

Supplementary Information

Catalytic Properties of a Cobalt Metal-Organic Framework with a Zwitterionic Ligand
Synthesized *In Situ*

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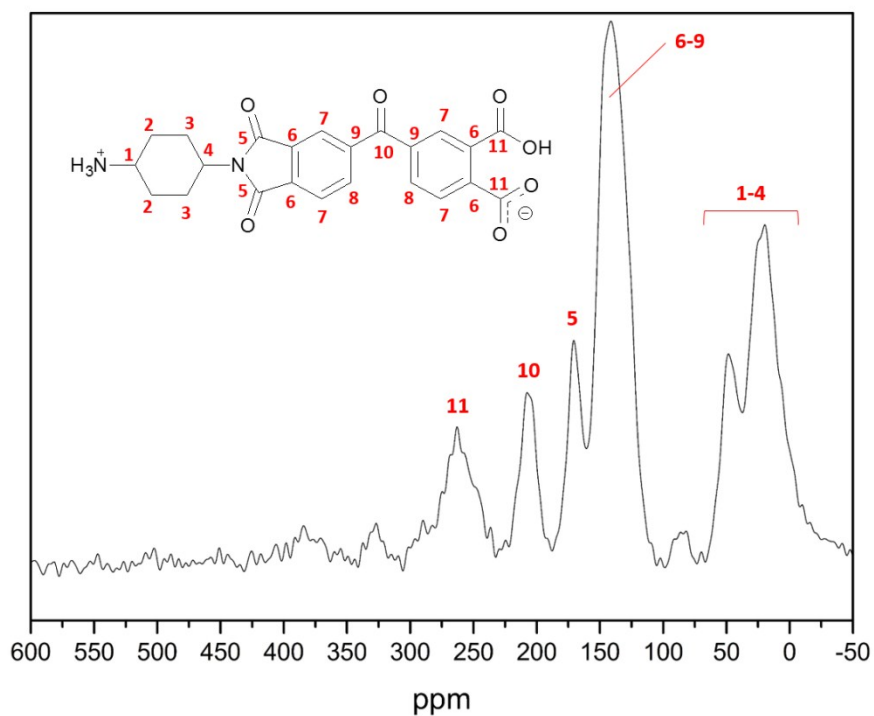


Figure S1. ^{13}C Nuclear magnetic resonance spectrum of the Co-MOF.

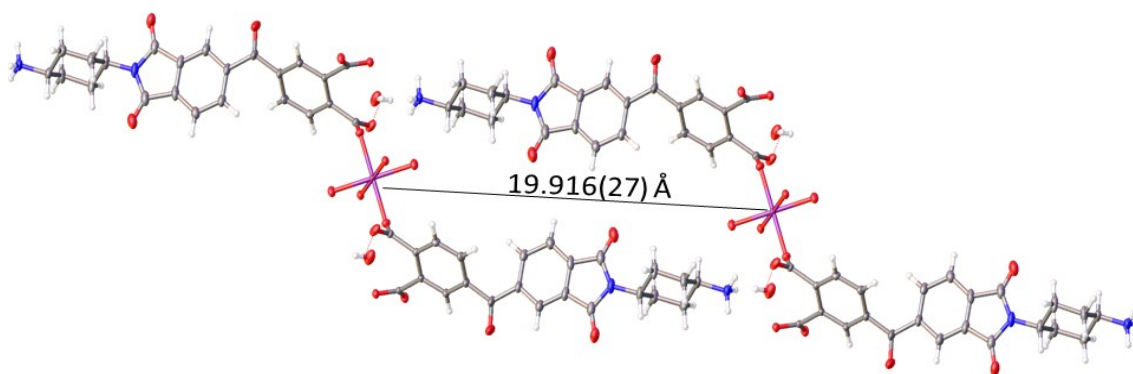


Figure S2. Crystallographic structure showing the distance between the cobalt centers of different 1D units (green) and hydrogen bonds between the ammonium ion and the oxygens of the coordination sphere of cobalt (yellow).

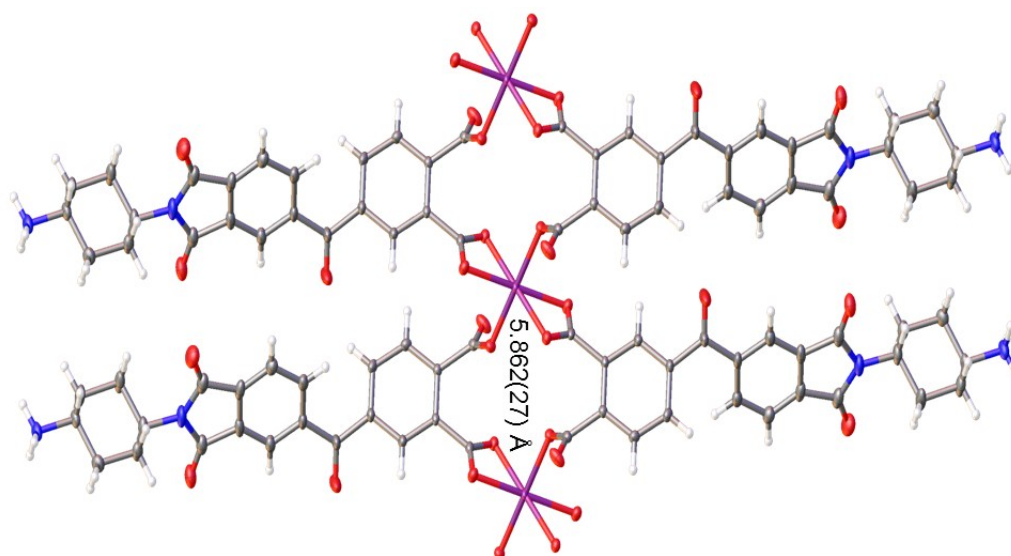


Figure S3. Crystallographic structure showing the distance between the cobalt centers of the same 1D unit.

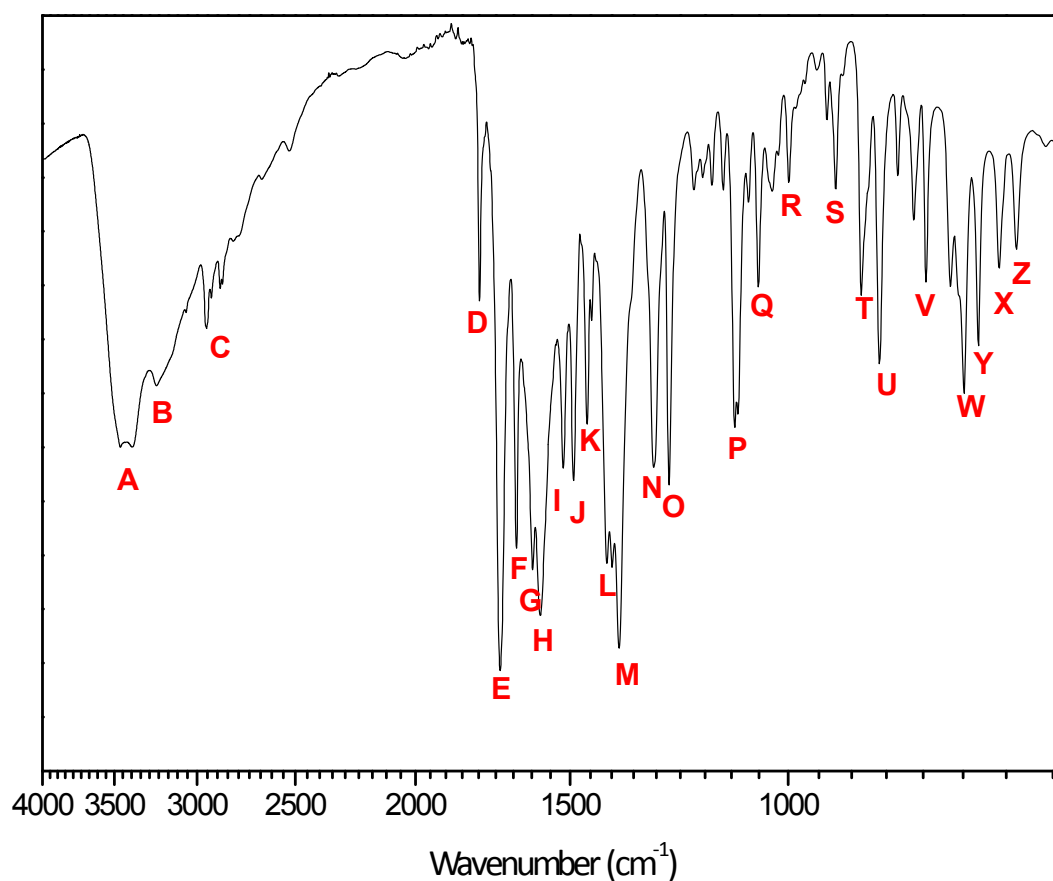


Figure S4. FT-IR spectrum of Co-MOF obtained on KBr optics. A) 3469-3400 cm^{-1} , B) 3238 cm^{-1} , C) 2949-2878 cm^{-1} , D) 1774 cm^{-1} , E) 1708 cm^{-1} , F) 1657 cm^{-1} , G) 1608 cm^{-1} , H) 1586 cm^{-1} , I) 1523 cm^{-1} , J) 1486 cm^{-1} , K) 1456 cm^{-1} , L) 1402 cm^{-1} , M) 1368 cm^{-1} , N) 1280 cm^{-1} , O) 1247 cm^{-1} , P) 1107 cm^{-1} , Q) 1057 cm^{-1} , R) 998 cm^{-1} , S) 919 cm^{-1} , T) 871 cm^{-1} , U) 845 cm^{-1} , V) 775 cm^{-1} , W) 772 cm^{-1} , Y) 702 cm^{-1} , X) 673 cm^{-1} and Z) 657 cm^{-1} .

