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Table 7. Torsion Angles (°) for OS21B. (Cont.)

C81 -C3 -C91 -C96	28.3(8)	C91 -C3 -C81 -C86	50.3(8)
C91 -C3 -C81 -C82	-133.6(6)	C3 -C81 -C86 -C85	174.7(6)
C3 -C81 -C82 -C83	-175.4(7)	C82 -C81 -C86 -C85	-2.(1)
C86 -C81 -C82 -C83	1.(1)	C81 -C82 -C83 -C84	0.(1)
C82 -C83 -C84 -C85	1.(1)	C83 -C84 -C85 -C86	-2.(1)
C84 -C85 -C86 -C81	2.(1)	C3 -C91 -C96 -C95	179.3(5)
C3 -C91 -C92 -C93	179.8(6)	C92 -C91 -C96 -C95	-0.2(8)
C96 -C91 -C92 -C93	-0.8(9)	C91 -C92 -C93 -C94	0.4(9)
C92 -C93 -C94 -C95	1.(1)	C93 -C94 -C95 -C96	-2.(1)
C94 -C95 -C96 -C91	1.5(9)		

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Table 8. Torsion angles (°) involving hydrogen atoms for OS21B.

C72 -Os -C73 -H73	121.4(7)	C71 -Os -C73 -H73	159.0(6)
C70 -Os -C73 -H73	-159.0(6)	P2 -Os -C73 -H73	7.6(6)
P1 -Os -C73 -H73	104.7(6)	C71 -Os -C72 -H72	121.1(7)
C70 -Os -C72 -H72	159.2(7)	P2 -Os -C72 -H72	-52.1(6)
P1 -Os -C72 -H72	46.7(6)	C70 -Os -C71 -H71	123.1(7)
P2 -Os -C71 -H71	-111.6(5)	P1 -Os -C71 -H71	-12.2(5)
C72 -Os -C71 -H71	-121.8(7)	C73 -Os -C71 -H71	-158.5(6)
C74 -Os -C71 -H71	159.6(6)	C1 -Os -C71 -H71	77.6(6)
C73 -Os -C72 -H72	-121.8(7)	C74 -Os -C72 -H72	-159.7(7)
C1 -Os -C72 -H72	162.3(6)	C74 -Os -C73 -H73	-122.8(7)
C1 -Os -C73 -H73	-92.6(6)	P1 -C11 -C16 -H16	0.2(8)
P1 -C11 -C12 -H12	0.(1)	C12 -C11 -C16 -H16	177.8(6)
C16 -C11 -C12 -H12	-177.9(7)	C11 -C12 -C13 -H13	178.9(8)
H12 -C12 -C13 -H13	-1.(1)	H12 -C12 -C13 -C14	178.9(8)
C12 -C13 -C14 -H14	179.9(8)	H13 -C13 -C14 -H14	0.(1)
H13 -C13 -C14 -C15	179.9(9)	C13 -C14 -C15 -H15	-179.9(8)
H14 -C14 -C15 -H15	0.(1)	H14 -C14 -C15 -C16	-179.9(8)
H15 -C15 -C16 -C11	-178.9(7)	C14 -C15 -C16 -H16	-178.9(7)
H15 -C15 -C16 -H16	1.(1)	P1 -C21 -C26 -H26	-2.2(9)
P1 -C21 -C22 -H22	2.2(8)	C22 -C21 -C26 -H26	-177.8(6)
C26 -C21 -C22 -H22	178.1(6)	C21 -C22 -C23 -H23	-179.5(7)
H22 -C22 -C23 -H23	0.(1)	H22 -C22 -C23 -C24	-179.5(7)
C22 -C23 -C24 -H24	-179.2(7)	H23 -C23 -C24 -H24	1.(1)
H23 -C23 -C24 -C25	-179.2(8)	C23 -C24 -C25 -H25	179.5(7)
H24 -C24 -C25 -H25	-1.(1)	H24 -C24 -C25 -C26	179.5(7)
