

Speciation of Uranyl Ion in Fulvic Acid and Humic Acid: A DFT exploration.

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Supporting Information

(i) Force Field Parameters used for the GROMACS Molecular Dynamics Simulations.

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; PRODRG - a tool for high-throughput crystallography
; of protein-ligand complexes.
; Acta Crystallogr. D60, 1355--1363.
;
;
; Include forcefield parameters
#include "ffG43a2.itp"
#include "spc.itp"
#include "ions.itp"

[ moleculetype ]
; Name nrexcl
xmo      3

[ atoms ]
;  nr      type  resnr  resid  atom  cgnr  charge  mass
  1         OA   1  xmo   OAA   1  -0.576698  15.9994
  2         H    1  xmo   HAA   1   0.459098   1.0080
  3         C    1  xmo   CAB   1   0.117712  12.0110
  4         C    1  xmo   CAC   1   0.347924  12.0110
  5         OA   1  xmo   OAD   1  -0.594066  15.9994
  6         H    1  xmo   HAD   1   0.461491   1.0080
  7        CR1   1  xmo   CAE   2  -0.369880  12.0110
  8         HC   1  xmo   HAE   2   0.188810   1.0080
  9         C    1  xmo   CAF   2  -0.038806  12.0110
 10         C    1  xmo   CAG   2   0.683461  12.0110
 11         OM   1  xmo   OAH   2  -0.744918  15.9994
 12         OM   1  xmo   OAI   2  -0.742148  15.9994
 13        CR1   1  xmo   CAJ   2  -0.273303  12.0110
 14         HC   1  xmo   HAJ   2   0.141299   1.0080
 15         C    1  xmo   CAK   3  -0.073693  12.0110
 16         C    1  xmo   CAL   3   0.141526  12.0110
 17         C    1  xmo   CAM   3   0.038367  12.0110
 18         OA   1  xmo   OAN   3  -0.465363  15.9994
 19         H    1  xmo   HAN   3   0.429890   1.0080
 20        CR1   1  xmo   CAO   4  -0.324247  12.0110
 21         HC   1  xmo   HAO   4   0.164959   1.0080
 22         C    1  xmo   CAP   4  -0.002151  12.0110
 23         C    1  xmo   CAQ   4   0.665930  12.0110
 24         OM   1  xmo   OAR   4  -0.733273  15.9994
 25         OM   1  xmo   OAS   4  -0.727512  15.9994
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26	CR1	1	xmo	CAT	4	-0.296356	12.0110
27	HC	1	xmo	HAT	4	0.181993	1.0080
28	C	1	xmo	CAU	4	0.228419	12.0110
29	O	1	xmo	OAV	5	-0.278177	15.9994
30	C	1	xmo	CAW	5	0.330069	12.0110
31	C	1	xmo	CAX	5	0.262581	12.0110
32	CR1	1	xmo	CAY	5	-0.158836	12.0110
33	HC	1	xmo	HAY	5	0.180102	1.0080
34	OA	1	xmo	OAZ	6	-0.522415	15.9994
35	H	1	xmo	HAZ	6	0.423136	1.0080
36	CR1	1	xmo	CBA	6	-0.525627	12.0110
37	HC	1	xmo	HBA	6	0.262224	1.0080
38	C	1	xmo	CBB	6	0.695849	12.0110
39	OA	1	xmo	OBC	6	-0.343367	15.9994
40	C	1	xmo	CBD	6	-0.525060	12.0110
41	C	1	xmo	CBE	6	0.853441	12.0110
42	OA	1	xmo	OBF	6	-0.529887	15.9994
43	H	1	xmo	HBF	6	0.497463	1.0080
44	C	1	xmo	CBG	7	-0.688654	12.0110
45	C	1	xmo	CBH	7	0.757080	12.0110
46	O	1	xmo	OBI	7	-0.462255	15.9994
47	C	1	xmo	CBJ	7	0.440209	12.0110
48	C	1	xmo	CBK	7	0.496020	12.0110
49	O	1	xmo	OBL	8	-0.448084	15.9994
50	CR1	1	xmo	CBM	8	-0.403051	12.0110
51	HC	1	xmo	HBM	8	0.218397	1.0080
52	C	1	xmo	CBN	8	0.073984	12.0110
53	OA	1	xmo	OBO	8	-0.284586	15.9994
54	C	1	xmo	CBP	8	-0.037937	12.0110
55	C	1	xmo	CBQ	8	0.395056	12.0110
56	CR1	1	xmo	CBR	8	-0.461153	12.0110
57	HC	1	xmo	HBR	8	0.205766	1.0080
58	OA	1	xmo	OBS	9	-0.581566	15.9994
59	H	1	xmo	HBS	9	0.466455	1.0080
60	C	1	xmo	CBT	9	0.272074	12.0110
61	N	1	xmo	N	9	-0.363977	14.0067
62	H	1	xmo	H	9	0.303412	1.0080
63	CH1	1	xmo	CA	9	0.048168	13.0190
64	C	1	xmo	C	9	0.638395	12.0110
65	O	1	xmo	O	9	-0.579295	15.9994
66	NT	1	xmo	NBY	9	-0.797435	14.0067
67	H	1	xmo	HKL	9	0.415355	1.0080
68	H	1	xmo	HBY	9	0.392692	1.0080
69	C	1	xmo	CBZ	10	-0.057018	12.0110
70	CR1	1	xmo	CCA	10	-0.136099	12.0110
71	HC	1	xmo	HCA	10	0.137495	1.0080
72	CR1	1	xmo	CCB	11	-0.334459	12.0110
73	HC	1	xmo	HCB	11	0.192255	1.0080
74	C	1	xmo	CCC	11	0.417734	12.0110
75	OA	1	xmo	OCD	12	-0.642320	15.9994
76	H	1	xmo	HCD	12	0.447045	1.0080
77	CR1	1	xmo	CCE	12	-0.255865	12.0110
78	HC	1	xmo	HCE	12	0.151400	1.0080
79	CR1	1	xmo	CCF	12	-0.164125	12.0110
80	HC	1	xmo	HCF	12	0.157382	1.0080
81	CR1	1	xmo	CCG	12	-0.404844	12.0110
82	HC	1	xmo	HCG	12	0.237614	1.0080

