

C10	C11	C12	C13	1.5(6)	.	.	.	.	?
C11	C12	C13	C14	-1.1(6)	.	.	.	.	?
C12	C13	C14	C15	-0.2(6)	.	.	.	.	?
C13	C14	C15	C10	1.0(6)	.	.	.	.	?
P2	C16	C17	C18	-176.6(6)	.	.	.	.	?
P2	C16	C21	C20	178.9(6)	.	.	.	.	?
C21	C16	C17	C18	53.4(5)	.	.	.	.	?
C17	C16	C21	C20	-54.6(5)	.	.	.	.	?
C16	C17	C18	C19	-52.7(6)	.	.	.	.	?
C17	C18	C19	C20	53.2(6)	.	.	.	.	?
C18	C19	C20	C21	-55.8(7)	.	.	.	.	?
C19	C20	C21	C16	56.5(6)	.	.	.	.	?
P2	C22	C23	C24	176.0(5)	.	.	.	.	?
P2	C22	C27	C26	-176.4(5)	.	.	.	.	?
C27	C22	C23	C24	-55.5(4)	.	.	.	.	?
C23	C22	C27	C26	55.9(5)	.	.	.	.	?
C22	C23	C24	C25	57.1(5)	.	.	.	.	?
C23	C24	C25	C26	-57.2(5)	.	.	.	.	?
C24	C25	C26	C27	56.7(5)	.	.	.	.	?
C25	C26	C27	C22	-57.2(5)	.	.	.	.	?
P2	C28	C29	P3	-38.2(3)	.	.	.	.	?
P3	C30	C31	C32	178.5(5)	.	.	.	.	?
P3	C30	C35	C34	179.5(5)	.	.	.	.	?
C35	C30	C31	C32	53.3(4)	.	.	.	.	?
C31	C30	C35	C34	-54.7(4)	.	.	.	.	?
C30	C31	C32	C33	-54.6(5)	.	.	.	.	?
C31	C32	C33	C34	56.4(5)	.	.	.	.	?
C32	C33	C34	C35	-58.1(5)	.	.	.	.	?
C33	C34	C35	C30	57.5(4)	.	.	.	.	?
P3	C36	C37	C38	177.1(5)	.	.	.	.	?
P3	C36	C41	C40	-173.1(5)	.	.	.	.	?
C41	C36	C37	C38	-55.7(4)	.	.	.	.	?
C37	C36	C41	C40	57.4(4)	.	.	.	.	?
C36	C37	C38	C39	55.0(4)	.	.	.	.	?
C37	C38	C39	C40	-54.1(4)	.	.	.	.	?
C38	C39	C40	C41	55.1(4)	.	.	.	.	?
C39	C40	C41	C36	-57.5(4)	.	.	.	.	?
Ni1	P2	C16	H16	-170.4(5)	.	.	.	.	?
Ni1	P2	C22	H22	70.7(3)	.	.	.	.	?
Ni1	P2	C28	H28A	152.8(4)	.	.	.	.	?
Ni1	P2	C28	H28B	-88.1(4)	.	.	.	.	?
C22	P2	C16	H16	-40.2(4)	.	.	.	.	?
C16	P2	C22	H22	-61.7(4)	.	.	.	.	?
C28	P2	C16	H16	69.1(4)	.	.	.	.	?
C16	P2	C28	H28A	-78.5(4)	.	.	.	.	?
C16	P2	C28	H28B	40.7(4)	.	.	.	.	?
C28	P2	C22	H22	-171.1(4)	.	.	.	.	?
C22	P2	C28	H28A	28.3(4)	.	.	.	.	?
C22	P2	C28	H28B	147.4(4)	.	.	.	.	?
Ni1	P3	C29	H29A	149.8(4)	.	.	.	.	?
Ni1	P3	C29	H29B	-91.3(3)	.	.	.	.	?
Ni1	P3	C30	H30	-176.3(4)	.	.	.	.	?
Ni1	P3	C36	H36	-66.6(3)	.	.	.	.	?
C29	P3	C30	H30	-56.0(3)	.	.	.	.	?
C30	P3	C29	H29A	23.9(3)	.	.	.	.	?
C30	P3	C29	H29B	142.8(4)	.	.	.	.	?
C29	P3	C36	H36	172.7(4)	.	.	.	.	?
C36	P3	C29	H29A	-84.2(4)	.	.	.	.	?

C30	P3	C36	H36	65.5(3)	.	.	.	.	?
Ni1	C1	C2	H2	-11.2(5)	.	.	.	.	?
P1	C1	C2	H2	-177.2(8)	.	.	.	.	?
C1	C2	C3	H3A	-179.7(7)	.	.	.	.	?
C1	C2	C3	H3B	-59.8(5)	.	.	.	.	?
C1	C2	C3	H3C	59.6(5)	.	.	.	.	?
H2	C2	C3	H3A	0.6(4)	.	.	.	.	?
H2	C2	C3	H3B	120.5(6)	.	.	.	.	?
H2	C2	C3	H3C	-120.1(6)	.	.	.	.	?
P1	C4	C5	H5	4.0(4)	.	.	.	.	?
P1	C4	C9	H9	-4.2(5)	.	.	.	.	?
C9	C4	C5	H5	-178.8(8)	.	.	.	.	?
C5	C4	C9	H9	178.5(8)	.	.	.	.	?
C4	C5	C6	H6	178.8(9)	.	.	.	.	?
H5	C5	C6	C7	-180.0(9)	.	.	.	.	?
H5	C5	C6	H6	0.1(6)	.	.	.	.	?
C5	C6	C7	H7	179.0(10)	.	.	.	.	?
H6	C6	C7	C8	179.7(10)	.	.	.	.	?
H6	C6	C7	H7	-1.0(6)	.	.	.	.	?
C6	C7	C8	H8	-178.6(11)	.	.	.	.	?
H7	C7	C8	C9	-178.8(11)	.	.	.	.	?
H7	C7	C8	H8	2.2(7)	.	.	.	.	?
C7	C8	C9	H9	-179.9(10)	.	.	.	.	?
H8	C8	C9	C4	179.9(10)	.	.	.	.	?
H8	C8	C9	H9	-0.9(7)	.	.	.	.	?
P1	C10	C11	H11	-3.3(5)	.	.	.	.	?
P1	C10	C15	H15	1.6(4)	.	.	.	.	?
C15	C10	C11	H11	177.2(8)	.	.	.	.	?
C11	C10	C15	H15	-179.0(7)	.	.	.	.	?
C10	C11	C12	H12	-178.6(10)	.	.	.	.	?
H11	C11	C12	C13	-176.4(10)	.	.	.	.	?
H11	C11	C12	H12	3.5(7)	.	.	.	.	?
C11	C12	C13	H13	-179.0(11)	.	.	.	.	?
H12	C12	C13	C14	179.1(11)	.	.	.	.	?
H12	C12	C13	H13	1.2(7)	.	.	.	.	?
C12	C13	C14	H14	179.4(10)	.	.	.	.	?
H13	C13	C14	C15	177.8(10)	.	.	.	.	?
H13	C13	C14	H14	-2.6(6)	.	.	.	.	?
C13	C14	C15	H15	179.4(9)	.	.	.	.	?
H14	C14	C15	C10	-178.6(9)	.	.	.	.	?
H14	C14	C15	H15	-0.2(6)	.	.	.	.	?
P2	C16	C17	H17A	-53.2(4)	.	.	.	.	?
P2	C16	C17	H17B	64.6(4)	.	.	.	.	?
P2	C16	C21	H21A	-60.7(5)	.	.	.	.	?
P2	C16	C21	H21B	58.6(5)	.	.	.	.	?
C21	C16	C17	H17A	176.8(6)	.	.	.	.	?
C21	C16	C17	H17B	-65.4(5)	.	.	.	.	?
C17	C16	C21	H21A	65.7(6)	.	.	.	.	?
C17	C16	C21	H21B	-175.0(7)	.	.	.	.	?
H16	C16	C17	C18	-59.2(5)	.	.	.	.	?
H16	C16	C17	H17A	64.2(5)	.	.	.	.	?
H16	C16	C17	H17B	-178.0(6)	.	.	.	.	?
H16	C16	C21	C20	59.6(5)	.	.	.	.	?
H16	C16	C21	H21A	180.0(7)	.	.	.	.	?
H16	C16	C21	H21B	-60.8(6)	.	.	.	.	?
C16	C17	C18	H18A	68.8(6)	.	.	.	.	?
C16	C17	C18	H18B	-172.1(8)	.	.	.	.	?
H17A	C17	C18	C19	-174.6(8)	.	.	.	.	?

H17B	C17	C18	C19	65.0(6)	.	.	.	.	?
H17B	C17	C18	H18A	-173.6(8)	.	.	.	.	?
H17B	C17	C18	H18B	-54.5(6)	.	.	.	.	?
C17	C18	C19	H19A	-67.1(7)	.	.	.	.	?
C17	C18	C19	H19B	173.9(9)	.	.	.	.	?
H18A	C18	C19	C20	-67.3(7)	.	.	.	.	?
H18A	C18	C19	H19A	172.4(10)	.	.	.	.	?
H18A	C18	C19	H19B	53.3(8)	.	.	.	.	?
H18B	C18	C19	C20	173.3(9)	.	.	.	.	?
H18B	C18	C19	H19A	53.1(8)	.	.	.	.	?
H18B	C18	C19	H19B	-66.0(8)	.	.	.	.	?
C18	C19	C20	H20A	-174.7(9)	.	.	.	.	?
C18	C19	C20	H20B	66.3(7)	.	.	.	.	?
H19A	C19	C20	C21	64.1(7)	.	.	.	.	?
H19A	C19	C20	H20A	-54.8(7)	.	.	.	.	?
H19A	C19	C20	H20B	-173.8(10)	.	.	.	.	?
H19B	C19	C20	C21	-176.0(9)	.	.	.	.	?
H19B	C19	C20	H20A	65.1(8)	.	.	.	.	?
H19B	C19	C20	H20B	-54.0(7)	.	.	.	.	?
C19	C20	C21	H21A	-63.1(7)	.	.	.	.	?
C19	C20	C21	H21B	176.7(8)	.	.	.	.	?
H20A	C20	C21	C16	174.3(8)	.	.	.	.	?
H20A	C20	C21	H21A	54.7(6)	.	.	.	.	?
H20A	C20	C21	H21B	-65.5(7)	.	.	.	.	?
H20B	C20	C21	C16	-66.4(6)	.	.	.	.	?
H20B	C20	C21	H21A	173.9(8)	.	.	.	.	?
H20B	C20	C21	H21B	53.8(6)	.	.	.	.	?
P2	C22	C23	H23A	-63.9(4)	.	.	.	.	?
P2	C22	C23	H23B	55.3(4)	.	.	.	.	?
P2	C22	C27	H27A	-54.9(4)	.	.	.	.	?
P2	C22	C27	H27B	63.6(4)	.	.	.	.	?
C27	C22	C23	H23A	64.6(5)	.	.	.	.	?
C27	C22	C23	H23B	-176.2(5)	.	.	.	.	?
C23	C22	C27	H27A	177.4(6)	.	.	.	.	?
C23	C22	C27	H27B	-64.1(5)	.	.	.	.	?
H22	C22	C23	C24	57.0(4)	.	.	.	.	?
H22	C22	C23	H23A	177.1(5)	.	.	.	.	?
H22	C22	C23	H23B	-63.8(5)	.	.	.	.	?
H22	C22	C27	C26	-57.1(5)	.	.	.	.	?
H22	C22	C27	H27A	64.3(5)	.	.	.	.	?
H22	C22	C27	H27B	-177.1(6)	.	.	.	.	?
C22	C23	C24	H24A	177.8(6)	.	.	.	.	?
C22	C23	C24	H24B	-62.1(5)	.	.	.	.	?
H23A	C23	C24	C25	-62.8(5)	.	.	.	.	?
H23A	C23	C24	H24A	58.0(5)	.	.	.	.	?
H23A	C23	C24	H24B	178.1(6)	.	.	.	.	?
H23B	C23	C24	C25	177.5(6)	.	.	.	.	?
H23B	C23	C24	H24A	-61.7(5)	.	.	.	.	?
H23B	C23	C24	H24B	58.4(5)	.	.	.	.	?
C23	C24	C25	H25A	61.7(5)	.	.	.	.	?
C23	C24	C25	H25B	-179.1(7)	.	.	.	.	?
H24A	C24	C25	C26	-178.2(7)	.	.	.	.	?
H24A	C24	C25	H25A	-59.3(6)	.	.	.	.	?
H24A	C24	C25	H25B	59.8(6)	.	.	.	.	?
H24B	C24	C25	C26	62.4(5)	.	.	.	.	?
H24B	C24	C25	H25A	-178.7(7)	.	.	.	.	?
H24B	C24	C25	H25B	-59.6(6)	.	.	.	.	?
H24B	C24	C25	H26A	-62.7(5)	.	.	.	.	?

H25A	C25	C26	H26A	179.3(7)	.	.	.	.	?
H25A	C25	C26	H26B	59.6(5)	.	.	.	.	?
H25B	C25	C26	C27	178.6(7)	.	.	.	.	?
H25B	C25	C26	H26A	59.2(6)	.	.	.	.	?
H25B	C25	C26	H26B	-60.6(6)	.	.	.	.	?
C25	C26	C27	H27A	-178.1(6)	.	.	.	.	?
C25	C26	C27	H27B	62.2(5)	.	.	.	.	?
H26A	C26	C27	C22	62.3(5)	.	.	.	.	?
H26A	C26	C27	H27A	-58.5(5)	.	.	.	.	?
H26A	C26	C27	H27B	-178.3(7)	.	.	.	.	?
H26B	C26	C27	C22	-177.9(6)	.	.	.	.	?
H26B	C26	C27	H27A	61.2(5)	.	.	.	.	?
H26B	C26	C27	H27B	-58.5(5)	.	.	.	.	?
P2	C28	C29	H29A	-159.0(5)	.	.	.	.	?
P2	C28	C29	H29B	80.8(4)	.	.	.	.	?
H28A	C28	C29	P3	-158.7(5)	.	.	.	.	?
H28A	C28	C29	H29A	80.5(5)	.	.	.	.	?
H28A	C28	C29	H29B	-39.7(4)	.	.	.	.	?
H28B	C28	C29	P3	81.8(4)	.	.	.	.	?
H28B	C28	C29	H29A	-39.1(4)	.	.	.	.	?
H28B	C28	C29	H29B	-159.2(5)	.	.	.	.	?
P3	C30	C31	H31A	-59.6(4)	.	.	.	.	?
P3	C30	C31	H31B	59.4(4)	.	.	.	.	?
P3	C30	C35	H35A	57.3(4)	.	.	.	.	?
P3	C30	C35	H35B	-61.6(4)	.	.	.	.	?
C35	C30	C31	H31A	175.2(5)	.	.	.	.	?
C35	C30	C31	H31B	-65.8(4)	.	.	.	.	?
C31	C30	C35	H35A	-176.8(5)	.	.	.	.	?
C31	C30	C35	H35B	64.2(4)	.	.	.	.	?
H30	C30	C31	C32	-62.5(4)	.	.	.	.	?
H30	C30	C31	H31A	59.4(4)	.	.	.	.	?
H30	C30	C31	H31B	178.4(5)	.	.	.	.	?
H30	C30	C35	C34	60.9(4)	.	.	.	.	?
H30	C30	C35	H35A	-61.2(4)	.	.	.	.	?
H30	C30	C35	H35B	179.8(5)	.	.	.	.	?
C30	C31	C32	H32A	64.0(5)	.	.	.	.	?
C30	C31	C32	H32B	-177.0(6)	.	.	.	.	?
H31A	C31	C32	C33	-176.4(6)	.	.	.	.	?
H31A	C31	C32	H32A	-57.7(5)	.	.	.	.	?
H31A	C31	C32	H32B	61.2(5)	.	.	.	.	?
H31B	C31	C32	C33	64.2(5)	.	.	.	.	?
H31B	C31	C32	H32A	-177.2(6)	.	.	.	.	?
H31B	C31	C32	H32B	-58.2(5)	.	.	.	.	?
C31	C32	C33	H33A	-62.2(5)	.	.	.	.	?
C31	C32	C33	H33B	178.2(7)	.	.	.	.	?
H32A	C32	C33	C34	-61.9(5)	.	.	.	.	?
H32A	C32	C33	H33A	179.5(7)	.	.	.	.	?
H32A	C32	C33	H33B	59.8(5)	.	.	.	.	?
H32B	C32	C33	C34	178.5(6)	.	.	.	.	?
H32B	C32	C33	H33A	59.9(5)	.	.	.	.	?
H32B	C32	C33	H33B	-59.7(6)	.	.	.	.	?
C32	C33	C34	H34A	-178.7(6)	.	.	.	.	?
C32	C33	C34	H34B	61.7(5)	.	.	.	.	?
H33A	C33	C34	C35	60.4(5)	.	.	.	.	?
H33A	C33	C34	H34A	-60.2(5)	.	.	.	.	?
H33A	C33	C34	H34B	-179.8(7)	.	.	.	.	?
H33B	C33	C34	C35	-179.8(6)	.	.	.	.	?
H33B	C33	C34	H34A	59.6(5)	.	.	.	.	?

