

Electronic Supplementary Information

Table 1S. The assignments of the selected vibrations in IR spectra of **I** and **II**

Table 2S. Theoretical energies (in cm^{-1}) $^{2S+1}L_J$ states of **II_{Eu1}** and **II_{Eu2}** obtained within CASSCF/CASPT2/RASSI calculations.

Table 3S. Cartesian coordinates (in Å) of the DFT optimized geometry of $\{\text{K}_4[\text{Eu}(\text{DOTP})]\}^-$ cluster representing **I_{Eu1}** and **II_{Eu1}** sites.

Table 1S. The assignments of the selected vibrations in IR spectra of I and II

Exp (I)	Exp (II)	Calc	Vibr
140	136	180	τ_{PO}, ν_{EuN}
		181	$\rho_{CH2}, \rho_{PO2}, \nu_{EuN}$
260	254	245	$\rho_{CH2}, \rho_{PO2}, \nu_{EuO}$
		245	$\nu_{PO}, \delta_{CH2}, \nu_{EuO}$
468	476	482	ν_{PO}
510	510	483	ν_{PO}
584	584	581	ρ_{CH2}, ω_{CH2}
755	755	767	δ_{PO}, τ_{CH2}
800	801	807	δ_{CH2}
	831	871	ω_{CH2}
930	930	871	ω_{CH2}
974	974	893	δ_{CH2}
		893	δ_{CH2}
974	974	935	$\delta_{PO\ sym}$
1057	1059	1003	ν_{CN}
		1004	δ_{CH2}
		1044	$\delta_{PO\ sym}$
		1044	$\delta_{PO\ sym}$
1057	1059	1068	ρ_{CH2}
		1106	ω_{CH2}
	1106	1107	τ_{CH2}
1070	1073	1178	$\rho_{CH2}, \nu_{PO}, \delta_{CH2}$
1121	1124	1182	ν_{PO}
		1194	ρ_{CH2}, ν_{PO}
2820	2822	2968	ν_{CH2}
2861	2860	2969	ν_{CH2}
	2926	2971	ν_{CH2}
	2963	2981	ν_{CH2}
		2982	ν_{CH2}
		2984	ν_{CH2}
		3102	ν_{CH2}

Table 2S. Theoretical energies (in cm^{-1}) $^{2S+1}L_J$ states of Π_{Eu1} and Π_{Eu2} obtained within CASSCF/CASPT2/RASSI calculations

Isomer Π_{Eu1}			
Level	(2S+1) L	Irrep	Energy (cm^{-1})
1	7F	1 A	0.000
2	7F	2 A	192.406
3	7F	1 E	520.384
4	7F	2 E	1090.796
5	7F	1 B	1110.748
6	7F	3 A	1115.541
7	7F	2 B	1362.143
8	7F	3 E	2014.914
9	7F	4 A	2043.122
10	7F	3 B	2083.971
11	7F	4 E	2110.068
12	7F	4 B	2138.497
13	7F	5 A	2869.430
14	7F	6 A	3057.714
15	7F	5 E	3064.412
16	7F	6 E	3152.168
17	7F	5 B	3216.174
18	7F	7 A	3217.592
19	7F	6 B	3353.287
20	7F	7 E	3993.078
21	7F	8 E	4169.391
22	7F	7 B	4199.036
23	7F	8 A	4259.326
24	7F	9 A	4290.863
25	7F	8 B	4409.077
26	7F	9 E	4485.949
27	7F	10 A	4537.285
28	7F	9 B	5036.972
29	7F	10 B	5037.959
30	7F	10 E	5231.685
31	7F	11 A	5473.394
32	7F	12 A	5503.881
33	7F	11 E	5589.148
34	7F	11 B	5611.124
35	7F	13 A	5719.395
36	7F	12 E	5731.584
37	7F	12 B	5743.334
38	5D	14 A	18168.792
39	5D	15 A	18895.808
40	5D	13 E	18961.388
41	5D	16 A	20529.463
42	5D	13 B	20534.530
43	5D	14 E	20580.666
44	5D	14 B	20601.392