83	C	1	xmo	CCH	12	0.065868	12.0110
84	C	1	xmo	CCI	12	0.287148	12.0110
85	NR	1	xmo	NCJ	12	-0.493665	14.0067
86	C	1	xmo	CCK	13	0.158466	12.0110
87	OA	1	xmo	OCL	13	-0.429410	15.9994
88	C	1	xmo	CCM	13	0.770176	12.0110
89	O	1	xmo	OCN	13	-0.560395	15.9994
90	CH1	1	xmo	CCO	13	0.189275	13.0190
91	OA	1	xmo	OCP	14	-0.626520	15.9994
92	H	1	xmo	HCP	14	0.410412	1.0080
93	CH1	1	xmo	CCQ	14	0.192882	13.0190
94	OA	1	xmo	OCR	14	-0.708073	15.9994
95	H	1	xmo	HCR	14	0.471070	1.0080
96	CH1	1	xmo	CCS	15	0.248365	13.0190
97	OA	1	xmo	OCT	15	-0.765117	15.9994
98	H	1	xmo	HCT	15	0.499635	1.0080
99	CH1	1	xmo	CCU	15	0.326333	13.0190
100	C	1	xmo	CCV	15	0.419672	13.0190
101	O	1	xmo	OCW	15	-0.458617	15.9994
102	OA	1	xmo	OCX	16	-0.691333	15.9994
103	H	1	xmo	HCX	16	0.439954	1.0080
104	CR1	1	xmo	CCY	16	-0.118707	12.0110
105	HC	1	xmo	HCY	16	0.179658	1.0080
106	C	1	xmo	CCZ	17	-0.137310	12.0110
107	CR1	1	xmo	CDA	18	-0.326130	12.0110
108	HC	1	xmo	HDA	18	0.180814	1.0080
109	C	1	xmo	CDB	18	0.271988	12.0110
110	C	1	xmo	CDC	18	0.383035	12.0110
111	OA	1	xmo	ODD	18	-0.641060	15.9994
112	CR1	1	xmo	CDE	18	-0.513396	12.0110
113	HC	1	xmo	HDE	18	0.197411	1.0080
114	C	1	xmo	CDF	18	0.290135	12.0110
115	OA	1	xmo	ODG	18	-0.330835	15.9994
116	C	1	xmo	CDH	19	0.091289	12.0110
117	CR1	1	xmo	CDI	20	-0.079589	12.0110
118	HC	1	xmo	HDI	20	0.144783	1.0080
119	C	1	xmo	CDJ	20	-0.259823	12.0110
120	C	1	xmo	CDK	21	0.457293	12.0110
121	O	1	xmo	ODL	21	-0.498103	15.9994
122	C	1	xmo	CDM	21	0.574311	12.0110
123	O	1	xmo	ODN	21	-0.563205	15.9994
124	C	1	xmo	CDO	21	-0.580216	12.0110
125	C	1	xmo	CDP	21	0.587727	12.0110
126	OA	1	xmo	ODQ	22	-0.605622	15.9994
127	H	1	xmo	HDQ	22	0.491349	1.0080
128	C	1	xmo	CDR	22	-0.234968	12.0110
129	C	1	xmo	CDS	22	-0.279350	12.0110
130	C	1	xmo	CDT	22	0.427840	12.0110
131	OA	1	xmo	ODU	22	-0.600857	15.9994
132	H	1	xmo	HDU	22	0.464519	1.0080
133	C	1	xmo	CDV	23	-0.332457	12.0110
134	C	1	xmo	CDW	23	0.704330	12.0110
135	OM	1	xmo	ODX	23	-0.726707	15.9994
136	OM	1	xmo	ODY	23	-0.720857	15.9994
137	C	1	xmo	CDZ	24	0.046345	12.0110
138	C	1	xmo	CEA	24	0.654597	12.0110
139	OM	1	xmo	OEB	24	-0.745638	15.9994

140	OM	1	xmo	OEC	24	-0.698017	15.9994
141	CR1	1	xmo	CED	24	-0.478709	12.0110
142	HC	1	xmo	HED	24	0.211517	1.0080
143	C	1	xmo	CEE	24	0.384116	12.0110
144	O	1	xmo	OEF	25	-0.305986	15.9994
145	C	1	xmo	CEG	25	0.402354	12.0110
146	CR1	1	xmo	CEH	25	-0.376119	12.0110
147	HC	1	xmo	HEH	25	0.195866	1.0080
148	C	1	xmo	CEI	25	0.166510	12.0110
149	C	1	xmo	CEJ	25	0.088889	12.0110
150	CR1	1	xmo	CEK	26	-0.367311	12.0110
151	HC	1	xmo	HEK	26	0.217046	1.0080
152	C	1	xmo	CEL	27	0.391685	12.0110
153	OA	1	xmo	OEM	27	-0.574029	15.9994
154	H	1	xmo	HEM	27	0.472237	1.0080

[bonds]

; ai	aj	fu	c0, c1, ...					
1	2	2	0.100	15700000.0	0.100	15700000.0	; OAA	HAA
3	1	2	0.136	10200000.0	0.136	10200000.0	; CAB	OAA
3	4	2	0.139	10800000.0	0.139	10800000.0	; CAB	CAC
3	15	2	0.139	10800000.0	0.139	10800000.0	; CAB	CAK
4	5	2	0.136	10200000.0	0.136	10200000.0	; CAC	OAD
4	7	2	0.139	10800000.0	0.139	10800000.0	; CAC	CAE
5	6	2	0.100	15700000.0	0.100	15700000.0	; OAD	HAD
7	8	2	0.109	12300000.0	0.109	12300000.0	; CAE	HAE
9	7	2	0.139	10800000.0	0.139	10800000.0	; CAF	CAE
9	10	2	0.139	10800000.0	0.139	10800000.0	; CAF	CAG
9	13	2	0.139	10800000.0	0.139	10800000.0	; CAF	CAJ
10	11	2	0.125	13400000.0	0.125	13400000.0	; CAG	OAH
10	12	2	0.125	13400000.0	0.125	13400000.0	; CAG	OAI
13	14	2	0.109	12300000.0	0.109	12300000.0	; CAJ	HAJ
15	13	2	0.139	10800000.0	0.139	10800000.0	; CAK	CAJ
15	16	2	0.139	10800000.0	0.139	10800000.0	; CAK	CAL
16	17	2	0.139	10800000.0	0.139	10800000.0	; CAL	CAM
16	20	2	0.139	10800000.0	0.139	10800000.0	; CAL	CAO
17	18	2	0.136	10200000.0	0.136	10200000.0	; CAM	OAN
17	28	2	0.139	10800000.0	0.139	10800000.0	; CAM	CAU
18	19	2	0.100	15700000.0	0.100	15700000.0	; OAN	HAN
20	21	2	0.109	12300000.0	0.109	12300000.0	; CAO	HAO
22	20	2	0.139	10800000.0	0.139	10800000.0	; CAP	CAO
22	23	2	0.139	10800000.0	0.139	10800000.0	; CAP	CAQ
22	26	2	0.139	10800000.0	0.139	10800000.0	; CAP	CAT
23	24	2	0.125	13400000.0	0.125	13400000.0	; CAQ	OAR
23	25	2	0.125	13400000.0	0.125	13400000.0	; CAQ	OAS
26	27	2	0.109	12300000.0	0.109	12300000.0	; CAT	HAT
28	26	2	0.139	10800000.0	0.139	10800000.0	; CAU	CAT
28	29	2	0.137	3682150.9	0.137	3682150.9	; CAU	OAV
30	29	2	0.137	3682150.9	0.137	3682150.9	; CAW	OAV
30	31	2	0.139	10800000.0	0.139	10800000.0	; CAW	CAX
30	36	2	0.139	10800000.0	0.139	10800000.0	; CAW	CBA
31	32	2	0.139	10800000.0	0.139	10800000.0	; CAX	CAY
31	34	2	0.136	10200000.0	0.136	10200000.0	; CAX	OAZ
32	33	2	0.109	12300000.0	0.109	12300000.0	; CAY	HAY
40	32	2	0.139	10800000.0	0.139	10800000.0	; CBD	CAY
34	35	2	0.100	15700000.0	0.100	15700000.0	; OAZ	HAZ
36	37	2	0.109	12300000.0	0.109	12300000.0	; CBA	HBA

