

Supplemental Information: Speciation analysis the complexation of uranyl nitrate with tri-n-butyl phosphate in supercritical CO₂

Zhu Liyang,^a Lan Youshi^{*a}, Liu Qian^a, Hao Xuan^a, Zhou Jin^a, and Yang Suliang^{*a}

^aDepartment of Radiochemistry, China Institute of Atomic Energy, Beijing, 102413, China.

1. Force field parameters

The RESP charge of TBP

	coordination			charge
C	-5.304029	-3.454731	-0.660390	-0.252491
C	-4.591919	-2.281919	0.013704	0.146218
C	-3.120940	-2.174084	-0.395331	-0.046190
C	-2.424705	-1.011397	0.280255	0.184638
O	-1.050243	-0.982518	-0.181025	-0.483229
P	0.000263	-0.001809	0.518082	1.259105
O	1.374121	-0.420393	-0.182702	-0.483229
C	2.086717	-1.597529	0.274586	0.184638
C	3.445410	-1.610755	-0.393897	-0.046190
C	4.275678	-2.831470	0.010186	0.146218
C	5.651133	-2.852394	-0.656681	-0.252491
O	0.000988	-0.001193	1.997497	-0.669935
O	-0.324220	1.397538	-0.182245	-0.483229
C	0.338983	2.602741	0.276195	0.184638
C	-0.325430	3.786754	-0.394486	-0.046190
C	0.317029	5.115291	0.011909	0.146218
C	-0.348907	6.318014	-0.656688	-0.252491
H	-2.430516	-1.115448	1.367809	0.020582
H	-2.895210	-0.059765	0.017072	0.020582
H	0.257592	2.658584	1.364286	0.020582
H	1.396964	2.535897	0.007055	0.020582
H	2.173914	-1.557408	1.362934	0.020582
H	1.501233	-2.480308	0.002284	0.020582
H	-0.267261	3.656569	-1.480262	0.035582
H	-1.389194	3.787666	-0.133498	0.035582
H	3.305280	-1.593060	-1.479856	0.035582
H	3.976545	-0.690091	-0.129379	0.035582
H	-3.039530	-2.052776	-1.480648	0.035582
H	-2.590635	-3.097985	-0.140602	0.035582
H	-4.662019	-2.387589	1.102717	-0.018004
H	-5.109609	-1.347779	-0.234614	-0.018004
H	0.267256	5.227607	1.101391	-0.018004
H	1.383281	5.098734	-0.243186	-0.018004
H	4.396454	-2.847362	1.099767	-0.018004
H	3.729721	-3.746590	-0.248167	-0.018004
H	-6.352179	-3.513731	-0.356249	0.059447
H	-5.279373	-3.359196	-1.750016	0.059447
H	-4.829757	-4.406402	-0.402695	0.059447
H	0.124493	7.255729	-0.354729	0.059447
H	-0.285494	6.250041	-1.746811	0.059447
H	-1.408620	6.381121	-0.392035	0.059447
H	6.227458	-3.731077	-0.356062	0.059447
H	5.562027	-2.870877	-1.746974	0.059447
H	6.233951	-1.965959	-0.389141	0.059447

Other parameters for TBP generated from Ambertool 18

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MASS

c3	12.010	0.878
os	16.000	0.465
p5	30.970	1.538
o	16.000	0.434
h1	1.008	0.135
hc	1.008	0.135

BOND

c3-c3	300.90	1.538
c3-hc	330.60	1.097
c3-os	308.60	1.432
c3-h1	330.60	1.097
os-p5	330.60	1.615
o -p5	479.50	1.487

ANGLE

c3-c3-c3	62.900	111.510
c3-c3-hc	46.300	109.800
c3-c3-os	68.000	107.970
c3-c3-h1	46.400	109.560
c3-os-p5	77.700	119.540
h1-c3-os	50.800	109.780
os-p5-os	45.000	101.840
o -p5-os	43.900	115.460
h1-c3-h1	39.200	108.460
hc-c3-hc	39.400	107.580