C33	C34	C35	H35B	-60.9(5)	.	.	.	.	?
H34A	C34	C35	C30	178.3(6)	.	.	.	.	?
H34A	C34	C35	H35A	-60.1(5)	.	.	.	.	?
H34A	C34	C35	H35B	59.9(5)	.	.	.	.	?
H34B	C34	C35	C30	-62.1(5)	.	.	.	.	?
H34B	C34	C35	H35A	59.4(5)	.	.	.	.	?
H34B	C34	C35	H35B	179.4(6)	.	.	.	.	?
P3	C36	C37	H37A	-63.8(4)	.	.	.	.	?
P3	C36	C37	H37B	55.4(4)	.	.	.	.	?
P3	C36	C41	H41A	-52.3(4)	.	.	.	.	?
P3	C36	C41	H41B	66.4(4)	.	.	.	.	?
C41	C36	C37	H37A	63.3(4)	.	.	.	.	?
C41	C36	C37	H37B	-177.5(5)	.	.	.	.	?
C37	C36	C41	H41A	178.2(5)	.	.	.	.	?
C37	C36	C41	H41B	-63.2(4)	.	.	.	.	?
H36	C36	C37	C38	57.8(4)	.	.	.	.	?
H36	C36	C37	H37A	176.9(5)	.	.	.	.	?
H36	C36	C37	H37B	-63.9(4)	.	.	.	.	?
H36	C36	C41	C40	-54.2(4)	.	.	.	.	?
H36	C36	C41	H41A	66.7(4)	.	.	.	.	?
H36	C36	C41	H41B	-174.7(5)	.	.	.	.	?
C36	C37	C38	H38A	-64.3(5)	.	.	.	.	?
C36	C37	C38	H38B	175.9(6)	.	.	.	.	?
H37A	C37	C38	C39	-64.1(5)	.	.	.	.	?
H37A	C37	C38	H38A	176.7(6)	.	.	.	.	?
H37A	C37	C38	H38B	56.9(5)	.	.	.	.	?
H37B	C37	C38	C39	176.5(6)	.	.	.	.	?
H37B	C37	C38	H38A	57.3(5)	.	.	.	.	?
H37B	C37	C38	H38B	-62.6(5)	.	.	.	.	?
C37	C38	C39	H39A	66.6(5)	.	.	.	.	?
C37	C38	C39	H39B	-174.4(6)	.	.	.	.	?
H38A	C38	C39	C40	65.3(5)	.	.	.	.	?
H38A	C38	C39	H39A	-174.0(6)	.	.	.	.	?
H38A	C38	C39	H39B	-55.0(5)	.	.	.	.	?
H38B	C38	C39	C40	-176.3(6)	.	.	.	.	?
H38B	C38	C39	H39A	-55.6(5)	.	.	.	.	?
H38B	C38	C39	H39B	63.4(5)	.	.	.	.	?
C38	C39	C40	H40A	-65.4(5)	.	.	.	.	?
C38	C39	C40	H40B	174.5(6)	.	.	.	.	?
H39A	C39	C40	C41	-64.6(5)	.	.	.	.	?
H39A	C39	C40	H40A	174.9(6)	.	.	.	.	?
H39A	C39	C40	H40B	54.8(5)	.	.	.	.	?
H39B	C39	C40	C41	175.3(6)	.	.	.	.	?
H39B	C39	C40	H40A	54.8(5)	.	.	.	.	?
H39B	C39	C40	H40B	-65.3(5)	.	.	.	.	?
C39	C40	C41	H41A	-177.3(6)	.	.	.	.	?
C39	C40	C41	H41B	62.4(5)	.	.	.	.	?
H40A	C40	C41	C36	63.4(5)	.	.	.	.	?
H40A	C40	C41	H41A	-56.4(5)	.	.	.	.	?
H40A	C40	C41	H41B	-176.7(6)	.	.	.	.	?
H40B	C40	C41	C36	-177.5(6)	.	.	.	.	?
H40B	C40	C41	H41A	62.7(5)	.	.	.	.	?
H40B	C40	C41	H41B	-57.6(5)	.	.	.	.	?

_geom_special_details

All standard uncertainties (except dihedral angles between l.s. planes) are estimated using the full covariance matrix.

angles and torsion angles. Angles between l.s. planes have standard uncertainties calculated from atomic positional standard uncertainties; the errors in cell dimensions are not used in this case.

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Ni1	P1	2.1860(10) . . ?
Ni1	P2	2.2270(10) . . ?
Ni1	P3	2.1700(10) . . ?
Ni1	C1	1.903(4) . . ?
P1	C1	1.747(4) . . ?
P1	C4	1.818(4) . . ?
P1	C10	1.821(4) . . ?
P2	C16	1.844(4) . . ?
P2	C22	1.851(4) . . ?
P2	C28	1.838(4) . . ?
P3	C29	1.840(4) . . ?
P3	C30	1.851(4) . . ?
P3	C36	1.841(4) . . ?
C1	C2	1.324(5) . . ?
C2	C3	1.500(6) . . ?
C4	C5	1.387(6) . . ?
C4	C9	1.385(6) . . ?
C5	C6	1.392(6) . . ?
C6	C7	1.360(8) . . ?
C7	C8	1.363(9) . . ?
C8	C9	1.395(8) . . ?
C10	C11	1.393(6) . . ?
C10	C15	1.372(6) . . ?
C11	C12	1.383(8) . . ?
C12	C13	1.347(8) . . ?
C13	C14	1.373(8) . . ?
C14	C15	1.387(6) . . ?
C16	C17	1.519(7) . . ?
C16	C21	1.508(7) . . ?
C17	C18	1.530(7) . . ?
C18	C19	1.489(10) . . ?
C19	C20	1.500(10) . . ?
C20	C21	1.530(8) . . ?
C22	C23	1.519(6) . . ?
C22	C27	1.530(6) . . ?
C23	C24	1.535(6) . . ?
C24	C25	1.520(7) . . ?
C25	C26	1.487(7) . . ?
C26	C27	1.520(6) . . ?
C28	C29	1.528(6) . . ?
C30	C31	1.530(6) . . ?
C30	C35	1.538(5) . . ?
C31	C32	1.523(6) . . ?
C32	C33	1.514(7) . . ?
C33	C34	1.513(7) . . ?

C36	C41	1.528(5)	. . ?
C37	C38	1.517(6)	. . ?
C38	C39	1.511(6)	. . ?
C39	C40	1.522(6)	. . ?
C40	C41	1.521(6)	. . ?
C2	H2	0.960(4)	. . ?
C3	H3A	0.960(4)	. . ?
C3	H3B	0.960(5)	. . ?
C3	H3C	0.959(5)	. . ?
C5	H5	0.960(5)	. . ?
C6	H6	0.959(6)	. . ?
C7	H7	0.960(5)	. . ?
C8	H8	0.960(6)	. . ?
C9	H9	0.960(6)	. . ?
C11	H11	0.961(6)	. . ?
C12	H12	0.959(6)	. . ?
C13	H13	0.960(5)	. . ?
C14	H14	0.960(6)	. . ?
C15	H15	0.960(5)	. . ?
C16	H16	0.959(4)	. . ?
C17	H17A	0.960(5)	. . ?
C17	H17B	0.961(5)	. . ?
C18	H18A	0.961(6)	. . ?
C18	H18B	0.959(8)	. . ?
C19	H19A	0.960(6)	. . ?
C19	H19B	0.960(6)	. . ?
C20	H20A	0.960(7)	. . ?
C20	H20B	0.960(5)	. . ?
C21	H21A	0.960(5)	. . ?
C21	H21B	0.960(6)	. . ?
C22	H22	0.960(4)	. . ?
C23	H23A	0.960(4)	. . ?
C23	H23B	0.960(4)	. . ?
C24	H24A	0.960(5)	. . ?
C24	H24B	0.959(5)	. . ?
C25	H25A	0.961(5)	. . ?
C25	H25B	0.960(4)	. . ?
C26	H26A	0.958(5)	. . ?
C26	H26B	0.960(5)	. . ?
C27	H27A	0.960(5)	. . ?
C27	H27B	0.960(6)	. . ?
C28	H28A	0.961(4)	. . ?
C28	H28B	0.960(4)	. . ?
C29	H29A	0.959(4)	. . ?
C29	H29B	0.961(4)	. . ?
C30	H30	0.960(4)	. . ?
C31	H31A	0.961(4)	. . ?
C31	H31B	0.960(4)	. . ?
C32	H32A	0.961(5)	. . ?
C32	H32B	0.960(5)	. . ?
C33	H33A	0.959(5)	. . ?
C33	H33B	0.960(4)	. . ?
C34	H34A	0.959(4)	. . ?
C34	H34B	0.960(5)	. . ?
C35	H35A	0.960(4)	. . ?
C35	H35B	0.961(4)	. . ?
C36	H36	0.960(4)	. . ?
C37	H37	0.960(4)	. . ?

C38	H38B	0.960(4)	. . ?
C39	H39A	0.961(4)	. . ?
C39	H39B	0.960(4)	. . ?
C40	H40A	0.959(4)	. . ?
C40	H40B	0.960(5)	. . ?
C41	H41A	0.961(4)	. . ?
C41	H41B	0.960(4)	. . ?

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P1	Ni1	P2	112.60(10)	. . . ?
P1	Ni1	P3	136.20(10)	. . . ?
P1	Ni1	C1	50.0(2)	. . . ?
P2	Ni1	P3	88.90(10)	. . . ?
P2	Ni1	C1	158.7(2)	. . . ?
P3	Ni1	C1	97.8(2)	. . . ?
Ni1	P1	C1	56.6(2)	. . . ?
Ni1	P1	C4	125.4(2)	. . . ?
Ni1	P1	C10	129.2(2)	. . . ?
C1	P1	C4	112.4(2)	. . . ?
C1	P1	C10	113.9(2)	. . . ?
C4	P1	C10	104.8(2)	. . . ?
Ni1	P2	C16	120.1(2)	. . . ?
Ni1	P2	C22	116.5(2)	. . . ?
Ni1	P2	C28	107.0(2)	. . . ?
C16	P2	C22	101.6(2)	. . . ?
C16	P2	C28	105.1(3)	. . . ?
C22	P2	C28	105.1(2)	. . . ?
Ni1	P3	C29	109.4(2)	. . . ?
Ni1	P3	C30	117.8(2)	. . . ?
Ni1	P3	C36	117.5(2)	. . . ?
C29	P3	C30	102.8(2)	. . . ?
C29	P3	C36	103.5(2)	. . . ?
C30	P3	C36	103.9(2)	. . . ?
Ni1	C1	P1	73.5(2)	. . . ?
Ni1	C1	C2	148.5(4)	. . . ?
P1	C1	C2	137.4(4)	. . . ?
C1	C2	C3	125.8(4)	. . . ?
P1	C4	C5	122.5(4)	. . . ?
P1	C4	C9	118.6(4)	. . . ?
C5	C4	C9	118.9(5)	. . . ?
C4	C5	C6	120.7(5)	. . . ?
C5	C6	C7	119.4(6)	. . . ?
C6	C7	C8	120.8(6)	. . . ?
C7	C8	C9	120.5(6)	. . . ?
C4	C9	C8	119.5(6)	. . . ?
P1	C10	C11	121.0(4)	. . . ?
P1	C10	C15	120.8(4)	. . . ?
C11	C10	C15	118.2(5)	. . . ?
C10	C11	C12	120.3(6)	. . . ?

C13	C14	C15	119.4(6)	. . . ?
C10	C15	C14	121.1(5)	. . . ?
P2	C16	C17	109.7(4)	. . . ?
P2	C16	C21	116.3(4)	. . . ?
C17	C16	C21	111.1(4)	. . . ?
C16	C17	C18	112.4(6)	. . . ?
C17	C18	C19	112.1(6)	. . . ?
C18	C19	C20	111.3(6)	. . . ?
C19	C20	C21	112.3(5)	. . . ?
C16	C21	C20	110.4(6)	. . . ?
P2	C22	C23	113.1(3)	. . . ?
P2	C22	C27	114.5(3)	. . . ?
C23	C22	C27	108.9(4)	. . . ?
C22	C23	C24	111.2(4)	. . . ?
C23	C24	C25	110.8(4)	. . . ?
C24	C25	C26	110.7(4)	. . . ?
C25	C26	C27	110.7(5)	. . . ?
C22	C27	C26	112.5(4)	. . . ?
P2	C28	C29	111.7(3)	. . . ?
P3	C29	C28	111.0(3)	. . . ?
P3	C30	C31	112.5(3)	. . . ?
P3	C30	C35	111.3(3)	. . . ?
C31	C30	C35	110.6(4)	. . . ?
C30	C31	C32	111.9(4)	. . . ?
C31	C32	C33	111.6(4)	. . . ?
C32	C33	C34	110.5(4)	. . . ?
C33	C34	C35	111.1(4)	. . . ?
C30	C35	C34	110.9(4)	. . . ?
P3	C36	C37	115.9(3)	. . . ?
P3	C36	C41	111.6(3)	. . . ?
C37	C36	C41	109.4(4)	. . . ?
C36	C37	C38	111.6(4)	. . . ?
C37	C38	C39	112.1(4)	. . . ?
C38	C39	C40	111.3(4)	. . . ?
C39	C40	C41	110.7(4)	. . . ?
C36	C41	C40	111.4(4)	. . . ?
C1	C2	H2	119.1(4)	. . . ?
C3	C2	H2	115.1(4)	. . . ?
C2	C3	H3A	110.5(5)	. . . ?
C2	C3	H3B	108.3(4)	. . . ?
C2	C3	H3C	109.4(5)	. . . ?
H3A	C3	H3B	109.5(5)	. . . ?
H3A	C3	H3C	109.5(5)	. . . ?
H3B	C3	H3C	109.6(5)	. . . ?
C4	C5	H5	119.5(5)	. . . ?
C6	C5	H5	119.8(6)	. . . ?
C5	C6	H6	120.5(7)	. . . ?
C7	C6	H6	120.1(6)	. . . ?
C6	C7	H7	117.9(8)	. . . ?
C8	C7	H7	121.3(8)	. . . ?
C7	C8	H8	118.8(7)	. . . ?
C9	C8	H8	120.7(8)	. . . ?
C4	C9	H9	121.1(5)	. . . ?
C8	C9	H9	119.3(6)	. . . ?
C10	C11	H11	120.4(5)	. . . ?
C12	C11	H11	119.3(6)	. . . ?
C11	C12	H12	120.9(8)	. . . ?
C13	C12	H12	118.6(7)	. . . ?