45	5D	15 B	23160.141
46	5D	15 E	23163.084
47	5D	16 B	23200.116
48	5D	16 E	23209.626
49	5D	17 A	23214.018
50	5D	18 A	26902.691
51	5D	19 A	26911.917
52	5D	17 E	26916.590
53	5D	17 B	26950.595
54	5D	18 B	26965.080
55	5D	18 E	27011.179
56	5D	20 A	27042.720
57	5G	19 B	27668.957
58	5G	19 E	27691.804
59	5G	20 B	27693.678
60	5G	21 A	27766.221
61	5G	20 E	27793.620
62	5G	22 A	27804.876
63	5G	23 A	27902.079
64	5G	21 B	27906.818
65	5G	21 E	27911.386
66	5G	22 B	27922.196
67	5G	24 A	27933.622
68	5G	22 E	28012.422
69	5G	23 B	28054.442
70	5G	23 E	28097.311
71	5G	24 B	28109.609
72	5G	25 A	28137.261
73	5G	24 E	28190.555
74	5G	26 A	28223.319
75	5G	25 E	28286.642
76	5G	27 A	28299.585
77	5G	28 A	28309.744
78	5G	25 B	28334.924
79	5G	26 E	28342.999
80	5G	26 B	28380.176
81	5L	27 B	28583.521
82	5L	27 E	28598.337
83	5L	29 A	28610.114
84	5L	28 B	28677.727
85	5L	29 B	28682.359
86	5L	28 E	28777.398
87	5L	30 B	28801.715
88	5L	30 A	28827.209
89	5L	29 E	28847.120
90	5L	31 A	28910.831
91	5G	31 B	29093.840
92	5G	32 B	29111.030
93	5L	32 A	29116.767

94	5L	30 E	29132.706
95	5L	33 B	29139.065
96	5G	31 E	29148.861
97	5G	33 A	29184.755
98	5G	34 A	29199.242
99	5G	32 E	29212.549
100	5L	33 E	29232.622
101	5G	34 B	29242.139
102	5L	35 B	29251.890
103	5L	34 E	29291.335
104	5L	35 A	29298.048
105	5L	36 A	29330.259
106	5L	36 B	29333.304
107	5L	35 E	29333.792
108	5L	37 B	29342.530
109	5L	38 B	29372.351
110	5L	36 E	29373.953
111	5L	37 A	29377.654
112	5L	38 A	29780.579
113	5L	39 B	29789.421
114	5L	37 E	29816.570
115	5L	39 A	29880.247
116	5L	40 A	29925.289
117	5L	40 B	29949.995
118	5L	38 E	29957.747
119	5L	41 A	29968.068
120	5L	39 E	30006.490
121	5L	42 A	30013.788
122	5L	41 B	30026.955
123	5L	40 E	30032.604
124	5L	42 B	30051.652
125	5L	43 A	30620.919
126	5L	41 E	30626.234
127	5L	43 B	30630.547
128	5L	42 E	30722.808
129	5L	44 A	30759.641
130	5L	44 B	30779.897
131	5L	43 E	30785.754
132	5L	45 A	30804.961
133	5L	46 A	30830.620
134	5L	47 A	30858.687
135	5L	45 B	30866.028
136	5L	44 E	30870.258
137	5L	45 E	30891.676
138	5L	46 B	30895.573
139	5L	47 B	31625.529
140	5L	46 E	31630.677
141	5L	48 A	31635.301
142	5L	48 B	31706.266

