8A	0.087(5)	0.054(4)	0.052(4)	0.039(3)	0.045(3)	0.033(3)
C9A	0.059(4)	0.042(3)	0.037(3)	0.027(3)	0.029(3)	0.018(2)
O1B	0.186(7)	0.144(6)	0.270(8)	0.051(5)	0.124(6)	0.090(6)
C2B	0.216(9)	0.229(10)	0.259(10)	0.121(8)	0.150(8)	0.106(8)
C3B	0.182(8)	0.177(9)	0.245(9)	0.066(6)	0.138(7)	0.110(7)
C4B	0.158(8)	0.194(9)	0.194(9)	0.083(7)	0.128(7)	0.037(6)
C5B	0.189(9)	0.209(10)	0.233(10)	0.118(8)	0.079(7)	0.088(8)

The Uij are the mean-square amplitudes of vibration in $Å^2$ from the general temperature factor expression

$$\exp[-2\pi^2(h^2a^{*2}U11 + k^2b^{*2}U22 + l^2c^{*2}U33 + 2hka^*b^*U12 + 2hla^*c^*U13 + 2klb^*c^*U23)]$$

Supplementary Table 4. Fractional coordinates and isotropic thermal parameters ($Å^2$) for the hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

Atom	x	y	z	U
H5	0.9250	0.7259	0.4941	0.053
H10	1.0060	1.0831	0.3012	0.052
H15	0.5401	0.9671	-0.0694	0.037
H20	0.2569	0.4897	-0.1211	0.038
H25A	0.5256	0.4045	0.4249	0.080
H25B	0.4310	0.4370	0.3557	0.080
H25C	0.4564	0.3449	0.3075	0.080
H26A	0.7006	0.5284	0.5478	0.074
H26B	0.8099	0.6379	0.5743	0.074
H27A	0.8815	0.5086	0.6101	0.13
H27B	0.7971	0.4347	0.4968	0.13
H27C	0.9072	0.5449	0.5235	0.13
H28A	1.2255	0.9411	0.5552	0.089
H28B	1.1318	0.8811	0.5923	0.089
H28C	1.1506	0.8147	0.5098	0.089
H29A	1.2434	1.0719	0.4922	0.069
H29B	1.1759	1.1247	0.4242	0.069
H30A	1.3034	1.0870	0.3634	0.12
H30B	1.2359	0.9647	0.3515	0.12
H30C	1.1679	1.0179	0.2830	0.12
H31A	1.0189	1.2291	0.2640	0.097
H31B	0.9723	1.2629	0.1688	0.097
H32A	1.1529	1.2537	0.1930	0.19
H32B	1.0928	1.1324	0.1870	0.19
H32C	1.0459	1.1665	0.0910	0.19
H33A	0.8074	1.2123	0.0177	0.056
H33B	0.6702	1.1329	-0.0392	0.056
H34A	0.7591	1.1291	-0.1508	0.10
H34B	0.8501	1.0964	-0.0773	0.10
H34C	0.7119	1.0164	-0.1346	0.10
H35A	0.3581	0.9009	-0.2020	0.044
H35B	0.2460	0.7928	-0.2768	0.044
H36A	0.3718	0.8511	-0.3542	0.072
H36B	0.4769	0.8495	-0.2633	0.072
H36C	0.3640	0.7406	-0.3386	0.072
H37A	0.1603	0.6139	-0.3082	0.069
H37B	0.2012	0.5241	-0.2846	0.069
H37C	0.1232	0.5532	-0.2371	0.069
H38A	0.2402	0.2409	-0.0878	0.048
H38B	0.2252	0.3229	-0.1444	0.048
H39A	0.0400	0.2130	-0.1540	0.13
H39B	0.0978	0.2508	-0.0353	0.13
H39C	0.0827	0.3336	-0.0925	0.13
H40A	0.2992	0.2259	0.0696	0.063

Supplementary Table 4. (continued).