Table S1. Bond Lengths

Number	Atom 1	Atom 2	Cyclicity	Length
1	Co	O1	acyclic	2.068
2	Co	O11	cyclic	2.133
3	Co	O12	cyclic	2.132
4	O1	C3	acyclic	1.264(3)
5	O2	C3	acyclic	1.240(4)
6	C3	C4	acyclic	1.511(4)
7	C4	C5	cyclic	1.382(4)
8	C4	C9	cyclic	1.404(4)
9	C5	H5	acyclic	0.950
10	C5	C6	cyclic	1.388(4)
11	C6	H6	acyclic	0.950
12	C6	C7	cyclic	1.396(4)
13	C7	C8	cyclic	1.399(4)
14	C7	C13	acyclic	1.488(4)
15	C8	H8	acyclic	0.950
16	C8	C9	cyclic	1.383(4)
17	C9	C10	acyclic	1.500(4)
18	C10	O11	acyclic	1.258(4)
19	C10	O12	acyclic	1.262(4)
20	C13	O14	acyclic	1.223(5)
21	C13	C15	acyclic	1.494(5)
22	C15	C16	cyclic	1.400(6)
23	C15	C20	cyclic	1.403(5)
24	C16	H16	acyclic	0.950
25	C16	C17	cyclic	1.403(5)
26	C17	H17	acyclic	0.950
27	C17	C18	cyclic	1.386(5)
28	C18	C19	cyclic	1.383(6)
29	C18	C21	cyclic	1.506(5)
30	C19	C20	cyclic	1.378(5)
31	C19	C24	cyclic	1.493(5)
32	C20	H20	acyclic	0.950
33	C21	O22	acyclic	1.203(6)
34	C21	N23	cyclic	1.410(5)
35	N23	C24	cyclic	1.400(5)
36	N23	C26	acyclic	1.476(4)
37	C24	O25	acyclic	1.203(5)
38	C26	H26	acyclic	1.05(5)
39	C26	C27	cyclic	1.528(5)
40	C26	C31	cyclic	1.520(5)
41	C27	H27A	acyclic	0.990
42	C27	H27B	acyclic	0.990
43	C27	C28	cyclic	1.541(5)
44	C28	H28A	acyclic	0.990
45	C28	H28B	acyclic	0.990
46	C28	C29	cyclic	1.520(5)
47	C29	H29	acyclic	1.01(5)

48	C29	C30	cyclic	1.502(5)
49	C29	N32	acyclic	1.501(4)
50	C30	H30A	acyclic	0.990
51	C30	H30B	acyclic	0.990
52	C30	C31	cyclic	1.523(5)
53	C31	H31A	acyclic	0.990
54	C31	H31B	acyclic	0.990
55	N32	H32A	acyclic	0.910
56	N32	H32B	acyclic	0.910
57	N32	H32C	acyclic	0.910
58	O100	H10A	acyclic	0.83(3)
59	O100	H10B	acyclic	0.84(3)

Table S2. Bond angles.

Number	Atom 1	Atom 2	Atom 3	Angle
1	O1	Co	O1	180.00
2	O1	Co	O11	93.32
3	O1	Co	O11	86.68
4	O1	Co	O12	86.10
5	O1	Co	O12	93.90
6	O1	Co	O11	86.68
7	O1	Co	O11	93.32
8	O1	Co	O12	93.90
9	O1	Co	O12	86.10
10	O11	Co	O11	180.00
11	O11	Co	O12	62.13
12	O11	Co	O12	117.87
13	O11	Co	O12	117.87
14	O11	Co	O12	62.13
15	O12	Co	O12	180.00
16	Co	O1	C3	124.3
17	O1	C3	O2	125.2(3)
18	O1	C3	C4	115.4(2)
19	O2	C3	C4	119.4(3)
20	C3	C4	C5	120.8(3)
21	C3	C4	C9	119.7(2)
22	C5	C4	C9	119.3(3)
23	C4	C5	H5	119.3
24	C4	C5	C6	121.5(3)
25	H5	C5	C6	119.3
26	C5	C6	H6	120.4
27	C5	C6	C7	119.3(3)
28	H6	C6	C7	120.3
29	C6	C7	C8	119.5(3)
30	C6	C7	C13	122.7(3)
31	C8	C7	C13	117.6(3)
32	C7	C8	H8	119.6
33	C7	C8	C9	120.8(3)
34	H8	C8	C9	119.6
35	C4	C9	C8	119.6(3)
36	C4	C9	C10	119.6(2)
37	C8	C9	C10	120.7(3)
38	C9	C10	O11	118.8(2)
39	C9	C10	O12	119.5(3)
40	O11	C10	O12	121.7(3)
41	C10	O11	Co	88.1
42	C10	O12	Co	88.1
43	C7	C13	O14	118.9(3)
44	C7	C13	C15	122.3(3)
45	O14	C13	C15	118.8(3)
46	C13	C15	C16	122.4(3)
47	C13	C15	C20	116.8(3)
48	C16	C15	C20	120.6(3)
49	C15	C16	H16	119.4

50	C15	C16	C17	121.2(3)
51	H16	C16	C17	119.4
52	C16	C17	H17	121.5
53	C16	C17	C18	117.0(3)
54	H17	C17	C18	121.5
55	C17	C18	C19	121.7(3)
56	C17	C18	C21	130.2(3)
57	C19	C18	C21	108.0(3)
58	C18	C19	C20	121.9(3)
59	C18	C19	C24	109.2(3)
60	C20	C19	C24	128.9(3)
61	C15	C20	C19	117.6(3)
62	C15	C20	H20	121.2
63	C19	C20	H20	121.2
64	C18	C21	O22	128.6(3)
65	C18	C21	N23	104.9(3)
66	O22	C21	N23	126.5(4)
67	C21	N23	C24	112.7(3)
68	C21	N23	C26	126.3(3)
69	C24	N23	C26	120.4(3)
70	C19	C24	N23	105.1(3)
71	C19	C24	O25	129.1(3)
72	N23	C24	O25	125.8(3)
73	N23	C26	H26	107(2)
74	N23	C26	C27	112.0(3)
75	N23	C26	C31	110.6(3)
76	H26	C26	C27	109(2)
77	H26	C26	C31	106(2)
78	C27	C26	C31	112.0(3)
79	C26	C27	H27A	109.8
80	C26	C27	H27B	109.8
81	C26	C27	C28	109.3(3)
82	H27A	C27	H27B	108.2
83	H27A	C27	C28	109.8
84	H27B	C27	C28	109.8
85	C27	C28	H28A	109.8
86	C27	C28	H28B	109.8
87	C27	C28	C29	109.3(3)
88	H28A	C28	H28B	108.3
89	H28A	C28	C29	109.8
90	H28B	C28	C29	109.8
91	C28	C29	H29	108(2)
92	C28	C29	C30	112.0(3)
93	C28	C29	N32	110.3(3)
94	H29	C29	C30	114(2)
95	H29	C29	N32	103(2)
96	C30	C29	N32	109.3(3)
97	C29	C30	H30A	109.6
98	C29	C30	H30B	109.6
99	C29	C30	C31	110.1(3)
100	H30A	C30	H30B	108.1

101	H30A	C30	C31	109.6
102	H30B	C30	C31	109.7
103	C26	C31	C30	111.1(3)
104	C26	C31	H31A	109.4
105	C26	C31	H31B	109.5
106	C30	C31	H31A	109.5
107	C30	C31	H31B	109.4
108	H31A	C31	H31B	108.0
109	C29	N32	H32A	109.5
110	C29	N32	H32B	109.5
111	C29	N32	H32C	109.5
112	H32A	N32	H32B	109.5
113	H32A	N32	H32C	109.4
114	H32B	N32	H32C	109.5
115	Co	O1	C3	124.3
116	O1	C3	O2	125.2(3)
117	O1	C3	C4	115.4(2)
118	O2	C3	C4	119.4(3)
119	C3	C4	C5	120.8(3)
120	C3	C4	C9	119.7(2)
121	C5	C4	C9	119.3(3)
122	C4	C5	H5	119.3
123	C4	C5	C6	121.5(3)
124	H5	C5	C6	119.3
125	C5	C6	H6	120.4
126	C5	C6	C7	119.3(3)
127	H6	C6	C7	120.3
128	C6	C7	C8	119.5(3)
129	C6	C7	C13	122.7(3)
130	C8	C7	C13	117.6(3)
131	C7	C8	H8	119.6
132	C7	C8	C9	120.8(3)
133	H8	C8	C9	119.6
134	C4	C9	C8	119.6(3)
135	C4	C9	C10	119.6(2)
136	C8	C9	C10	120.7(3)
137	C9	C10	O11	118.8(2)
138	C9	C10	O12	119.5(3)
139	O11	C10	O12	121.7(3)
140	C10	O11	Co	88.1
141	C10	O12	Co	88.1
142	C7	C13	O14	118.9(3)
143	C7	C13	C15	122.3(3)
144	O14	C13	C15	118.8(3)
145	C13	C15	C16	122.4(3)
146	C13	C15	C20	116.8(3)
147	C16	C15	C20	120.6(3)
148	C15	C16	H16	119.4
149	C15	C16	C17	121.2(3)
150	H16	C16	C17	119.4
151	C16	C17	H17	121.5

152	C16	C17	C18	117.0(3)
153	H17	C17	C18	121.5
154	C17	C18	C19	121.7(3)
155	C17	C18	C21	130.2(3)
156	C19	C18	C21	108.0(3)
157	C18	C19	C20	121.9(3)
158	C18	C19	C24	109.2(3)
159	C20	C19	C24	128.9(3)
160	C15	C20	C19	117.6(3)
161	C15	C20	H20	121.2
162	C19	C20	H20	121.2
163	C18	C21	O22	128.6(3)
164	C18	C21	N23	104.9(3)
165	O22	C21	N23	126.5(4)
166	C21	N23	C24	112.7(3)
167	C21	N23	C26	126.3(3)
168	C24	N23	C26	120.4(3)
169	C19	C24	N23	105.1(3)
170	C19	C24	O25	129.1(3)
171	N23	C24	O25	125.8(3)
172	N23	C26	H26	107(2)
173	N23	C26	C27	112.0(3)
174	N23	C26	C31	110.6(3)
175	H26	C26	C27	109(2)
176	H26	C26	C31	106(2)
177	C27	C26	C31	112.0(3)
178	C26	C27	H27A	109.8
179	C26	C27	H27B	109.8
180	C26	C27	C28	109.3(3)
181	H27A	C27	H27B	108.2
182	H27A	C27	C28	109.8
183	H27B	C27	C28	109.8
184	C27	C28	H28A	109.8
185	C27	C28	H28B	109.8
186	C27	C28	C29	109.3(3)
187	H28A	C28	H28B	108.3
188	H28A	C28	C29	109.8
189	H28B	C28	C29	109.8
190	C28	C29	H29	108(2)
191	C28	C29	C30	112.0(3)
192	C28	C29	N32	110.3(3)
193	H29	C29	C30	114(2)
194	H29	C29	N32	103(2)
195	C30	C29	N32	109.3(3)
196	C29	C30	H30A	109.6
197	C29	C30	H30B	109.6
198	C29	C30	C31	110.1(3)
199	H30A	C30	H30B	108.1
200	H30A	C30	C31	109.6
201	H30B	C30	C31	109.7
202	C26	C31	C30	111.1(3)

203	C26	C31	H31A	109.4
204	C26	C31	H31B	109.5
205	C30	C31	H31A	109.5
206	C30	C31	H31B	109.4
207	H31A	C31	H31B	108.0
208	C29	N32	H32A	109.5
209	C29	N32	H32B	109.5
210	C29	N32	H32C	109.5
211	H32A	N32	H32B	109.5
212	H32A	N32	H32C	109.4
213	H32B	N32	H32C	109.5
214	O11	Co	O12	62.13
215	O11	Co	O1	86.68
216	O11	Co	O1	93.32
217	O11	Co	O11	180.00
218	O11	Co	O12	117.87
219	O12	Co	O1	93.90
220	O12	Co	O1	86.10
221	O12	Co	O11	117.87
222	O12	Co	O12	180.00
223	O1	Co	O1	180.00
224	O1	Co	O11	93.32
225	O1	Co	O12	86.10
226	O1	Co	O11	86.68
227	O1	Co	O12	93.90
228	O11	Co	O12	62.13
229	O11	Co	O12	62.13
230	O11	Co	O1	93.32
231	O11	Co	O1	86.68
232	O11	Co	O11	180.00
233	O11	Co	O12	117.87
234	O12	Co	O1	86.10
235	O12	Co	O1	93.90
236	O12	Co	O11	117.87
237	O12	Co	O12	180.00
238	O1	Co	O1	180.00
239	O1	Co	O11	86.68
240	O1	Co	O12	93.90
241	O1	Co	O11	93.32
242	O1	Co	O12	86.10
243	O11	Co	O12	62.13
244	Co	O11	C10	88.1
245	Co	O11	C10	88.1
246	Co	O12	C10	88.1
247	Co	O12	C10	88.1
248	Co	O1	C3	124.3
249	Co	O1	C3	124.3
250	O1	C3	O2	125.2(3)
251	O1	C3	C4	115.4(2)
252	O2	C3	C4	119.4(3)
253	C3	C4	C5	120.8(3)