C13	C14	H14	118.9(6)	.	.	.	?
C15	C14	H14	121.8(7)	.	.	.	?
C10	C15	H15	119.0(5)	.	.	.	?
C14	C15	H15	119.9(6)	.	.	.	?
P2	C16	H16	108.6(4)	.	.	.	?
C17	C16	H16	106.5(5)	.	.	.	?
C21	C16	H16	104.0(5)	.	.	.	?
C16	C17	H17A	108.6(5)	.	.	.	?
C16	C17	H17B	106.6(5)	.	.	.	?
C18	C17	H17A	111.1(5)	.	.	.	?
C18	C17	H17B	108.5(5)	.	.	.	?
H17A	C17	H17B	109.5(6)	.	.	.	?
C17	C18	H18A	108.3(5)	.	.	.	?
C17	C18	H18B	109.1(7)	.	.	.	?
C19	C18	H18A	109.9(8)	.	.	.	?
C19	C18	H18B	108.0(6)	.	.	.	?
H18A	C18	H18B	109.5(7)	.	.	.	?
C18	C19	H19A	108.6(8)	.	.	.	?
C18	C19	H19B	108.8(8)	.	.	.	?
C20	C19	H19A	109.2(8)	.	.	.	?
C20	C19	H19B	109.4(8)	.	.	.	?
H19A	C19	H19B	109.5(6)	.	.	.	?
C19	C20	H20A	106.8(6)	.	.	.	?
C19	C20	H20B	110.6(8)	.	.	.	?
C21	C20	H20A	108.6(7)	.	.	.	?
C21	C20	H20B	109.1(6)	.	.	.	?
H20A	C20	H20B	109.5(6)	.	.	.	?
C16	C21	H21A	108.6(5)	.	.	.	?
C16	C21	H21B	109.2(5)	.	.	.	?
C20	C21	H21A	109.8(5)	.	.	.	?
C20	C21	H21B	109.5(5)	.	.	.	?
H21A	C21	H21B	109.4(7)	.	.	.	?
P2	C22	H22	108.8(3)	.	.	.	?
C23	C22	H22	105.9(4)	.	.	.	?
C27	C22	H22	105.0(4)	.	.	.	?
C22	C23	H23A	108.7(4)	.	.	.	?
C22	C23	H23B	108.9(4)	.	.	.	?
C24	C23	H23A	109.1(4)	.	.	.	?
C24	C23	H23B	109.5(5)	.	.	.	?
H23A	C23	H23B	109.4(5)	.	.	.	?
C23	C24	H24A	109.8(5)	.	.	.	?
C23	C24	H24B	109.0(5)	.	.	.	?
C25	C24	H24A	109.2(5)	.	.	.	?
C25	C24	H24B	108.4(5)	.	.	.	?
H24A	C24	H24B	109.6(5)	.	.	.	?
C24	C25	H25A	107.5(5)	.	.	.	?
C24	C25	H25B	109.9(5)	.	.	.	?
C26	C25	H25A	108.9(5)	.	.	.	?
C26	C25	H25B	110.2(5)	.	.	.	?
H25A	C25	H25B	109.5(5)	.	.	.	?
C25	C26	H26A	108.9(5)	.	.	.	?
C25	C26	H26B	109.4(5)	.	.	.	?
C27	C26	H26A	108.6(5)	.	.	.	?
C27	C26	H26B	109.6(5)	.	.	.	?
H26A	C26	H26B	109.6(5)	.	.	.	?
C22	C27	H27A	108.5(5)	.	.	.	?
C22	C27	H27B	107.8(5)	.	.	.	?
C27	C27	H27A	109.6(5)	.	.	.	?

P2	C28	H28A	108.7(4)	.	.	.	?
P2	C28	H28B	108.8(4)	.	.	.	?
C29	C28	H28A	109.6(4)	.	.	.	?
C29	C28	H28B	108.6(4)	.	.	.	?
H28A	C28	H28B	109.5(4)	.	.	.	?
P3	C29	H29A	108.9(3)	.	.	.	?
P3	C29	H29B	108.3(3)	.	.	.	?
C28	C29	H29A	110.4(4)	.	.	.	?
C28	C29	H29B	108.8(4)	.	.	.	?
H29A	C29	H29B	109.5(4)	.	.	.	?
P3	C30	H30	108.7(3)	.	.	.	?
C31	C30	H30	106.5(4)	.	.	.	?
C35	C30	H30	107.0(4)	.	.	.	?
C30	C31	H31A	109.5(4)	.	.	.	?
C30	C31	H31B	107.8(4)	.	.	.	?
C32	C31	H31A	109.7(4)	.	.	.	?
C32	C31	H31B	108.4(4)	.	.	.	?
H31A	C31	H31B	109.4(5)	.	.	.	?
C31	C32	H32A	107.7(5)	.	.	.	?
C31	C32	H32B	109.7(5)	.	.	.	?
C33	C32	H32A	108.3(5)	.	.	.	?
C33	C32	H32B	110.2(5)	.	.	.	?
H32A	C32	H32B	109.4(5)	.	.	.	?
C32	C33	H33A	108.2(5)	.	.	.	?
C32	C33	H33B	110.0(5)	.	.	.	?
C34	C33	H33A	108.5(5)	.	.	.	?
C34	C33	H33B	110.1(5)	.	.	.	?
H33A	C33	H33B	109.5(5)	.	.	.	?
C33	C34	H34A	109.4(5)	.	.	.	?
C33	C34	H34B	108.7(5)	.	.	.	?
C35	C34	H34A	109.2(5)	.	.	.	?
C35	C34	H34B	108.9(5)	.	.	.	?
H34A	C34	H34B	109.5(5)	.	.	.	?
C30	C35	H35A	109.5(4)	.	.	.	?
C30	C35	H35B	107.9(4)	.	.	.	?
C34	C35	H35A	110.5(4)	.	.	.	?
C34	C35	H35B	108.6(4)	.	.	.	?
H35A	C35	H35B	109.4(4)	.	.	.	?
P3	C36	H36	109.0(3)	.	.	.	?
C37	C36	H36	103.7(4)	.	.	.	?
C41	C36	H36	106.7(4)	.	.	.	?
C36	C37	H37A	108.2(4)	.	.	.	?
C36	C37	H37B	109.5(4)	.	.	.	?
C38	C37	H37A	108.3(4)	.	.	.	?
C38	C37	H37B	109.8(4)	.	.	.	?
H37A	C37	H37B	109.4(5)	.	.	.	?
C37	C38	H38A	108.4(4)	.	.	.	?
C37	C38	H38B	110.4(5)	.	.	.	?
C39	C38	H38A	108.1(5)	.	.	.	?
C39	C38	H38B	108.3(4)	.	.	.	?
H38A	C38	H38B	109.4(5)	.	.	.	?
C38	C39	H39A	108.1(5)	.	.	.	?
C38	C39	H39B	108.9(5)	.	.	.	?
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C40	C39	H39B	109.1(5)	.	.	.	?
H39A	C39	H39B	109.5(5)	.	.	.	?
C39	C40	H40A	109.8(5)	.	.	.	?
C39	C40	H40B	109.4(4)	.	.	.	?

H40A	C40	H40B	109.4(5)	. . . ?
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C14	H9	2.910(5)	1_555	2_656 ?
C14	H28B	3.115(5)	1_555	4_566 ?
C14	H29A	2.946(5)	1_555	4_566 ?
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C15	C29	3.662(5)	1_555	4_566 ?
C15	H29A	2.966(4)	1_555	4_566 ?
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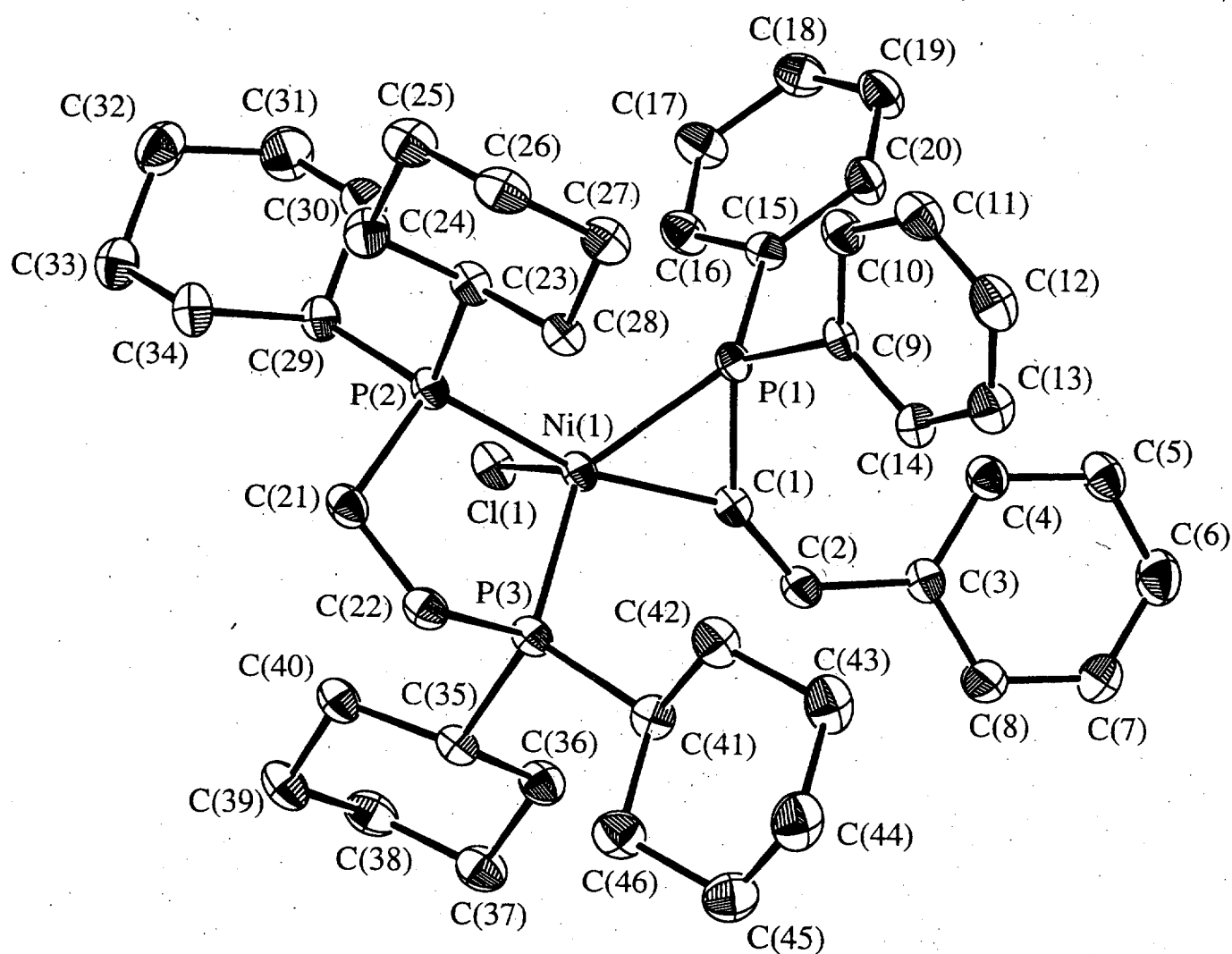
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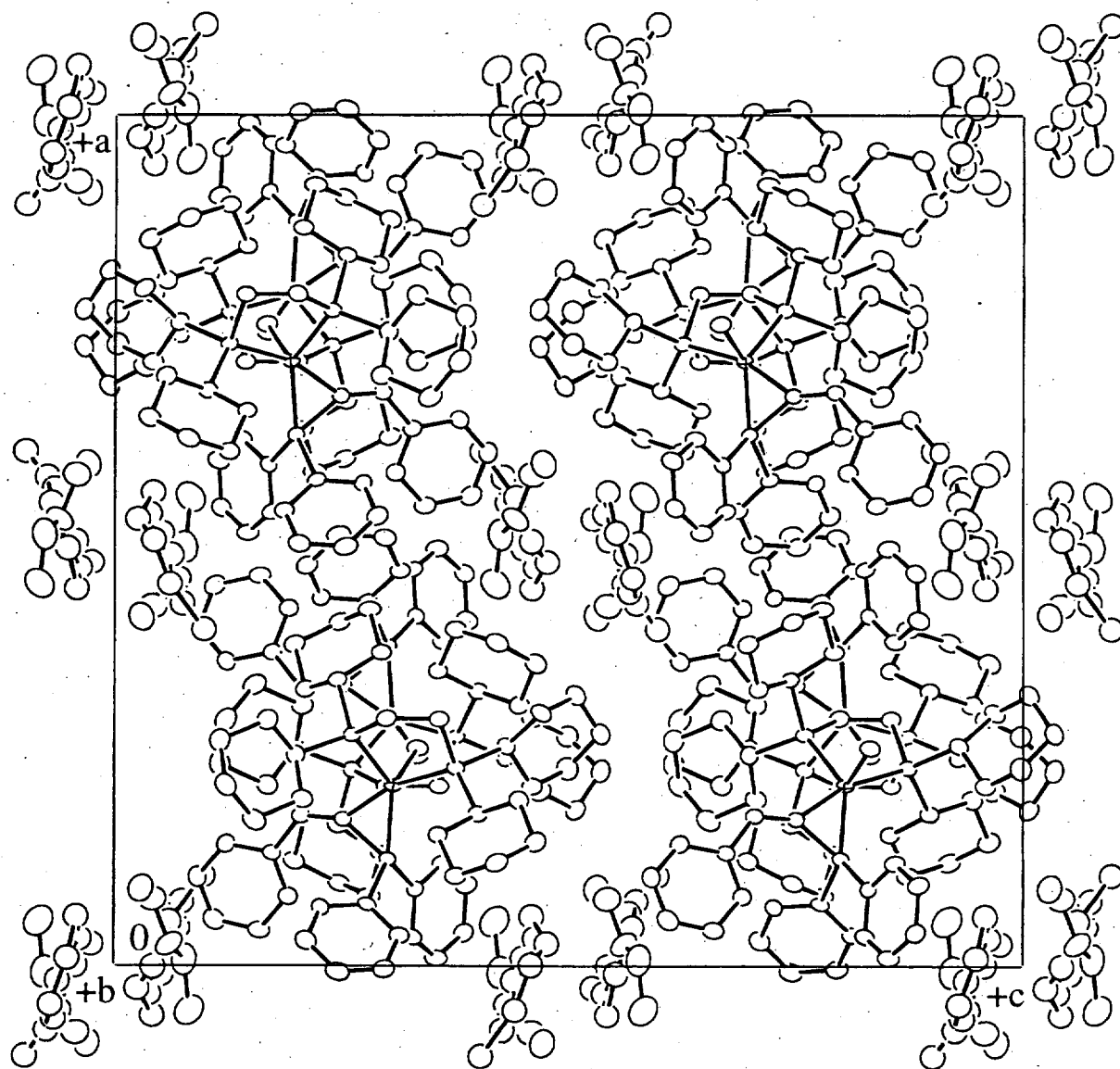
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$(2\text{c}\cdot 1.5\text{C}_4\text{H}_{10}\text{O}\cdot 0.5\text{C}_6\text{D}_6)$





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multi-scan from symmetry-related measurements
Sortav (Blessing 1995)

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CCD data collecting conditions-
psi scan and omega scans of 0.8 deg / frame,
crystal-detector distance 35mm, 110 sec/deg,
multiple scan sets so over 95 percent of data collected with 6-fold
redundancy or more.