38	36	2	0.139	10800000.0	0.139	10800000.0 ;	CBB	CBA
38	39	2	0.136	10200000.0	0.136	10200000.0 ;	CBB	OBC
38	40	2	0.139	10800000.0	0.139	10800000.0 ;	CBB	CBD
47	39	2	0.136	10200000.0	0.136	10200000.0 ;	CBJ	OBC
40	41	2	0.139	10800000.0	0.139	10800000.0 ;	CBD	CBE
41	42	2	0.136	10200000.0	0.136	10200000.0 ;	CBE	OBF
41	44	2	0.139	10800000.0	0.139	10800000.0 ;	CBE	CBG
42	43	2	0.100	15700000.0	0.100	15700000.0 ;	OBF	HBF
44	45	2	0.139	10800000.0	0.139	10800000.0 ;	CBG	CBH
44	47	2	0.139	10800000.0	0.139	10800000.0 ;	CBG	CBJ
45	46	2	0.123	16600000.0	0.123	16600000.0 ;	CBH	OBI
45	52	2	0.139	10800000.0	0.139	10800000.0 ;	CBH	CBN
47	48	2	0.139	10800000.0	0.139	10800000.0 ;	CBJ	CBK
48	49	2	0.123	16600000.0	0.123	16600000.0 ;	CBK	OBL
48	50	2	0.139	10800000.0	0.139	10800000.0 ;	CBK	CBM
50	51	2	0.109	12300000.0	0.109	12300000.0 ;	CBM	HBM
52	50	2	0.139	10800000.0	0.139	10800000.0 ;	CBN	CBM
52	53	2	0.136	10200000.0	0.136	10200000.0 ;	CBN	OBO
54	53	2	0.136	10200000.0	0.136	10200000.0 ;	CBP	OBO
54	55	2	0.139	10800000.0	0.139	10800000.0 ;	CBP	CBQ
54	60	2	0.139	10800000.0	0.139	10800000.0 ;	CBP	CBT
55	56	2	0.139	10800000.0	0.139	10800000.0 ;	CBQ	CBR
55	58	2	0.136	10200000.0	0.136	10200000.0 ;	CBQ	OBS
56	57	2	0.109	12300000.0	0.109	12300000.0 ;	CBR	HBR
83	56	2	0.139	10800000.0	0.139	10800000.0 ;	CCH	CBR
58	59	2	0.100	15700000.0	0.100	15700000.0 ;	OBS	HBS
60	61	2	0.133	10600000.0	0.133	10600000.0 ;	CBT	N
60	81	2	0.139	10800000.0	0.139	10800000.0 ;	CBT	CCG
61	62	2	0.100	18700000.0	0.100	18700000.0 ;	N	H
63	61	2	0.147	8710000.0	0.147	8710000.0 ;	CA	N
63	64	2	0.153	7150000.0	0.153	7150000.0 ;	CA	C
69	63	2	0.139	8660000.0	0.139	8660000.0 ;	CBZ	CA
64	65	2	0.123	16600000.0	0.123	16600000.0 ;	C	O
64	66	2	0.133	10600000.0	0.133	10600000.0 ;	C	NBY
66	67	2	0.100	18700000.0	0.100	18700000.0 ;	NBY	HKL
66	68	2	0.100	18700000.0	0.100	18700000.0 ;	NBY	HBY
69	70	2	0.139	10800000.0	0.139	10800000.0 ;	CBZ	CCA
69	79	2	0.139	10800000.0	0.139	10800000.0 ;	CBZ	CCF
70	71	2	0.109	12300000.0	0.109	12300000.0 ;	CCA	HCA
70	72	2	0.139	10800000.0	0.139	10800000.0 ;	CCA	CCB
72	73	2	0.109	12300000.0	0.109	12300000.0 ;	CCB	HCB
74	72	2	0.139	10800000.0	0.139	10800000.0 ;	CCC	CCB
74	75	2	0.136	10200000.0	0.136	10200000.0 ;	CCC	OCD
74	77	2	0.139	10800000.0	0.139	10800000.0 ;	CCC	CCE
75	76	2	0.100	15700000.0	0.100	15700000.0 ;	OCD	HCD
77	78	2	0.109	12300000.0	0.109	12300000.0 ;	CCE	HCE
77	79	2	0.139	10800000.0	0.139	10800000.0 ;	CCE	CCF
79	80	2	0.109	12300000.0	0.109	12300000.0 ;	CCF	HCF
81	82	2	0.109	12300000.0	0.109	12300000.0 ;	CCG	HCG
83	81	2	0.139	10800000.0	0.139	10800000.0 ;	CCH	CCG
83	84	2	0.139	10800000.0	0.139	10800000.0 ;	CCH	CCI
84	85	2	0.134	11700000.0	0.134	11700000.0 ;	CCI	NCJ
84	86	2	0.139	10800000.0	0.139	10800000.0 ;	CCI	CCK
109	85	2	0.134	11700000.0	0.134	11700000.0 ;	CDB	NCJ
86	87	2	0.136	10200000.0	0.136	10200000.0 ;	CCK	OCL
86	104	2	0.139	10800000.0	0.139	10800000.0 ;	CCK	CCY
88	87	2	0.136	10200000.0	0.136	10200000.0 ;	CCM	OCL

88	89	2	0.123	16600000.0	0.123	16600000.0	;	CCM	OCN
90	88	2	0.153	7150000.0	0.153	7150000.0	;	CCO	CCM
90	91	2	0.143	8180000.0	0.143	8180000.0	;	CCO	OCP
90	93	2	0.153	7150000.0	0.153	7150000.0	;	CCO	CCQ
91	92	2	0.100	15700000.0	0.100	15700000.0	;	OCP	HCP
93	94	2	0.143	8180000.0	0.143	8180000.0	;	CCQ	OCR
93	96	2	0.153	7150000.0	0.153	7150000.0	;	CCQ	CCS
94	95	2	0.100	15700000.0	0.100	15700000.0	;	OCR	HCR
96	97	2	0.143	8180000.0	0.143	8180000.0	;	CCS	OCT
96	99	2	0.153	7150000.0	0.153	7150000.0	;	CCS	CCU
97	98	2	0.100	15700000.0	0.100	15700000.0	;	OCT	HCT
99	100	2	0.153	7150000.0	0.153	7150000.0	;	CCU	CCV
99	102	2	0.143	8180000.0	0.143	8180000.0	;	CCU	OCX
100	101	2	0.123	16600000.0	0.123	16600000.0	;	CCV	OCW
102	103	2	0.100	15700000.0	0.100	15700000.0	;	OCX	HCX
104	105	2	0.109	12300000.0	0.109	12300000.0	;	CCY	HCY
106	104	2	0.139	10800000.0	0.139	10800000.0	;	CCZ	CCY
106	107	2	0.139	10800000.0	0.139	10800000.0	;	CCZ	CDA
106	109	2	0.139	10800000.0	0.139	10800000.0	;	CCZ	CDB
107	108	2	0.109	12300000.0	0.109	12300000.0	;	CDA	HDA
114	107	2	0.139	10800000.0	0.139	10800000.0	;	CDF	CDA
109	110	2	0.139	10800000.0	0.139	10800000.0	;	CDB	CDC
110	111	2	0.136	10200000.0	0.136	10200000.0	;	CDC	ODD
110	112	2	0.139	10800000.0	0.139	10800000.0	;	CDC	CDE
112	113	2	0.109	12300000.0	0.109	12300000.0	;	CDE	HDE
114	112	2	0.139	10800000.0	0.139	10800000.0	;	CDF	CDE
114	115	2	0.136	10200000.0	0.136	10200000.0	;	CDF	ODG
116	115	2	0.136	10200000.0	0.136	10200000.0	;	CDH	ODG
116	117	2	0.139	10800000.0	0.139	10800000.0	;	CDH	CDI
116	152	2	0.139	10800000.0	0.139	10800000.0	;	CDH	CEL
117	118	2	0.109	12300000.0	0.109	12300000.0	;	CDI	HDI
119	117	2	0.139	10800000.0	0.139	10800000.0	;	CDJ	CDI
119	120	2	0.139	10800000.0	0.139	10800000.0	;	CDJ	CDK
119	149	2	0.139	10800000.0	0.139	10800000.0	;	CDJ	CEJ
120	121	2	0.123	16600000.0	0.123	16600000.0	;	CDK	ODL
120	122	2	0.139	10800000.0	0.139	10800000.0	;	CDK	CDM
122	123	2	0.123	16600000.0	0.123	16600000.0	;	CDM	ODN
122	124	2	0.139	10800000.0	0.139	10800000.0	;	CDM	CDO
124	125	2	0.139	10800000.0	0.139	10800000.0	;	CDO	CDP
124	148	2	0.139	10800000.0	0.139	10800000.0	;	CDO	CEI
125	126	2	0.136	10200000.0	0.136	10200000.0	;	CDP	ODQ
125	128	2	0.133	11800000.0	0.133	11800000.0	;	CDP	CDR
126	127	2	0.100	15700000.0	0.100	15700000.0	;	ODQ	HDQ
128	129	2	0.133	11800000.0	0.133	11800000.0	;	CDR	CDS
128	145	2	0.133	11800000.0	0.133	11800000.0	;	CDR	CEG
129	130	2	0.133	11800000.0	0.133	11800000.0	;	CDS	CDT
129	143	2	0.133	11800000.0	0.133	11800000.0	;	CDS	CEE
130	131	2	0.136	10200000.0	0.136	10200000.0	;	CDT	ODU
130	133	2	0.139	10800000.0	0.139	10800000.0	;	CDT	CDV
131	132	2	0.100	15700000.0	0.100	15700000.0	;	ODU	HDU
133	134	2	0.139	10800000.0	0.139	10800000.0	;	CDV	CDW
133	137	2	0.139	10800000.0	0.139	10800000.0	;	CDV	CDZ
134	135	2	0.125	13400000.0	0.125	13400000.0	;	CDW	ODX
134	136	2	0.125	13400000.0	0.125	13400000.0	;	CDW	ODY
137	138	2	0.139	10800000.0	0.139	10800000.0	;	CDZ	CEA
137	141	2	0.139	10800000.0	0.139	10800000.0	;	CDZ	CED
138	139	2	0.125	13400000.0	0.125	13400000.0	;	CEA	OEB