Atom	x	y	z	U
H40B	0.4389	0.2726	0.1365	0.063
H40C	0.3571	0.2906	0.1852	0.063
H5A	0.4475	0.9370	0.3259	0.062
H6A	0.3896	0.8950	0.4524	0.086
H7A	0.4250	0.7608	0.5162	0.076
H8A	0.5156	0.6692	0.4535	0.066
H9A	0.5741	0.7131	0.3288	0.050
H2BA	0.1167	0.6092	0.2699	0.25
H2BB	-0.0036	0.5614	0.1698	0.25
H3BA	0.2100	0.7073	0.1987	0.22
H3BB	0.0966	0.6404	0.0942	0.22
H4BA	0.2900	0.6244	0.1461	0.20
H4BB	0.1652	0.5358	0.0604	0.20
H5BA	0.2075	0.4422	0.1617	0.25
H5BB	0.2612	0.5426	0.2576	0.25
H2N	0.787(5)	0.825(4)	0.298(4)	0.05(2)
H3N	0.680(4)	0.888(4)	0.149(4)	0.06(2)
H4N	0.509(3)	0.758(3)	0.052(3)	0.019(11)
H5N	0.521(4)	0.635(4)	0.140(3)	0.043(14)

Supplementary Table 5. Bond Lengths (Å) and Angles (°) for the non-hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

1	2	3	1-2	1-2-3
C1	N1	C4	1.355(6)	105.4(4)
C4	N1		1.362(6)	
C6	N2	C9	1.388(7)	108.9(4)
C9	N2		1.381(7)	
C11	N3	C14	1.375(5)	109.1(4)
C14	N3		1.382(7)	
C16	N4	C19	1.373(7)	110.0(4)
C19	N4		1.380(4)	
C21	N5	C24	1.368(5)	110.5(4)
C24	N5		1.371(7)	
C2	C1	C24	1.458(8)	129.9(4)
C2	C1	N1		111.7(4)
C24	C1	N1	1.422(6)	118.4(5)
C3	C2	C25	1.363(6)	126.6(5)
C3	C2	C1		105.3(5)
C25	C2	C1	1.507(8)	127.4(4)
C4	C3	C26	1.452(8)	125.7(4)
C4	C3	C2		106.5(5)
C26	C3	C2	1.504(8)	127.7(5)
C5	C4	N1	1.381(6)	123.3(5)
C5	C4	C3		125.6(5)
N1	C4	C3		111.1(4)
C6	C5	C4	1.396(8)	129.9(5)
C7	C6	N2	1.421(7)	107.7(5)
C7	C6	C5		126.0(5)
N2	C6	C5		126.3(4)
C8	C7	C28	1.365(9)	127.4(5)
C8	C7	C6		108.1(5)
C28	C7	C6	1.506(8)	124.5(5)
C9	C8	C29	1.436(7)	125.2(5)
C9	C8	C7		108.1(4)
C29	C8	C7	1.499(7)	126.3(5)
C10	C9	N2	1.400(8)	131.0(4)
C10	C9	C8		121.8(5)
N2	C9	C8		107.2(5)
C11	C10	C9	1.386(7)	139.8(4)
C12	C11	N3	1.432(8)	107.1(4)
C12	C11	C10		123.2(4)
N3	C11	C10		129.6(5)
C13	C12	C31	1.354(7)	127.0(6)
C13	C12	C11		108.5(4)
C31	C12	C11	1.525(7)	124.5(5)
C14	C13	C33	1.430(7)	124.3(4)
C14	C13	C12		107.8(5)
C33	C13	C12	1.509(8)	127.6(5)
C15	C14	N3	1.378(5)	128.1(4)
C15	C14	C13		124.4(5)

Supplementary Table 5. (continued).