DIHE

c3-c3-c3-c3	1	0.180	0.000	-3.000
c3-c3-c3-c3	1	0.250	180.000	-2.000
c3-c3-c3-c3	1	0.200	180.000	1.000
c3-c3-c3-hc	1	0.160	0.000	3.000
c3-c3-c3-os	9	1.400	0.000	3.000
c3-c3-c3-h1	9	1.400	0.000	3.000
c3-c3-os-p5	3	1.150	0.000	-3.000
c3-c3-os-p5	1	3.950	180.000	1.000
c3-os-p5-os	1	0.250	0.000	-3.000
c3-os-p5-os	1	1.200	0.000	2.000
c3-os-p5-o	1	0.800	0.000	-2.000
c3-os-p5-o	1	0.550	0.000	3.000
hc-c3-c3-os	1	0.000	0.000	-3.000
hc-c3-c3-os	1	0.250	0.000	1.000
h1-c3-os-p5	3	1.150	0.000	3.000
h1-c3-c3-hc	9	1.400	0.000	3.000
hc-c3-c3-hc	1	0.150	0.000	3.000

IMPROPER**NONBON**

c3	1.9080	0.1094
os	1.6837	0.1700
p5	2.1000	0.2000
o	1.6612	0.2100
h1	1.3870	0.0157
hc	1.4870	0.0157

The parameters for CO₂

Table S1. The parameters of CO₂ in different model.

	GAFF	GAFF2	EPM2	EMP2-flex ^a	Literature ^b	Literature ^{c, d}
ϵ_C (kcal·mol ⁻¹)	0.2100	0.1596	0.0559	0.0559	0.0559	0.0927
ϵ_O (kcal·mol ⁻¹)	0.2100	0.1463	0.1600	0.1598	0.1598	0.1521
σ_C (Å)	1.928	1.9525	1.5473	1.5714	1.5714	2.1663
σ_O (Å)	1.6612	1.7107	1.7022	1.6994	1.6994	1.8857
$L_{C=O}$ (Å)	1.172	1.172	1.140	1.162	1.162	1.162
θ (degree)	180	180	180	180	180	180
k_S (kcal·mol ⁻¹ ·Å ⁻²)	758.1	794.18	/	143.40	2017.9	700
k_B (kcal·mol ⁻¹ ·rad ⁻²)	77.94	118.8	/	26.29	108.0	300
q_C (e)	0.6516	0.6516	0.6516	0.6516	0.6512	0.7200
q_O (e)	-0.3258	-0.3258	-0.3258	-0.3258	-0.3256	-0.3600
ρ (g·ml ⁻¹) (20MPa, 323K)	1.195	0.993	0.764	0.787	0.778	0.736

Note: the density ρ was the average value after the equilibration reached.

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- R.T. Cygan, V.N. Romanov, E.M. Myshakin. Molecular simulation of carbon dioxide capture by montmorillonite using an accurate and flexible force field. The Journal of Physical Chemistry C, 2012, 116(24), 13079–13091.
- A.G. Sanchez, C.O. Ania J.B., Parra, et al. Transferable force field for carbon dioxide adsorption in zeolites. The Journal of Physical Chemistry C, 2009, 113(20): 8814–8820.
- G. Maurin, P.L. Llewellyn, R.G. Bell. Adsorption mechanism of carbon dioxide in faujasites: grand canonical Monte Carlo simulations and microcalorimetry measurements. The Journal of Physical Chemistry B, 2005, 109(33): 16084-16091.

The other parameters for UO₂(NO₃)₂ generated by MCPB.py

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REMARK GOES HERE, THIS FILE IS GENERATED BY MCPB.PY
MASS
M1 238.0          U ion
Y1 16.00          0.465      Ether and ester oxygen
Y2 16.00          0.465      Ether and ester oxygen
Y3 16.00          0.434      Oxygen with one connected atom
Y4 16.00          0.434      Oxygen with one connected atom
Y5 16.00          0.434      Oxygen with one connected atom
Y6 16.00          0.434      Oxygen with one connected atom