H25 -C25 -C26 -C21	179.1(7)	C24 -C25 -C26 -H26	179.0(7)
H25 -C25 -C26 -H26	-1.(1)	P1 -C31 -C36 -H36	-4.4(8)
P1 -C31 -C32 -H32	5.9(9)	C32 -C31 -C36 -H36	-179.3(6)
C36 -C31 -C32 -H32	-179.1(6)	C31 -C32 -C33 -H33	178.2(7)
H32 -C32 -C33 -H33	-2.(1)	H32 -C32 -C33 -C34	178.2(7)
C32 -C33 -C34 -H34	-178.8(7)	H33 -C33 -C34 -H34	1.(1)
H33 -C33 -C34 -C35	-178.8(7)	C33 -C34 -C35 -H35	-179.7(7)
H34 -C34 -C35 -H35	0.(1)	H34 -C34 -C35 -C36	-179.7(7)
H35 -C35 -C36 -C31	178.7(7)	C34 -C35 -C36 -H36	178.7(7)
H35 -C35 -C36 -H36	-1.(1)	P2 -C41 -C46 -H46	7.3(8)
P2 -C41 -C42 -H42	-7.2(7)	C42 -C41 -C46 -H46	179.9(6)
C46 -C41 -C42 -H42	179.9(6)	C41 -C42 -C43 -H43	-178.6(6)
H42 -C42 -C43 -H43	1.(1)	H42 -C42 -C43 -C44	-178.7(6)
C42 -C43 -C44 -H44	177.7(6)	H43 -C43 -C44 -H44	-2.(1)
H43 -C43 -C44 -C45	177.7(6)	C43 -C44 -C45 -H45	-177.9(6)
H44 -C44 -C45 -H45	2.(1)	H44 -C44 -C45 -C46	-177.9(6)
H45 -C45 -C46 -C41	179.1(6)	C44 -C45 -C46 -H46	179.1(6)
H45 -C45 -C46 -H46	-1.(1)	P2 -C51 -C56 -H56	0.0(8)
P2 -C51 -C52 -H52	-0.3(9)	C52 -C51 -C56 -H56	176.5(6)
C56 -C51 -C52 -H52	-176.6(6)	C51 -C52 -C53 -H53	178.1(7)
H52 -C52 -C53 -H53	-2.(1)	H52 -C52 -C53 -C54	178.1(7)
C52 -C53 -C54 -H54	-179.5(7)	H53 -C53 -C54 -H54	0.(1)
H53 -C53 -C54 -C55	-179.5(7)	C53 -C54 -C55 -H55	179.4(7)
H54 -C54 -C55 -H55	-1.(1)	H54 -C54 -C55 -C56	179.4(7)
H55 -C55 -C56 -C51	-177.8(7)	C54 -C55 -C56 -H56	-177.8(7)
H55 -C55 -C56 -H56	2.(1)	P2 -C61 -C66 -H66	-3.8(8)
P2 -C61 -C62 -H62	3.2(8)	C62 -C61 -C66 -H66	-178.2(6)
C66 -C61 -C62 -H62	177.4(6)	C61 -C62 -C63 -H63	-178.5(7)
H62 -C62 -C63 -H63	1.(1)	H62 -C62 -C63 -C64	-178.5(6)
C62 -C63 -C64 -H64	-179.6(7)	H63 -C63 -C64 -H64	0.(1)
H63 -C63 -C64 -C65	-179.6(7)	C63 -C64 -C65 -H65	178.7(7)
H64 -C64 -C65 -H65	-1.(1)	H64 -C64 -C65 -C66	178.7(7)
H65 -C65 -C66 -C61	-179.9(6)	C64 -C65 -C66 -H66	-179.9(6)
H65 -C65 -C66 -H66	0.(1)	Os -C70 -C78 -H78	90.7(7)
Os -C70 -C71 -H71	-114.1(7)	C74 -C70 -C78 -H78	-178.9(6)

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Table 8. Torsion angles (°) involving hydrogen atoms for OS21B.
(Cont.)