1	2	3	1-2	1-2-3
N3	C14	C13		107.4(4)
C16	C15	C14	1.398(6)	133.1(5)
C17	C16	N4	1.434(5)	107.0(3)
C17	C16	C15		124.8(5)
N4	C16	C15		127.8(4)
C18	C17	C35	1.368(7)	126.6(3)
C18	C17	C16		108.0(4)
C35	C17	C16	1.506(8)	125.3(4)
C19	C18	C37	1.430(7)	124.9(4)
C19	C18	C17		108.1(3)
C37	C18	C17	1.491(5)	126.9(5)
C20	C19	N4	1.388(7)	128.6(4)
C20	C19	C18		124.4(3)
N4	C19	C18		106.9(4)
C21	C20	C19	1.392(7)	134.9(3)
C22	C21	N5	1.431(7)	106.5(4)
C22	C21	C20		124.2(3)
N5	C21	C20		129.3(4)
C23	C22	C38	1.380(7)	127.1(4)
C23	C22	C21		108.2(3)
C38	C22	C21	1.510(5)	124.6(4)
C24	C23	C40	1.422(5)	127.2(4)
C24	C23	C22		107.3(4)
C40	C23	C22	1.500(8)	125.2(3)
N5	C24	C1		119.6(4)
N5	C24	C23		107.4(4)
C1	C24	C23		132.7(5)
C27	C26	C3	1.529(12)	112.6(6)
C30	C29	C8	1.514(11)	113.0(4)
C32	C31	C12	1.495(14)	111.9(6)
C34	C33	C13	1.520(10)	111.9(6)
C36	C35	C17	1.518(9)	112.1(5)
C39	C38	C22	1.508(9)	114.4(5)
C2A	O1A		1.291(7)	
O3A	C2A	C4A	1.238(7)	118.6(5)
O3A	C2A	O1A		123.9(5)
C4A	C2A	O1A	1.510(8)	117.5(5)
C5A	C4A	C9A	1.382(10)	118.9(6)
C5A	C4A	C2A		120.5(5)
C9A	C4A	C2A	1.377(8)	120.6(6)
C6A	C5A	C4A	1.389(10)	120.5(6)
C7A	C6A	C5A	1.370(11)	120.0(8)
C8A	C7A	C6A	1.370(12)	119.9(7)
C9A	C8A	C7A	1.389(9)	120.3(6)
C4A	C9A	C8A		120.5(6)
C2B	O1B	C5B	1.37(2)	101.2(12)
C5B	O1B		1.39(2)	
C3B	C2B	O1B	1.49(2)	107.(2)

Supplementary Table 5. (continued).

1	2	3	1-2	1-2-3
C4B	C3B	C2B	1.37(2)	105.0(14)
C5B	C4B	C3B	1.45(2)	103.(2)
O1B	C5B	C4B		105.4(14)

Supplementary Table 6. Bond Lengths (Å) and Angles (°) for the hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

1	2	3	1-2	1-2-3
H2N	N2	C6	0.89(5)	121.(4)
H2N	N2	C9		128.(4)
H3N	N3	C11	0.97(6)	125.(3)
H3N	N3	C14		122.(3)
H4N	N4	C16	0.90(4)	123.(3)
H4N	N4	C19		126.(3)
H5N	N5	C21	0.92(4)	132.(3)
H5N	N5	C24		118.(3)
H5	C5	C6	0.96	115.2(5)
H5	C5	C4		114.8(6)
H10	C10	C11	0.96	109.8(6)
H10	C10	C9		110.4(6)
H15	C15	C16	0.96	113.1(4)
H15	C15	C14		113.7(5)
H20	C20	C21	0.96	112.6(5)
H20	C20	C19		112.5(6)
H25A	C25	H25B	0.96	109.5(9)
H25A	C25	H25C		109.5(8)
H25A	C25	C2		108.9(5)
H25B	C25	H25C	0.96	109.5(7)
H25B	C25	C2		109.2(7)
H25C	C25	C2	0.96	110.3(7)
H26A	C26	H26B	0.96	108.3(9)
H26A	C26	C27		109.1(8)
H26A	C26	C3		109.4(6)
H26B	C26	C27	0.96	108.4(7)
H26B	C26	C3		109.0(7)
H27A	C27	H27B	0.96	109.5(10)
H27A	C27	H27C		109.5(8)
H27A	C27	C26		111.6(9)
H27B	C27	H27C	0.96	109.5(10)
H27B	C27	C26		108.0(8)
H27C	C27	C26	0.96	108.8(9)
H28A	C28	H28B	0.96	109.5(6)
H28A	C28	H28C		109.5(9)
H28A	C28	C7		109.5(7)
H28B	C28	H28C	0.96	109.5(9)
H28B	C28	C7		110.0(7)
H28C	C28	C7	0.96	109.0(5)
H29A	C29	H29B	0.96	108.2(7)
H29A	C29	C30		108.8(8)
H29A	C29	C8		108.2(7)
H29B	C29	C30	0.96	108.9(7)
H29B	C29	C8		109.7(7)
H30A	C30	H30B	0.96	109.5(10)
H30A	C30	H30C		109.4(10)