254	C3	C4	C9	119.7(2)
255	C5	C4	C9	119.3(3)
256	C4	C5	H5	119.3
257	C4	C5	C6	121.5(3)
258	H5	C5	C6	119.3
259	C4	C9	C8	119.6(3)
260	C4	C9	C10	119.6(2)
261	C8	C9	C10	120.7(3)
262	C5	C6	H6	120.4
263	C5	C6	C7	119.3(3)
264	H6	C6	C7	120.3
265	C6	C7	C8	119.5(3)
266	C6	C7	C13	122.7(3)
267	C8	C7	C13	117.6(3)
268	C9	C8	C7	120.8(3)
269	C9	C8	H8	119.6
270	C7	C8	H8	119.6
271	C7	C13	O14	118.9(3)
272	C7	C13	C15	122.3(3)
273	O14	C13	C15	118.8(3)
274	O11	C10	O12	121.7(3)
275	O11	C10	C9	118.8(2)
276	O12	C10	C9	119.5(3)
277	C13	C15	C16	122.4(3)
278	C13	C15	C20	116.8(3)
279	C16	C15	C20	120.6(3)
280	C15	C16	H16	119.4
281	C15	C16	C17	121.2(3)
282	H16	C16	C17	119.4
283	C15	C20	C19	117.6(3)
284	C15	C20	H20	121.2
285	C19	C20	H20	121.2
286	C16	C17	H17	121.5
287	C16	C17	C18	117.0(3)
288	H17	C17	C18	121.5
289	C17	C18	C19	121.7(3)
290	C17	C18	C21	130.2(3)
291	C19	C18	C21	108.0(3)
292	C20	C19	C18	121.9(3)
293	C20	C19	C24	128.9(3)
294	C18	C19	C24	109.2(3)
295	C18	C21	O22	128.6(3)
296	C18	C21	N23	104.9(3)
297	O22	C21	N23	126.5(4)
298	C19	C24	N23	105.1(3)
299	C19	C24	O25	129.1(3)
300	N23	C24	O25	125.8(3)
301	C21	N23	C24	112.7(3)
302	C21	N23	C26	126.3(3)
303	C24	N23	C26	120.4(3)
304	N23	C26	H26	107(2)

305	N23	C26	C27	112.0(3)
306	N23	C26	C31	110.6(3)
307	H26	C26	C27	109(2)
308	H26	C26	C31	106(2)
309	C27	C26	C31	112.0(3)
310	C26	C27	H27A	109.8
311	C26	C27	H27B	109.8
312	C26	C27	C28	109.3(3)
313	H27A	C27	H27B	108.2
314	H27A	C27	C28	109.8
315	H27B	C27	C28	109.8
316	C26	C31	C30	111.1(3)
317	C26	C31	H31A	109.4
318	C26	C31	H31B	109.5
319	C30	C31	H31A	109.5
320	C30	C31	H31B	109.4
321	H31A	C31	H31B	108.0
322	C27	C28	H28A	109.8
323	C27	C28	H28B	109.8
324	C27	C28	C29	109.3(3)
325	H28A	C28	H28B	108.3
326	H28A	C28	C29	109.8
327	H28B	C28	C29	109.8
328	C28	C29	H29	108(2)
329	C28	C29	C30	112.0(3)
330	C28	C29	N32	110.3(3)
331	H29	C29	C30	114(2)
332	H29	C29	N32	103(2)
333	C30	C29	N32	109.3(3)
334	C31	C30	C29	110.1(3)
335	C31	C30	H30A	109.6
336	C31	C30	H30B	109.7
337	C29	C30	H30A	109.6
338	C29	C30	H30B	109.6
339	H30A	C30	H30B	108.1
340	C29	N32	H32A	109.5
341	C29	N32	H32B	109.5
342	C29	N32	H32C	109.5
343	H32A	N32	H32B	109.5
344	H32A	N32	H32C	109.4
345	H32B	N32	H32C	109.5
346	O1	C3	O2	125.2(3)
347	O1	C3	C4	115.4(2)
348	O2	C3	C4	119.4(3)
349	C3	C4	C5	120.8(3)
350	C3	C4	C9	119.7(2)
351	C5	C4	C9	119.3(3)
352	C4	C5	H5	119.3
353	C4	C5	C6	121.5(3)
354	H5	C5	C6	119.3
355	C4	C9	C8	119.6(3)

356	C4	C9	C10	119.6(2)
357	C8	C9	C10	120.7(3)
358	C5	C6	H6	120.4
359	C5	C6	C7	119.3(3)
360	H6	C6	C7	120.3
361	C6	C7	C8	119.5(3)
362	C6	C7	C13	122.7(3)
363	C8	C7	C13	117.6(3)
364	C9	C8	C7	120.8(3)
365	C9	C8	H8	119.6
366	C7	C8	H8	119.6
367	C7	C13	O14	118.9(3)
368	C7	C13	C15	122.3(3)
369	O14	C13	C15	118.8(3)
370	C9	C10	O11	118.8(2)
371	C9	C10	O12	119.5(3)
372	O11	C10	O12	121.7(3)
373	C10	O11	Co	88.1
374	C10	O12	Co	88.1
375	O11	Co	O12	62.13
376	C13	C15	C16	122.4(3)
377	C13	C15	C20	116.8(3)
378	C16	C15	C20	120.6(3)
379	C15	C16	H16	119.4
380	C15	C16	C17	121.2(3)
381	H16	C16	C17	119.4
382	C15	C20	C19	117.6(3)
383	C15	C20	H20	121.2
384	C19	C20	H20	121.2
385	C16	C17	H17	121.5
386	C16	C17	C18	117.0(3)
387	H17	C17	C18	121.5
388	C17	C18	C19	121.7(3)
389	C17	C18	C21	130.2(3)
390	C19	C18	C21	108.0(3)
391	C20	C19	C18	121.9(3)
392	C20	C19	C24	128.9(3)
393	C18	C19	C24	109.2(3)
394	C18	C21	O22	128.6(3)
395	C18	C21	N23	104.9(3)
396	O22	C21	N23	126.5(4)
397	C19	C24	N23	105.1(3)
398	C19	C24	O25	129.1(3)
399	N23	C24	O25	125.8(3)
400	C21	N23	C24	112.7(3)
401	C21	N23	C26	126.3(3)
402	C24	N23	C26	120.4(3)
403	N23	C26	H26	107(2)
404	N23	C26	C27	112.0(3)
405	N23	C26	C31	110.6(3)
406	H26	C26	C27	109(2)

407	H26	C26	C31	106(2)
408	C27	C26	C31	112.0(3)
409	C26	C27	H27A	109.8
410	C26	C27	H27B	109.8
411	C26	C27	C28	109.3(3)
412	H27A	C27	H27B	108.2
413	H27A	C27	C28	109.8
414	H27B	C27	C28	109.8
415	C26	C31	C30	111.1(3)
416	C26	C31	H31A	109.4
417	C26	C31	H31B	109.5
418	C30	C31	H31A	109.5
419	C30	C31	H31B	109.4
420	H31A	C31	H31B	108.0
421	C27	C28	H28A	109.8
422	C27	C28	H28B	109.8
423	C27	C28	C29	109.3(3)
424	H28A	C28	H28B	108.3
425	H28A	C28	C29	109.8
426	H28B	C28	C29	109.8
427	C28	C29	H29	108(2)
428	C28	C29	C30	112.0(3)
429	C28	C29	N32	110.3(3)
430	H29	C29	C30	114(2)
431	H29	C29	N32	103(2)
432	C30	C29	N32	109.3(3)
433	C31	C30	C29	110.1(3)
434	C31	C30	H30A	109.6
435	C31	C30	H30B	109.7
436	C29	C30	H30A	109.6
437	C29	C30	H30B	109.6
438	H30A	C30	H30B	108.1
439	C29	N32	H32A	109.5
440	C29	N32	H32B	109.5
441	C29	N32	H32C	109.5
442	H32A	N32	H32B	109.5
443	H32A	N32	H32C	109.4
444	H32B	N32	H32C	109.5
445	Co	O1	C3	124.3
446	Co	O1	C3	124.3
447	O1	C3	O2	125.2(3)
448	O1	C3	C4	115.4(2)
449	O2	C3	C4	119.4(3)
450	C3	C4	C5	120.8(3)
451	C3	C4	C9	119.7(2)
452	C5	C4	C9	119.3(3)
453	C4	C5	H5	119.3
454	C4	C5	C6	121.5(3)
455	H5	C5	C6	119.3
456	C4	C9	C8	119.6(3)
457	C4	C9	C10	119.6(2)

458	C8	C9	C10	120.7(3)
459	C5	C6	H6	120.4
460	C5	C6	C7	119.3(3)
461	H6	C6	C7	120.3
462	C6	C7	C8	119.5(3)
463	C6	C7	C13	122.7(3)
464	C8	C7	C13	117.6(3)
465	C9	C8	C7	120.8(3)
466	C9	C8	H8	119.6
467	C7	C8	H8	119.6
468	C7	C13	O14	118.9(3)
469	C7	C13	C15	122.3(3)
470	O14	C13	C15	118.8(3)
471	C9	C10	O11	118.8(2)
472	C9	C10	O12	119.5(3)
473	O11	C10	O12	121.7(3)
474	C10	O11	Co	88.1
475	C10	O12	Co	88.1
476	O11	Co	O12	62.13
477	C13	C15	C16	122.4(3)
478	C13	C15	C20	116.8(3)
479	C16	C15	C20	120.6(3)
480	C15	C16	H16	119.4
481	C15	C16	C17	121.2(3)
482	H16	C16	C17	119.4
483	C15	C20	C19	117.6(3)
484	C15	C20	H20	121.2
485	C19	C20	H20	121.2
486	C16	C17	H17	121.5
487	C16	C17	C18	117.0(3)
488	H17	C17	C18	121.5
489	C17	C18	C19	121.7(3)
490	C17	C18	C21	130.2(3)
491	C19	C18	C21	108.0(3)
492	C20	C19	C18	121.9(3)
493	C20	C19	C24	128.9(3)
494	C18	C19	C24	109.2(3)
495	C18	C21	O22	128.6(3)
496	C18	C21	N23	104.9(3)
497	O22	C21	N23	126.5(4)
498	C19	C24	N23	105.1(3)
499	C19	C24	O25	129.1(3)
500	N23	C24	O25	125.8(3)
501	C21	N23	C24	112.7(3)
502	C21	N23	C26	126.3(3)
503	C24	N23	C26	120.4(3)
504	N23	C26	H26	107(2)
505	N23	C26	C27	112.0(3)
506	N23	C26	C31	110.6(3)
507	H26	C26	C27	109(2)
508	H26	C26	C31	106(2)