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O1	.47482(12)	.09641(18)	.56028(12)	.077(2)	1.0000	Uani	?	?	
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C48	.4828(3)	.1738(3)	.5768(3)	.099(4)	1.0000	Uani	?	?	

C49	.4220(2)	.0883(4)	.5418(2)	.104(4)	1.0000	Uani	?	?
C50	.4095(2)	.0035(5)	.5293(2)	.122(5)	1.0000	Uani	?	?
O10	.0167(2)	.1134(3)	.5618(2)	.0810(8)	0.495(4)	Uiso	?	?
C101	.1052(3)	.1300(5)	.5974(4)	.0810(8)	0.495(4)	Uiso	?	?
C102	.0615(3)	.1684(4)	.5662(4)	.0810(8)	0.495(4)	Uiso	?	?
C103	-.0255(3)	.1311(5)	.5252(3)	.0810(8)	0.495(4)	Uiso	?	?
C104	-.0576(4)	.2056(6)	.5418(4)	.0810(8)	0.495(4)	Uiso	?	?
C201	.0517(3)	.0921(2)	.5600(3)	.0810(8)	0.505(4)	Uiso	?	?
C202	-.0008(3)	.0890(2)	.5425(2)	.0810(8)	0.505(4)	Uiso	?	?
C203	-.0318(2)	.1620(3)	.5381(2)	.0810(8)	0.505(4)	Uiso	?	?
C204	-.0091(2)	.2355(3)	.5515(2)	.0810(8)	0.505(4)	Uiso	?	?
C205	.0449(3)	.2387(3)	.5695(3)	.0810(8)	0.505(4)	Uiso	?	?
C206	.0751(2)	.1678(3)	.5738(3)	.0810(8)	0.505(4)	Uiso	?	?
H1	.28933	.27995	.69093	.10000	1.0000	Uiso	?	?
H2	.42800	.32464	.72655	.10000	1.0000	Uiso	?	?
H3	.49347	.38237	.67257	.10000	1.0000	Uiso	?	?
H4	.47268	.41004	.58752	.10000	1.0000	Uiso	?	?
H5	.38790	.37921	.55589	.10000	1.0000	Uiso	?	?
H6	.32202	.32180	.60854	.10000	1.0000	Uiso	?	?
H7	.46238	.13472	.84909	.10000	1.0000	Uiso	?	?
H8	.52820	.04324	.82137	.10000	1.0000	Uiso	?	?
H9	.53414	.00724	.73505	.10000	1.0000	Uiso	?	?
H10	.47260	.05999	.67618	.10000	1.0000	Uiso	?	?
H11	.40744	.15486	.70257	.10000	1.0000	Uiso	?	?
H12	.34178	.35556	.86328	.10000	1.0000	Uiso	?	?
H13	.38463	.46164	.90682	.10000	1.0000	Uiso	?	?
H14	.47871	.47798	.90182	.10000	1.0000	Uiso	?	?
H15	.52902	.38877	.85110	.10000	1.0000	Uiso	?	?
H16	.48724	.28298	.80703	.10000	1.0000	Uiso	?	?
H17	.21361	.00406	.87497	.10000	1.0000	Uiso	?	?
H18	.17752	.08006	.86557	.10000	1.0000	Uiso	?	?
H19	.17425	.01924	.78962	.10000	1.0000	Uiso	?	?
H20	.23455	-.00770	.79242	.10000	1.0000	Uiso	?	?
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H22	.29363	.03025	.97181	.10000	1.0000	Uiso	?	?
H23	.27794	-.03813	.93337	.10000	1.0000	Uiso	?	?
H24	.38139	-.01789	.97611	.10000	1.0000	Uiso	?	?
H25	.34253	-.08950	.98880	.10000	1.0000	Uiso	?	?
H26	.41059	-.12925	.93231	.10000	1.0000	Uiso	?	?
H27	.35344	-.14164	.90843	.10000	1.0000	Uiso	?	?
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H30	.35742	.03522	.82777	.10000	1.0000	Uiso	?	?
H31	.31907	-.03582	.84287	.10000	1.0000	Uiso	?	?
H32	.22318	.22423	.91519	.10000	1.0000	Uiso	?	?
H33	.30990	.18154	.97665	.10000	1.0000	Uiso	?	?
H34	.31241	.24858	.93463	.10000	1.0000	Uiso	?	?
H35	.29869	.30510	1.01660	.10000	1.0000	Uiso	?	?
H36	.25164	.32746	.97948	.10000	1.0000	Uiso	?	?
H37	.24675	.20668	1.05490	.10000	1.0000	Uiso	?	?
H38	.21391	.28728	1.05598	.10000	1.0000	Uiso	?	?
H39	.15950	.17894	1.03118	.10000	1.0000	Uiso	?	?
H40	.16221	.24450	.98824	.10000	1.0000	Uiso	?	?
H41	.22168	.09873	.98707	.10000	1.0000	Uiso	?	?
H42	.17362	.11772	.95036	.10000	1.0000	Uiso	?	?
H43	.14313	.13722	.72626	.10000	1.0000	Uiso	?	?
H44	.20003	.28491	.72689	.10000	1.0000	Uiso	?	?
H45	.19097	.23082	.67867	.10000	1.0000	Uiso	?	?
H46	.13096	.34204	.67754	.10000	1.0000	Uiso	?	?
H47	.09856	.26110	.67988	.10000	1.0000	Uiso	?	?
H48	.12080	.35693	.76623	.10000	1.0000	Uiso	?	?
H49	.06427	.35303	.73998	.10000	1.0000	Uiso	?	?
H50	.06523	.26779	.81135	.10000	1.0000	Uiso	?	?
H51	.05686	.21651	.76181	.10000	1.0000	Uiso	?	?
H52	.15528	.23039	.81539	.10000	1.0000	Uiso	?	?
H53	.12138	.15106	.81099	.10000	1.0000	Uiso	?	?
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H55	.33091	.06297	.72607	.10000	1.0000	Uiso	?	?
H56	.29647	-.01612	.72492	.10000	1.0000	Uiso	?	?
H57	.33875	.05926	.63625	.10000	1.0000	Uiso	?	?
H58	.36105	-.02158	.65881	.10000	1.0000	Uiso	?	?
H59	.30329	-.04829	.58922	.10000	1.0000	Uiso	?	?
H60	.28028	-.08692	.63918	.10000	1.0000	Uiso	?	?
H61	.24392	.05916	.59653	.10000	1.0000	Uiso	?	?
H62	.21074	-.02114	.59717	.10000	1.0000	Uiso	?	?
H63	.18032	.06745	.66308	.10000	1.0000	Uiso	?	?
H64	.20204	-.01299	.68669	.10000	1.0000	Uiso	?	?
H65	.56166	.13293	.60720	.10000	1.0000	Uiso	?	?
H66	.56797	.15991	.55027	.10000	1.0000	Uiso	?	?
H67	.56384	.22483	.59349	.10000	1.0000	Uiso	?	?
H68	.48291	.21368	.55197	.10000	1.0000	Uiso	?	?
H69	.47660	.18670	.60890	.10000	1.0000	Uiso	?	?
H70	.39735	.10686	.56732	.10000	1.0000	Uiso	?	?
H71	.41815	.12047	.51159	.10000	1.0000	Uiso	?	?
H72	.43417	-.01514	.50373	.10000	1.0000	Uiso	?	?
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P1	.0270(4)	.0260(4)	.0386(5)	-.0009(3)	.0023(3)	-.0006(3)
P2	.0288(4)	.0276(4)	.0428(5)	-.0002(3)	.0024(4)	.0042(4)
P3	.0309(4)	.0278(4)	.0442(5)	-.0008(3)	-.0015(4)	.0013(4)
C1	.0296(16)	.0266(15)	.0414(19)	.0010(13)	.0007(13)	.0005(14)
C2	.0298(17)	.0375(18)	.045(2)	.0015(14)	-.0000(14)	.0035(15)
C3	.0358(17)	.0256(16)	.0456(19)	-.0005(13)	.0033(15)	.0057(14)
C4	.0398(19)	.0403(19)	.049(2)	-.0054(16)	.0012(16)	.0073(16)
C5	.040(2)	.041(2)	.064(3)	-.0062(16)	.0030(17)	.0082(18)
C6	.059(3)	.063(3)	.063(3)	-.008(2)	.012(2)	.016(2)
C7	.061(3)	.110(4)	.046(2)	-.012(3)	.002(2)	.023(2)
C8	.047(2)	.074(3)	.047(2)	-.011(2)	-.0051(17)	.015(2)
C9	.0253(16)	.0252(15)	.047(2)	-.0010(12)	.0065(14)	.0018(14)
C10	.0352(18)	.0379(19)	.053(2)	.0019(15)	.0015(15)	.0045(16)
C11	.041(2)	.042(2)	.066(3)	.0074(17)	-.0044(17)	.0089(18)
C12	.042(2)	.038(2)	.079(3)	.0102(17)	.009(2)	-.005(2)
C13	.050(2)	.040(2)	.061(2)	.0044(17)	.0086(18)	-.0099(18)
C14	.0371(18)	.0361(18)	.042(2)	-.0007(14)	.0042(15)	-.0009(15)
C15	.0339(17)	.0278(16)	.0377(18)	-.0028(13)	-.0027(14)	.0021(14)
C16	.0347(18)	.0388(18)	.059(2)	.0044(15)	-.0030(16)	-.0083(17)
C17	.044(2)	.044(2)	.064(2)	.0042(17)	-.0081(17)	-.0145(18)
C18	.049(2)	.039(2)	.053(2)	-.0051(17)	-.0066(17)	-.0062(17)
C19	.0354(19)	.056(2)	.068(3)	-.0124(18)	.0024(18)	-.012(2)
C20	.0356(18)	.044(2)	.053(2)	-.0074(15)	.0081(16)	-.0116(17)
C21	.0333(18)	.0374(18)	.052(2)	-.0074(15)	-.0011(15)	.0118(16)
C22	.0382(19)	.0311(18)	.052(2)	-.0078(14)	-.0038(15)	.0023(15)
C23	.0342(18)	.0297(16)	.048(2)	.0015(14)	.0010(14)	.0041(15)
C24	.048(2)	.049(2)	.053(2)	.0102(17)	.0035(17)	.0186(18)
C25	.054(2)	.040(2)	.063(3)	.0069(17)	-.0089(19)	.0117(18)
C26	.049(2)	.038(2)	.071(3)	.0089(17)	-.0134(19)	.0054(19)
C27	.041(2)	.0381(19)	.061(2)	.0105(16)	-.0024(17)	-.0021(17)
C28	.0340(17)	.0316(17)	.048(2)	.0003(14)	.0001(14)	-.0015(15)
C29	.0383(18)	.0326(18)	.044(2)	.0000(14)	.0055(15)	.0022(14)
C30	.042(2)	.048(2)	.056(2)	.0006(16)	.0005(17)	-.0011(18)
C31	.067(3)	.059(2)	.064(3)	-.004(2)	.003(2)	-.016(2)
C32	.068(3)	.071(3)	.048(2)	.016(2)	.008(2)	-.006(2)
C33	.052(2)	.051(2)	.052(2)	.0050(18)	.0111(18)	.0002(18)

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C34 .046(2) .044(2) .057(2) .0030(16) .0142(17) .0045(18)
C35 .0310(17) .0353(17) .047(2) -.0010(14) -.0037(14) .0008(15)
C36 .0390(19) .0416(19) .051(2) .0033(16) -.0033(15) .0073(17)
C37 .044(2) .044(2) .060(2) .0055(16) -.0075(17) .0060(18)
C38 .041(2) .045(2) .067(3) .0087(16) -.0109(18) -.0008(18)
C39 .0314(18) .044(2) .071(3) .0041(16) -.0022(17) .0027(19)
C40 .0316(17) .041(2) .055(2) .0031(15) -.0007(15) .0035(16)
C41 .046(2) .0318(17) .045(2) -.0009(15) .0006(16) -.0015(15)
C42 .046(2) .039(2) .063(2) .0067(16) .0039(17) -.0087(18)
C43 .058(2) .048(2) .074(3) -.0005(19) .015(2) -.019(2)
C44 .073(3) .059(3) .066(3) -.001(2) .014(2) -.023(2)
C45 .074(3) .069(3) .057(3) -.009(2) -.003(2) -.018(2)
C46 .057(2) .047(2) .060(3) -.0050(18) -.0041(19) -.014(2)
O1 .076(2) .0604(19) .094(2) .0096(15) -.0332(18) -.0074(17)
C47 .131(5) .084(4) .118(5) -.037(4) -.029(4) .005(3)
C48 .139(5) .048(3) .083(4) .011(3) -.009(3) .010(2)
C49 .078(4) .129(5) .104(4) -.002(4) -.005(3) .044(4)
C50 .105(4) .177(7) .085(4) -.084(5) -.012(3) .015(4)

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The structure solves to reveal the Ni-species and two regions of solvation. One of these solvate regions is simply a molecule of diethylether, the other appears to be disorder of molecules of diethylether and benzene (roughly 1:1). In the latter region, restraints were placed on bond distances and angles of the ether and on bonds, angles and dihedral angles of the benzene, all these atom sites were given a common isotropic displacement factor and the relative occupancies of the two units were refined.