143	5L	49 B	31713.806
144	5L	47 E	31763.243
145	5L	49 A	31770.679
146	5L	50 B	31786.185
147	5L	48 E	31806.315
148	5L	50 A	31880.691
149	5L	51 B	31913.678
150	5L	51 A	31916.514
151	5L	49 E	31919.011
152	5L	52 A	31965.488
153	5L	52 B	31967.300
154	5L	50 E	31971.535
155	5H	53 B	33331.418
156	5H	51 E	33352.926
157	5H	54 B	33382.912
158	5H	52 E	33469.107
159	5H	53 A	33537.295
160	5H	53 E	33604.450
161	5H	54 A	33625.088
162	5H	55 B	33636.413
163	5H	55 A	33659.263
164	5H	56 B	33690.515
165	5H	54 E	33708.082
166	5H	56 A	33726.314
167	5H	57 A	33789.181
168	5H	55 E	33798.533
169	5H	58 A	33815.659
170	5H	57 B	33819.377
171	5H	59 A	33852.468
172	5H	56 E	33860.265
173	5H	57 E	33869.978
174	5H	58 B	33874.157
175	5H	60 A	33896.456
176	5H	59 B	33901.269
177	5H	58 E	33906.917
178	5H	60 B	33942.178
179	5H	61 B	33963.259
180	5H	61 A	33984.662
181	5H	59 E	33990.484
182	5H	60 E	34044.197
183	5H	62 A	34068.133
184	5H	62 B	34082.849
185	5H	61 E	34094.602
186	5H	63 A	34103.670
187	5H	63 B	34117.540
188	5H	62 E	34129.103
189	5H	64 B	34143.805
190	5H	63 E	34161.001
191	5H	64 A	34173.687

192	5H	65 B	34243.682
193	5H	64 E	34252.705
194	5H	65 A	34271.516
195	5H	66 B	34273.730
196	5F	65 E	36354.043
197	5F	66 A	36509.133
198	5F	67 B	36764.532
199	5F	66 E	36831.682
200	5F	68 B	36835.445
201	5F	67 A	36850.231
202	5F	69 B	37286.780
203	5F	67 E	37295.103
204	5F	68 A	37308.969
205	5F	68 E	37372.374
206	5F	70 B	37389.383
207	5F	69 A	37721.024
208	5F	70 A	37722.564
209	5F	71 B	37812.785
210	5I	71 A	37821.079
211	5F	69 E	37839.382
212	5F	72 B	37848.017
213	5F	70 E	37857.471
214	5F	71 E	37884.982
215	5I	72 A	37901.877
216	5I	73 B	37907.239
217	5F	73 A	37919.693
218	5I	72 E	37919.894
219	5I	74 B	37927.639
220	5I	73 E	37953.372
221	5I	74 A	38009.667
222	5F	75 A	38059.323
223	5F	76 A	38080.358
224	5F	75 B	38113.994
225	5F	74 E	38134.625
226	5F	77 A	38138.841
227	5F	75 E	38161.227
228	5F	76 B	38165.832
229	5I	77 B	38235.349
230	5I	78 A	38255.900
231	5I	76 E	38273.394
232	5I	79 A	38283.986
233	5I	78 B	38299.979
234	5I	77 E	38330.718
235	5I	80 A	38383.341
236	5I	78 E	38401.270
237	5I	79 B	38516.049
238	5I	79 E	38518.435
239	5I	80 B	38523.124
240	5I	81 A	38538.549

241	5I	81 B	38552.873
242	5I	82 A	38572.930
243	5I	80 E	38573.282
244	5I	81 E	38602.345
245	5I	82 B	38629.560
246	5I	83 A	38652.079
247	5I	82 E	38654.942
248	5I	83 B	38655.365
249	5I	84 A	38665.479
250	5I	85 A	38683.347
251	5I	86 A	38695.057
252	5I	83 E	38700.129
253	5I	84 E	38728.651
254	5I	84 B	38732.955
255	5I	85 B	38751.466
256	5I	85 E	38780.022
257	5I	86 B	38782.950
258	5I	87 B	38802.945
259	5I	87 A	38814.544
260	5I	88 A	38844.207
261	5I	86 E	38868.988
262	5I	89 A	38892.519
263	5I	87 E	38900.567
264	5I	90 A	38902.896
265	5I	88 B	38914.254
266	5I	89 B	38917.220
267	5I	88 E	38939.620
268	5I	90 B	38946.221
269	5I	91 A	38960.971
270	5I	89 E	38987.293
271	5K	90 E	41883.349
272	5K	92 A	41946.778
273	5K	93 A	41954.269
274	5K	91 B	41954.759
275	5K	91 E	41978.054
276	5K	94 A	42050.199
277	5K	92 E	42112.137
278	5K	92 B	42131.354
279	5K	93 B	42791.053
280	5K	94 B	42811.770
281	5K	93 E	42877.705
282	5K	95 A	42936.705
283	5K	95 B	42948.996
284	5K	96 A	42962.395
285	5K	94 E	42970.204
286	5K	95 E	42995.818
287	5K	96 B	42999.237
288	5K	97 A	43001.327
289	5K	96 E	43665.677