509	C27	C26	C31	112.0(3)
510	C26	C27	H27A	109.8
511	C26	C27	H27B	109.8
512	C26	C27	C28	109.3(3)
513	H27A	C27	H27B	108.2
514	H27A	C27	C28	109.8
515	H27B	C27	C28	109.8
516	C26	C31	C30	111.1(3)
517	C26	C31	H31A	109.4
518	C26	C31	H31B	109.5
519	C30	C31	H31A	109.5
520	C30	C31	H31B	109.4
521	H31A	C31	H31B	108.0
522	C27	C28	H28A	109.8
523	C27	C28	H28B	109.8
524	C27	C28	C29	109.3(3)
525	H28A	C28	H28B	108.3
526	H28A	C28	C29	109.8
527	H28B	C28	C29	109.8
528	C28	C29	H29	108(2)
529	C28	C29	C30	112.0(3)
530	C28	C29	N32	110.3(3)
531	H29	C29	C30	114(2)
532	H29	C29	N32	103(2)
533	C30	C29	N32	109.3(3)
534	C31	C30	C29	110.1(3)
535	C31	C30	H30A	109.6
536	C31	C30	H30B	109.7
537	C29	C30	H30A	109.6
538	C29	C30	H30B	109.6
539	H30A	C30	H30B	108.1
540	C29	N32	H32A	109.5
541	C29	N32	H32B	109.5
542	C29	N32	H32C	109.5
543	H32A	N32	H32B	109.5
544	H32A	N32	H32C	109.4
545	H32B	N32	H32C	109.5
546	O1	C3	O2	125.2(3)
547	O1	C3	C4	115.4(2)
548	O2	C3	C4	119.4(3)
549	C3	C4	C5	120.8(3)
550	C3	C4	C9	119.7(2)
551	C5	C4	C9	119.3(3)
552	C4	C5	H5	119.3
553	C4	C5	C6	121.5(3)
554	H5	C5	C6	119.3
555	C4	C9	C8	119.6(3)
556	C4	C9	C10	119.6(2)
557	C8	C9	C10	120.7(3)
558	C5	C6	H6	120.4
559	C5	C6	C7	119.3(3)

560	H6	C6	C7	120.3
561	C6	C7	C8	119.5(3)
562	C6	C7	C13	122.7(3)
563	C8	C7	C13	117.6(3)
564	C9	C8	C7	120.8(3)
565	C9	C8	H8	119.6
566	C7	C8	H8	119.6
567	C7	C13	O14	118.9(3)
568	C7	C13	C15	122.3(3)
569	O14	C13	C15	118.8(3)
570	O11	C10	O12	121.7(3)
571	O11	C10	C9	118.8(2)
572	O12	C10	C9	119.5(3)
573	C13	C15	C16	122.4(3)
574	C13	C15	C20	116.8(3)
575	C16	C15	C20	120.6(3)
576	C15	C16	H16	119.4
577	C15	C16	C17	121.2(3)
578	H16	C16	C17	119.4
579	C15	C20	C19	117.6(3)
580	C15	C20	H20	121.2
581	C19	C20	H20	121.2
582	C16	C17	H17	121.5
583	C16	C17	C18	117.0(3)
584	H17	C17	C18	121.5
585	C17	C18	C19	121.7(3)
586	C17	C18	C21	130.2(3)
587	C19	C18	C21	108.0(3)
588	C20	C19	C18	121.9(3)
589	C20	C19	C24	128.9(3)
590	C18	C19	C24	109.2(3)
591	C18	C21	O22	128.6(3)
592	C18	C21	N23	104.9(3)
593	O22	C21	N23	126.5(4)
594	C19	C24	N23	105.1(3)
595	C19	C24	O25	129.1(3)
596	N23	C24	O25	125.8(3)
597	C21	N23	C24	112.7(3)
598	C21	N23	C26	126.3(3)
599	C24	N23	C26	120.4(3)
600	N23	C26	H26	107(2)
601	N23	C26	C27	112.0(3)
602	N23	C26	C31	110.6(3)
603	H26	C26	C27	109(2)
604	H26	C26	C31	106(2)
605	C27	C26	C31	112.0(3)
606	C26	C27	H27A	109.8
607	C26	C27	H27B	109.8
608	C26	C27	C28	109.3(3)
609	H27A	C27	H27B	108.2
610	H27A	C27	C28	109.8

611	H27B	C27	C28	109.8
612	C26	C31	C30	111.1(3)
613	C26	C31	H31A	109.4
614	C26	C31	H31B	109.5
615	C30	C31	H31A	109.5
616	C30	C31	H31B	109.4
617	H31A	C31	H31B	108.0
618	C27	C28	H28A	109.8
619	C27	C28	H28B	109.8
620	C27	C28	C29	109.3(3)
621	H28A	C28	H28B	108.3
622	H28A	C28	C29	109.8
623	H28B	C28	C29	109.8
624	C28	C29	H29	108(2)
625	C28	C29	C30	112.0(3)
626	C28	C29	N32	110.3(3)
627	H29	C29	C30	114(2)
628	H29	C29	N32	103(2)
629	C30	C29	N32	109.3(3)
630	C31	C30	C29	110.1(3)
631	C31	C30	H30A	109.6
632	C31	C30	H30B	109.7
633	C29	C30	H30A	109.6
634	C29	C30	H30B	109.6
635	H30A	C30	H30B	108.1
636	C29	N32	H32A	109.5
637	C29	N32	H32B	109.5
638	C29	N32	H32C	109.5
639	H32A	N32	H32B	109.5
640	H32A	N32	H32C	109.4
641	H32B	N32	H32C	109.5
642	H10A	O100	H10B	102(4)

Table S3. Bond torsion.

Number	Atom 1	Atom 2	Atom 3	Atom 4	Torsion
1	O1	Co	O1	C3	Undefined
2	O11	Co	O1	C3	19.8
3	O11	Co	O1	C3	-160.2
4	O12	Co	O1	C3	81.6
5	O12	Co	O1	C3	-98.4
6	O1	Co	O1	C3	Undefined
7	O11	Co	O1	C3	160.2
8	O11	Co	O1	C3	-19.8
9	O12	Co	O1	C3	98.4
10	O12	Co	O1	C3	-81.6
11	O1	Co	O11	C10	83.7
12	O1	Co	O11	C10	-96.3
13	O11	Co	O11	C10	Undefined
14	O12	Co	O11	C10	-0.2
15	O12	Co	O11	C10	179.8
16	O1	Co	O11	C10	96.3
17	O1	Co	O11	C10	-83.7
18	O11	Co	O11	C10	Undefined
19	O12	Co	O11	C10	-179.8
20	O12	Co	O11	C10	0.2
21	O1	Co	O12	C10	-95.7
22	O1	Co	O12	C10	84.3
23	O11	Co	O12	C10	0.1
24	O11	Co	O12	C10	-179.9
25	O12	Co	O12	C10	Undefined
26	O1	Co	O12	C10	-84.3
27	O1	Co	O12	C10	95.7
28	O11	Co	O12	C10	179.9
29	O11	Co	O12	C10	-0.1
30	O12	Co	O12	C10	Undefined
31	Co	O1	C3	O2	44.1
32	Co	O1	C3	C4	-134.9
33	O1	C3	C4	C5	117.9(3)
34	O1	C3	C4	C9	-56.2(4)
35	O2	C3	C4	C5	-61.2(4)
36	O2	C3	C4	C9	124.7(3)
37	C3	C4	C5	H5	7.0
38	C3	C4	C5	C6	-173.0(3)
39	C9	C4	C5	H5	-178.9
40	C9	C4	C5	C6	1.1(4)
41	C3	C4	C9	C8	173.6(3)
42	C3	C4	C9	C10	-9.4(4)
43	C5	C4	C9	C8	-0.5(4)
44	C5	C4	C9	C10	176.4(3)
45	C4	C5	C6	H6	179.1
46	C4	C5	C6	C7	-0.9(4)
47	H5	C5	C6	H6	-0.9
48	H5	C5	C6	C7	179.0
49	C5	C6	C7	C8	0.2(4)

50	C5	C6	C7	C13	-174.1(3)
51	H6	C6	C7	C8	-179.8
52	H6	C6	C7	C13	5.9
53	C6	C7	C8	H8	-179.7
54	C6	C7	C8	C9	0.3(5)
55	C13	C7	C8	H8	-5.1
56	C13	C7	C8	C9	174.9(3)
57	C6	C7	C13	O14	138.6(4)
58	C6	C7	C13	C15	-42.1(5)
59	C8	C7	C13	O14	-35.8(5)
60	C8	C7	C13	C15	143.5(3)
61	C7	C8	C9	C4	-0.1(4)
62	C7	C8	C9	C10	-177.1(3)
63	H8	C8	C9	C4	179.8
64	H8	C8	C9	C10	2.9
65	C4	C9	C10	O11	-45.2(4)
66	C4	C9	C10	O12	135.1(3)
67	C8	C9	C10	O11	131.8(3)
68	C8	C9	C10	O12	-47.9(4)
69	C9	C10	O11	Co	-179.4
70	O12	C10	O11	Co	0.3
71	C9	C10	O12	Co	179.4
72	O11	C10	O12	Co	-0.3
73	C10	O11	Co	O12	-0.2
74	C10	O11	Co	O1	83.7
75	C10	O11	Co	O1	-96.3
76	C10	O11	Co	O11	Undefined
77	C10	O11	Co	O12	179.8
78	C10	O12	Co	O11	0.1
79	C10	O12	Co	O1	-95.7
80	C10	O12	Co	O1	84.3
81	C10	O12	Co	O11	-179.9
82	C10	O12	Co	O12	Undefined
83	C7	C13	C15	C16	-22.3(5)
84	C7	C13	C15	C20	162.6(3)
85	O14	C13	C15	C16	156.9(4)
86	O14	C13	C15	C20	-18.2(5)
87	C13	C15	C16	H16	6.6
88	C13	C15	C16	C17	-173.5(3)
89	C20	C15	C16	H16	-178.6
90	C20	C15	C16	C17	1.4(5)
91	C13	C15	C20	C19	174.5(3)
92	C13	C15	C20	H20	-5.6
93	C16	C15	C20	C19	-0.7(5)
94	C16	C15	C20	H20	179.3
95	C15	C16	C17	H17	179.0
96	C15	C16	C17	C18	-1.0(5)
97	H16	C16	C17	H17	-1.1
98	H16	C16	C17	C18	178.9
99	C16	C17	C18	C19	0.0(5)
100	C16	C17	C18	C21	176.2(3)