Supplementary Table 6. (continued).

1	2	3	1-2	1-2-3
H30A	C30	C29		111.2(7)
H30B	C30	H30C	0.96	109.5(8)
H30B	C30	C29		108.7(9)
H30C	C30	C29	0.96	108.5(9)
H31A	C31	H31B	0.96	108.3(9)
H31A	C31	C32		108.8(8)
H31A	C31	C12		108.9(8)
H31B	C31	C32	0.96	109.2(9)
H31B	C31	C12		109.7(6)
H32A	C32	H32B	0.96	109.5(11)
H32A	C32	H32C		109.4(13)
H32A	C32	C31		111.3(11)
H32B	C32	H32C	0.96	109.5(13)
H32B	C32	C31		108.8(11)
H32C	C32	C31	0.96	108.3(9)
H33A	C33	H33B	0.96	108.3(8)
H33A	C33	C34		107.8(7)
H33A	C33	C13		109.8(5)
H33B	C33	C34	0.96	109.8(6)
H33B	C33	C13		109.2(7)
H34A	C34	H34B	0.96	109.5(10)
H34A	C34	H34C		109.5(7)
H34A	C34	C33		111.5(9)
H34B	C34	H34C	0.96	109.5(10)
H34B	C34	C33		109.5(6)
H34C	C34	C33	0.96	107.4(8)
H35A	C35	H35B	0.96	108.3(8)
H35A	C35	C36		109.7(6)
H35A	C35	C17		109.1(5)
H35B	C35	C36	0.96	108.2(5)
H35B	C35	C17		109.3(6)
H36A	C36	H36B	0.96	109.5(7)
H36A	C36	H36C		109.5(6)
H36A	C36	C35		111.4(8)
H36B	C36	H36C	0.96	109.5(9)
H36B	C36	C35		107.8(6)
H36C	C36	C35	0.96	109.3(7)
H37A	C37	H37B	0.96	109.5(7)
H37A	C37	H37C		109.5(8)
H37A	C37	C18		109.7(5)
H37B	C37	H37C	0.96	109.5(7)
H37B	C37	C18		109.1(6)
H37C	C37	C18	0.96	109.6(5)
H38A	C38	H38B	0.96	107.8(8)
H38A	C38	C39		108.4(6)
H38A	C38	C22		108.6(5)
H38B	C38	C39	0.96	108.5(6)
H38B	C38	C22		108.9(5)

Supplementary Table 6. (continued).