138	140	2	0.125	13400000.0	0.125	13400000.0	;	CEA	OEC
141	142	2	0.109	12300000.0	0.109	12300000.0	;	CED	HED
143	141	2	0.133	11800000.0	0.133	11800000.0	;	CEE	CED
143	144	2	0.137	3682150.9	0.137	3682150.9	;	CEE	OEF
145	144	2	0.137	3682150.9	0.137	3682150.9	;	CEG	OEF
145	146	2	0.133	11800000.0	0.133	11800000.0	;	CEG	CEH
146	147	2	0.109	12300000.0	0.109	12300000.0	;	CEH	HEH
148	146	2	0.139	10800000.0	0.139	10800000.0	;	CEI	CEH
148	149	2	0.139	10800000.0	0.139	10800000.0	;	CEI	CEJ
149	150	2	0.139	10800000.0	0.139	10800000.0	;	CEJ	CEK
150	151	2	0.109	12300000.0	0.109	12300000.0	;	CEK	HEK
152	150	2	0.139	10800000.0	0.139	10800000.0	;	CEL	CEK
152	153	2	0.136	10200000.0	0.136	10200000.0	;	CEL	OEM
153	154	2	0.100	15700000.0	0.100	15700000.0	;	OEM	HEM

[pairs]

;	ai	aj	fu	c0, c1, ...					
	1	5	1		;	OAA	OAD		
	1	7	1		;	OAA	CAE		
	1	13	1		;	OAA	CAJ		
	1	16	1		;	OAA	CAL		
	2	4	1		;	HAA	CAC		
	2	15	1		;	HAA	CAK		
	3	6	1		;	CAB	HAD		
	3	8	1		;	CAB	HAE		
	3	9	1		;	CAB	CAF		
	3	14	1		;	CAB	HAJ		
	3	17	1		;	CAB	CAM		
	3	20	1		;	CAB	CAO		
	4	10	1		;	CAC	CAG		
	4	13	1		;	CAC	CAJ		
	4	16	1		;	CAC	CAL		
	5	8	1		;	OAD	HAE		
	5	9	1		;	OAD	CAF		
	5	15	1		;	OAD	CAK		
	6	7	1		;	HAD	CAE		
	7	11	1		;	CAE	OAH		
	7	12	1		;	CAE	OAI		
	7	14	1		;	CAE	HAJ		
	7	15	1		;	CAE	CAK		
	8	10	1		;	HAE	CAG		
	8	13	1		;	HAE	CAJ		
	9	16	1		;	CAF	CAL		
	10	14	1		;	CAG	HAJ		
	10	15	1		;	CAG	CAK		
	11	13	1		;	OAH	CAJ		
	12	13	1		;	OAI	CAJ		
	13	17	1		;	CAJ	CAM		
	13	20	1		;	CAJ	CAO		
	14	16	1		;	HAJ	CAL		
	15	18	1		;	CAK	OAN		
	15	21	1		;	CAK	HAO		
	15	22	1		;	CAK	CAP		
	15	28	1		;	CAK	CAU		
	16	19	1		;	CAL	HAN		
	16	23	1		;	CAL	CAQ		
	16	26	1		;	CAL	CAT		

16	29	1	;	CAL	OAV
17	21	1	;	CAM	HAO
17	22	1	;	CAM	CAP
17	27	1	;	CAM	HAT
17	30	1	;	CAM	CAW
18	20	1	;	OAN	CAO
18	26	1	;	OAN	CAT
18	29	1	;	OAN	OAV
19	28	1	;	HAN	CAU
20	24	1	;	CAO	OAR
20	25	1	;	CAO	OAS
20	27	1	;	CAO	HAT
20	28	1	;	CAO	CAU
21	23	1	;	HAO	CAQ
21	26	1	;	HAO	CAT
22	29	1	;	CAP	OAV
23	27	1	;	CAQ	HAT
23	28	1	;	CAQ	CAU
24	26	1	;	OAR	CAT
25	26	1	;	OAS	CAT
26	30	1	;	CAT	CAW
27	29	1	;	HAT	OAV
28	31	1	;	CAU	CAX
28	36	1	;	CAU	CBA
29	32	1	;	OAV	CAY
29	34	1	;	OAV	OAZ
29	37	1	;	OAV	HBA
29	38	1	;	OAV	CBB
30	33	1	;	CAW	HAY
30	35	1	;	CAW	HAZ
30	39	1	;	CAW	OBC
30	40	1	;	CAW	CBD
31	37	1	;	CAX	HBA
31	38	1	;	CAX	CBB
31	41	1	;	CAX	CBE
32	35	1	;	CAY	HAZ
32	36	1	;	CAY	CBA
32	39	1	;	CAY	OBC
32	42	1	;	CAY	OBF
32	44	1	;	CAY	CBG
33	34	1	;	HAY	OAZ
33	38	1	;	HAY	CBB
33	41	1	;	HAY	CBE
34	36	1	;	OAZ	CBA
34	40	1	;	OAZ	CBD
36	41	1	;	CBA	CBE
36	47	1	;	CBA	CBJ
37	39	1	;	HBA	OBC
37	40	1	;	HBA	CBD
38	42	1	;	CBB	OBF
38	44	1	;	CBB	CBG
38	48	1	;	CBB	CBK
39	41	1	;	OBC	CBE
39	45	1	;	OBC	CBH
39	49	1	;	OBC	OBL
39	50	1	;	OBC	CBM
40	43	1	;	CBD	HBF

40	45	1	;	CBD	CBH
40	47	1	;	CBD	CBJ
41	46	1	;	CBE	OBI
41	48	1	;	CBE	CBK
41	52	1	;	CBE	CBN
42	45	1	;	OBF	CBH
42	47	1	;	OBF	CBJ
43	44	1	;	HBF	CBG
44	49	1	;	CBG	OBL
44	50	1	;	CBG	CBM
44	53	1	;	CBG	OBO
45	48	1	;	CBH	CBK
45	51	1	;	CBH	HBM
45	54	1	;	CBH	CBP
46	47	1	;	OBI	CBJ
46	50	1	;	OBI	CBM
46	53	1	;	OBI	OBO
47	51	1	;	CBJ	HBM
47	52	1	;	CBJ	CBN
48	53	1	;	CBK	OBO
49	51	1	;	OBL	HBM
49	52	1	;	OBL	CBN
50	54	1	;	CBM	CBP
51	53	1	;	HBM	OBO
52	55	1	;	CBN	CBQ
52	60	1	;	CBN	CBT
53	56	1	;	OBO	CBR
53	58	1	;	OBO	OBS
53	61	1	;	OBO	N
53	81	1	;	OBO	CCG
54	57	1	;	CBP	HBR
54	59	1	;	CBP	HBS
54	62	1	;	CBP	H
54	63	1	;	CBP	CA
54	82	1	;	CBP	HCG
54	83	1	;	CBP	CCH
55	61	1	;	CBQ	N
55	81	1	;	CBQ	CCG
55	84	1	;	CBQ	CCI
56	59	1	;	CBR	HBS
56	60	1	;	CBR	CBT
56	82	1	;	CBR	HCG
56	85	1	;	CBR	NCJ
56	86	1	;	CBR	CCK
57	58	1	;	HBR	OBS
57	81	1	;	HBR	CCG
57	84	1	;	HBR	CCI
58	60	1	;	OBS	CBT
58	83	1	;	OBS	CCH
60	64	1	;	CBT	C
60	69	1	;	CBT	CBZ
60	84	1	;	CBT	CCI
61	65	1	;	N	O
61	66	1	;	N	NBY
61	70	1	;	N	CCA
61	79	1	;	N	CCF
61	82	1	;	N	HCG