Hydrogen atoms were placed at calculated positions for the Ni-species and for the ordered ether. Hydrogen atoms were not included in the disordered region [which accounts for the mis-match in the number of expected:found H atoms by checkcif].

Refinement in the disordered region of the structure is very slow to converge. The largest shifts in the last cycle of refinement are for atoms in this region.

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Ni1	P1	2.1734(8)	?	
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Ni1	P3	2.1952(9)	?	
Ni1	C1	1.903(3)	?	
P1	C1	1.751(3)	?	
P1	C9	1.824(3)	?	
P1	C15	1.826(3)	?	
P2	C21	1.854(3)	?	
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P2	C29	1.846(3)	?	
P3	C22	1.839(3)	?	
P3	C35	1.852(3)	?	
P3	C41	1.845(3)	?	
C1	C2	1.328(5)	?	
C2	C3	1.478(4)	?	
C2	H1	.950(3)	?	
C3	C4	1.390(5)	?	
C3	C8	1.381(5)	?	
C4	C5	1.395(5)	?	
C4	H2	.950(3)	?	
C5	C6	1.360(6)	?	
C5	H3	.950(3)	?	
C6	C7	1.356(6)	?	
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C7	C8	1.385(6)	?	
C7	H5	.950(4)	?	
C8	H6	.950(4)	?	
C9	C10	1.401(5)	?	
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C10	C11	1.378(5)	?	
C10	H7	.950(4)	?	
C11	C12	1.376(6)	?	
C11	H8	.950(4)	?	
C12	C13	1.372(5)	?	
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C16	C17	1.386(5)	?	
C16	H12	.950(3)	?	
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C18	H14	.950(3)	?	
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C20	H16	.950(3)	?	
C21	C22	1.517(5)	?	
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C22	H19	.950(3)	?	
C22	H20	.950(3)	?	
C23	C24	1.540(5)	?	
C23	C28	1.538(5)	?	
C23	H21	.950(3)	?	
C24	C25	1.530(5)	?	
C24	H22	.950(4)	?	
C24	H23	.950(4)	?	

C25	C26	1.497(5)	.	.	?
C25	H24	.950(4)	.	.	?
C25	H25	.950(4)	.	.	?
C26	C27	1.522(5)	.	.	?
C26	H26	.950(4)	.	.	?
C26	H27	.950(4)	.	.	?
C27	C28	1.529(5)	.	.	?
C27	H28	.950(3)	.	.	?
C27	H29	.950(4)	.	.	?
C28	H30	.950(3)	.	.	?
C28	H31	.950(3)	.	.	?
C29	C30	1.523(5)	.	.	?
C29	C34	1.549(5)	.	.	?
C29	H32	.950(3)	.	.	?
C30	C31	1.523(6)	.	.	?
C30	H33	.950(4)	.	.	?
C30	H34	.950(4)	.	.	?
C31	C32	1.520(6)	.	.	?
C31	H35	.950(4)	.	.	?
C31	H36	.950(4)	.	.	?
C32	C33	1.504(6)	.	.	?
C32	H37	.950(4)	.	.	?
C32	H38	.950(4)	.	.	?
C33	C34	1.533(5)	.	.	?
C33	H39	.950(4)	.	.	?
C33	H40	.950(4)	.	.	?
C34	H41	.950(4)	.	.	?
C34	H42	.950(4)	.	.	?
C35	C36	1.545(5)	.	.	?
C35	C40	1.535(5)	.	.	?
C35	H43	.950(3)	.	.	?
C36	C37	1.536(5)	.	.	?
C36	H44	.950(3)	.	.	?
C36	H45	.950(4)	.	.	?
C37	C38	1.512(5)	.	.	?
C37	H46	.950(4)	.	.	?
C37	H47	.950(4)	.	.	?
C38	C39	1.517(5)	.	.	?
C38	H48	.950(4)	.	.	?
C38	H49	.950(4)	.	.	?
C39	C40	1.538(5)	.	.	?
C39	H50	.950(4)	.	.	?
C39	H51	.950(4)	.	.	?
C40	H52	.950(3)	.	.	?
C40	H53	.950(3)	.	.	?
C41	C42	1.531(5)	.	.	?
C41	C46	1.533(5)	.	.	?
C41	H54	.950(3)	.	.	?
C42	C43	1.540(6)	.	.	?
C42	H55	.950(4)	.	.	?
C42	H56	.950(4)	.	.	?
C43	C44	1.525(6)	.	.	?
C43	H57	.950(4)	.	.	?
C43	H58	.950(4)	.	.	?
C44	C45	1.514(6)	.	.	?
C44	H59	.950(4)	.	.	?
C44	H60	.950(4)	.	.	?
C45	C46	1.549(6)	.	.	?
C45	H61	.950(4)	.	.	?
C45	H62	.950(4)	.	.	?
C46	H63	.950(4)	.	.	?
C46	H64	.950(4)	.	.	?
O1	C48	1.413(6)	.	.	?
O1	C49	1.393(6)	.	.	?
C47	C48	1.457(10)	.	.	?
C47	H65	.950(6)	.	.	?
C47	H66	.950(7)	.	.	?

C47 H67 .950(6) . . . ?
 C48 H68 .950(5) . . . ?
 C48 H69 .950(6) . . . ?
 C49 C50 1.463(10) . . . ?
 C49 H70 .950(6) . . . ?
 C49 H71 .950(6) . . . ?
 C50 H72 .950(6) . . . ?
 C50 H73 .950(7) . . . ?
 C50 H74 .950(6) . . . ?
 O10 C102 1.430(10) . . . ?
 O10 C103 1.439(10) . . . ?
 O10 C201 .931(8) . . . ?
 O10 C202 .775(8) . . . ?
 O10 C203 1.564(8) . . . ?
 C101 C102 1.487(13) . . . ?
 C101 C206 1.145(11) . . . ?
 C102 C201 1.286(8) . . . ?
 C102 C205 1.227(9) . . . ?
 C102 C206 .388(11) . . . ?
 C103 C104 1.519(12) . . . ?
 C103 C202 1.024(9) . . . ?
 C103 C203 .627(9) . . . ?
 C104 C203 .962(10) . . . ?
 C104 C204 1.316(11) . . . ?
 C201 C202 1.373(10) . . . ?
 C201 C206 1.415(7) . . . ?
 C202 C203 1.426(7) . . . ?
 C203 C204 1.376(7) . . . ?
 C204 C205 1.411(9) . . . ?
 C205 C206 1.385(7) . . . ?

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C11 Ni1 P1 106.24(3) . . . ?
 C11 Ni1 P2 98.07(3) . . . ?
 C11 Ni1 P3 108.44(3) . . . ?
 C11 Ni1 C1 94.78(9) . . . ?
 P1 Ni1 P2 112.49(3) . . . ?
 P1 Ni1 P3 135.96(4) . . . ?
 P1 Ni1 C1 50.34(9) . . . ?
 P2 Ni1 P3 88.62(3) . . . ?
 P2 Ni1 C1 161.28(9) . . . ?
 P3 Ni1 C1 100.19(10) . . . ?
 Ni1 P1 C1 56.79(10) . . . ?
 Ni1 P1 C9 126.73(10) . . . ?
 Ni1 P1 C15 126.37(10) . . . ?
 C1 P1 C9 111.44(15) . . . ?
 C1 P1 C15 117.29(14) . . . ?
 C9 P1 C15 105.65(14) . . . ?
 Ni1 P2 C21 107.45(12) . . . ?
 Ni1 P2 C22 116.22(11) . . . ?

Ni1	P2	C29	113.63(11)	.	.	.	?
C21	P2	C23	106.21(14)	.	.	.	?
C21	P2	C29	105.18(15)	.	.	.	?
C23	P2	C29	107.35(15)	.	.	.	?
Ni1	P3	C22	108.67(11)	.	.	.	?
Ni1	P3	C35	117.32(11)	.	.	.	?
Ni1	P3	C41	116.64(11)	.	.	.	?
C22	P3	C35	104.29(14)	.	.	.	?
C22	P3	C41	104.50(15)	.	.	.	?
C35	P3	C41	104.05(16)	.	.	.	?
Ni1	C1	P1	72.87(12)	.	.	.	?
Ni1	C1	C2	144.3(2)	.	.	.	?
P1	C1	C2	142.8(2)	.	.	.	?
C1	C2	C3	129.2(3)	.	.	.	?
C1	C2	H1	115.4(3)	.	.	.	?
C3	C2	H1	115.4(3)	.	.	.	?
C2	C3	C4	123.6(3)	.	.	.	?
C2	C3	C8	119.1(3)	.	.	.	?
C4	C3	C8	117.2(3)	.	.	.	?
C3	C4	C5	121.2(3)	.	.	.	?
C3	C4	H2	119.4(3)	.	.	.	?
C5	C4	H2	119.4(3)	.	.	.	?
C4	C5	C6	119.8(3)	.	.	.	?
C4	C5	H3	120.1(4)	.	.	.	?
C6	C5	H3	120.1(4)	.	.	.	?
C5	C6	C7	119.8(4)	.	.	.	?
C5	C6	H4	120.1(4)	.	.	.	?
C7	C6	H4	120.1(4)	.	.	.	?
C6	C7	C8	121.0(4)	.	.	.	?
C6	C7	H5	119.5(4)	.	.	.	?
C8	C7	H5	119.5(4)	.	.	.	?
C3	C8	C7	120.8(3)	.	.	.	?
C3	C8	H6	119.6(4)	.	.	.	?
C7	C8	H6	119.6(4)	.	.	.	?
P1	C9	C10	119.5(2)	.	.	.	?
P1	C9	C14	121.2(2)	.	.	.	?
C10	C9	C14	119.2(3)	.	.	.	?
C9	C10	C11	119.9(3)	.	.	.	?
C9	C10	H7	120.1(3)	.	.	.	?
C11	C10	H7	120.1(3)	.	.	.	?
C10	C11	C12	120.6(3)	.	.	.	?
C10	C11	H8	119.7(4)	.	.	.	?
C12	C11	H8	119.7(4)	.	.	.	?
C11	C12	C13	119.9(3)	.	.	.	?
C11	C12	H9	120.1(4)	.	.	.	?
C13	C12	H9	120.1(4)	.	.	.	?
C12	C13	C14	120.3(4)	.	.	.	?
C12	C13	H10	119.8(4)	.	.	.	?
C14	C13	H10	119.8(4)	.	.	.	?
C9	C14	C13	120.1(3)	.	.	.	?
C9	C14	H11	120.0(3)	.	.	.	?
C13	C14	H11	120.0(3)	.	.	.	?
P1	C15	C16	118.0(2)	.	.	.	?
P1	C15	C20	123.1(2)	.	.	.	?
C16	C15	C20	118.9(3)	.	.	.	?
C15	C16	C17	120.1(3)	.	.	.	?
C15	C16	H12	120.0(3)	.	.	.	?
C17	C16	H12	120.0(3)	.	.	.	?
C16	C17	C18	120.8(3)	.	.	.	?
C16	C17	H13	119.6(3)	.	.	.	?
C18	C17	H13	119.6(4)	.	.	.	?
C17	C18	C19	118.7(3)	.	.	.	?
C17	C18	H14	120.7(4)	.	.	.	?
C19	C18	H14	120.7(4)	.	.	.	?
C18	C19	C20	121.3(3)	.	.	.	?
C18	C19	H15	119.4(4)	.	.	.	?

C15	C20	C19	120.1(3)	.	.	.	?
C15	C20	H16	119.9(3)	.	.	.	?
C19	C20	H16	119.9(3)	.	.	.	?
P2	C21	C22	112.2(2)	.	.	.	?
P2	C21	H17	108.8(2)	.	.	.	?
P2	C21	H18	108.8(3)	.	.	.	?
C22	C21	H17	108.8(3)	.	.	.	?
C22	C21	H18	108.8(3)	.	.	.	?
H17	C21	H18	109.5(3)	.	.	.	?
P3	C22	C21	111.1(2)	.	.	.	?
P3	C22	H19	109.1(3)	.	.	.	?
P3	C22	H20	109.1(2)	.	.	.	?
C21	C22	H19	109.1(3)	.	.	.	?
C21	C22	H20	109.0(3)	.	.	.	?
H19	C22	H20	109.5(3)	.	.	.	?
P2	C23	C24	115.4(2)	.	.	.	?
P2	C23	C28	111.2(2)	.	.	.	?
P2	C23	H21	106.8(2)	.	.	.	?
C24	C23	C28	109.5(3)	.	.	.	?
C24	C23	H21	106.8(3)	.	.	.	?
C28	C23	H21	106.8(3)	.	.	.	?
C23	C24	C25	111.1(3)	.	.	.	?
C23	C24	H22	109.1(3)	.	.	.	?
C23	C24	H23	109.1(3)	.	.	.	?
C25	C24	H22	109.1(3)	.	.	.	?
C25	C24	H23	109.1(3)	.	.	.	?
H22	C24	H23	109.5(3)	.	.	.	?
C24	C25	C26	112.1(3)	.	.	.	?
C24	C25	H24	108.8(3)	.	.	.	?
C24	C25	H25	108.8(3)	.	.	.	?
C26	C25	H24	108.8(3)	.	.	.	?
C26	C25	H25	108.8(3)	.	.	.	?
H24	C25	H25	109.5(4)	.	.	.	?
C25	C26	C27	111.0(3)	.	.	.	?
C25	C26	H26	109.1(4)	.	.	.	?
C25	C26	H27	109.1(3)	.	.	.	?
C27	C26	H26	109.1(3)	.	.	.	?
C27	C26	H27	109.1(4)	.	.	.	?
H26	C26	H27	109.5(3)	.	.	.	?
C26	C27	C28	111.3(3)	.	.	.	?
C26	C27	H28	109.0(3)	.	.	.	?
C26	C27	H29	109.0(3)	.	.	.	?
C28	C27	H28	109.0(3)	.	.	.	?
C28	C27	H29	109.0(3)	.	.	.	?
H28	C27	H29	109.5(3)	.	.	.	?
C23	C28	C27	110.0(3)	.	.	.	?
C23	C28	H30	109.3(3)	.	.	.	?
C23	C28	H31	109.3(3)	.	.	.	?
C27	C28	H30	109.3(3)	.	.	.	?
C27	C28	H31	109.3(3)	.	.	.	?
H30	C28	H31	109.5(3)	.	.	.	?
P2	C29	C30	111.6(2)	.	.	.	?
P2	C29	C34	119.1(2)	.	.	.	?
P2	C29	H32	104.8(3)	.	.	.	?
C30	C29	C34	110.3(3)	.	.	.	?
C30	C29	H32	104.8(3)	.	.	.	?
C34	C29	H32	104.8(3)	.	.	.	?
C29	C30	C31	111.7(3)	.	.	.	?
C29	C30	H33	108.9(3)	.	.	.	?
C29	C30	H34	108.9(3)	.	.	.	?
C31	C30	H33	108.9(3)	.	.	.	?
C31	C30	H34	108.9(3)	.	.	.	?
H33	C30	H34	109.5(3)	.	.	.	?
C30	C31	C32	110.9(3)	.	.	.	?
C30	C31	H35	109.1(4)	.	.	.	?
C30	C31	H36	109.1(4)	.	.	.	?