1	2	3	1-2	1-2-3
H39A	C39	H39B	0.96	109.5(9)
H39A	C39	H39C		109.5(9)
H39A	C39	C38		110.7(9)
H39B	C39	H39C	0.96	109.5(11)
H39B	C39	C38		108.9(7)
H39C	C39	C38	0.96	108.8(7)
H40A	C40	H40B	0.96	109.5(7)
H40A	C40	H40C		109.5(7)
H40A	C40	C23		109.5(6)
H40B	C40	H40C	0.96	109.5(7)
H40B	C40	C23		109.0(6)
H40C	C40	C23	0.96	109.9(6)
H5A	C5A	C6A	0.96	121.4(9)
H5A	C5A	C4A		118.1(8)
H6A	C6A	C7A	0.96	120.3(9)
H6A	C6A	C5A		119.6(9)
H7A	C7A	C8A	0.96	119.6(9)
H7A	C7A	C6A		120.6(10)
H8A	C8A	C9A	0.96	119.4(9)
H8A	C8A	C7A		120.4(8)
H9A	C9A	C4A	0.96	118.8(7)
H9A	C9A	C8A		120.7(7)
H2BA	C2B	H2BB	0.96	109.(3)
H2BA	C2B	C3B		107.(2)
H2BA	C2B	O1B		109.(2)
H2BB	C2B	C3B	0.96	112.(2)
H2BB	C2B	O1B		113.(2)
H3BA	C3B	H3BB	0.96	109.(2)
H3BA	C3B	C4B		109.(2)
H3BA	C3B	C2B		115.(2)
H3BB	C3B	C4B	0.96	111.(2)
H3BB	C3B	C2B		108.(2)
H4BA	C4B	H4BB	0.96	109.(2)
H4BA	C4B	C5B		114.(2)
H4BA	C4B	C3B		112.(2)
H4BB	C4B	C5B	0.96	108.2(15)
H4BB	C4B	C3B		110.(2)
H5BA	C5B	H5BB	0.96	109.(2)
H5BA	C5B	O1B		111.(2)
H5BA	C5B	C4B		112.(2)
H5BB	C5B	O1B	0.96	112.(2)
H5BB	C5B	C4B		108.(2)

Supplementary Table 7. Torsion Angles (°) for the non-hydrogen atoms of $(C_{40}H_{50}N_5)^{1+}$ $(C_6H_5CO_2)^{1-}$ (C_4H_8O).