C71 -C70 -C78 -H78	-4.(1)	C74 -C70 -C71 -H71	-176.7(6)
C78 -C70 -C71 -H71	8.(1)	H71 -C71 -C72 -Os	112.2(7)
C70 -C71 -C72 -H72	174.7(7)	Os -C71 -C72 -H72	-117.5(7)
H71 -C71 -C72 -H72	-5.(1)	H71 -C71 -C72 -C73	174.7(6)
H72 -C72 -C73 -Os	118.3(7)	C71 -C72 -C73 -H73	-174.7(7)
Os -C72 -C73 -H73	-113.0(7)	H72 -C72 -C73 -H73	5.(1)
H72 -C72 -C73 -C74	-174.7(7)	H73 -C73 -C74 -Os	114.9(7)
H73 -C73 -C74 -C70	176.7(7)	H73 -C73 -C74 -C75	-5.(1)
C73 -C74 -C75 -H75	3.(1)	C70 -C74 -C75 -H75	-179.1(6)
Os -C74 -C75 -H75	-90.1(7)	C74 -C75 -C76 -H76	-179.1(7)
H75 -C75 -C76 -H76	1.(1)	H75 -C75 -C76 -C77	-179.1(7)
C75 -C76 -C77 -H77	178.2(7)	H76 -C76 -C77 -H77	-2.(1)
H76 -C76 -C77 -C78	178.2(7)	H77 -C77 -C78 -C70	-179.3(7)
C76 -C77 -C78 -H78	-179.3(6)	H77 -C77 -C78 -H78	1.(1)
C3 -C81 -C86 -H86	-5.(1)	C3 -C81 -C82 -H82	5.(1)
C82 -C81 -C86 -H86	178.4(8)	C86 -C81 -C82 -H82	-179.1(8)
C81 -C82 -C83 -H83	180.(1)	H82 -C82 -C83 -H83	-1.(2)
H82 -C82 -C83 -C84	180.(1)	C82 -C83 -C84 -H84	-179.(1)
H83 -C83 -C84 -H84	1.(2)	H83 -C83 -C84 -C85	-179.(1)
C83 -C84 -C85 -H85	178.(1)	H84 -C84 -C85 -H85	-2.(2)
H84 -C84 -C85 -C86	178.(1)	H85 -C85 -C86 -C81	-178.1(9)
C84 -C85 -C86 -H86	-178.1(9)	H85 -C85 -C86 -H86	2.(1)
C3 -C91 -C96 -H96	-1.(1)	C3 -C91 -C92 -H92	0.(1)
C92 -C91 -C96 -H96	179.8(7)	C96 -C91 -C92 -H92	179.2(7)
C91 -C92 -C93 -H93	-179.6(8)	H92 -C92 -C93 -H93	0.(1)
H92 -C92 -C93 -C94	-179.6(7)	C92 -C93 -C94 -H94	-179.0(8)
H93 -C93 -C94 -H94	1.(1)	H93 -C93 -C94 -C95	-179.0(8)
C93 -C94 -C95 -H95	178.0(8)	H94 -C94 -C95 -H95	-2.(1)
H94 -C94 -C95 -C96	178.0(8)	H95 -C95 -C96 -C91	-178.5(7)
C94 -C95 -C96 -H96	-178.4(7)	H95 -C95 -C96 -H96	2.(1)

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Table 9. Slip parameter Δ^a , selected bond length [Å], selected angles, FA^a , HA^a , CA^a , DA^a [°].

Δ			0.095(4)
Os	-C*		1.950(5)
C*	-Os	-C1	123.1(2)
C*	-Os	-P1	122.2(1)
C*	-Os	-P2	120.6(2)
FA			172.1(3)
HA			174.7(3)
CA			9.4(2)
DA			16.8(2)

C* = CENTROID (C70, C71, C72, C73, C74)

C** = CENTROID (C70, C74, C75, C76, C77, C78)