101	H17	C17	C18	C19	-180.0
102	H17	C17	C18	C21	-3.8
103	C17	C18	C19	C20	0.6(5)
104	C17	C18	C19	C24	-179.9(3)
105	C21	C18	C19	C20	-176.3(3)
106	C21	C18	C19	C24	3.2(4)
107	C17	C18	C21	O22	-1.4(7)
108	C17	C18	C21	N23	179.4(4)
109	C19	C18	C21	O22	175.1(4)
110	C19	C18	C21	N23	-4.0(4)
111	C18	C19	C20	C15	-0.3(5)
112	C18	C19	C20	H20	179.7
113	C24	C19	C20	C15	-179.6(3)
114	C24	C19	C20	H20	0.4
115	C18	C19	C24	N23	-1.1(4)
116	C18	C19	C24	O25	179.2(4)
117	C20	C19	C24	N23	178.3(4)
118	C20	C19	C24	O25	-1.4(7)
119	C18	C21	N23	C24	3.5(4)
120	C18	C21	N23	C26	174.7(3)
121	O22	C21	N23	C24	-175.7(4)
122	O22	C21	N23	C26	-4.5(6)
123	C21	N23	C24	C19	-1.6(4)
124	C21	N23	C24	O25	178.1(4)
125	C26	N23	C24	C19	-173.5(3)
126	C26	N23	C24	O25	6.3(6)
127	C21	N23	C26	H26	179(2)
128	C21	N23	C26	C27	59.8(5)
129	C21	N23	C26	C31	-66.0(5)
130	C24	N23	C26	H26	-10(2)
131	C24	N23	C26	C27	-129.6(3)
132	C24	N23	C26	C31	104.6(4)
133	N23	C26	C27	H27A	58.1
134	N23	C26	C27	H27B	-60.9
135	N23	C26	C27	C28	178.6(3)
136	H26	C26	C27	H27A	-60
137	H26	C26	C27	H27B	-179
138	H26	C26	C27	C28	60(2)
139	C31	C26	C27	H27A	-177.0
140	C31	C26	C27	H27B	64.1
141	C31	C26	C27	C28	-56.4(4)
142	N23	C26	C31	C30	-178.7(3)
143	N23	C26	C31	H31A	60.3
144	N23	C26	C31	H31B	-57.8
145	H26	C26	C31	C30	-63(2)
146	H26	C26	C31	H31A	176
147	H26	C26	C31	H31B	58
148	C27	C26	C31	C30	55.5(4)
149	C27	C26	C31	H31A	-65.4
150	C27	C26	C31	H31B	176.5
151	C26	C27	C28	H28A	177.8

152	C26	C27	C28	H28B	-63.3
153	C26	C27	C28	C29	57.3(4)
154	H27A	C27	C28	H28A	-61.7
155	H27A	C27	C28	H28B	57.3
156	H27A	C27	C28	C29	177.8
157	H27B	C27	C28	H28A	57.2
158	H27B	C27	C28	H28B	176.2
159	H27B	C27	C28	C29	-63.3
160	C27	C28	C29	H29	67(3)
161	C27	C28	C29	C30	-59.6(4)
162	C27	C28	C29	N32	178.3(3)
163	H28A	C28	C29	H29	-53
164	H28A	C28	C29	C30	179.9
165	H28A	C28	C29	N32	57.8
166	H28B	C28	C29	H29	-172
167	H28B	C28	C29	C30	61.0
168	H28B	C28	C29	N32	-61.1
169	C28	C29	C30	H30A	-62.6
170	C28	C29	C30	H30B	178.9
171	C28	C29	C30	C31	58.1(4)
172	H29	C29	C30	H30A	174
173	H29	C29	C30	H30B	56
174	H29	C29	C30	C31	-65(3)
175	N32	C29	C30	H30A	60.1
176	N32	C29	C30	H30B	-58.5
177	N32	C29	C30	C31	-179.2(3)
178	C28	C29	N32	H32A	66.1
179	C28	C29	N32	H32B	-54.0
180	C28	C29	N32	H32C	-174.0
181	H29	C29	N32	H32A	-179
182	H29	C29	N32	H32B	61
183	H29	C29	N32	H32C	-59
184	C30	C29	N32	H32A	-57.6
185	C30	C29	N32	H32B	-177.6
186	C30	C29	N32	H32C	62.3
187	C29	C30	C31	C26	-55.1(4)
188	C29	C30	C31	H31A	65.8
189	C29	C30	C31	H31B	-176.0
190	H30A	C30	C31	C26	65.6
191	H30A	C30	C31	H31A	-173.5
192	H30A	C30	C31	H31B	-55.3
193	H30B	C30	C31	C26	-175.8
194	H30B	C30	C31	H31A	-54.9
195	H30B	C30	C31	H31B	63.3
196	Co	O1	C3	O2	-44.1
197	Co	O1	C3	C4	134.9
198	O1	C3	C4	C5	-117.9(3)
199	O1	C3	C4	C9	56.2(4)
200	O2	C3	C4	C5	61.2(4)
201	O2	C3	C4	C9	-124.7(3)
202	C3	C4	C5	H5	-7.0

203	C3	C4	C5	C6	173.0(3)
204	C9	C4	C5	H5	178.9
205	C9	C4	C5	C6	-1.1(4)
206	C3	C4	C9	C8	-173.6(3)
207	C3	C4	C9	C10	9.4(4)
208	C5	C4	C9	C8	0.5(4)
209	C5	C4	C9	C10	-176.4(3)
210	C4	C5	C6	H6	-179.1
211	C4	C5	C6	C7	0.9(4)
212	H5	C5	C6	H6	0.9
213	H5	C5	C6	C7	-179.0
214	C5	C6	C7	C8	-0.2(4)
215	C5	C6	C7	C13	174.1(3)
216	H6	C6	C7	C8	179.8
217	H6	C6	C7	C13	-5.9
218	C6	C7	C8	H8	179.7
219	C6	C7	C8	C9	-0.3(5)
220	C13	C7	C8	H8	5.1
221	C13	C7	C8	C9	-174.9(3)
222	C6	C7	C13	O14	-138.6(4)
223	C6	C7	C13	C15	42.1(5)
224	C8	C7	C13	O14	35.8(5)
225	C8	C7	C13	C15	-143.5(3)
226	C7	C8	C9	C4	0.1(4)
227	C7	C8	C9	C10	177.1(3)
228	H8	C8	C9	C4	-179.8
229	H8	C8	C9	C10	-2.9
230	C4	C9	C10	O11	45.2(4)
231	C4	C9	C10	O12	-135.1(3)
232	C8	C9	C10	O11	-131.8(3)
233	C8	C9	C10	O12	47.9(4)
234	C9	C10	O11	Co	179.4
235	O12	C10	O11	Co	-0.3
236	C9	C10	O12	Co	-179.4
237	O11	C10	O12	Co	0.3
238	C10	O11	Co	O12	0.2
239	C10	O11	Co	O1	96.3
240	C10	O11	Co	O1	-83.7
241	C10	O11	Co	O11	Undefined
242	C10	O11	Co	O12	-179.8
243	C10	O12	Co	O11	-0.1
244	C10	O12	Co	O1	-84.3
245	C10	O12	Co	O1	95.7
246	C10	O12	Co	O11	179.9
247	C10	O12	Co	O12	Undefined
248	C7	C13	C15	C16	22.3(5)
249	C7	C13	C15	C20	-162.6(3)
250	O14	C13	C15	C16	-156.9(4)
251	O14	C13	C15	C20	18.2(5)
252	C13	C15	C16	H16	-6.6
253	C13	C15	C16	C17	173.5(3)

254	C20	C15	C16	H16	178.6
255	C20	C15	C16	C17	-1.4(5)
256	C13	C15	C20	C19	-174.5(3)
257	C13	C15	C20	H20	5.6
258	C16	C15	C20	C19	0.7(5)
259	C16	C15	C20	H20	-179.3
260	C15	C16	C17	H17	-179.0
261	C15	C16	C17	C18	1.0(5)
262	H16	C16	C17	H17	1.1
263	H16	C16	C17	C18	-178.9
264	C16	C17	C18	C19	-0.0(5)
265	C16	C17	C18	C21	-176.2(3)
266	H17	C17	C18	C19	180.0
267	H17	C17	C18	C21	3.8
268	C17	C18	C19	C20	-0.6(5)
269	C17	C18	C19	C24	179.9(3)
270	C21	C18	C19	C20	176.3(3)
271	C21	C18	C19	C24	-3.2(4)
272	C17	C18	C21	O22	1.4(7)
273	C17	C18	C21	N23	-179.4(4)
274	C19	C18	C21	O22	-175.1(4)
275	C19	C18	C21	N23	4.0(4)
276	C18	C19	C20	C15	0.3(5)
277	C18	C19	C20	H20	-179.7
278	C24	C19	C20	C15	179.6(3)
279	C24	C19	C20	H20	-0.4
280	C18	C19	C24	N23	1.1(4)
281	C18	C19	C24	O25	-179.2(4)
282	C20	C19	C24	N23	-178.3(4)
283	C20	C19	C24	O25	1.4(7)
284	C18	C21	N23	C24	-3.5(4)
285	C18	C21	N23	C26	-174.7(3)
286	O22	C21	N23	C24	175.7(4)
287	O22	C21	N23	C26	4.5(6)
288	C21	N23	C24	C19	1.6(4)
289	C21	N23	C24	O25	-178.1(4)
290	C26	N23	C24	C19	173.5(3)
291	C26	N23	C24	O25	-6.3(6)
292	C21	N23	C26	H26	-179(2)
293	C21	N23	C26	C27	-59.8(5)
294	C21	N23	C26	C31	66.0(5)
295	C24	N23	C26	H26	10(2)
296	C24	N23	C26	C27	129.6(3)
297	C24	N23	C26	C31	-104.6(4)
298	N23	C26	C27	H27A	-58.1
299	N23	C26	C27	H27B	60.9
300	N23	C26	C27	C28	-178.6(3)
301	H26	C26	C27	H27A	60
302	H26	C26	C27	H27B	179
303	H26	C26	C27	C28	-60(2)
304	C31	C26	C27	H27A	177.0