C32	C31	H36	109.1(4)	.	.	.	?
H35	C31	H36	109.5(4)	.	.	.	?
C31	C32	C33	112.2(3)	.	.	.	?
C31	C32	H37	108.8(4)	.	.	.	?
C31	C32	H38	108.8(4)	.	.	.	?
C33	C32	H37	108.8(4)	.	.	.	?
C33	C32	H38	108.8(4)	.	.	.	?
H37	C32	H38	109.5(4)	.	.	.	?
C32	C33	C34	111.3(3)	.	.	.	?
C32	C33	H39	109.0(3)	.	.	.	?
C32	C33	H40	109.0(3)	.	.	.	?
C34	C33	H39	109.0(3)	.	.	.	?
C34	C33	H40	109.0(3)	.	.	.	?
H39	C33	H40	109.5(4)	.	.	.	?
C29	C34	C33	109.6(3)	.	.	.	?
C29	C34	H41	109.4(3)	.	.	.	?
C29	C34	H42	109.4(3)	.	.	.	?
C33	C34	H41	109.4(3)	.	.	.	?
C33	C34	H42	109.4(3)	.	.	.	?
H41	C34	H42	109.5(4)	.	.	.	?
P3	C35	C36	109.4(2)	.	.	.	?
P3	C35	C40	111.8(2)	.	.	.	?
P3	C35	H43	107.9(2)	.	.	.	?
C36	C35	C40	111.7(3)	.	.	.	?
C36	C35	H43	107.9(3)	.	.	.	?
C40	C35	H43	107.9(3)	.	.	.	?
C35	C36	C37	111.3(3)	.	.	.	?
C35	C36	H44	109.0(3)	.	.	.	?
C35	C36	H45	109.0(3)	.	.	.	?
C37	C36	H44	109.0(3)	.	.	.	?
C37	C36	H45	109.0(3)	.	.	.	?
H44	C36	H45	109.5(3)	.	.	.	?
C36	C37	C38	109.8(3)	.	.	.	?
C36	C37	H46	109.4(3)	.	.	.	?
C36	C37	H47	109.4(3)	.	.	.	?
C38	C37	H46	109.4(3)	.	.	.	?
C38	C37	H47	109.4(3)	.	.	.	?
H46	C37	H47	109.5(4)	.	.	.	?
C37	C38	C39	109.9(3)	.	.	.	?
C37	C38	H48	109.3(3)	.	.	.	?
C37	C38	H49	109.4(4)	.	.	.	?
C39	C38	H48	109.4(3)	.	.	.	?
C39	C38	H49	109.4(3)	.	.	.	?
H48	C38	H49	109.5(4)	.	.	.	?
C38	C39	C40	111.2(3)	.	.	.	?
C38	C39	H50	109.0(3)	.	.	.	?
C38	C39	H51	109.1(3)	.	.	.	?
C40	C39	H50	109.0(3)	.	.	.	?
C40	C39	H51	109.1(3)	.	.	.	?
H50	C39	H51	109.5(3)	.	.	.	?
C35	C40	C39	111.9(3)	.	.	.	?
C35	C40	H52	108.9(3)	.	.	.	?
C35	C40	H53	108.9(3)	.	.	.	?
C39	C40	H52	108.9(3)	.	.	.	?
C39	C40	H53	108.9(3)	.	.	.	?
H52	C40	H53	109.5(3)	.	.	.	?
P3	C41	C42	111.2(2)	.	.	.	?
P3	C41	C46	116.1(2)	.	.	.	?
P3	C41	H54	106.3(3)	.	.	.	?
C42	C41	C46	109.9(3)	.	.	.	?
C42	C41	H54	106.3(3)	.	.	.	?
C46	C41	H54	106.4(3)	.	.	.	?
C41	C42	C43	109.8(3)	.	.	.	?
C41	C42	H55	109.4(3)	.	.	.	?
C41	C42	H56	109.4(3)	.	.	.	?
C43	C42	H55	109.4(3)	.	.	.	?
C43	C42	H56	109.4(3)	.	.	.	?

H55	C42	H56	109.5(4)	.	.	.	?
C42	C43	C44	110.2(3)	.	.	.	?
C42	C43	H57	109.3(3)	.	.	.	?
C42	C43	H58	109.3(4)	.	.	.	?
C44	C43	H57	109.3(4)	.	.	.	?
C44	C43	H58	109.3(4)	.	.	.	?
H57	C43	H58	109.5(4)	.	.	.	?
C43	C44	C45	110.8(3)	.	.	.	?
C43	C44	H59	109.2(4)	.	.	.	?
C43	C44	H60	109.1(4)	.	.	.	?
C45	C44	H59	109.1(4)	.	.	.	?
C45	C44	H60	109.1(4)	.	.	.	?
H59	C44	H60	109.5(4)	.	.	.	?
C44	C45	C46	111.2(3)	.	.	.	?
C44	C45	H61	109.0(4)	.	.	.	?
C44	C45	H62	109.0(4)	.	.	.	?
C46	C45	H61	109.1(4)	.	.	.	?
C46	C45	H62	109.1(4)	.	.	.	?
H61	C45	H62	109.5(4)	.	.	.	?
C41	C46	C45	109.7(3)	.	.	.	?
C41	C46	H63	109.4(3)	.	.	.	?
C41	C46	H64	109.4(3)	.	.	.	?
C45	C46	H63	109.4(4)	.	.	.	?
C45	C46	H64	109.4(4)	.	.	.	?
H63	C46	H64	109.5(4)	.	.	.	?
C48	O1	C49	119.0(4)	.	.	.	?
C48	C47	H65	109.5(6)	.	.	.	?
C48	C47	H66	109.5(6)	.	.	.	?
C48	C47	H67	109.5(6)	.	.	.	?
H65	C47	H66	109.5(6)	.	.	.	?
H65	C47	H67	109.5(7)	.	.	.	?
H66	C47	H67	109.5(6)	.	.	.	?
O1	C48	C47	109.4(4)	.	.	.	?
O1	C48	H68	109.5(5)	.	.	.	?
O1	C48	H69	109.5(5)	.	.	.	?
C47	C48	H68	109.5(5)	.	.	.	?
C47	C48	H69	109.5(6)	.	.	.	?
H68	C48	H69	109.5(5)	.	.	.	?
O1	C49	C50	111.4(5)	.	.	.	?
O1	C49	H70	109.0(5)	.	.	.	?
O1	C49	H71	109.0(5)	.	.	.	?
C50	C49	H70	109.0(5)	.	.	.	?
C50	C49	H71	109.0(5)	.	.	.	?
H70	C49	H71	109.5(6)	.	.	.	?
C49	C50	H72	109.0(6)	.	.	.	?
C49	C50	H73	109.0(6)	.	.	.	?
C49	C50	H74	111.4(6)	.	.	.	?
H72	C50	H73	109.4(7)	.	.	.	?
H72	C50	H74	109.0(6)	.	.	.	?
H73	C50	H74	109.0(6)	.	.	.	?
C102	O10	C103	118.8(6)	.	.	.	?
C102	O10	C201	61.8(5)	.	.	.	?
C102	O10	C202	144.0(9)	.	.	.	?
C102	O10	C203	107.3(5)	.	.	.	?
C103	O10	C201	135.4(8)	.	.	.	?
C103	O10	C202	43.3(6)	.	.	.	?
C103	O10	C203	23.6(4)	.	.	.	?
C201	O10	C202	106.8(9)	.	.	.	?
C201	O10	C203	151.5(7)	.	.	.	?
C202	O10	C203	65.3(6)	.	.	.	?
C102	C101	C206	8.0(4)	.	.	.	?
O10	C102	C101	109.4(6)	.	.	.	?
O10	C102	C201	39.6(4)	.	.	.	?
O10	C102	C205	110.1(7)	.	.	.	?
O10	C102	C206	133.4(16)	.	.	.	?
C101	C102	C201	77.9(6)	.	.	.	?
C101	C102	C205	127.0(9)	.	.	.	?

C101	C102	C206	24.4(11)	.	.	.	?
C201	C102	C205	149.6(9)	.	.	.	?
C201	C102	C206	101.4(13)	.	.	.	?
C205	C102	C206	106.1(15)	.	.	.	?
O10	C103	C104	110.6(6)	.	.	.	?
O10	C103	C202	31.3(4)	.	.	.	?
O10	C103	C203	89.4(9)	.	.	.	?
C104	C103	C202	136.8(8)	.	.	.	?
C104	C103	C203	21.3(8)	.	.	.	?
C202	C103	C203	117.4(11)	.	.	.	?
C103	C104	C203	13.7(5)	.	.	.	?
C103	C104	C204	83.3(6)	.	.	.	?
C203	C104	C204	72.4(7)	.	.	.	?
O10	C201	C102	78.6(6)	.	.	.	?
O10	C201	C202	32.7(5)	.	.	.	?
O10	C201	C206	92.0(5)	.	.	.	?
C102	C201	C202	104.8(5)	.	.	.	?
C102	C201	C206	15.6(5)	.	.	.	?
C202	C201	C206	120.0(4)	.	.	.	?
O10	C202	C103	105.4(7)	.	.	.	?
O10	C202	C201	40.5(6)	.	.	.	?
O10	C202	C203	85.1(6)	.	.	.	?
C103	C202	C201	132.8(6)	.	.	.	?
C103	C202	C203	23.0(5)	.	.	.	?
C201	C202	C203	119.9(4)	.	.	.	?
O10	C203	C103	66.9(9)	.	.	.	?
O10	C203	C104	147.7(8)	.	.	.	?
O10	C203	C202	29.6(3)	.	.	.	?
O10	C203	C204	92.1(4)	.	.	.	?
C103	C203	C104	145.0(12)	.	.	.	?
C103	C203	C202	39.6(8)	.	.	.	?
C103	C203	C204	138.1(10)	.	.	.	?
C104	C203	C202	166.3(8)	.	.	.	?
C104	C203	C204	65.8(7)	.	.	.	?
C202	C203	C204	120.0(5)	.	.	.	?
C104	C204	C203	41.8(5)	.	.	.	?
C104	C204	C205	158.9(6)	.	.	.	?
C203	C204	C205	120.0(5)	.	.	.	?
C102	C205	C204	104.8(6)	.	.	.	?
C102	C205	C206	15.6(5)	.	.	.	?
C204	C205	C206	120.0(5)	.	.	.	?
C101	C206	C102	147.6(14)	.	.	.	?
C101	C206	C201	85.6(6)	.	.	.	?
C101	C206	C205	147.7(8)	.	.	.	?
C102	C206	C201	63.0(12)	.	.	.	?
C102	C206	C205	58.3(12)	.	.	.	?
C201	C206	C205	120.0(6)	.	.	.	?

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C11	Ni1	P1	C1	-82.60(12)	.	.	.	?
C11	Ni1	P1	C9	-175.84(13)	.	.	.	?
C11	Ni1	P1	C15	18.86(14)	.	.	.	?
P2	Ni1	P1	C1	171.21(12)	.	.	.	?
P2	Ni1	P1	C9	77.97(14)	.	.	.	?
P2	Ni1	P1	C15	-87.33(13)	.	.	.	?
P3	Ni1	P1	C1	58.23(13)	.	.	.	?
P3	Ni1	P1	C9	25.01(15)	.	.	.	?

P3	Ni1	P1	C15	159.69(13)	?
C1	Ni1	P1	C1	-.00(17)	?
C1	Ni1	P1	C9	-93.25(18)	?
C1	Ni1	P1	C15	101.45(18)	?
C11	Ni1	P2	C21	102.32(11)	?
C11	Ni1	P2	C23	-138.93(12)	?
C11	Ni1	P2	C29	-13.59(12)	?
P1	Ni1	P2	C21	-146.31(11)	?
P1	Ni1	P2	C23	-27.55(12)	?
P1	Ni1	P2	C29	97.78(12)	?
P3	Ni1	P2	C21	-6.12(11)	?
P3	Ni1	P2	C23	112.64(12)	?
P3	Ni1	P2	C29	-122.03(12)	?
C1	Ni1	P2	C21	-124.8(3)	?
C1	Ni1	P2	C23	-6.1(3)	?
C1	Ni1	P2	C29	119.3(3)	?
C11	Ni1	P3	C22	-110.06(11)	?
C11	Ni1	P3	C35	7.83(13)	?
C11	Ni1	P3	C41	132.22(12)	?
P1	Ni1	P3	C22	109.67(12)	?
P1	Ni1	P3	C35	-132.43(13)	?
P1	Ni1	P3	C41	-8.04(14)	?
P2	Ni1	P3	C22	-12.02(11)	?
P2	Ni1	P3	C35	105.87(13)	?
P2	Ni1	P3	C41	-129.74(12)	?
C1	Ni1	P3	C22	151.36(14)	?
C1	Ni1	P3	C35	-90.75(15)	?
C1	Ni1	P3	C41	33.64(15)	?
C11	Ni1	C1	P1	107.18(8)	?
C11	Ni1	C1	C2	-70.7(4)	?
P1	Ni1	C1	P1	.00(4)	?
P1	Ni1	C1	C2	-177.9(5)	?
P2	Ni1	C1	P1	-26.1(4)	?
P2	Ni1	C1	C2	156.1(3)	?
P3	Ni1	C1	P1	-143.09(7)	?
P3	Ni1	C1	C2	39.0(4)	?
Ni1	P1	C1	Ni1	-.000(19)	?
Ni1	P1	C1	C2	177.9(5)	?
C9	P1	C1	Ni1	120.72(12)	?
C9	P1	C1	C2	-61.4(4)	?
C15	P1	C1	Ni1	-117.37(13)	?
C15	P1	C1	C2	60.6(5)	?
Ni1	P1	C9	C10	-107.9(2)	?
Ni1	P1	C9	C14	69.8(3)	?
C1	P1	C9	C10	-171.7(2)	?
C1	P1	C9	C14	6.0(3)	?
C15	P1	C9	C10	59.9(3)	?
C15	P1	C9	C14	-122.4(3)	?
Ni1	P1	C15	C16	.4(3)	?
Ni1	P1	C15	C20	177.5(2)	?
C1	P1	C15	C16	67.7(3)	?
C1	P1	C15	C20	-115.2(3)	?
C9	P1	C15	C16	-167.4(3)	?
C9	P1	C15	C20	9.7(3)	?
Ni1	P2	C21	C22	27.7(2)	?
Ni1	P2	C21	H17	148.1(2)	?
Ni1	P2	C21	H18	-92.7(3)	?
C23	P2	C21	C22	-97.3(2)	?
C23	P2	C21	H17	23.1(3)	?
C23	P2	C21	H18	142.3(3)	?
C29	P2	C21	C22	149.1(2)	?
C29	P2	C21	H17	-90.5(3)	?
C29	P2	C21	H18	28.7(3)	?
Ni1	P2	C23	C24	-176.4(2)	?
Ni1	P2	C23	C28	-51.0(2)	?
Ni1	P2	C23	H21	65.1(3)	?