290	5K	97 B	43725.127
291	5K	98 B	43735.416
292	5K	97 E	43797.128
293	5K	98 A	43808.531
294	5K	99 B	43809.025
295	5K	99 A	43841.676
296	5K	98 E	43843.997
297	5K	100 A	43849.207
298	5K	100 B	43857.448
299	5K	99 E	43871.565
300	5K	101 A	44461.861
301	5K	102 A	44462.990
302	5K	100 E	44498.613
303	5K	101 B	44519.538
304	5K	102 B	44540.710
305	5K	101 E	44560.087
306	5K	103 B	44575.976
307	5K	103 A	44583.123
308	5K	102 E	44607.264
309	5K	104 A	44617.023
310	5K	105 A	44673.285
311	5K	104 B	44673.589
312	5K	103 E	44676.948
313	5K	106 A	45133.636
314	5K	104 E	45136.745
315	5K	105 B	45150.144
316	5K	105 E	45153.271
317	5K	107 A	45159.887
318	5K	106 B	45170.702
319	5K	108 A	45199.678
320	5K	106 E	45209.279
321	5K	107 B	45256.203
322	5K	107 E	45289.903
323	5K	109 A	45317.795
324	5K	110 A	45446.393
325	5K	108 E	45463.635
326	5K	108 B	45476.958

Isomer II_{Eu2}

Level	(2S+1) L	Irrep	Energy (cm ⁻¹)
1	7F	1 A	0
2	7F	2 A	206.401
3	7F	1 E	507.453
4	7F	2 E	1078.547
5	7F	3 A	1107.401
6	7F	1 B	1110.631
7	7F	2 B	1332.736
8	7F	3 E	2005.537
9	7F	4 A	2033.496

10	7F	3 B	2069.38
11	7F	4 E	2093.288
12	7F	4 B	2127.633
13	7F	5 A	2863.882
14	7F	6 A	3047.889
15	7F	5 E	3049.801
16	7F	6 E	3134.294
17	7F	7 A	3196.324
18	7F	5 B	3199.846
19	7F	6 B	3338.002
20	7F	7 E	3994.823
21	7F	8 E	4158.038
22	7F	7 B	4179.629
23	7F	8 A	4257.099
24	7F	9 A	4282.282
25	7F	8 B	4371.328
26	7F	9 E	4453.681
27	7F	10 A	4503.056
28	7F	9 B	5065.764
29	7F	10 B	5066.632
30	7F	10 E	5218.276
31	7F	11 A	5446.771
32	7F	12 A	5471.712
33	7F	11 E	5559.678
34	7F	11 B	5582.748
35	7F	13 A	5680.937
36	7F	12 E	5691.209
37	7F	12 B	5701.577
38	5D	14 A	18156.489
39	5D	15 A	18884.968
40	5D	13 E	18948.412
41	5D	16 A	20512.5
42	5D	13 B	20524.847
43	5D	14 E	20570.688
44	5D	14 B	20586.729
45	5D	15 B	23143.769
46	5D	15 E	23156.609
47	5D	16 B	23180.856
48	5D	16 E	23196.685
49	5D	17 A	23204.566
50	5D	18 A	26893.823
51	5D	19 A	26903.946
52	5D	17 E	26909.016
53	5D	17 B	26938.543
54	5D	18 B	26952.72
55	5D	18 E	26994.984
56	5D	20 A	27025.681
57	5G	19 B	27672.923
58	5G	19 E	27699.417