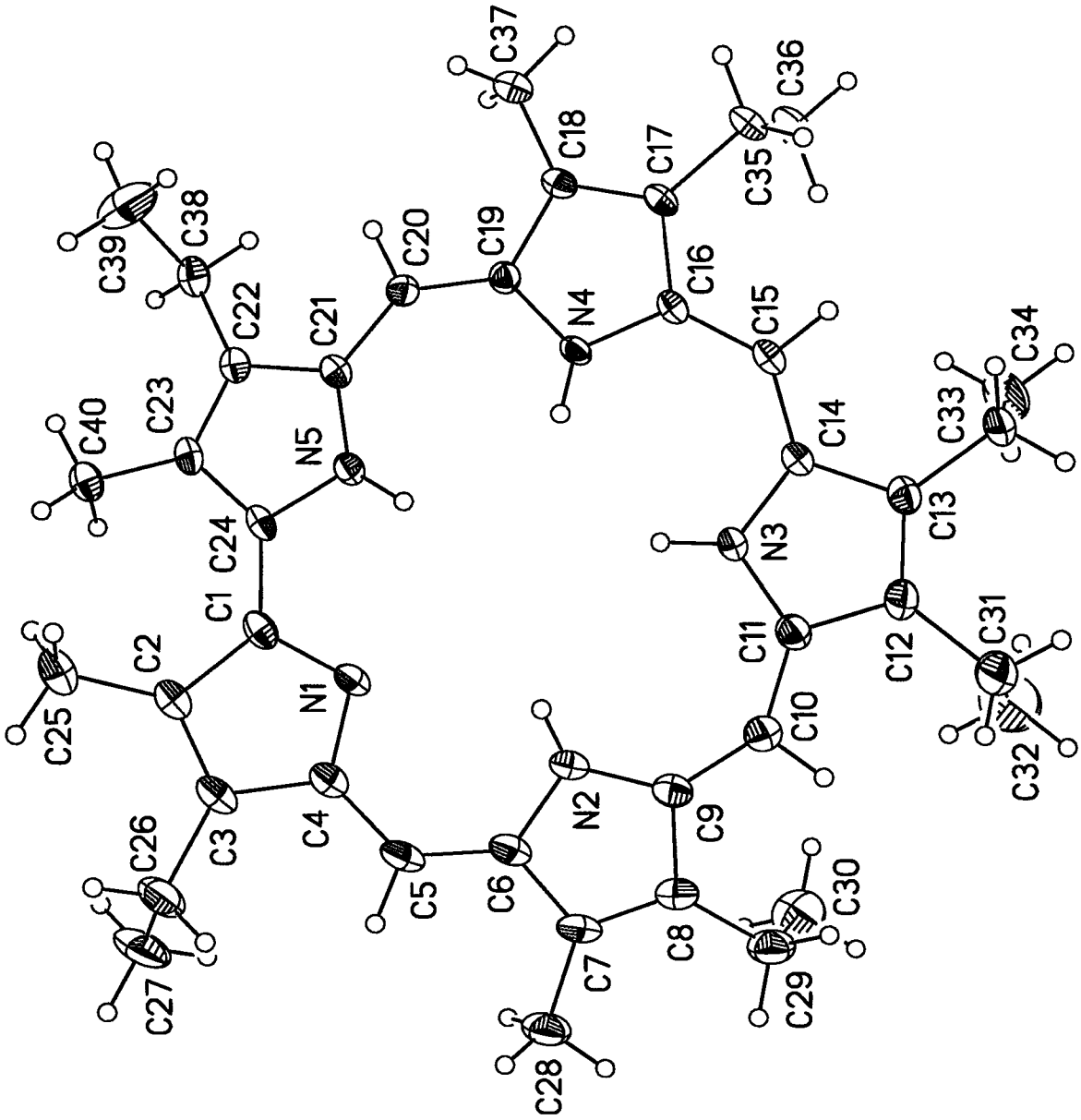
1	2	3	4	1-2-3-4
C1	N1	C4	C3	-1.4(7)
C1	N1	C4	C5	179.2(7)
C4	N1	C1	C2	2.5(7)
C4	N1	C1	C24	179.4(6)
C6	N2	C9	C8	2.0(7)
C6	N2	C9	C10	-176.8(7)
C9	N2	C6	C5	177.1(6)
C9	N2	C6	C7	-2.0(7)
C11	N3	C14	C13	1.2(7)
C11	N3	C14	C15	178.1(6)
C14	N3	C11	C10	-176.4(7)
C14	N3	C11	C12	-0.5(7)
C16	N4	C19	C18	-0.4(7)
C16	N4	C19	C20	175.3(6)
C19	N4	C16	C15	-171.3(6)
C19	N4	C16	C17	0.8(7)
C21	N5	C24	C1	175.6(6)
C21	N5	C24	C23	0.8(7)
C24	N5	C21	C20	175.8(6)
C24	N5	C21	C22	-2.0(7)
C2	C1	C24	N5	153.8(7)
C2	C1	C24	C23	-33.1(12)
C24	C1	C2	C3	-179.1(7)
C24	C1	C2	C25	-8.1(11)
N1	C1	C2	C3	-2.7(8)
N1	C1	C2	C25	168.2(6)
N1	C1	C24	N5	-22.3(9)
N1	C1	C24	C23	150.8(7)
C25	C2	C3	C4	-169.4(6)
C25	C2	C3	C26	8.0(12)
C1	C2	C3	C4	1.7(8)
C1	C2	C3	C26	179.1(7)
C4	C3	C26	C27	-84.3(8)
C26	C3	C4	N1	-177.7(7)
C26	C3	C4	C5	1.7(12)
C2	C3	C4	N1	-0.3(9)
C2	C3	C4	C5	179.1(7)
C2	C3	C26	C27	98.9(9)
N1	C4	C5	C6	11.8(12)
C3	C4	C5	C6	-167.5(7)
C4	C5	C6	N2	12.8(12)
C4	C5	C6	C7	-168.3(7)
N2	C6	C7	C8	1.2(7)
N2	C6	C7	C28	-177.1(6)
C5	C6	C7	C8	-177.8(6)
C5	C6	C7	C28	3.8(10)
C28	C7	C8	C9	178.2(6)

Supplementary Table 7. (continued).