61	83	1	;	N	CCH
62	64	1	;	H	C
62	69	1	;	H	CBZ
62	81	1	;	H	CCG
63	67	1	;	CA	HKL
63	68	1	;	CA	HBV
63	71	1	;	CA	HCA
63	72	1	;	CA	CCB
63	77	1	;	CA	CCE
63	80	1	;	CA	HCF
63	81	1	;	CA	CCG
64	70	1	;	C	CCA
64	79	1	;	C	CCF
65	67	1	;	O	HKL
65	68	1	;	O	HBV
65	69	1	;	O	CBZ
66	69	1	;	NBY	CBZ
69	73	1	;	CBZ	HCN
69	74	1	;	CBZ	CCC
69	78	1	;	CBZ	HCE
70	75	1	;	CCA	OCN
70	77	1	;	CCA	CCE
70	80	1	;	CCA	HCF
71	73	1	;	HCA	HCN
71	74	1	;	HCA	CCC
71	79	1	;	HCA	CCF
72	76	1	;	CCB	HCD
72	78	1	;	CCB	HCE
72	79	1	;	CCB	CCF
73	75	1	;	HCN	OCN
73	77	1	;	HCN	CCE
74	80	1	;	CCC	HCF
75	78	1	;	OCN	HCE
75	79	1	;	OCN	CCF
76	77	1	;	HCD	CCE
78	80	1	;	HCE	HCF
81	85	1	;	CCG	NCJ
81	86	1	;	CCG	CCK
82	84	1	;	HCG	CCI
83	87	1	;	CCH	OCL
83	104	1	;	CCH	CCY
83	109	1	;	CCH	CDB
84	88	1	;	CCI	CCM
84	105	1	;	CCI	HCY
84	106	1	;	CCI	CCZ
84	110	1	;	CCI	CDC
85	87	1	;	NCJ	OCL
85	104	1	;	NCJ	CCY
85	107	1	;	NCJ	CDA
85	111	1	;	NCJ	ODD
85	112	1	;	NCJ	CDE
86	89	1	;	CCK	OCN
86	90	1	;	CCK	CCO
86	107	1	;	CCK	CDA
86	109	1	;	CCK	CDB
87	91	1	;	OCL	OCP
87	93	1	;	OCL	CCQ

87	105	1	;	OCL	HCY
87	106	1	;	OCL	CCZ
88	92	1	;	CCM	HCP
88	94	1	;	CCM	OCR
88	96	1	;	CCM	CCS
88	104	1	;	CCM	CCY
89	91	1	;	OCN	OCP
89	93	1	;	OCN	CCQ
90	95	1	;	CCO	HCR
90	97	1	;	CCO	OCT
90	99	1	;	CCO	CCU
91	94	1	;	OCP	OCR
91	96	1	;	OCP	CCS
92	93	1	;	HCP	CCQ
93	98	1	;	CCQ	HCT
93	100	1	;	CCQ	CCV
93	102	1	;	CCQ	OCX
94	97	1	;	OCR	OCT
94	99	1	;	OCR	CCU
95	96	1	;	HCR	CCS
96	101	1	;	CCS	OCW
96	103	1	;	CCS	HCX
97	100	1	;	OCT	CCV
97	102	1	;	OCT	OCX
98	99	1	;	HCT	CCU
100	103	1	;	CCV	HCX
101	102	1	;	OCW	OCX
104	108	1	;	CCY	HDA
104	110	1	;	CCY	CDC
104	114	1	;	CCY	CDF
105	107	1	;	HCY	CDA
105	109	1	;	HCY	CDB
106	111	1	;	CCZ	ODD
106	112	1	;	CCZ	CDE
106	115	1	;	CCZ	ODG
107	110	1	;	CDA	CDC
107	113	1	;	CDA	HDE
107	116	1	;	CDA	CDH
108	109	1	;	HDA	CDB
108	112	1	;	HDA	CDE
108	115	1	;	HDA	ODG
109	113	1	;	CDB	HDE
109	114	1	;	CDB	CDF
110	115	1	;	CDC	ODG
111	113	1	;	ODD	HDE
111	114	1	;	ODD	CDF
112	116	1	;	CDE	CDH
113	115	1	;	HDE	ODG
114	117	1	;	CDF	CDI
114	152	1	;	CDF	CEL
115	118	1	;	ODG	HDI
115	119	1	;	ODG	CDJ
115	150	1	;	ODG	CEK
115	153	1	;	ODG	OEM
116	120	1	;	CDH	CDK
116	149	1	;	CDH	CEJ
116	151	1	;	CDH	HEK

116	154	1	;	CDH	HEM
117	121	1	;	CDI	ODL
117	122	1	;	CDI	CDM
117	148	1	;	CDI	CEI
117	150	1	;	CDI	CEK
117	153	1	;	CDI	OEM
118	120	1	;	HDI	CDK
118	149	1	;	HDI	CEJ
118	152	1	;	HDI	CEL
119	123	1	;	CDJ	ODN
119	124	1	;	CDJ	CDO
119	146	1	;	CDJ	CEH
119	151	1	;	CDJ	HEK
119	152	1	;	CDJ	CEL
120	125	1	;	CDK	CDP
120	148	1	;	CDK	CEI
120	150	1	;	CDK	CEK
121	123	1	;	ODL	ODN
121	124	1	;	ODL	CDO
121	149	1	;	ODL	CEJ
122	126	1	;	CDM	ODQ
122	128	1	;	CDM	CDR
122	146	1	;	CDM	CEH
122	149	1	;	CDM	CEJ
123	125	1	;	ODN	CDP
123	148	1	;	ODN	CEI
124	127	1	;	CDO	HDQ
124	129	1	;	CDO	CDS
124	145	1	;	CDO	CEG
124	147	1	;	CDO	HEH
124	150	1	;	CDO	CEK
125	130	1	;	CDP	CDT
125	143	1	;	CDP	CEE
125	144	1	;	CDP	OEF
125	146	1	;	CDP	CEH
125	149	1	;	CDP	CEJ
126	129	1	;	ODQ	CDS
126	145	1	;	ODQ	CEG
126	148	1	;	ODQ	CEI
127	128	1	;	HDQ	CDR
128	131	1	;	CDR	ODU
128	133	1	;	CDR	CDV
128	141	1	;	CDR	CED
128	147	1	;	CDR	HEH
128	148	1	;	CDR	CEI
129	132	1	;	CDS	HDU
129	134	1	;	CDS	CDW
129	137	1	;	CDS	CDZ
129	142	1	;	CDS	HED
129	146	1	;	CDS	CEH
130	135	1	;	CDT	ODX
130	136	1	;	CDT	ODY
130	138	1	;	CDT	CEA
130	141	1	;	CDT	CED
130	144	1	;	CDT	OEF
130	145	1	;	CDT	CEG
131	134	1	;	ODU	CDW