305	C31	C26	C27	H27B	-64.1
306	C31	C26	C27	C28	56.4(4)
307	N23	C26	C31	C30	178.7(3)
308	N23	C26	C31	H31A	-60.3
309	N23	C26	C31	H31B	57.8
310	H26	C26	C31	C30	63(2)
311	H26	C26	C31	H31A	-176
312	H26	C26	C31	H31B	-58
313	C27	C26	C31	C30	-55.5(4)
314	C27	C26	C31	H31A	65.4
315	C27	C26	C31	H31B	-176.5
316	C26	C27	C28	H28A	-177.8
317	C26	C27	C28	H28B	63.3
318	C26	C27	C28	C29	-57.3(4)
319	H27A	C27	C28	H28A	61.7
320	H27A	C27	C28	H28B	-57.3
321	H27A	C27	C28	C29	-177.8
322	H27B	C27	C28	H28A	-57.2
323	H27B	C27	C28	H28B	-176.2
324	H27B	C27	C28	C29	63.3
325	C27	C28	C29	H29	-67(3)
326	C27	C28	C29	C30	59.6(4)
327	C27	C28	C29	N32	-178.3(3)
328	H28A	C28	C29	H29	53
329	H28A	C28	C29	C30	-179.9
330	H28A	C28	C29	N32	-57.8
331	H28B	C28	C29	H29	172
332	H28B	C28	C29	C30	-61.0
333	H28B	C28	C29	N32	61.1
334	C28	C29	C30	H30A	62.6
335	C28	C29	C30	H30B	-178.9
336	C28	C29	C30	C31	-58.1(4)
337	H29	C29	C30	H30A	-174
338	H29	C29	C30	H30B	-56
339	H29	C29	C30	C31	65(3)
340	N32	C29	C30	H30A	-60.1
341	N32	C29	C30	H30B	58.5
342	N32	C29	C30	C31	179.2(3)
343	C28	C29	N32	H32A	-66.1
344	C28	C29	N32	H32B	54.0
345	C28	C29	N32	H32C	174.0
346	H29	C29	N32	H32A	179
347	H29	C29	N32	H32B	-61
348	H29	C29	N32	H32C	59
349	C30	C29	N32	H32A	57.6
350	C30	C29	N32	H32B	177.6
351	C30	C29	N32	H32C	-62.3
352	C29	C30	C31	C26	55.1(4)
353	C29	C30	C31	H31A	-65.8
354	C29	C30	C31	H31B	176.0
355	H30A	C30	C31	C26	-65.6

356	H30A	C30	C31	H31A	173.5
357	H30A	C30	C31	H31B	55.3
358	H30B	C30	C31	C26	175.8
359	H30B	C30	C31	H31A	54.9
360	H30B	C30	C31	H31B	-63.3
361	O11	Co	O1	C3	-160.2
362	O12	Co	O1	C3	-98.4
363	O1	Co	O1	C3	Undefined
364	O11	Co	O1	C3	19.8
365	O12	Co	O1	C3	81.6
366	O11	Co	O1	C3	-19.8
367	O12	Co	O1	C3	-81.6
368	O1	Co	O1	C3	Undefined
369	O11	Co	O1	C3	160.2
370	O12	Co	O1	C3	98.4
371	O11	Co	O1	C3	19.8
372	O12	Co	O1	C3	81.6
373	O1	Co	O1	C3	Undefined
374	O11	Co	O1	C3	-160.2
375	O12	Co	O1	C3	-98.4
376	O11	Co	O1	C3	160.2
377	O12	Co	O1	C3	98.4
378	O1	Co	O1	C3	Undefined
379	O11	Co	O1	C3	-19.8
380	O12	Co	O1	C3	-81.6
381	Co	O11	C10	O12	0.3
382	Co	O11	C10	C9	-179.4
383	Co	O11	C10	O12	-0.3
384	Co	O11	C10	C9	179.4
385	Co	O12	C10	O11	-0.3
386	Co	O12	C10	C9	179.4
387	Co	O12	C10	O11	0.3
388	Co	O12	C10	C9	-179.4
389	Co	O1	C3	O2	44.1
390	Co	O1	C3	C4	-134.9
391	Co	O1	C3	O2	-44.1
392	Co	O1	C3	C4	134.9
393	O1	C3	C4	C5	117.9(3)
394	O1	C3	C4	C9	-56.2(4)
395	O2	C3	C4	C5	-61.2(4)
396	O2	C3	C4	C9	124.7(3)
397	C3	C4	C5	H5	7.0
398	C3	C4	C5	C6	-173.0(3)
399	C9	C4	C5	H5	-178.9
400	C9	C4	C5	C6	1.1(4)
401	C3	C4	C9	C8	173.6(3)
402	C3	C4	C9	C10	-9.4(4)
403	C5	C4	C9	C8	-0.5(4)
404	C5	C4	C9	C10	176.4(3)
405	C4	C5	C6	H6	179.1
406	C4	C5	C6	C7	-0.9(4)

407	H5	C5	C6	H6	-0.9
408	H5	C5	C6	C7	179.0
409	C4	C9	C8	C7	-0.1(4)
410	C4	C9	C8	H8	179.8
411	C10	C9	C8	C7	-177.1(3)
412	C10	C9	C8	H8	2.9
413	C4	C9	C10	O11	-45.2(4)
414	C4	C9	C10	O12	135.1(3)
415	C8	C9	C10	O11	131.8(3)
416	C8	C9	C10	O12	-47.9(4)
417	C5	C6	C7	C8	0.2(4)
418	C5	C6	C7	C13	-174.1(3)
419	H6	C6	C7	C8	-179.8
420	H6	C6	C7	C13	5.9
421	C6	C7	C8	C9	0.3(5)
422	C6	C7	C8	H8	-179.7
423	C13	C7	C8	C9	174.9(3)
424	C13	C7	C8	H8	-5.1
425	C6	C7	C13	O14	138.6(4)
426	C6	C7	C13	C15	-42.1(5)
427	C8	C7	C13	O14	-35.8(5)
428	C8	C7	C13	C15	143.5(3)
429	C7	C13	C15	C16	-22.3(5)
430	C7	C13	C15	C20	162.6(3)
431	O14	C13	C15	C16	156.9(4)
432	O14	C13	C15	C20	-18.2(5)
433	C13	C15	C16	H16	6.6
434	C13	C15	C16	C17	-173.5(3)
435	C20	C15	C16	H16	-178.6
436	C20	C15	C16	C17	1.4(5)
437	C13	C15	C20	C19	174.5(3)
438	C13	C15	C20	H20	-5.6
439	C16	C15	C20	C19	-0.7(5)
440	C16	C15	C20	H20	179.3
441	C15	C16	C17	H17	179.0
442	C15	C16	C17	C18	-1.0(5)
443	H16	C16	C17	H17	-1.1
444	H16	C16	C17	C18	178.9
445	C15	C20	C19	C18	-0.3(5)
446	C15	C20	C19	C24	-179.6(3)
447	H20	C20	C19	C18	179.7
448	H20	C20	C19	C24	0.4
449	C16	C17	C18	C19	0.0(5)
450	C16	C17	C18	C21	176.2(3)
451	H17	C17	C18	C19	-180.0
452	H17	C17	C18	C21	-3.8
453	C17	C18	C19	C20	0.6(5)
454	C17	C18	C19	C24	-179.9(3)
455	C21	C18	C19	C20	-176.3(3)
456	C21	C18	C19	C24	3.2(4)
457	C17	C18	C21	O22	-1.4(7)

458	C17	C18	C21	N23	179.4(4)
459	C19	C18	C21	O22	175.1(4)
460	C19	C18	C21	N23	-4.0(4)
461	C20	C19	C24	N23	178.3(4)
462	C20	C19	C24	O25	-1.4(7)
463	C18	C19	C24	N23	-1.1(4)
464	C18	C19	C24	O25	179.2(4)
465	C18	C21	N23	C24	3.5(4)
466	C18	C21	N23	C26	174.7(3)
467	O22	C21	N23	C24	-175.7(4)
468	O22	C21	N23	C26	-4.5(6)
469	C19	C24	N23	C21	-1.6(4)
470	C19	C24	N23	C26	-173.5(3)
471	O25	C24	N23	C21	178.1(4)
472	O25	C24	N23	C26	6.3(6)
473	C21	N23	C26	H26	179(2)
474	C21	N23	C26	C27	59.8(5)
475	C21	N23	C26	C31	-66.0(5)
476	C24	N23	C26	H26	-10(2)
477	C24	N23	C26	C27	-129.6(3)
478	C24	N23	C26	C31	104.6(4)
479	N23	C26	C27	H27A	58.1
480	N23	C26	C27	H27B	-60.9
481	N23	C26	C27	C28	178.6(3)
482	H26	C26	C27	H27A	-60
483	H26	C26	C27	H27B	-179
484	H26	C26	C27	C28	60(2)
485	C31	C26	C27	H27A	-177.0
486	C31	C26	C27	H27B	64.1
487	C31	C26	C27	C28	-56.4(4)
488	N23	C26	C31	C30	-178.7(3)
489	N23	C26	C31	H31A	60.3
490	N23	C26	C31	H31B	-57.8
491	H26	C26	C31	C30	-63(2)
492	H26	C26	C31	H31A	176
493	H26	C26	C31	H31B	58
494	C27	C26	C31	C30	55.5(4)
495	C27	C26	C31	H31A	-65.4
496	C27	C26	C31	H31B	176.5
497	C26	C27	C28	H28A	177.8
498	C26	C27	C28	H28B	-63.3
499	C26	C27	C28	C29	57.3(4)
500	H27A	C27	C28	H28A	-61.7
501	H27A	C27	C28	H28B	57.3
502	H27A	C27	C28	C29	177.8
503	H27B	C27	C28	H28A	57.2
504	H27B	C27	C28	H28B	176.2
505	H27B	C27	C28	C29	-63.3
506	C26	C31	C30	C29	-55.1(4)
507	C26	C31	C30	H30A	65.6
508	C26	C31	C30	H30B	-175.8

509	H31A	C31	C30	C29	65.8
510	H31A	C31	C30	H30A	-173.5
511	H31A	C31	C30	H30B	-54.9
512	H31B	C31	C30	C29	-176.0
513	H31B	C31	C30	H30A	-55.3
514	H31B	C31	C30	H30B	63.3
515	C27	C28	C29	H29	67(3)
516	C27	C28	C29	C30	-59.6(4)
517	C27	C28	C29	N32	178.3(3)
518	H28A	C28	C29	H29	-53
519	H28A	C28	C29	C30	179.9
520	H28A	C28	C29	N32	57.8
521	H28B	C28	C29	H29	-172
522	H28B	C28	C29	C30	61.0
523	H28B	C28	C29	N32	-61.1
524	C28	C29	C30	C31	58.1(4)
525	C28	C29	C30	H30A	-62.6
526	C28	C29	C30	H30B	178.9
527	H29	C29	C30	C31	-65(3)
528	H29	C29	C30	H30A	174
529	H29	C29	C30	H30B	56
530	N32	C29	C30	C31	-179.2(3)
531	N32	C29	C30	H30A	60.1
532	N32	C29	C30	H30B	-58.5
533	C28	C29	N32	H32A	66.1
534	C28	C29	N32	H32B	-54.0
535	C28	C29	N32	H32C	-174.0
536	H29	C29	N32	H32A	-179
537	H29	C29	N32	H32B	61
538	H29	C29	N32	H32C	-59
539	C30	C29	N32	H32A	-57.6
540	C30	C29	N32	H32B	-177.6
541	C30	C29	N32	H32C	62.3
542	O1	C3	C4	C5	-117.9(3)
543	O1	C3	C4	C9	56.2(4)
544	O2	C3	C4	C5	61.2(4)
545	O2	C3	C4	C9	-124.7(3)
546	C3	C4	C5	H5	-7.0
547	C3	C4	C5	C6	173.0(3)
548	C9	C4	C5	H5	178.9
549	C9	C4	C5	C6	-1.1(4)
550	C3	C4	C9	C8	-173.6(3)
551	C3	C4	C9	C10	9.4(4)
552	C5	C4	C9	C8	0.5(4)
553	C5	C4	C9	C10	-176.4(3)
554	C4	C5	C6	H6	-179.1
555	C4	C5	C6	C7	0.9(4)
556	H5	C5	C6	H6	0.9
557	H5	C5	C6	C7	-179.0
558	C4	C9	C8	C7	0.1(4)
559	C4	C9	C8	H8	-179.8