C21	P2	C23	C28	68.4(2)	?
C21	P2	C23	H21	-175.5(2)	?
C29	P2	C23	C24	55.1(3)	?
C29	P2	C23	C28	-179.5(2)	?
C29	P2	C23	H21	-63.4(3)	?
Ni1	P2	C29	C30	-78.2(2)	?
Ni1	P2	C29	C34	151.4(2)	?
Ni1	P2	C29	H32	34.7(3)	?
C21	P2	C29	C30	164.5(2)	?
C21	P2	C29	C34	34.1(3)	?
C21	P2	C29	H32	-82.6(3)	?
C23	P2	C29	C30	51.7(3)	?
C23	P2	C29	C34	-78.7(3)	?
C23	P2	C29	H32	164.6(2)	?
Ni1	P3	C22	C21	32.3(2)	?
Ni1	P3	C22	H19	152.5(2)	?
Ni1	P3	C22	H20	-88.0(2)	?
C35	P3	C22	C21	-93.6(2)	?
C35	P3	C22	H19	26.6(3)	?
C35	P3	C22	H20	146.2(2)	?
C41	P3	C22	C21	157.4(2)	?
C41	P3	C22	H19	-82.3(3)	?
C41	P3	C22	H20	37.2(3)	?
Ni1	P3	C35	C36	63.4(2)	?
Ni1	P3	C35	C40	-60.9(2)	?
Ni1	P3	C35	H43	-179.5(2)	?
C22	P3	C35	C36	-176.4(2)	?
C22	P3	C35	C40	59.3(2)	?
C22	P3	C35	H43	-59.3(3)	?
C41	P3	C35	C36	-67.1(3)	?
C41	P3	C35	C40	168.6(2)	?
C41	P3	C35	H43	50.0(3)	?
Ni1	P3	C41	C42	54.4(3)	?
Ni1	P3	C41	C46	-179.0(2)	?
Ni1	P3	C41	H54	-60.9(3)	?
C22	P3	C41	C42	-65.6(3)	?
C22	P3	C41	C46	61.0(3)	?
C22	P3	C41	H54	179.1(2)	?
C35	P3	C41	C42	-174.7(2)	?
C35	P3	C41	C46	-48.1(3)	?
C35	P3	C41	H54	70.0(3)	?
Ni1	C1	C2	C3	176.8(3)	?
Ni1	C1	C2	H1	-3.2(6)	?
P1	C1	C2	C3	.2(7)	?
P1	C1	C2	H1	-179.8(3)	?
C1	C2	C3	C4	-12.2(5)	?
C1	C2	C3	C8	167.0(4)	?
H1	C2	C3	C4	167.8(3)	?
H1	C2	C3	C8	-13.0(5)	?
C2	C3	C4	C5	179.4(3)	?
C2	C3	C4	H2	-.6(5)	?
C8	C3	C4	C5	.1(5)	?
C8	C3	C4	H2	-179.9(3)	?
C2	C3	C8	C7	-179.4(4)	?
C2	C3	C8	H6	.5(6)	?
C4	C3	C8	C7	-.1(6)	?
C4	C3	C8	H6	179.8(4)	?
C3	C4	C5	C6	.1(5)	?
C3	C4	C5	H3	-179.9(3)	?
H2	C4	C5	C6	-179.8(4)	?
H2	C4	C5	H3	.1(6)	?
C4	C5	C6	C7	-.4(6)	?
C4	C5	C6	H4	179.6(4)	?
H3	C5	C6	C7	179.6(4)	?
H3	C5	C6	H4	-.3(6)	?
C5	C6	C7	C8	.4(7)	?
C5	C6	C7	H5	-179.6(4)	?

H4	C6	C7	C8	-179.6(4)	?
H4	C6	C7	H5	.4(8)	?
C6	C7	C8	C3	-.1(7)	?
C6	C7	C8	H6	179.9(4)	?
H5	C7	C8	C3	179.9(4)	?
H5	C7	C8	H6	-.1(8)	?
P1	C9	C10	C11	177.8(3)	?
P1	C9	C10	H7	-2.3(4)	?
C14	C9	C10	C11	.0(5)	?
C14	C9	C10	H7	180.0(3)	?
P1	C9	C14	C13	-176.8(3)	?
P1	C9	C14	H11	3.2(4)	?
C10	C9	C14	C13	.9(5)	?
C10	C9	C14	H11	-179.1(3)	?
C9	C10	C11	C12	-.1(5)	?
C9	C10	C11	H8	179.9(3)	?
H7	C10	C11	C12	179.9(3)	?
H7	C10	C11	H8	-.1(6)	?
C10	C11	C12	C13	-.7(5)	?
C10	C11	C12	H9	179.3(3)	?
H8	C11	C12	C13	179.2(3)	?
H8	C11	C12	H9	-.8(6)	?
C11	C12	C13	C14	1.6(5)	?
C11	C12	C13	H10	-178.4(3)	?
H9	C12	C13	C14	-178.4(3)	?
H9	C12	C13	H10	1.6(6)	?
C12	C13	C14	C9	-1.8(5)	?
C12	C13	C14	H11	178.3(3)	?
H10	C13	C14	C9	178.3(3)	?
H10	C13	C14	H11	-1.7(6)	?
P1	C15	C16	C17	176.5(3)	?
P1	C15	C16	H12	-3.4(5)	?
C20	C15	C16	C17	-.7(5)	?
C20	C15	C16	H12	179.3(3)	?
P1	C15	C20	C19	-176.2(3)	?
P1	C15	C20	H16	3.8(5)	?
C16	C15	C20	C19	.9(5)	?
C16	C15	C20	H16	-179.1(3)	?
C15	C16	C17	C18	-.1(6)	?
C15	C16	C17	H13	179.9(3)	?
H12	C16	C17	C18	179.8(4)	?
H12	C16	C17	H13	-.2(6)	?
C16	C17	C18	C19	.8(6)	?
C16	C17	C18	H14	-179.2(4)	?
H13	C17	C18	C19	-179.2(4)	?
H13	C17	C18	H14	.8(6)	?
C17	C18	C19	C20	-.6(6)	?
C17	C18	C19	H15	179.3(4)	?
H14	C18	C19	C20	179.4(4)	?
H14	C18	C19	H15	-.7(6)	?
C18	C19	C20	C15	-.2(6)	?
C18	C19	C20	H16	179.8(4)	?
H15	C19	C20	C15	179.8(4)	?
H15	C19	C20	H16	-.1(6)	?
P2	C21	C22	P3	-38.3(3)	?
P2	C21	C22	H19	-158.5(2)	?
P2	C21	C22	H20	82.0(3)	?
H17	C21	C22	P3	-158.7(2)	?
H17	C21	C22	H19	81.1(4)	?
H17	C21	C22	H20	-38.4(4)	?
H18	C21	C22	P3	82.1(3)	?
H18	C21	C22	H19	-38.1(4)	?
H18	C21	C22	H20	-157.6(3)	?
P2	C23	C24	C25	-177.5(2)	?
P2	C23	C24	H22	-57.2(4)	?
P2	C23	C24	H23	62.3(4)	?
C28	C23	C24	C25	56.2(4)	?

C28	C23	C24	H22	176.5(3)	?
C28	C23	C24	H23	-64.0(4)	?
H21	C23	C24	C25	-59.0(4)	?
H21	C23	C24	H22	61.2(4)	?
H21	C23	C24	H23	-179.3(3)	?
P2	C23	C28	C27	173.9(2)	?
P2	C23	C28	H30	53.8(3)	?
P2	C23	C28	H31	-66.0(3)	?
C24	C23	C28	C27	-57.5(3)	?
C24	C23	C28	H30	-177.6(3)	?
C24	C23	C28	H31	62.6(4)	?
H21	C23	C28	C27	57.8(3)	?
H21	C23	C28	H30	-62.3(4)	?
H21	C23	C28	H31	177.9(3)	?
C23	C24	C25	C26	-55.6(4)	?
C23	C24	C25	H24	64.8(4)	?
C23	C24	C25	H25	-175.9(3)	?
H22	C24	C25	C26	-175.8(3)	?
H22	C24	C25	H24	-55.4(4)	?
H22	C24	C25	H25	63.8(4)	?
H23	C24	C25	C26	64.7(4)	?
H23	C24	C25	H24	-174.9(3)	?
H23	C24	C25	H25	-55.7(4)	?
C24	C25	C26	C27	55.0(4)	?
C24	C25	C26	H26	175.2(3)	?
C24	C25	C26	H27	-65.3(4)	?
H24	C25	C26	C27	-65.4(4)	?
H24	C25	C26	H26	54.8(4)	?
H24	C25	C26	H27	174.3(3)	?
H25	C25	C26	C27	175.4(3)	?
H25	C25	C26	H26	-64.4(4)	?
H25	C25	C26	H27	55.1(5)	?
C25	C26	C27	C28	-56.5(4)	?
C25	C26	C27	H28	63.8(4)	?
C25	C26	C27	H29	-176.7(3)	?
H26	C26	C27	C28	-176.7(3)	?
H26	C26	C27	H28	-56.4(4)	?
H26	C26	C27	H29	63.0(4)	?
H27	C26	C27	C28	63.8(4)	?
H27	C26	C27	H28	-176.0(3)	?
H27	C26	C27	H29	-56.5(4)	?
C26	C27	C28	C23	58.0(3)	?
C26	C27	C28	H30	178.1(3)	?
C26	C27	C28	H31	-62.1(4)	?
H28	C27	C28	C23	-62.3(4)	?
H28	C27	C28	H30	57.8(4)	?
H28	C27	C28	H31	177.6(3)	?
H29	C27	C28	C23	178.3(3)	?
H29	C27	C28	H30	-61.6(4)	?
H29	C27	C28	H31	58.2(4)	?
P2	C29	C30	C31	168.7(3)	?
P2	C29	C30	H33	-71.0(4)	?
P2	C29	C30	H34	48.3(4)	?
C34	C29	C30	C31	-56.5(4)	?
C34	C29	C30	H33	63.8(4)	?
C34	C29	C30	H34	-176.9(3)	?
H32	C29	C30	C31	55.8(4)	?
H32	C29	C30	H33	176.1(3)	?
H32	C29	C30	H34	-64.6(4)	?
P2	C29	C34	C33	-172.2(2)	?
P2	C29	C34	H41	67.8(4)	?
P2	C29	C34	H42	-52.2(4)	?
C30	C29	C34	C33	56.8(4)	?
C30	C29	C34	H41	-63.2(4)	?
C30	C29	C34	H42	176.8(3)	?
H32	C29	C34	C33	-55.5(4)	?
H32	C29	C34	H41	175.6(3)	?

H32	C29	C34	H42	64.5(4)	?
C29	C30	C31	C32	54.9(4)	?
C29	C30	C31	H35	175.1(3)	?
C29	C30	C31	H36	-65.3(4)	?
H33	C30	C31	C32	-65.5(4)	?
H33	C30	C31	H35	54.8(5)	?
H33	C30	C31	H36	174.3(4)	?
H34	C30	C31	C32	175.2(3)	?
H34	C30	C31	H35	-64.6(5)	?
H34	C30	C31	H36	55.0(5)	?
C30	C31	C32	C33	-54.5(4)	?
C30	C31	C32	H37	65.9(5)	?
C30	C31	C32	H38	-174.9(3)	?
H35	C31	C32	C33	-174.8(4)	?
H35	C31	C32	H37	-54.4(5)	?
H35	C31	C32	H38	64.8(5)	?
H36	C31	C32	C33	65.7(5)	?
H36	C31	C32	H37	-173.9(4)	?
H36	C31	C32	H38	-54.7(5)	?
C31	C32	C33	C34	56.2(4)	?
C31	C32	C33	H39	176.5(3)	?
C31	C32	C33	H40	-64.1(4)	?
H37	C32	C33	C34	-64.2(4)	?
H37	C32	C33	H39	56.0(5)	?
H37	C32	C33	H40	175.5(4)	?
H38	C32	C33	C34	176.6(3)	?
H38	C32	C33	H39	-63.1(5)	?
H38	C32	C33	H40	56.3(5)	?
C32	C33	C34	C29	-56.8(4)	?
C32	C33	C34	H41	63.3(4)	?
C32	C33	C34	H42	-176.8(3)	?
H39	C33	C34	C29	-177.0(3)	?
H39	C33	C34	H41	-57.0(4)	?
H39	C33	C34	H42	62.9(4)	?
H40	C33	C34	C29	63.5(4)	?
H40	C33	C34	H41	-176.4(3)	?
H40	C33	C34	H42	-56.5(4)	?
P3	C35	C36	C37	-176.6(2)	?
P3	C35	C36	H44	-56.3(3)	?
P3	C35	C36	H45	63.1(3)	?
C40	C35	C36	C37	-52.2(4)	?
C40	C35	C36	H44	68.1(4)	?
C40	C35	C36	H45	-172.5(3)	?
H43	C35	C36	C37	66.3(4)	?
H43	C35	C36	H44	-173.4(3)	?
H43	C35	C36	H45	-54.0(4)	?
P3	C35	C40	C39	173.0(2)	?
P3	C35	C40	H52	52.7(3)	?
P3	C35	C40	H53	-66.6(3)	?
C36	C35	C40	C39	50.1(4)	?
C36	C35	C40	H52	-70.3(4)	?
C36	C35	C40	H53	170.4(3)	?
H43	C35	C40	C39	-68.4(4)	?
H43	C35	C40	H52	171.2(3)	?
H43	C35	C40	H53	51.9(4)	?
C35	C36	C37	C38	57.8(4)	?
C35	C36	C37	H46	177.9(3)	?
C35	C36	C37	H47	-62.3(4)	?
H44	C36	C37	C38	-62.5(4)	?
H44	C36	C37	H46	57.6(4)	?
H44	C36	C37	H47	177.5(3)	?
H45	C36	C37	C38	178.1(3)	?
H45	C36	C37	H46	-61.9(4)	?
H45	C36	C37	H47	58.0(4)	?
C36	C37	C38	C39	-61.3(4)	?
C36	C37	C38	H48	58.7(4)	?
C36	C37	C38	H49	178.6(3)	?