1	2	3	4	1-2-3-4
C28	C7	C8	C29	5.0(11)
C6	C7	C8	C9	0.0(6)
C6	C7	C8	C29	-173.3(6)
C9	C8	C29	C30	-76.8(9)
C29	C8	C9	N2	172.2(6)
C29	C8	C9	C10	-8.9(10)
C7	C8	C9	N2	-1.2(7)
C7	C8	C9	C10	177.8(6)
C7	C8	C29	C30	95.3(8)
N2	C9	C10	C11	-10.0(14)
C8	C9	C10	C11	171.3(8)
C9	C10	C11	N3	1.2(14)
C9	C10	C11	C12	-174.2(8)
N3	C11	C12	C13	-0.4(8)
N3	C11	C12	C31	177.4(6)
C10	C11	C12	C13	175.8(6)
C10	C11	C12	C31	-6.4(11)
C13	C12	C31	C32	-99.7(9)
C31	C12	C13	C14	-176.6(7)
C31	C12	C13	C33	8.5(12)
C11	C12	C13	C14	1.1(8)
C11	C12	C13	C33	-173.7(6)
C11	C12	C31	C32	82.9(9)
C14	C13	C33	C34	-81.2(7)
C33	C13	C14	N3	173.6(6)
C33	C13	C14	C15	-3.4(10)
C12	C13	C14	N3	-1.5(7)
C12	C13	C14	C15	-178.5(6)
C12	C13	C33	C34	92.8(7)
N3	C14	C15	C16	-7.5(11)
C13	C14	C15	C16	168.9(6)
C14	C15	C16	N4	5.2(11)
C14	C15	C16	C17	-165.6(7)
N4	C16	C17	C18	-0.8(7)
N4	C16	C17	C35	-177.0(6)
C15	C16	C17	C18	171.6(6)
C15	C16	C17	C35	-4.6(10)
C18	C17	C35	C36	-88.8(7)
C35	C17	C18	C19	176.7(6)
C35	C17	C18	C37	-1.9(10)
C16	C17	C18	C19	0.6(7)
C16	C17	C18	C37	-178.0(6)
C16	C17	C35	C36	86.7(6)
C37	C18	C19	N4	178.5(6)
C37	C18	C19	C20	2.6(10)
C17	C18	C19	N4	-0.1(5)
C17	C18	C19	C20	-176.0(6)
N4	C19	C20	C21	3.1(12)

Supplementary Table 7. (continued).

1	2	3	4	1-2-3-4
C18	C19	C20	C21	178.1(7)
C19	C20	C21	N5	5.0(12)
C19	C20	C21	C22	-177.6(7)
N5	C21	C22	C23	2.3(7)
N5	C21	C22	C38	-173.8(6)
C20	C21	C22	C23	-175.5(6)
C20	C21	C22	C38	8.3(10)
C23	C22	C38	C39	88.4(8)
C38	C22	C23	C24	174.2(6)
C38	C22	C23	C40	-0.3(11)
C21	C22	C23	C24	-1.8(7)
C21	C22	C23	C40	-176.3(6)
C21	C22	C38	C39	-96.2(7)
C40	C23	C24	N5	175.0(6)
C40	C23	C24	C1	1.3(12)
C22	C23	C24	N5	0.7(8)
C22	C23	C24	C1	-173.1(7)
O3A	C2A	C4A	C5A	-2.5(5)
O3A	C2A	C4A	C9A	176.5(3)
O1A	C2A	C4A	C5A	179.4(3)
O1A	C2A	C4A	C9A	-1.6(5)
C5A	C4A	C9A	C8A	0.9(6)
C9A	C4A	C5A	C6A	-1.0(6)
C2A	C4A	C5A	C6A	178.0(4)
C2A	C4A	C9A	C8A	-178.1(4)
C4A	C5A	C6A	C7A	0.1(10)
C5A	C6A	C7A	C8A	0.9(7)
C6A	C7A	C8A	C9A	-1.0(7)
C7A	C8A	C9A	C4A	0.1(8)
C2B	O1B	C5B	C4B	-42.6(14)
C5B	O1B	C2B	C3B	31.2(13)
O1B	C2B	C3B	C4B	-8.5(12)
C2B	C3B	C4B	C5B	-17.1(11)
C3B	C4B	C5B	O1B	38.0(12)