17	16	20	2	120.0	560.0	120.0	560.0 ;	CAM	CAL	CAO
16	17	18	2	115.0	610.0	115.0	610.0 ;	CAL	CAM	OAN
16	17	28	2	120.0	560.0	120.0	560.0 ;	CAL	CAM	CAU
18	17	28	2	115.0	610.0	115.0	610.0 ;	OAN	CAM	CAU
17	18	19	2	109.5	450.0	109.5	450.0 ;	CAM	OAN	HAN
16	20	21	2	120.0	505.0	120.0	505.0 ;	CAL	CAO	HAO
16	20	22	2	120.0	505.0	120.0	505.0 ;	CAL	CAO	CAP
21	20	22	2	120.0	505.0	120.0	505.0 ;	HAO	CAO	CAP
20	22	23	2	120.0	560.0	120.0	560.0 ;	CAO	CAP	CAQ
20	22	26	2	120.0	560.0	120.0	560.0 ;	CAO	CAP	CAT
23	22	26	2	120.0	560.0	120.0	560.0 ;	CAQ	CAP	CAT
22	23	24	2	126.0	770.0	126.0	770.0 ;	CAP	CAQ	OAR
22	23	25	2	126.0	770.0	126.0	770.0 ;	CAP	CAQ	OAS
24	23	25	2	126.0	770.0	126.0	770.0 ;	OAR	CAQ	OAS
22	26	27	2	120.0	505.0	120.0	505.0 ;	CAP	CAT	HAT
22	26	28	2	120.0	505.0	120.0	505.0 ;	CAP	CAT	CAU
27	26	28	2	120.0	505.0	120.0	505.0 ;	HAT	CAT	CAU
17	28	26	2	120.0	560.0	120.0	560.0 ;	CAM	CAU	CAT
17	28	29	2	121.0	685.0	121.0	685.0 ;	CAM	CAU	OAV
26	28	29	2	120.0	560.0	120.0	560.0 ;	CAT	CAU	OAV
28	29	30	2	108.5	418.7	108.5	418.7 ;	CAU	OAV	CAW
29	30	31	2	121.0	685.0	121.0	685.0 ;	OAV	CAW	CAX
29	30	36	2	120.0	560.0	120.0	560.0 ;	OAV	CAW	CBA
31	30	36	2	120.0	560.0	120.0	560.0 ;	CAX	CAW	CBA
30	31	32	2	120.0	560.0	120.0	560.0 ;	CAW	CAX	CAY
30	31	34	2	115.0	610.0	115.0	610.0 ;	CAW	CAX	OAZ
32	31	34	2	120.0	560.0	120.0	560.0 ;	CAY	CAX	OAZ
31	32	33	2	120.0	505.0	120.0	505.0 ;	CAX	CAY	HAY
31	32	40	2	120.0	505.0	120.0	505.0 ;	CAX	CAY	CBD
33	32	40	2	120.0	505.0	120.0	505.0 ;	HAY	CAY	CBD
31	34	35	2	109.5	450.0	109.5	450.0 ;	CAX	OAZ	HAZ
30	36	37	2	120.0	505.0	120.0	505.0 ;	CAW	CBA	HBA
30	36	38	2	120.0	505.0	120.0	505.0 ;	CAW	CBA	CBB
37	36	38	2	120.0	505.0	120.0	505.0 ;	HBA	CBA	CBB
36	38	39	2	120.0	560.0	120.0	560.0 ;	CBA	CBB	OBC
36	38	40	2	120.0	560.0	120.0	560.0 ;	CBA	CBB	CBD
39	38	40	2	115.0	610.0	115.0	610.0 ;	OBC	CBB	CBD
38	39	47	2	109.5	380.0	109.5	380.0 ;	CBB	OBC	CBJ
32	40	38	2	120.0	560.0	120.0	560.0 ;	CAY	CBD	CBB
32	40	41	2	120.0	560.0	120.0	560.0 ;	CAY	CBD	CBE
38	40	41	2	120.0	560.0	120.0	560.0 ;	CBB	CBD	CBE
40	41	42	2	115.0	610.0	115.0	610.0 ;	CBD	CBE	OBF
40	41	44	2	120.0	560.0	120.0	560.0 ;	CBD	CBE	CBG
42	41	44	2	115.0	610.0	115.0	610.0 ;	OBF	CBE	CBG
41	42	43	2	109.5	450.0	109.5	450.0 ;	CBE	OBF	HBF
41	44	45	2	120.0	560.0	120.0	560.0 ;	CBE	CBG	CBH
41	44	47	2	120.0	560.0	120.0	560.0 ;	CBE	CBG	CBJ
45	44	47	2	120.0	560.0	120.0	560.0 ;	CBH	CBG	CBJ
44	45	46	2	121.0	685.0	121.0	685.0 ;	CBG	CBH	OBI
44	45	52	2	120.0	560.0	120.0	560.0 ;	CBG	CBH	CBN
46	45	52	2	121.0	685.0	121.0	685.0 ;	OBI	CBH	CBN
39	47	44	2	115.0	610.0	115.0	610.0 ;	OBC	CBJ	CBG
39	47	48	2	115.0	610.0	115.0	610.0 ;	OBC	CBJ	CBK
44	47	48	2	120.0	560.0	120.0	560.0 ;	CBG	CBJ	CBK
47	48	49	2	121.0	685.0	121.0	685.0 ;	CBJ	CBK	OBL
47	48	50	2	120.0	560.0	120.0	560.0 ;	CBJ	CBK	CBM
49	48	50	2	120.0	560.0	120.0	560.0 ;	OBL	CBK	CBM