59	5G	20 B	27703.989
60	5G	21 A	27751.889
61	5G	20 E	27767.169
62	5G	22 A	27789.341
63	5G	23 A	27866.504
64	5G	21 E	27868.804
65	5G	21 B	27882.286
66	5G	24 A	27889.173
67	5G	22 B	27898.058
68	5G	22 E	27978.584
69	5G	23 B	28011.347
70	5G	24 B	28066.568
71	5G	23 E	28069.959
72	5G	25 A	28096.788
73	5G	24 E	28167.685
74	5G	26 A	28191.518
75	5G	25 E	28256.903
76	5G	27 A	28266.503
77	5G	28 A	28280.342
78	5G	25 B	28294.786
79	5G	26 E	28308.698
80	5G	26 B	28339.782
81	5L	27 B	28537.168
82	5L	27 E	28555.113
83	5L	29 A	28564.81
84	5L	28 B	28608.157
85	5L	29 B	28617.956
86	5L	28 E	28746.942
87	5L	30 B	28760.742
88	5L	30 A	28805.887
89	5L	29 E	28807.742
90	5L	31 A	28875.883
91	5L	31 B	29065.454
92	5L	32 A	29077.893
93	5L	30 E	29091.265
94	5G	32 B	29104.064
95	5G	33 B	29113.966
96	5G	31 E	29127.913
97	5G	33 A	29148.051
98	5L	32 E	29155.569
99	5G	34 A	29160.959
100	5G	33 E	29184.756
101	5G	34 B	29208.438
102	5L	35 B	29217.758
103	5L	34 E	29253.863
104	5G	35 A	29278.457
105	5L	36 B	29294.798
106	5L	36 A	29296.98
107	5L	35 E	29299.19

108	5L	37 B	29302.983
109	5L	38 B	29332.129
110	5L	37 A	29333.309
111	5L	36 E	29344.521
112	5L	37 E	29752.035
113	5L	39 B	29758.488
114	5L	38 A	29762.865
115	5L	39 A	29798.305
116	5L	40 A	29867.977
117	5L	40 B	29913.169
118	5L	38 E	29915.728
119	5L	41 A	29941.108
120	5L	39 E	29966.029
121	5L	42 A	29980.159
122	5L	40 E	29990.866
123	5L	41 B	29996
124	5L	42 B	30023.47
125	5L	43 A	30577.319
126	5L	41 E	30580.156
127	5L	43 B	30584.075
128	5L	42 E	30651.749
129	5L	44 A	30735.898
130	5L	44 B	30740.548
131	5L	43 E	30743.533
132	5L	45 A	30764.466
133	5L	46 A	30793.601
134	5L	47 A	30816.043
135	5L	45 B	30834.905
136	5L	44 E	30834.782
137	5L	45 E	30854.758
138	5L	46 B	30863.645
139	5L	47 B	31576.715
140	5L	46 E	31579.757
141	5L	48 A	31582.191
142	5L	48 B	31635.039
143	5L	49 B	31638.755
144	5L	47 E	31726.426
145	5L	49 A	31735.815
146	5L	50 B	31753.147
147	5L	48 E	31766.615
148	5L	50 A	31849.623
149	5L	49 E	31886.902
150	5L	51 A	31887.587
151	5L	51 B	31888.058
152	5L	52 A	31922.681
153	5L	52 B	31926.094
154	5L	50 E	31934.62
155	5H	53 B	33302.983
156	5H	54 B	33348.489