560	C10	C9	C8	C7	177.1(3)
561	C10	C9	C8	H8	-2.9
562	C4	C9	C10	O11	45.2(4)
563	C4	C9	C10	O12	-135.1(3)
564	C8	C9	C10	O11	-131.8(3)
565	C8	C9	C10	O12	47.9(4)
566	C5	C6	C7	C8	-0.2(4)
567	C5	C6	C7	C13	174.1(3)
568	H6	C6	C7	C8	179.8
569	H6	C6	C7	C13	-5.9
570	C6	C7	C8	C9	-0.3(5)
571	C6	C7	C8	H8	179.7
572	C13	C7	C8	C9	-174.9(3)
573	C13	C7	C8	H8	5.1
574	C6	C7	C13	O14	-138.6(4)
575	C6	C7	C13	C15	42.1(5)
576	C8	C7	C13	O14	35.8(5)
577	C8	C7	C13	C15	-143.5(3)
578	C7	C13	C15	C16	22.3(5)
579	C7	C13	C15	C20	-162.6(3)
580	O14	C13	C15	C16	-156.9(4)
581	O14	C13	C15	C20	18.2(5)
582	C9	C10	O11	Co	179.4
583	O12	C10	O11	Co	-0.3
584	C9	C10	O12	Co	-179.4
585	O11	C10	O12	Co	0.3
586	C10	O11	Co	O12	0.2
587	C10	O12	Co	O11	-0.1
588	C13	C15	C16	H16	-6.6
589	C13	C15	C16	C17	173.5(3)
590	C20	C15	C16	H16	178.6
591	C20	C15	C16	C17	-1.4(5)
592	C13	C15	C20	C19	-174.5(3)
593	C13	C15	C20	H20	5.6
594	C16	C15	C20	C19	0.7(5)
595	C16	C15	C20	H20	-179.3
596	C15	C16	C17	H17	-179.0
597	C15	C16	C17	C18	1.0(5)
598	H16	C16	C17	H17	1.1
599	H16	C16	C17	C18	-178.9
600	C15	C20	C19	C18	0.3(5)
601	C15	C20	C19	C24	179.6(3)
602	H20	C20	C19	C18	-179.7
603	H20	C20	C19	C24	-0.4
604	C16	C17	C18	C19	-0.0(5)
605	C16	C17	C18	C21	-176.2(3)
606	H17	C17	C18	C19	180.0
607	H17	C17	C18	C21	3.8
608	C17	C18	C19	C20	-0.6(5)
609	C17	C18	C19	C24	179.9(3)
610	C21	C18	C19	C20	176.3(3)

611	C21	C18	C19	C24	-3.2(4)
612	C17	C18	C21	O22	1.4(7)
613	C17	C18	C21	N23	-179.4(4)
614	C19	C18	C21	O22	-175.1(4)
615	C19	C18	C21	N23	4.0(4)
616	C20	C19	C24	N23	-178.3(4)
617	C20	C19	C24	O25	1.4(7)
618	C18	C19	C24	N23	1.1(4)
619	C18	C19	C24	O25	-179.2(4)
620	C18	C21	N23	C24	-3.5(4)
621	C18	C21	N23	C26	-174.7(3)
622	O22	C21	N23	C24	175.7(4)
623	O22	C21	N23	C26	4.5(6)
624	C19	C24	N23	C21	1.6(4)
625	C19	C24	N23	C26	173.5(3)
626	O25	C24	N23	C21	-178.1(4)
627	O25	C24	N23	C26	-6.3(6)
628	C21	N23	C26	H26	-179(2)
629	C21	N23	C26	C27	-59.8(5)
630	C21	N23	C26	C31	66.0(5)
631	C24	N23	C26	H26	10(2)
632	C24	N23	C26	C27	129.6(3)
633	C24	N23	C26	C31	-104.6(4)
634	N23	C26	C27	H27A	-58.1
635	N23	C26	C27	H27B	60.9
636	N23	C26	C27	C28	-178.6(3)
637	H26	C26	C27	H27A	60
638	H26	C26	C27	H27B	179
639	H26	C26	C27	C28	-60(2)
640	C31	C26	C27	H27A	177.0
641	C31	C26	C27	H27B	-64.1
642	C31	C26	C27	C28	56.4(4)
643	N23	C26	C31	C30	178.7(3)
644	N23	C26	C31	H31A	-60.3
645	N23	C26	C31	H31B	57.8
646	H26	C26	C31	C30	63(2)
647	H26	C26	C31	H31A	-176
648	H26	C26	C31	H31B	-58
649	C27	C26	C31	C30	-55.5(4)
650	C27	C26	C31	H31A	65.4
651	C27	C26	C31	H31B	-176.5
652	C26	C27	C28	H28A	-177.8
653	C26	C27	C28	H28B	63.3
654	C26	C27	C28	C29	-57.3(4)
655	H27A	C27	C28	H28A	61.7
656	H27A	C27	C28	H28B	-57.3
657	H27A	C27	C28	C29	-177.8
658	H27B	C27	C28	H28A	-57.2
659	H27B	C27	C28	H28B	-176.2
660	H27B	C27	C28	C29	63.3
661	C26	C31	C30	C29	55.1(4)

662	C26	C31	C30	H30A	-65.6
663	C26	C31	C30	H30B	175.8
664	H31A	C31	C30	C29	-65.8
665	H31A	C31	C30	H30A	173.5
666	H31A	C31	C30	H30B	54.9
667	H31B	C31	C30	C29	176.0
668	H31B	C31	C30	H30A	55.3
669	H31B	C31	C30	H30B	-63.3
670	C27	C28	C29	H29	-67(3)
671	C27	C28	C29	C30	59.6(4)
672	C27	C28	C29	N32	-178.3(3)
673	H28A	C28	C29	H29	53
674	H28A	C28	C29	C30	-179.9
675	H28A	C28	C29	N32	-57.8
676	H28B	C28	C29	H29	172
677	H28B	C28	C29	C30	-61.0
678	H28B	C28	C29	N32	61.1
679	C28	C29	C30	C31	-58.1(4)
680	C28	C29	C30	H30A	62.6
681	C28	C29	C30	H30B	-178.9
682	H29	C29	C30	C31	65(3)
683	H29	C29	C30	H30A	-174
684	H29	C29	C30	H30B	-56
685	N32	C29	C30	C31	179.2(3)
686	N32	C29	C30	H30A	-60.1
687	N32	C29	C30	H30B	58.5
688	C28	C29	N32	H32A	-66.1
689	C28	C29	N32	H32B	54.0
690	C28	C29	N32	H32C	174.0
691	H29	C29	N32	H32A	179
692	H29	C29	N32	H32B	-61
693	H29	C29	N32	H32C	59
694	C30	C29	N32	H32A	57.6
695	C30	C29	N32	H32B	177.6
696	C30	C29	N32	H32C	-62.3
697	Co	O1	C3	O2	44.1
698	Co	O1	C3	C4	-134.9
699	Co	O1	C3	O2	-44.1
700	Co	O1	C3	C4	134.9
701	O1	C3	C4	C5	117.9(3)
702	O1	C3	C4	C9	-56.2(4)
703	O2	C3	C4	C5	-61.2(4)
704	O2	C3	C4	C9	124.7(3)
705	C3	C4	C5	H5	7.0
706	C3	C4	C5	C6	-173.0(3)
707	C9	C4	C5	H5	-178.9
708	C9	C4	C5	C6	1.1(4)
709	C3	C4	C9	C8	173.6(3)
710	C3	C4	C9	C10	-9.4(4)
711	C5	C4	C9	C8	-0.5(4)
712	C5	C4	C9	C10	176.4(3)

713	C4	C5	C6	H6	179.1
714	C4	C5	C6	C7	-0.9(4)
715	H5	C5	C6	H6	-0.9
716	H5	C5	C6	C7	179.0
717	C4	C9	C8	C7	-0.1(4)
718	C4	C9	C8	H8	179.8
719	C10	C9	C8	C7	-177.1(3)
720	C10	C9	C8	H8	2.9
721	C4	C9	C10	O11	-45.2(4)
722	C4	C9	C10	O12	135.1(3)
723	C8	C9	C10	O11	131.8(3)
724	C8	C9	C10	O12	-47.9(4)
725	C5	C6	C7	C8	0.2(4)
726	C5	C6	C7	C13	-174.1(3)
727	H6	C6	C7	C8	-179.8
728	H6	C6	C7	C13	5.9
729	C6	C7	C8	C9	0.3(5)
730	C6	C7	C8	H8	-179.7
731	C13	C7	C8	C9	174.9(3)
732	C13	C7	C8	H8	-5.1
733	C6	C7	C13	O14	138.6(4)
734	C6	C7	C13	C15	-42.1(5)
735	C8	C7	C13	O14	-35.8(5)
736	C8	C7	C13	C15	143.5(3)
737	C7	C13	C15	C16	-22.3(5)
738	C7	C13	C15	C20	162.6(3)
739	O14	C13	C15	C16	156.9(4)
740	O14	C13	C15	C20	-18.2(5)
741	C9	C10	O11	Co	-179.4
742	O12	C10	O11	Co	0.3
743	C9	C10	O12	Co	179.4
744	O11	C10	O12	Co	-0.3
745	C10	O11	Co	O12	-0.2
746	C10	O12	Co	O11	0.1
747	C13	C15	C16	H16	6.6
748	C13	C15	C16	C17	-173.5(3)
749	C20	C15	C16	H16	-178.6
750	C20	C15	C16	C17	1.4(5)
751	C13	C15	C20	C19	174.5(3)
752	C13	C15	C20	H20	-5.6
753	C16	C15	C20	C19	-0.7(5)
754	C16	C15	C20	H20	179.3
755	C15	C16	C17	H17	179.0
756	C15	C16	C17	C18	-1.0(5)
757	H16	C16	C17	H17	-1.1
758	H16	C16	C17	C18	178.9
759	C15	C20	C19	C18	-0.3(5)
760	C15	C20	C19	C24	-179.6(3)
761	H20	C20	C19	C18	179.7
762	H20	C20	C19	C24	0.4
763	C16	C17	C18	C19	0.0(5)