48	50	51	2	120.0	505.0	120.0	505.0 ;	CBK	CBM	HBM
48	50	52	2	120.0	505.0	120.0	505.0 ;	CBK	CBM	CBN
51	50	52	2	120.0	505.0	120.0	505.0 ;	HBM	CBM	CBN
45	52	50	2	120.0	560.0	120.0	560.0 ;	CBH	CBN	CBM
45	52	53	2	115.0	610.0	115.0	610.0 ;	CBH	CBN	OBO
50	52	53	2	120.0	560.0	120.0	560.0 ;	CBM	CBN	OBO
52	53	54	2	109.5	380.0	109.5	380.0 ;	CBN	OBO	CBP
53	54	55	2	115.0	610.0	115.0	610.0 ;	OBO	CBP	CBQ
53	54	60	2	115.0	610.0	115.0	610.0 ;	OBO	CBP	CBT
55	54	60	2	120.0	560.0	120.0	560.0 ;	CBQ	CBP	CBT
54	55	56	2	120.0	560.0	120.0	560.0 ;	CBP	CBQ	CBR
54	55	58	2	115.0	610.0	115.0	610.0 ;	CBP	CBQ	OBS
56	55	58	2	120.0	560.0	120.0	560.0 ;	CBR	CBQ	OBS
55	56	57	2	120.0	505.0	120.0	505.0 ;	CBQ	CBR	HBR
55	56	83	2	120.0	505.0	120.0	505.0 ;	CBQ	CBR	CCH
57	56	83	2	120.0	505.0	120.0	505.0 ;	HBR	CBR	CCH
55	58	59	2	109.5	450.0	109.5	450.0 ;	CBQ	OBS	HBS
54	60	61	2	115.0	610.0	115.0	610.0 ;	CBP	CBT	N
54	60	81	2	120.0	560.0	120.0	560.0 ;	CBP	CBT	CCG
61	60	81	2	120.0	560.0	120.0	560.0 ;	N	CBT	CCG
60	61	62	2	123.0	415.0	123.0	415.0 ;	CBT	N	H
60	61	63	2	122.0	700.0	122.0	700.0 ;	CBT	N	CA
62	61	63	2	120.0	505.0	120.0	505.0 ;	H	N	CA
61	63	64	2	109.5	520.0	109.5	520.0 ;	N	CA	C
61	63	69	2	109.5	520.0	109.5	520.0 ;	N	CA	CBZ
64	63	69	2	109.5	520.0	109.5	520.0 ;	C	CA	CBZ
63	64	65	2	121.0	685.0	121.0	685.0 ;	CA	C	O
63	64	66	2	115.0	610.0	115.0	610.0 ;	CA	C	NBY
65	64	66	2	124.0	730.0	124.0	730.0 ;	O	C	NBY
64	66	67	2	120.0	390.0	120.0	390.0 ;	C	NBY	HKL
64	66	68	2	120.0	390.0	120.0	390.0 ;	C	NBY	HBV
67	66	68	2	120.0	445.0	120.0	445.0 ;	HKL	NBY	HBV
63	69	70	2	120.0	560.0	120.0	560.0 ;	CA	CBZ	CCA
63	69	79	2	120.0	560.0	120.0	560.0 ;	CA	CBZ	CCF
70	69	79	2	120.0	560.0	120.0	560.0 ;	CCA	CBZ	CCF
69	70	71	2	120.0	505.0	120.0	505.0 ;	CBZ	CCA	HCA
69	70	72	2	120.0	505.0	120.0	505.0 ;	CBZ	CCA	CCB
71	70	72	2	120.0	505.0	120.0	505.0 ;	HCA	CCA	CCB
70	72	73	2	120.0	505.0	120.0	505.0 ;	CCA	CCB	HCB
70	72	74	2	120.0	505.0	120.0	505.0 ;	CCA	CCB	CCC
73	72	74	2	120.0	505.0	120.0	505.0 ;	HCB	CCB	CCC
72	74	75	2	120.0	560.0	120.0	560.0 ;	CCB	CCC	OCD
72	74	77	2	120.0	560.0	120.0	560.0 ;	CCB	CCC	CCE
75	74	77	2	120.0	560.0	120.0	560.0 ;	OCD	CCC	CCE
74	75	76	2	109.5	450.0	109.5	450.0 ;	CCC	OCD	HCD
74	77	78	2	120.0	505.0	120.0	505.0 ;	CCC	CCE	HCE
74	77	79	2	120.0	505.0	120.0	505.0 ;	CCC	CCE	CCF
78	77	79	2	120.0	505.0	120.0	505.0 ;	HCE	CCE	CCF
69	79	77	2	120.0	505.0	120.0	505.0 ;	CBZ	CCF	CCE
69	79	80	2	120.0	505.0	120.0	505.0 ;	CBZ	CCF	HCF
77	79	80	2	120.0	505.0	120.0	505.0 ;	CCE	CCF	HCF
60	81	82	2	120.0	505.0	120.0	505.0 ;	CBT	CCG	HCG
60	81	83	2	120.0	505.0	120.0	505.0 ;	CBT	CCG	CCH
82	81	83	2	120.0	505.0	120.0	505.0 ;	HCG	CCG	CCH
56	83	81	2	120.0	560.0	120.0	560.0 ;	CBR	CCH	CCG
56	83	84	2	120.0	560.0	120.0	560.0 ;	CBR	CCH	CCI
81	83	84	2	120.0	560.0	120.0	560.0 ;	CCG	CCH	CCI

83	84	85	2	120.0	560.0	120.0	560.0 ;	CCH	CCI	NCJ
83	84	86	2	120.0	560.0	120.0	560.0 ;	CCH	CCI	CCK
85	84	86	2	120.0	560.0	120.0	560.0 ;	NCJ	CCI	CCK
84	85	109	2	120.0	560.0	120.0	560.0 ;	CCI	NCJ	CDB
84	86	87	2	115.0	610.0	115.0	610.0 ;	CCI	CCK	OCL
84	86	104	2	120.0	560.0	120.0	560.0 ;	CCI	CCK	CCY
87	86	104	2	120.0	560.0	120.0	560.0 ;	OCL	CCK	CCY
86	87	88	2	109.5	380.0	109.5	380.0 ;	CCK	OCL	CCM
87	88	89	2	124.0	730.0	124.0	730.0 ;	OCL	CCM	OCN
87	88	90	2	115.0	610.0	115.0	610.0 ;	OCL	CCM	CCO
89	88	90	2	121.0	685.0	121.0	685.0 ;	OCN	CCM	CCO
88	90	91	2	109.5	520.0	109.5	520.0 ;	CCM	CCO	OCP
88	90	93	2	109.5	520.0	109.5	520.0 ;	CCM	CCO	CCQ
91	90	93	2	109.5	520.0	109.5	520.0 ;	OCP	CCO	CCQ
90	91	92	2	109.5	450.0	109.5	450.0 ;	CCO	OCP	HCP
90	93	94	2	109.5	520.0	109.5	520.0 ;	CCO	CCQ	OCR
90	93	96	2	109.5	520.0	109.5	520.0 ;	CCO	CCQ	CCS
94	93	96	2	109.5	520.0	109.5	520.0 ;	OCR	CCQ	CCS
93	94	95	2	109.5	450.0	109.5	450.0 ;	CCQ	OCR	HCR
93	96	97	2	109.5	520.0	109.5	520.0 ;	CCQ	CCS	OCT
93	96	99	2	109.5	520.0	109.5	520.0 ;	CCQ	CCS	CCU
97	96	99	2	109.5	520.0	109.5	520.0 ;	OCT	CCS	CCU
96	97	98	2	109.5	450.0	109.5	450.0 ;	CCS	OCT	HCT
96	99	100	2	109.5	520.0	109.5	520.0 ;	CCS	CCU	CCV
96	99	102	2	109.5	520.0	109.5	520.0 ;	CCS	CCU	OCX
100	99	102	2	109.5	520.0	109.5	520.0 ;	CCV	CCU	OCX
99	100	101	2	121.0	685.0	121.0	685.0 ;	CCU	CCV	OCW
99	102	103	2	109.5	450.0	109.5	450.0 ;	CCU	OCX	HCX
86	104	105	2	120.0	505.0	120.0	505.0 ;	CCK	CCY	HCY
86	104	106	2	120.0	505.0	120.0	505.0 ;	CCK	CCY	CCZ
105	104	106	2	120.0	505.0	120.0	505.0 ;	HCY	CCY	CCZ
104	106	107	2	120.0	560.0	120.0	560.0 ;	CCY	CCZ	CDA
104	106	109	2	120.0	560.0	120.0	560.0 ;	CCY	CCZ	CDB
107	106	109	2	120.0	560.0	120.0	560.0 ;	CDA	CCZ	CDB
106	107	108	2	120.0	505.0	120.0	505.0 ;	CCZ	CDA	HDA
106	107	114	2	120.0	505.0	120.0	505.0 ;	CCZ	CDA	CDF
108	107	114	2	120.0	505.0	120.0	505.0 ;	HDA	CDA	CDF
85	109	106	2	120.0	560.0	120.0	560.0 ;	NCJ	CDB	CCZ
85	109	110	2	120.0	560.0	120.0	560.0 ;	NCJ	CDB	CDC
106	109	110	2	120.0	560.0	120.0	560.0 ;	CCZ	CDB	CDC
109	110	111	2	115.0	610.0	115.0	610.0 ;	CDB	CDC	ODD
109	110	112	2	120.0	560.0	120.0	560.0 ;	CDB	CDC	CDE
111	110	112	2	120.0	560.0	120.0	560.0 ;	ODD	CDC	CDE
110	112	113	2	120.0	505.0	120.0	505.0 ;	CDC	CDE	HDE
110	112	114	2	120.0	505.0	120.0	505.0 ;	CDC	CDE	CDF
113	112	114	2	120.0	505.0	120.0	505.0 ;	HDE	CDE	CDF
107	114	112	2	120.0	560.0	120.0	560.0 ;	CDA	CDF	CDE
107	114	115	2	120.0	560.0	120.0	560.0 ;	CDA	CDF	ODG
112	114	115	2	120.0	560.0	120.0	560.0 ;	CDE	CDF	ODG
114	115	116	2	109.5	380.0	109.5	380.0 ;	CDF	ODG	CDH
115	116	117	2	120.0	560.0	120.0	560.0 ;	ODG	CDH	CDI
115	116	152	2	115.0	610.0	115.0	610.0 ;	ODG	CDH	CEL
117	116	152	2	120.0	560.0	120.0	560.0 ;	CDI	CDH	CEL
116	117	118	2	120.0	505.0	120.0	505.0 ;	CDH	CDI	HDI
116	117	119	2	120.0	505.0	120.0	505.0 ;	CDH	CDI	CDJ
118	117	119	2	120.0	505.0	120.0	505.0 ;	HDI	CDI	CDJ
117	119	120	2	120.0	560.0	120.0	560.0 ;	CDI	CDJ	CDK