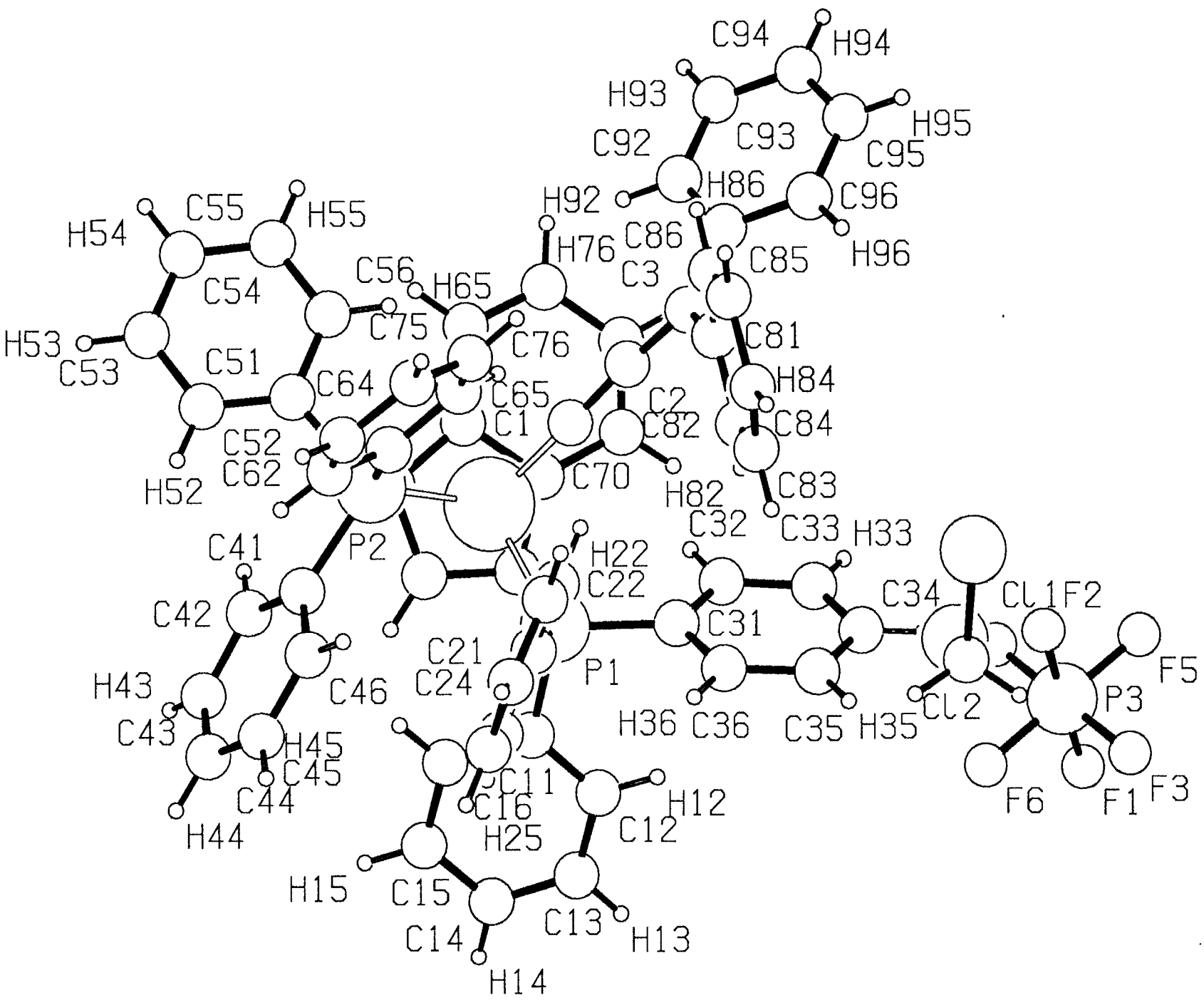
^a $\Delta = d [\text{Os} - \text{C74}, \text{C70}] - d [\text{Os} - \text{C71}, \text{C73}]$

Fold angle (FA) = angle between normals to least-squares planes defined by C71, C72, C73 and C70, C74, C75, C76, C77, C78.