157	5H	51 E	33353.618
158	5H	52 E	33454.495
159	5H	53 A	33520.511
160	5H	53 E	33579.735
161	5H	55 B	33608.346
162	5H	54 A	33610.991
163	5H	55 A	33647.299
164	5H	56 B	33659.281
165	5H	54 E	33688.565
166	5H	56 A	33717.77
167	5H	57 A	33775.163
168	5H	55 E	33781.198
169	5H	58 A	33786.25
170	5H	57 B	33797.832
171	5H	59 A	33820.871
172	5H	56 E	33827.629
173	5H	58 B	33842.447
174	5H	57 E	33846.319
175	5H	60 A	33867.234
176	5H	59 B	33869.825
177	5H	58 E	33887.273
178	5H	60 B	33917.619
179	5H	61 B	33940.866
180	5H	61 A	33964.011
181	5H	59 E	33984.517
182	5H	60 E	34025.759
183	5H	62 A	34033.91
184	5H	62 B	34068.871
185	5H	61 E	34072.056
186	5H	63 A	34079.739
187	5H	63 B	34095.396
188	5H	62 E	34103.121
189	5H	64 A	34126.313
190	5H	64 B	34128.576
191	5H	63 E	34151.824
192	5H	65 B	34219.677
193	5H	64 E	34229.06
194	5H	65 A	34240.41
195	5H	66 B	34243.554
196	5F	65 E	36340.842
197	5F	66 A	36478.749
198	5F	67 B	36749.547
199	5F	66 E	36804.299
200	5F	68 B	36813.104
201	5F	67 A	36828.58
202	5F	69 B	37264.243
203	5F	67 E	37276.013
204	5F	68 A	37286.705
205	5F	68 E	37351.863

206	5F	70 B	37361.297
207	5F	69 A	37714.683
208	5F	70 A	37716.093
209	5F	71 B	37784.958
210	5I	71 A	37804.346
211	5F	69 E	37828.796
212	5F	72 B	37829.379
213	5F	70 E	37842.726
214	5F	71 E	37866.873
215	5I	72 A	37880.962
216	5I	73 B	37893.715
217	5I	74 B	37899.653
218	5F	73 A	37902.524
219	5I	72 E	37903.197
220	5I	73 E	37942.33
221	5F	74 A	37989.458
222	5F	75 A	38028.547
223	5F	76 A	38050.757
224	5F	75 B	38086.42
225	5F	77 A	38101.922
226	5F	74 E	38105.354
227	5F	75 E	38126.673
228	5F	76 B	38132.838
229	5I	77 B	38223.236
230	5I	78 A	38233.048
231	5I	79 A	38257.555
232	5I	76 E	38265.234
233	5I	78 B	38278.996
234	5I	77 E	38307.314
235	5I	80 A	38369.495
236	5I	78 E	38379.178
237	5I	79 B	38497.892
238	5I	80 B	38501.742
239	5I	79 E	38511.643
240	5I	81 A	38541.093
241	5I	81 B	38556.296
242	5I	82 A	38561.756
243	5I	80 E	38568.779
244	5I	81 E	38588.618
245	5I	82 B	38623.687
246	5I	83 A	38625.222
247	5I	83 B	38633.181
248	5I	82 E	38638.503
249	5I	84 A	38648.78
250	5I	85 A	38659.453
251	5I	86 A	38667.831
252	5I	83 E	38678.509
253	5I	84 B	38702.15
254	5I	84 E	38715.305