764	C16	C17	C18	C21	176.2(3)
765	H17	C17	C18	C19	-180.0
766	H17	C17	C18	C21	-3.8
767	C17	C18	C19	C20	0.6(5)
768	C17	C18	C19	C24	-179.9(3)
769	C21	C18	C19	C20	-176.3(3)
770	C21	C18	C19	C24	3.2(4)
771	C17	C18	C21	O22	-1.4(7)
772	C17	C18	C21	N23	179.4(4)
773	C19	C18	C21	O22	175.1(4)
774	C19	C18	C21	N23	-4.0(4)
775	C20	C19	C24	N23	178.3(4)
776	C20	C19	C24	O25	-1.4(7)
777	C18	C19	C24	N23	-1.1(4)
778	C18	C19	C24	O25	179.2(4)
779	C18	C21	N23	C24	3.5(4)
780	C18	C21	N23	C26	174.7(3)
781	O22	C21	N23	C24	-175.7(4)
782	O22	C21	N23	C26	-4.5(6)
783	C19	C24	N23	C21	-1.6(4)
784	C19	C24	N23	C26	-173.5(3)
785	O25	C24	N23	C21	178.1(4)
786	O25	C24	N23	C26	6.3(6)
787	C21	N23	C26	H26	179(2)
788	C21	N23	C26	C27	59.8(5)
789	C21	N23	C26	C31	-66.0(5)
790	C24	N23	C26	H26	-10(2)
791	C24	N23	C26	C27	-129.6(3)
792	C24	N23	C26	C31	104.6(4)
793	N23	C26	C27	H27A	58.1
794	N23	C26	C27	H27B	-60.9
795	N23	C26	C27	C28	178.6(3)
796	H26	C26	C27	H27A	-60
797	H26	C26	C27	H27B	-179
798	H26	C26	C27	C28	60(2)
799	C31	C26	C27	H27A	-177.0
800	C31	C26	C27	H27B	64.1
801	C31	C26	C27	C28	-56.4(4)
802	N23	C26	C31	C30	-178.7(3)
803	N23	C26	C31	H31A	60.3
804	N23	C26	C31	H31B	-57.8
805	H26	C26	C31	C30	-63(2)
806	H26	C26	C31	H31A	176
807	H26	C26	C31	H31B	58
808	C27	C26	C31	C30	55.5(4)
809	C27	C26	C31	H31A	-65.4
810	C27	C26	C31	H31B	176.5
811	C26	C27	C28	H28A	177.8
812	C26	C27	C28	H28B	-63.3
813	C26	C27	C28	C29	57.3(4)
814	H27A	C27	C28	H28A	-61.7

815	H27A	C27	C28	H28B	57.3
816	H27A	C27	C28	C29	177.8
817	H27B	C27	C28	H28A	57.2
818	H27B	C27	C28	H28B	176.2
819	H27B	C27	C28	C29	-63.3
820	C26	C31	C30	C29	-55.1(4)
821	C26	C31	C30	H30A	65.6
822	C26	C31	C30	H30B	-175.8
823	H31A	C31	C30	C29	65.8
824	H31A	C31	C30	H30A	-173.5
825	H31A	C31	C30	H30B	-54.9
826	H31B	C31	C30	C29	-176.0
827	H31B	C31	C30	H30A	-55.3
828	H31B	C31	C30	H30B	63.3
829	C27	C28	C29	H29	67(3)
830	C27	C28	C29	C30	-59.6(4)
831	C27	C28	C29	N32	178.3(3)
832	H28A	C28	C29	H29	-53
833	H28A	C28	C29	C30	179.9
834	H28A	C28	C29	N32	57.8
835	H28B	C28	C29	H29	-172
836	H28B	C28	C29	C30	61.0
837	H28B	C28	C29	N32	-61.1
838	C28	C29	C30	C31	58.1(4)
839	C28	C29	C30	H30A	-62.6
840	C28	C29	C30	H30B	178.9
841	H29	C29	C30	C31	-65(3)
842	H29	C29	C30	H30A	174
843	H29	C29	C30	H30B	56
844	N32	C29	C30	C31	-179.2(3)
845	N32	C29	C30	H30A	60.1
846	N32	C29	C30	H30B	-58.5
847	C28	C29	N32	H32A	66.1
848	C28	C29	N32	H32B	-54.0
849	C28	C29	N32	H32C	-174.0
850	H29	C29	N32	H32A	-179
851	H29	C29	N32	H32B	61
852	H29	C29	N32	H32C	-59
853	C30	C29	N32	H32A	-57.6
854	C30	C29	N32	H32B	-177.6
855	C30	C29	N32	H32C	62.3
856	O1	C3	C4	C5	-117.9(3)
857	O1	C3	C4	C9	56.2(4)
858	O2	C3	C4	C5	61.2(4)
859	O2	C3	C4	C9	-124.7(3)
860	C3	C4	C5	H5	-7.0
861	C3	C4	C5	C6	173.0(3)
862	C9	C4	C5	H5	178.9
863	C9	C4	C5	C6	-1.1(4)
864	C3	C4	C9	C8	-173.6(3)
865	C3	C4	C9	C10	9.4(4)

866	C5	C4	C9	C8	0.5(4)
867	C5	C4	C9	C10	-176.4(3)
868	C4	C5	C6	H6	-179.1
869	C4	C5	C6	C7	0.9(4)
870	H5	C5	C6	H6	0.9
871	H5	C5	C6	C7	-179.0
872	C4	C9	C8	C7	0.1(4)
873	C4	C9	C8	H8	-179.8
874	C10	C9	C8	C7	177.1(3)
875	C10	C9	C8	H8	-2.9
876	C4	C9	C10	O11	45.2(4)
877	C4	C9	C10	O12	-135.1(3)
878	C8	C9	C10	O11	-131.8(3)
879	C8	C9	C10	O12	47.9(4)
880	C5	C6	C7	C8	-0.2(4)
881	C5	C6	C7	C13	174.1(3)
882	H6	C6	C7	C8	179.8
883	H6	C6	C7	C13	-5.9
884	C6	C7	C8	C9	-0.3(5)
885	C6	C7	C8	H8	179.7
886	C13	C7	C8	C9	-174.9(3)
887	C13	C7	C8	H8	5.1
888	C6	C7	C13	O14	-138.6(4)
889	C6	C7	C13	C15	42.1(5)
890	C8	C7	C13	O14	35.8(5)
891	C8	C7	C13	C15	-143.5(3)
892	C7	C13	C15	C16	22.3(5)
893	C7	C13	C15	C20	-162.6(3)
894	O14	C13	C15	C16	-156.9(4)
895	O14	C13	C15	C20	18.2(5)
896	C13	C15	C16	H16	-6.6
897	C13	C15	C16	C17	173.5(3)
898	C20	C15	C16	H16	178.6
899	C20	C15	C16	C17	-1.4(5)
900	C13	C15	C20	C19	-174.5(3)
901	C13	C15	C20	H20	5.6
902	C16	C15	C20	C19	0.7(5)
903	C16	C15	C20	H20	-179.3
904	C15	C16	C17	H17	-179.0
905	C15	C16	C17	C18	1.0(5)
906	H16	C16	C17	H17	1.1
907	H16	C16	C17	C18	-178.9
908	C15	C20	C19	C18	0.3(5)
909	C15	C20	C19	C24	179.6(3)
910	H20	C20	C19	C18	-179.7
911	H20	C20	C19	C24	-0.4
912	C16	C17	C18	C19	-0.0(5)
913	C16	C17	C18	C21	-176.2(3)
914	H17	C17	C18	C19	180.0
915	H17	C17	C18	C21	3.8
916	C17	C18	C19	C20	-0.6(5)

917	C17	C18	C19	C24	179.9(3)
918	C21	C18	C19	C20	176.3(3)
919	C21	C18	C19	C24	-3.2(4)
920	C17	C18	C21	O22	1.4(7)
921	C17	C18	C21	N23	-179.4(4)
922	C19	C18	C21	O22	-175.1(4)
923	C19	C18	C21	N23	4.0(4)
924	C20	C19	C24	N23	-178.3(4)
925	C20	C19	C24	O25	1.4(7)
926	C18	C19	C24	N23	1.1(4)
927	C18	C19	C24	O25	-179.2(4)
928	C18	C21	N23	C24	-3.5(4)
929	C18	C21	N23	C26	-174.7(3)
930	O22	C21	N23	C24	175.7(4)
931	O22	C21	N23	C26	4.5(6)
932	C19	C24	N23	C21	1.6(4)
933	C19	C24	N23	C26	173.5(3)
934	O25	C24	N23	C21	-178.1(4)
935	O25	C24	N23	C26	-6.3(6)
936	C21	N23	C26	H26	-179(2)
937	C21	N23	C26	C27	-59.8(5)
938	C21	N23	C26	C31	66.0(5)
939	C24	N23	C26	H26	10(2)
940	C24	N23	C26	C27	129.6(3)
941	C24	N23	C26	C31	-104.6(4)
942	N23	C26	C27	H27A	-58.1
943	N23	C26	C27	H27B	60.9
944	N23	C26	C27	C28	-178.6(3)
945	H26	C26	C27	H27A	60
946	H26	C26	C27	H27B	179
947	H26	C26	C27	C28	-60(2)
948	C31	C26	C27	H27A	177.0
949	C31	C26	C27	H27B	-64.1
950	C31	C26	C27	C28	56.4(4)
951	N23	C26	C31	C30	178.7(3)
952	N23	C26	C31	H31A	-60.3
953	N23	C26	C31	H31B	57.8
954	H26	C26	C31	C30	63(2)
955	H26	C26	C31	H31A	-176
956	H26	C26	C31	H31B	-58
957	C27	C26	C31	C30	-55.5(4)
958	C27	C26	C31	H31A	65.4
959	C27	C26	C31	H31B	-176.5
960	C26	C27	C28	H28A	-177.8
961	C26	C27	C28	H28B	63.3
962	C26	C27	C28	C29	-57.3(4)
963	H27A	C27	C28	H28A	61.7
964	H27A	C27	C28	H28B	-57.3
965	H27A	C27	C28	C29	-177.8
966	H27B	C27	C28	H28A	-57.2
967	H27B	C27	C28	H28B	-176.2

968	H27B	C27	C28	C29	63.3
969	C26	C31	C30	C29	55.1(4)
970	C26	C31	C30	H30A	-65.6
971	C26	C31	C30	H30B	175.8
972	H31A	C31	C30	C29	-65.8
973	H31A	C31	C30	H30A	173.5
974	H31A	C31	C30	H30B	54.9
975	H31B	C31	C30	C29	176.0
976	H31B	C31	C30	H30A	55.3
977	H31B	C31	C30	H30B	-63.3
978	C27	C28	C29	H29	-67(3)
979	C27	C28	C29	C30	59.6(4)
980	C27	C28	C29	N32	-178.3(3)
981	H28A	C28	C29	H29	53
982	H28A	C28	C29	C30	-179.9
983	H28A	C28	C29	N32	-57.8
984	H28B	C28	C29	H29	172
985	H28B	C28	C29	C30	-61.0
986	H28B	C28	C29	N32	61.1
987	C28	C29	C30	C31	-58.1(4)
988	C28	C29	C30	H30A	62.6
989	C28	C29	C30	H30B	-178.9
990	H29	C29	C30	C31	65(3)
991	H29	C29	C30	H30A	-174
992	H29	C29	C30	H30B	-56
993	N32	C29	C30	C31	179.2(3)
994	N32	C29	C30	H30A	-60.1
995	N32	C29	C30	H30B	58.5
996	C28	C29	N32	H32A	-66.1
997	C28	C29	N32	H32B	54.0
998	C28	C29	N32	H32C	174.0
999	H29	C29	N32	H32A	179
1000	H29	C29	N32	H32B	-61
1001	H29	C29	N32	H32C	59
1002	C30	C29	N32	H32A	57.6
1003	C30	C29	N32	H32B	177.6
1004	C30	C29	N32	H32C	-62.3