117	119	149	2	120.0	560.0	120.0	560.0 ;	CDI	CDJ	CEJ
120	119	149	2	120.0	560.0	120.0	560.0 ;	CDK	CDJ	CEJ
119	120	121	2	121.0	685.0	121.0	685.0 ;	CDJ	CDK	ODL
119	120	122	2	120.0	560.0	120.0	560.0 ;	CDJ	CDK	CDM
121	120	122	2	121.0	685.0	121.0	685.0 ;	ODL	CDK	CDM
120	122	123	2	121.0	685.0	121.0	685.0 ;	CDK	CDM	ODN
120	122	124	2	120.0	560.0	120.0	560.0 ;	CDK	CDM	CDO
123	122	124	2	121.0	685.0	121.0	685.0 ;	ODN	CDM	CDO
122	124	125	2	120.0	560.0	120.0	560.0 ;	CDM	CDO	CDP
122	124	148	2	120.0	560.0	120.0	560.0 ;	CDM	CDO	CEI
125	124	148	2	120.0	560.0	120.0	560.0 ;	CDP	CDO	CEI
124	125	126	2	115.0	610.0	115.0	610.0 ;	CDO	CDP	ODQ
124	125	128	2	120.0	560.0	120.0	560.0 ;	CDO	CDP	CDR
126	125	128	2	115.0	610.0	115.0	610.0 ;	ODQ	CDP	CDR
125	126	127	2	109.5	450.0	109.5	450.0 ;	CDP	ODQ	HDQ
125	128	129	2	132.0	760.0	132.0	760.0 ;	CDP	CDR	CDS
125	128	145	2	120.0	560.0	120.0	560.0 ;	CDP	CDR	CEG
129	128	145	2	108.0	465.0	108.0	465.0 ;	CDS	CDR	CEG
128	129	130	2	132.0	760.0	132.0	760.0 ;	CDR	CDS	CDT
128	129	143	2	108.0	465.0	108.0	465.0 ;	CDR	CDS	CEE
130	129	143	2	120.0	560.0	120.0	560.0 ;	CDT	CDS	CEE
129	130	131	2	115.0	610.0	115.0	610.0 ;	CDS	CDT	ODU
129	130	133	2	120.0	560.0	120.0	560.0 ;	CDS	CDT	CDV
131	130	133	2	115.0	610.0	115.0	610.0 ;	ODU	CDT	CDV
130	131	132	2	109.5	450.0	109.5	450.0 ;	CDT	ODU	HDU
130	133	134	2	120.0	560.0	120.0	560.0 ;	CDT	CDV	CDW
130	133	137	2	120.0	560.0	120.0	560.0 ;	CDT	CDV	CDZ
134	133	137	2	120.0	560.0	120.0	560.0 ;	CDW	CDV	CDZ
133	134	135	2	126.0	770.0	126.0	770.0 ;	CDV	CDW	ODX
133	134	136	2	126.0	770.0	126.0	770.0 ;	CDV	CDW	ODY
135	134	136	2	126.0	770.0	126.0	770.0 ;	ODX	CDW	ODY
133	137	138	2	120.0	560.0	120.0	560.0 ;	CDV	CDZ	CEA
133	137	141	2	120.0	560.0	120.0	560.0 ;	CDV	CDZ	CED
138	137	141	2	120.0	560.0	120.0	560.0 ;	CEA	CDZ	CED
137	138	139	2	126.0	770.0	126.0	770.0 ;	CDZ	CEA	OEB
137	138	140	2	126.0	770.0	126.0	770.0 ;	CDZ	CEA	OEC
139	138	140	2	126.0	770.0	126.0	770.0 ;	OEB	CEA	OEC
137	141	142	2	120.0	505.0	120.0	505.0 ;	CDZ	CED	HED
137	141	143	2	120.0	505.0	120.0	505.0 ;	CDZ	CED	CEE
142	141	143	2	120.0	505.0	120.0	505.0 ;	HED	CED	CEE
129	143	141	2	120.0	560.0	120.0	560.0 ;	CDS	CEE	CED
129	143	144	2	108.0	465.0	108.0	465.0 ;	CDS	CEE	OEF
141	143	144	2	132.0	760.0	132.0	760.0 ;	CED	CEE	OEF
143	144	145	2	108.5	418.7	108.5	418.7 ;	CEE	OEF	CEG
128	145	144	2	108.0	465.0	108.0	465.0 ;	CDR	CEG	OEF
128	145	146	2	120.0	560.0	120.0	560.0 ;	CDR	CEG	CEH
144	145	146	2	132.0	760.0	132.0	760.0 ;	OEF	CEG	CEH
145	146	147	2	120.0	505.0	120.0	505.0 ;	CEG	CEH	HEH
145	146	148	2	120.0	505.0	120.0	505.0 ;	CEG	CEH	CEI
147	146	148	2	120.0	505.0	120.0	505.0 ;	HEH	CEH	CEI
124	148	146	2	120.0	560.0	120.0	560.0 ;	CDO	CEI	CEH
124	148	149	2	120.0	560.0	120.0	560.0 ;	CDO	CEI	CEJ
146	148	149	2	120.0	560.0	120.0	560.0 ;	CEH	CEI	CEJ
119	149	148	2	120.0	560.0	120.0	560.0 ;	CDJ	CEJ	CEI
119	149	150	2	120.0	560.0	120.0	560.0 ;	CDJ	CEJ	CEK
148	149	150	2	120.0	560.0	120.0	560.0 ;	CEI	CEJ	CEK
149	150	151	2	120.0	505.0	120.0	505.0 ;	CEJ	CEK	HEK

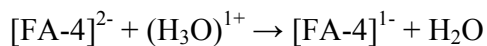
152	116	115	114	1	180.0	16.7	2	180.0	16.7	2 ; dih	CEL	CDH
ODG	ODG	CDF										
124	125	126	127	1	180.0	7.1	2	180.0	7.1	2 ; dih	CDO	CDP
ODQ	ODQ	HDQ										
129	130	131	132	1	180.0	7.1	2	180.0	7.1	2 ; dih	CDS	CDT
ODU	ODU	HDU										
136	134	133	130	1	180.0	5.9	2	180.0	5.9	2 ; dih	ODY	CDW
CDV	CDV	CDT										
140	138	137	133	1	180.0	5.9	2	180.0	5.9	2 ; dih	OEC	CEA
CDZ	CDZ	CDV										
116	152	153	154	1	180.0	7.1	2	180.0	7.1	2 ; dih	CDH	CEL
OEM	OEM	HEM										

[system]
; Name
xmo in water

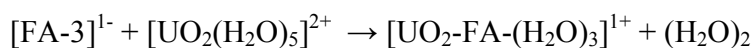
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SOL 7751
NA+ 4

(ii) Binding energy Evaluation:

Uranyl binding at FA-4 originates by doubly deprotonating the hydroxo groups, whereas in the other three binding sites of FA, they are singly deprotonated. Hence, due to the differing charges, binding energy comparison cannot be made directly within the four models. However, energetics comparison has been performed by adding and subtracting hydronium ions and water to balance the equation. By doing this the energetics of all four structures can be cross compared.



Binding energies are computed using the following equation,



Prior to uranyl binding, FA-3 is the lowest energy species, and hence all binding energies are evaluated with respect to FA-3 only.

Similarly binding energy were also carried out for HA models.