255	5I	85 B	38727.033
256	5I	85 E	38757.239
257	5I	86 B	38760.284
258	5I	87 B	38786.11
259	5I	87 A	38787.392
260	5I	88 A	38807.088
261	5I	86 E	38844.018
262	5I	89 A	38847.854
263	5I	90 A	38856.387
264	5I	87 E	38871.669
265	5I	88 B	38880.329
266	5I	89 B	38888.147
267	5I	90 B	38905.313
268	5I	88 E	38914.747
269	5I	91 A	38939.765
270	5I	89 E	38955.452
271	5K	90 E	41855.8
272	5K	92 A	41909.201
273	5K	93 A	41918.806
274	5K	91 B	41928.842
275	5K	91 E	41952.472
276	5K	94 A	42026.046
277	5K	92 E	42078.413
278	5K	92 B	42096.725
279	5K	93 B	42765.794
280	5K	94 B	42783.281
281	5K	93 E	42849.738
282	5K	95 A	42907.479
283	5K	95 B	42923.556
284	5K	96 A	42929.46
285	5K	94 E	42939.303
286	5K	96 B	42964.725
287	5K	95 E	42964.943
288	5K	97 A	42967.204
289	5K	96 E	43639.362
290	5K	97 B	43696.392
291	5K	98 B	43709.097
292	5K	97 E	43765.099
293	5K	98 A	43779.869
294	5K	99 B	43785.772
295	5K	99 A	43805.409
296	5K	98 E	43812.454
297	5K	100 A	43818.196
298	5K	100 B	43821.299
299	5K	99 E	43842.038
300	5K	101 A	44436.012
301	5K	102 A	44437.777
302	5K	100 E	44467.62
303	5K	101 B	44487.245

304	5K	102 B	44507.838
305	5K	101 E	44532.925
306	5K	103 B	44548.781
307	5K	103 A	44552.746
308	5K	104 A	44577.995
309	5K	102 E	44579.945
310	5K	105 A	44639.804
311	5K	104 B	44642.884
312	5K	103 E	44643.457
313	5K	104 E	45103.079
314	5K	106 A	45105.581
315	5K	105 B	45115.205
316	5K	107 A	45124.263
317	5K	105 E	45127.51
318	5K	106 B	45133.189
319	5K	108 A	45172.688
320	5K	106 E	45188.528
321	5K	107 B	45233.22
322	5K	107 E	45260.046
323	5K	109 A	45283.72
324	5K	110 A	45407.929
325	5K	108 E	45423.395
326	5K	108 B	45435.526

Table 3S. Cartesian coordinates (in Å) of the DFT optimized geometry of $\{K_4[Eu(DOTP)]\}^-$ cluster representing I_{Eu1} and II_{Eu1} sites.

Atom	I_{Eu1}		
	x	y	z
Eu	-0.04178	-0.02604	-0.29251
O	-3.77901	2.71597	-1.26817
O	-4.30950	0.48148	0.02434
O	-2.04955	0.83048	-1.13638
C	-2.46064	2.30022	1.06153
H	-1.87376	3.14015	0.68010
H	-3.21233	2.71754	1.75441
N	-1.53696	1.39028	1.79018
C	-0.65810	2.18207	2.67574
H	-1.24623	2.96107	3.19467
H	-0.27343	1.52360	3.46025
C	0.50371	2.86050	1.95222
H	0.13989	3.52406	1.16288
H	1.03778	3.50000	2.68072
P	-3.29550	1.54027	-0.42055
K	-3.67882	-1.34183	-1.73820
O	3.34395	-2.98710	-1.77790
O	4.15718	-0.57640	-1.09075
O	1.67309	-1.06508	-1.49935
C	2.71476	-2.14186	0.71773
H	2.06597	-3.02037	0.66573
H	3.63941	-2.45140	1.23588
N	2.00763	-1.09697	1.50530
C	1.42920	-1.70153	2.72328
H	2.15742	-2.39324	3.18510
H	1.26145	-0.90789	3.45745
C	0.12929	-2.46603	2.47979
H	0.27581	-3.26500	1.74773
H	-0.16542	-2.95637	3.42722
P	3.08601	-1.67082	-1.04618
K	3.01684	0.92930	-2.89665
O	-3.00715	-3.68355	-0.80882
O	-0.54882	-4.30062	-0.08714
O	-1.10693	-1.97837	-1.02101
C	-2.04810	-2.49685	1.42957
H	-2.94081	-1.88367	1.27965
H	-2.31233	-3.28180	2.15985
N	-0.97855	-1.62113	1.97845
C	-1.53140	-0.78556	3.06460
H	-2.18402	-1.39498	3.71632
H	-0.70476	-0.44914	3.69744