C37
C36
C18
C17
C35
C38
C39
C20
C19
C22
C21
N4
C16
C15
C34
C40
C23
N5
C14
C33
C24
C13
N3
C1
C2
C11
C12
C31
C25
N1
C10
C32
C26
C3
C4
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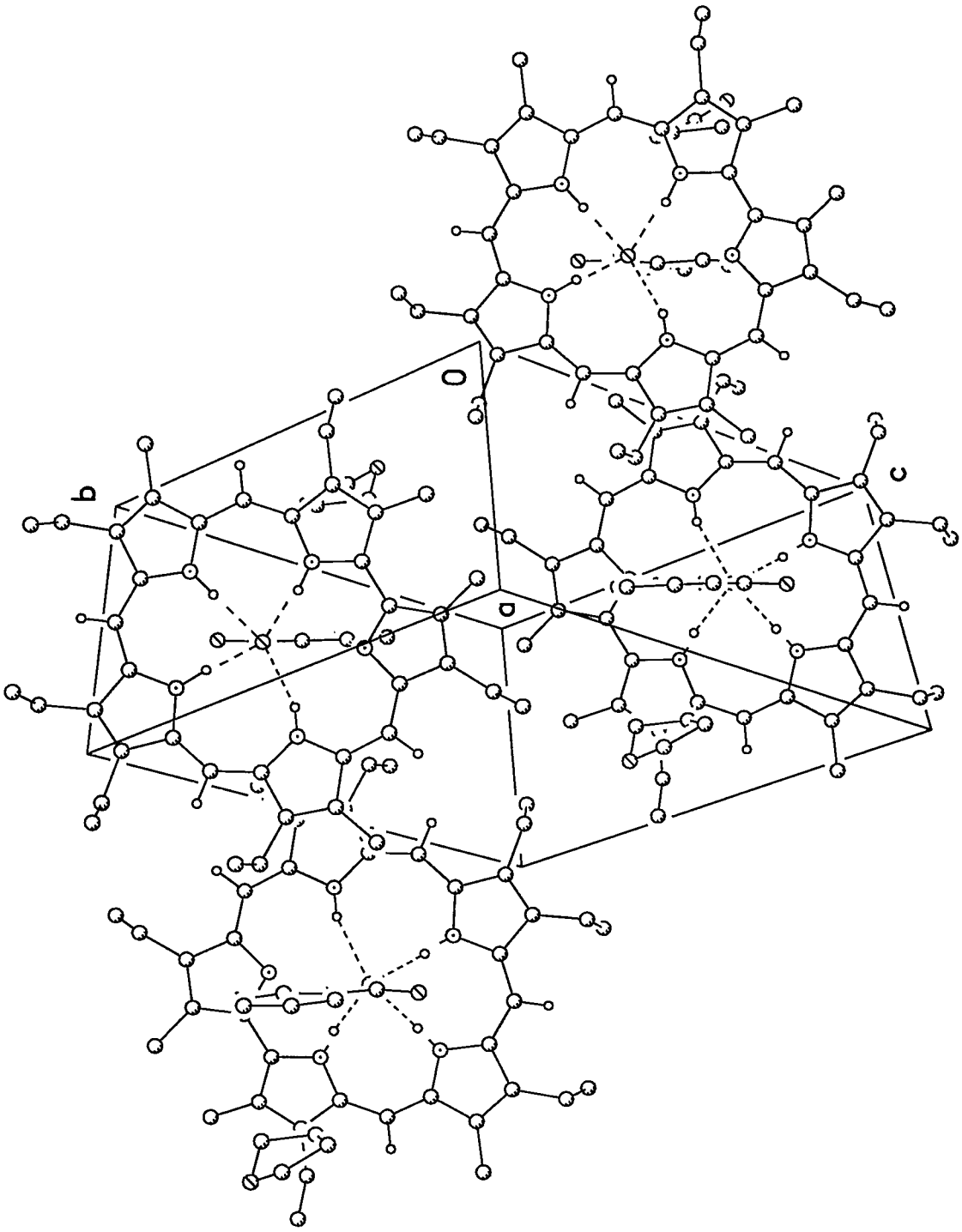
C9
C5
C6
C30
C8
C7
C29
C27
C28


b
c
a