H46	C37	C38	C39	178.6(3)	.	.	.	.	?
H46	C37	C38	H48	-61.3(4)	.	.	.	.	?
H46	C37	C38	H49	58.5(4)	.	.	.	.	?
H47	C37	C38	C39	58.7(4)	.	.	.	.	?
H47	C37	C38	H48	178.8(3)	.	.	.	.	?
H47	C37	C38	H49	-61.4(4)	.	.	.	.	?
C37	C38	C39	C40	59.6(4)	.	.	.	.	?
C37	C38	C39	H50	179.8(3)	.	.	.	.	?
C37	C38	C39	H51	-60.7(4)	.	.	.	.	?
H48	C38	C39	C40	-60.4(4)	.	.	.	.	?
H48	C38	C39	H50	59.8(4)	.	.	.	.	?
H48	C38	C39	H51	179.3(3)	.	.	.	.	?
H49	C38	C39	C40	179.7(3)	.	.	.	.	?
H49	C38	C39	H50	-60.1(4)	.	.	.	.	?
H49	C38	C39	H51	59.4(4)	.	.	.	.	?
C38	C39	C40	C35	-54.0(4)	.	.	.	.	?
C38	C39	C40	H52	66.4(4)	.	.	.	.	?
C38	C39	C40	H53	-174.3(3)	.	.	.	.	?
H50	C39	C40	C35	-174.2(3)	.	.	.	.	?
H50	C39	C40	H52	-53.9(4)	.	.	.	.	?
H50	C39	C40	H53	65.4(4)	.	.	.	.	?
H51	C39	C40	C35	66.3(4)	.	.	.	.	?
H51	C39	C40	H52	-173.3(3)	.	.	.	.	?
H51	C39	C40	H53	-54.0(4)	.	.	.	.	?
P3	C41	C42	C43	-170.4(2)	.	.	.	.	?
P3	C41	C42	H55	-50.4(4)	.	.	.	.	?
P3	C41	C42	H56	69.5(4)	.	.	.	.	?
C46	C41	C42	C43	59.6(4)	.	.	.	.	?
C46	C41	C42	H55	179.7(3)	.	.	.	.	?
C46	C41	C42	H56	-60.4(4)	.	.	.	.	?
H54	C41	C42	C43	-55.1(4)	.	.	.	.	?
H54	C41	C42	H55	65.0(4)	.	.	.	.	?
H54	C41	C42	H56	-175.1(3)	.	.	.	.	?
P3	C41	C46	C45	174.6(3)	.	.	.	.	?
P3	C41	C46	H63	54.6(4)	.	.	.	.	?
P3	C41	C46	H64	-65.3(4)	.	.	.	.	?
C42	C41	C46	C45	-58.1(4)	.	.	.	.	?
C42	C41	C46	H63	-178.2(3)	.	.	.	.	?
C42	C41	C46	H64	61.9(4)	.	.	.	.	?
H54	C41	C46	C45	56.6(4)	.	.	.	.	?
H54	C41	C46	H63	-63.5(4)	.	.	.	.	?
H54	C41	C46	H64	176.6(3)	.	.	.	.	?
C41	C42	C43	C44	-59.0(4)	.	.	.	.	?
C41	C42	C43	H57	61.1(4)	.	.	.	.	?
C41	C42	C43	H58	-179.1(3)	.	.	.	.	?
H55	C42	C43	C44	-179.0(3)	.	.	.	.	?
H55	C42	C43	H57	-58.9(5)	.	.	.	.	?
H55	C42	C43	H58	60.8(4)	.	.	.	.	?
H56	C42	C43	C44	61.1(4)	.	.	.	.	?
H56	C42	C43	H57	-178.8(3)	.	.	.	.	?
H56	C42	C43	H58	-59.0(5)	.	.	.	.	?
C42	C43	C44	C45	57.5(4)	.	.	.	.	?
C42	C43	C44	H59	177.7(3)	.	.	.	.	?
C42	C43	C44	H60	-62.7(5)	.	.	.	.	?
H57	C43	C44	C45	-62.5(5)	.	.	.	.	?
H57	C43	C44	H59	57.7(5)	.	.	.	.	?
H57	C43	C44	H60	177.3(4)	.	.	.	.	?
H58	C43	C44	C45	177.7(4)	.	.	.	.	?
H58	C43	C44	H59	-62.1(5)	.	.	.	.	?
H58	C43	C44	H60	57.5(5)	.	.	.	.	?
C43	C44	C45	C46	-56.7(5)	.	.	.	.	?
C43	C44	C45	H61	63.6(5)	.	.	.	.	?
C43	C44	C45	H62	-177.0(4)	.	.	.	.	?
H59	C44	C45	C46	-176.9(4)	.	.	.	.	?
H59	C44	C45	H61	-56.6(5)	.	.	.	.	?
H59	C44	C45	H62	62.8(5)	.	.	.	.	?

H60	C44	C45	H61	-176.2(4)	?
H60	C44	C45	H62	-56.8(5)	?
C44	C45	C46	C41	56.9(4)	?
C44	C45	C46	H63	176.9(3)	?
C44	C45	C46	H64	-63.1(5)	?
H61	C45	C46	C41	-63.4(4)	?
H61	C45	C46	H63	56.7(5)	?
H61	C45	C46	H64	176.6(4)	?
H62	C45	C46	C41	177.2(3)	?
H62	C45	C46	H63	-62.8(5)	?
H62	C45	C46	H64	57.1(5)	?
C49	O1	C48	C47	-166.2(5)	?
C49	O1	C48	H68	-46.3(7)	?
C49	O1	C48	H69	73.8(6)	?
C48	O1	C49	C50	-176.8(4)	?
C48	O1	C49	H70	-56.5(7)	?
C48	O1	C49	H71	62.9(7)	?
H65	C47	C48	O1	-60.0(7)	?
H65	C47	C48	H68	-180.0(5)	?
H65	C47	C48	H69	60.0(7)	?
H66	C47	C48	O1	60.0(6)	?
H66	C47	C48	H68	-60.0(6)	?
H66	C47	C48	H69	180.0(5)	?
H67	C47	C48	O1	180.0(5)	?
H67	C47	C48	H68	60.0(7)	?
H67	C47	C48	H69	-60.0(7)	?
O1	C49	C50	H72	-59.7(7)	?
O1	C49	C50	H73	59.7(7)	?
O1	C49	C50	H74	180.0(5)	?
H70	C49	C50	H72	-180.0(5)	?
H70	C49	C50	H73	-60.6(7)	?
H70	C49	C50	H74	59.7(7)	?
H71	C49	C50	H72	60.6(7)	?
H71	C49	C50	H73	180.0(5)	?
H71	C49	C50	H74	-59.7(7)	?
C103	O10	C102	C101	-168.0(7)	?
C103	O10	C102	C201	-128.8(9)	?
C103	O10	C102	C205	48.0(11)	?
C103	O10	C102	C206	-173(3)	?
C201	O10	C102	C101	-39.2(8)	?
C201	O10	C102	C201	.0(7)	?
C201	O10	C102	C205	176.9(11)	?
C201	O10	C102	C206	-44(3)	?
C202	O10	C102	C101	-118.9(14)	?
C202	O10	C102	C201	-79.7(14)	?
C202	O10	C102	C205	97.1(15)	?
C202	O10	C102	C206	-124(3)	?
C203	O10	C102	C101	169.5(6)	?
C203	O10	C102	C201	-151.3(8)	?
C203	O10	C102	C205	25.5(10)	?
C203	O10	C102	C206	164(3)	?
C102	O10	C103	C104	-68.4(9)	?
C102	O10	C103	C202	139.6(11)	?
C102	O10	C103	C203	-65.8(11)	?
C201	O10	C103	C104	-146.3(9)	?
C201	O10	C103	C202	61.7(11)	?
C201	O10	C103	C203	-143.7(11)	?
C202	O10	C103	C104	151.9(11)	?
C202	O10	C103	C202	-.0(9)	?
C202	O10	C103	C203	154.6(13)	?
C203	O10	C103	C104	-2.7(7)	?
C203	O10	C103	C202	-154.6(13)	?
C203	O10	C103	C203	.0(7)	?
C102	O10	C201	C102	-.0(7)	?
C102	O10	C201	C202	-142.8(9)	?
C102	O10	C201	C206	8.0(6)	?

C103	O10	C201	C202	-39.1(8)	.	.	.	.	?
C103	O10	C201	C206	111.7(9)	.	.	.	.	?
C202	O10	C201	C102	142.8(9)	.	.	.	.	?
C202	O10	C201	C202	.0(5)	.	.	.	.	?
C202	O10	C201	C206	150.8(7)	.	.	.	.	?
C203	O10	C201	C102	73.8(14)	.	.	.	.	?
C203	O10	C201	C202	-69.0(13)	.	.	.	.	?
C203	O10	C201	C206	81.8(14)	.	.	.	.	?
C102	O10	C202	C103	-74.8(15)	.	.	.	.	?
C102	O10	C202	C201	65.0(12)	.	.	.	.	?
C102	O10	C202	C203	-85.7(13)	.	.	.	.	?
C103	O10	C202	C103	.0(6)	.	.	.	.	?
C103	O10	C202	C201	139.8(8)	.	.	.	.	?
C103	O10	C202	C203	-10.9(6)	.	.	.	.	?
C201	O10	C202	C103	-139.8(8)	.	.	.	.	?
C201	O10	C202	C201	-.0(5)	.	.	.	.	?
C201	O10	C202	C203	-150.7(7)	.	.	.	.	?
C203	O10	C202	C103	10.9(6)	.	.	.	.	?
C203	O10	C202	C201	150.7(7)	.	.	.	.	?
C203	O10	C202	C203	.0(3)	.	.	.	.	?
C102	O10	C203	C103	123.2(10)	.	.	.	.	?
C102	O10	C203	C104	-64.2(15)	.	.	.	.	?
C102	O10	C203	C202	142.1(9)	.	.	.	.	?
C102	O10	C203	C204	-19.4(7)	.	.	.	.	?
C103	O10	C203	C103	-.0(11)	.	.	.	.	?
C103	O10	C203	C104	172.6(19)	.	.	.	.	?
C103	O10	C203	C202	18.9(10)	.	.	.	.	?
C103	O10	C203	C204	-142.6(10)	.	.	.	.	?
C201	O10	C203	C103	60.7(16)	.	.	.	.	?
C201	O10	C203	C104	-126.6(17)	.	.	.	.	?
C201	O10	C203	C202	79.6(14)	.	.	.	.	?
C201	O10	C203	C204	-81.8(14)	.	.	.	.	?
C202	O10	C203	C103	-18.9(10)	.	.	.	.	?
C202	O10	C203	C104	153.7(15)	.	.	.	.	?
C202	O10	C203	C202	-.0(7)	.	.	.	.	?
C202	O10	C203	C204	-161.5(7)	.	.	.	.	?
C206	C101	C102	O10	-171(4)	.	.	.	.	?
C206	C101	C102	C201	165(4)	.	.	.	.	?
C206	C101	C102	C205	-35(3)	.	.	.	.	?
C206	C101	C102	C206	0(4)	.	.	.	.	?
C102	C101	C206	C102	0(4)	.	.	.	.	?
C102	C101	C206	C201	-13(4)	.	.	.	.	?
C102	C101	C206	C205	131(5)	.	.	.	.	?
O10	C102	C201	O10	.0(5)	.	.	.	.	?
O10	C102	C201	C202	19.7(5)	.	.	.	.	?
O10	C102	C201	C206	-149(2)	.	.	.	.	?
C101	C102	C201	O10	142.5(8)	.	.	.	.	?
C101	C102	C201	C202	162.2(6)	.	.	.	.	?
C101	C102	C201	C206	-6.3(18)	.	.	.	.	?
C205	C102	C201	O10	-6(2)	.	.	.	.	?
C205	C102	C201	C202	14(2)	.	.	.	.	?
C205	C102	C201	C206	-155(4)	.	.	.	.	?
C206	C102	C201	O10	149(2)	.	.	.	.	?
C206	C102	C201	C202	169(2)	.	.	.	.	?
C206	C102	C201	C206	-.0(15)	.	.	.	.	?
O10	C102	C205	C204	-17.9(10)	.	.	.	.	?
O10	C102	C205	C206	150(3)	.	.	.	.	?
C101	C102	C205	C204	-153.9(9)	.	.	.	.	?
C101	C102	C205	C206	14.1(15)	.	.	.	.	?
C201	C102	C205	C204	-14(2)	.	.	.	.	?
C201	C102	C205	C206	154(4)	.	.	.	.	?
C206	C102	C205	C204	-168(2)	.	.	.	.	?
C206	C102	C205	C206	.0(15)	.	.	.	.	?
O10	C102	C206	C101	12(5)	.	.	.	.	?
O10	C102	C206	C201	27.1(15)	.	.	.	.	?
O10	C102	C206	C205	-140(3)	.	.	.	.	?
C101	C102	C206	C101	.0(12)	.	.	.	.	?

C101	C102	C206	C201	15(4)	?
C101	C102	C206	C205	-152(3)	?
C201	C102	C206	C101	-15(4)	?
C201	C102	C206	C201	.0(4)	?
C201	C102	C206	C205	-167.0(18)	?
C205	C102	C206	C101	152(3)	?
C205	C102	C206	C201	167.0(18)	?
C205	C102	C206	C205	-.0(5)	?
O10	C103	C104	C203	7.3(19)	?
O10	C103	C104	C204	44.2(7)	?
C202	C103	C104	C203	28(2)	?
C202	C103	C104	C204	65.1(13)	?
C203	C103	C104	C203	.0(19)	?
C203	C103	C104	C204	36.9(19)	?
O10	C103	C202	O10	-.0(6)	?
O10	C103	C202	C201	-34.9(7)	?
O10	C103	C202	C203	28.9(15)	?
C104	C103	C202	O10	-40.1(15)	?
C104	C103	C202	C201	-74.9(15)	?
C104	C103	C202	C203	-11.2(8)	?
C203	C103	C202	O10	-28.9(15)	?
C203	C103	C202	C201	-63.7(16)	?
C203	C103	C202	C203	-.0(8)	?
O10	C103	C203	O10	.0(3)	?
O10	C103	C203	C104	-173.1(17)	?
O10	C103	C203	C202	-14.5(8)	?
O10	C103	C203	C204	65.5(14)	?
C104	C103	C203	O10	173.1(17)	?
C104	C103	C203	C104	-.0(14)	?
C104	C103	C203	C202	158.6(15)	?
C104	C103	C203	C204	-121(3)	?
C202	C103	C203	O10	14.5(8)	?
C202	C103	C203	C104	-158.6(15)	?
C202	C103	C203	C202	.0(6)	?
C202	C103	C203	C204	80.0(17)	?
C103	C104	C203	O10	-168(3)	?
C103	C104	C203	C103	.0(17)	?
C103	C104	C203	C202	-101(4)	?
C103	C104	C203	C204	141(2)	?
C204	C104	C203	O10	50.6(14)	?
C204	C104	C203	C103	-141(2)	?
C204	C104	C203	C202	118(3)	?
C204	C104	C203	C204	-.0(4)	?
C103	C104	C204	C203	-8.6(5)	?
C103	C104	C204	C205	-44(2)	?
C203	C104	C204	C203	.0(5)	?
C203	C104	C204	C205	-36(2)	?
O10	C201	C202	O10	.0(9)	?
O10	C201	C202	C103	58.1(11)	?
O10	C201	C202	C203	34.3(9)	?
C102	C201	C202	O10	-37.8(9)	?
C102	C201	C202	C103	20.3(12)	?
C102	C201	C202	C203	-3.5(9)	?
C206	C201	C202	O10	-34.3(9)	?
C206	C201	C202	C103	23.9(12)	?
C206	C201	C202	C203	.0(9)	?
O10	C201	C206	C101	141.4(8)	?
O10	C201	C206	C102	-31(2)	?
O10	C201	C206	C205	-17.7(10)	?
C102	C201	C206	C101	172(2)	?
C102	C201	C206	C102	0(2)	?
C102	C201	C206	C205	12.8(18)	?
C202	C201	C206	C101	159.1(8)	?
C202	C201	C206	C102	-13(2)	?
C202	C201	C206	C205	-.0(11)	?
O10	C202	C203	O10	.0(6)	?
O10	C202	C203	C103	152.1(15)	?