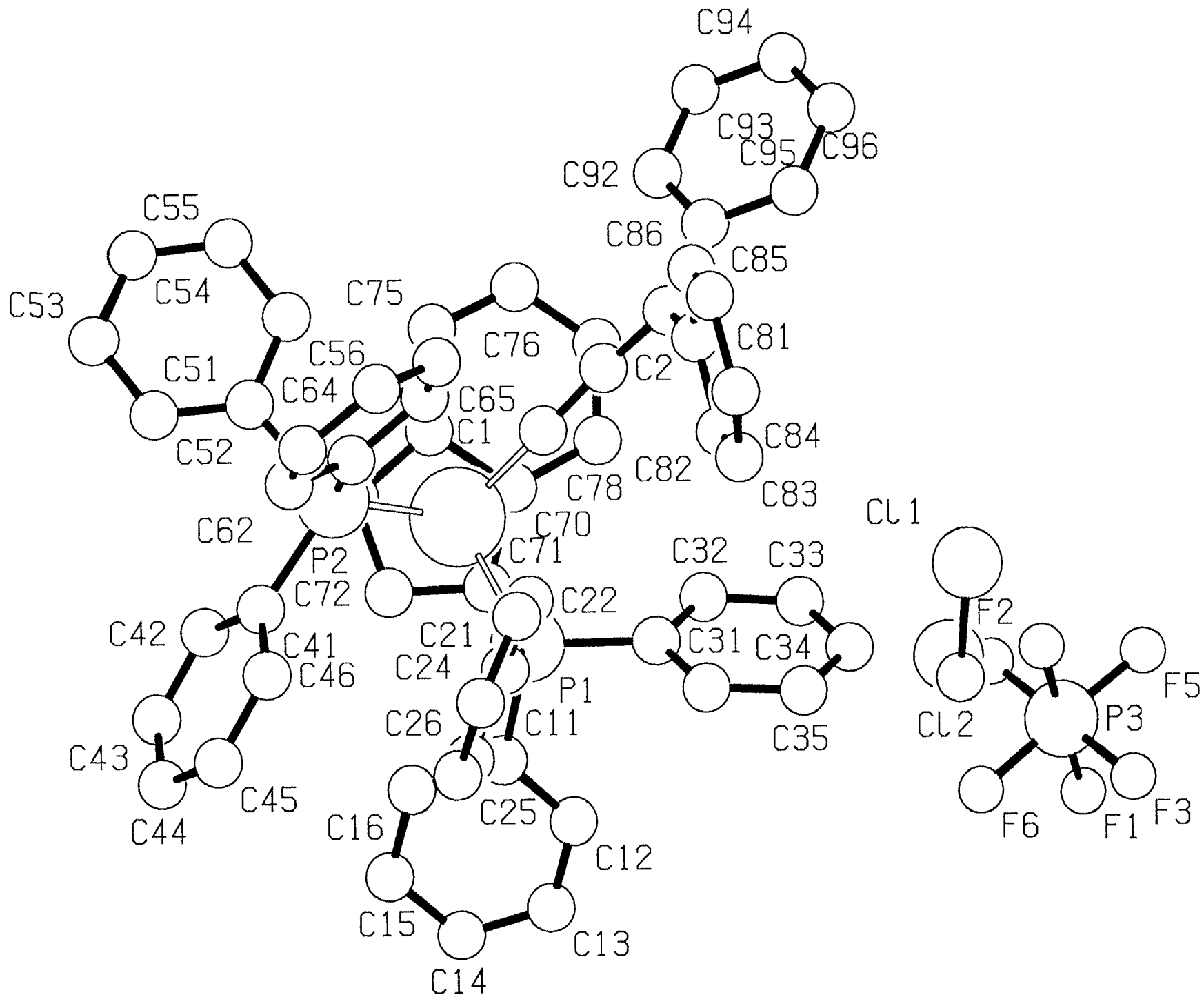
Hinge angle (HA) = angle between normals to least-squares planes defined by C71, C72, C73 and C71, C74, C70, C73.

Conformational angle (CA) = angle between normals to least-squares planes defined by C**, C*, Os and C*, Os, C1.

Dihedral angle (DA) = angle between normals to least-squares planes defined by C*, Os, C1 and C1, C2, C3, C81, C91.



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Ca14246