C	-2.33299	0.41900	2.57468
H	-3.16528	0.10370	1.93937
H	-2.78000	0.91765	3.45584
P	-1.66057	-3.25585	-0.22718
K	0.83967	-3.58925	-2.18352
O	2.57209	3.41243	-2.23725
O	0.39651	4.20570	-0.97927
O	0.73048	1.74377	-1.61473
C	2.30221	2.65521	0.34968
H	3.13302	2.00345	0.06618
H	2.73942	3.54795	0.83044
N	1.44922	1.91444	1.31702
C	2.30251	1.26610	2.33441
H	3.09520	1.96281	2.66345
H	1.69277	1.06485	3.22026
C	2.96598	-0.02453	1.85733
H	3.58098	0.15536	0.97124
H	3.65236	-0.37401	2.65211
P	1.45108	3.12530	-1.23955
K	-1.50165	3.17672	-2.45133

Atom	x	\parallel_{Eu1}	
		y	z
Eu	0.00000	-0.00018	-0.00791
O	2.72398	-3.33932	0.22574
O	1.79650	-1.08565	1.02089
O	4.31694	-1.49237	1.22395
C	3.26043	-1.00695	-1.21873
H	4.02099	-1.52303	-1.83090
H	3.65145	-0.01054	-0.99551
N	2.00041	-0.84220	-1.99103
C	2.19808	0.16152	-3.05647
H	3.17056	-0.00232	-3.55624
H	1.43451	0.00472	-3.82427
C	2.14789	1.60831	-2.56673
H	2.40183	2.26878	-3.41794
H	2.90346	1.78823	-1.79713
K	3.50480	0.84296	2.02772
P	3.06680	-1.85961	0.42618
O	-2.72407	3.33904	0.22626
O	-1.79636	1.08528	1.02077
O	-4.31679	1.49182	1.22430
C	-3.26051	1.00690	-1.21867
H	-4.02088	1.52324	-1.83086
H	-3.65176	0.01054	-0.99564
N	-2.00043	0.84201	-1.99086
C	-2.19810	-0.16169	-3.05634

H	-3.17061	0.00214	-3.55606
H	-1.43458	-0.00480	-3.82417
C	-2.14786	-1.60851	-2.56672
H	-2.40188	-2.26890	-3.41797
H	-2.90337	-1.78849	-1.79708
K	-3.50463	-0.84351	2.02759
P	-3.06679	1.85928	0.42640
O	3.33926	2.72410	0.22626
O	1.08564	1.79607	1.02080
O	1.49181	4.31656	1.22433
C	1.00703	3.26033	-1.21861
H	1.52329	4.02079	-1.83074
H	0.01066	3.65151	-0.99549
N	0.84217	2.00032	-1.99090
C	-0.16160	2.19806	-3.05630
H	0.00220	3.17060	-3.55598
H	-0.00477	1.43459	-3.82419
C	-1.60837	2.14778	-2.56657
H	-2.26885	2.40181	-3.41775
H	-1.78830	2.90328	-1.79690
K	-0.84320	3.50388	2.02815
P	1.85945	3.06662	0.42643
O	-3.33925	-2.72434	0.22585
O	-1.08556	-1.79662	1.02063
O	-1.49213	-4.31705	1.22410
C	-1.00700	-3.26072	-1.21884
H	-1.52329	-4.02112	-1.83105
H	-0.01064	-3.65195	-0.99576
N	-0.84211	-2.00064	-1.99102
C	0.16163	-2.19829	-3.05646
H	-0.00214	-3.17081	-3.55619
H	0.00475	-1.43478	-3.82430
C	1.60842	-2.14799	-2.56674
H	2.26890	-2.40199	-3.41793
H	1.78836	-2.90348	-1.79706
K	0.84313	-3.50470	2.02755
P	-1.85950	-3.06704	0.42616