BOND
M1-Y1  595.9      1.7519      Created by Seminario method using MCPB.py
M1-Y2  595.9      1.7519      Created by Seminario method using MCPB.py
M1-Y3  57.1       2.4200      Created by Seminario method using MCPB.py
M1-Y4  57.1       2.4199      Created by Seminario method using MCPB.py
M1-Y5  57.1       2.4200      Created by Seminario method using MCPB.py
M1-Y6  57.1       2.4199      Created by Seminario method using MCPB.py
no-Y3  741.8      1.2260      SOURCE1_SOURCE5  4403  0.0099
no-Y4  741.8      1.2260      SOURCE1_SOURCE5  4403  0.0099
no-Y5  741.8      1.2260      SOURCE1_SOURCE5  4403  0.0099
no-Y6  741.8      1.2260      SOURCE1_SOURCE5  4403  0.0099

ANGL
M1-Y3-no  111.73    96.75      Created by Seminario method using MCPB.py
M1-Y4-no  111.73    96.75      Created by Seminario method using MCPB.py
M1-Y5-no  111.68    96.75      Created by Seminario method using MCPB.py
M1-Y6-no  111.78    96.75      Created by Seminario method using MCPB.py
Y2-M1-Y1  47.15     179.98     Created by Seminario method using MCPB.py
Y3-M1-Y1  67.08     90.01      Created by Seminario method using MCPB.py
Y3-M1-Y2  67.06     89.99      Created by Seminario method using MCPB.py
Y4-M1-Y1  66.99     90.02      Created by Seminario method using MCPB.py
Y4-M1-Y2  67.00     89.99      Created by Seminario method using MCPB.py
Y4-M1-Y3  113.42    53.07      Created by Seminario method using MCPB.py
Y5-M1-Y1  66.99     90.00      Created by Seminario method using MCPB.py
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Y5-M1-Y2	67.01	89.99	Created by Seminario method using MCPB.py		
Y5-M1-Y3	113.28	127.02	Created by Seminario method using MCPB.py		
Y5-M1-Y4	123.97	179.91	Created by Seminario method using MCPB.py		
Y6-M1-Y1	67.06	90.01	Created by Seminario method using MCPB.py		
Y6-M1-Y2	67.04	90.00	Created by Seminario method using MCPB.py		
Y6-M1-Y3	122.47	179.91	Created by Seminario method using MCPB.py		
Y6-M1-Y4	113.40	126.84	Created by Seminario method using MCPB.py		
Y6-M1-Y5	113.27	53.07	Created by Seminario method using MCPB.py		
Y4-no-Y3	76.7	125.08	SOURCE4_SOURCE5	1464	0.8585
Y6-no-Y5	76.7	125.08	SOURCE4_SOURCE5	1464	0.8585
o -no-Y3	76.7	125.08	SOURCE4_SOURCE5	1464	0.8585
o -no-Y4	76.7	125.08	SOURCE4_SOURCE5	1464	0.8585
o -no-Y5	76.7	125.08	SOURCE4_SOURCE5	1464	0.8585
o -no-Y6	76.7	125.08	SOURCE4_SOURCE5	1464	0.8585
DIHE					
M1-Y3-no-Y4	3	0.00	0.00	3.0	Treat as zero by MCPB.py
M1-Y3-no-o	3	0.00	0.00	3.0	Treat as zero by MCPB.py
M1-Y4-no-Y3	3	0.00	0.00	3.0	Treat as zero by MCPB.py
M1-Y4-no-o	3	0.00	0.00	3.0	Treat as zero by MCPB.py
M1-Y5-no-Y6	3	0.00	0.00	3.0	Treat as zero by MCPB.py
M1-Y5-no-o	3	0.00	0.00	3.0	Treat as zero by MCPB.py
M1-Y6-no-Y5	3	0.00	0.00	3.0	Treat as zero by MCPB.py
M1-Y6-no-o	3	0.00	0.00	3.0	Treat as zero by MCPB.py
Y4-M1-Y3-no	3	0.00	0.00	3.0	Treat as zero by MCPB.py
Y5-M1-Y3-no	3	0.00	0.00	3.0	Treat as zero by MCPB.py
Y5-M1-Y4-no	3	0.00	0.00	3.0	Treat as zero by MCPB.py
Y6-M1-Y3-no	3	0.00	0.00	3.0	Treat as zero by MCPB.py
Y6-M1-Y4-no	3	0.00	0.00	3.0	Treat as zero by MCPB.py
Y6-M1-Y5-no	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y3-M1-Y1	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y3-M1-Y2	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y4-M1-Y1	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y4-M1-Y2	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y4-M1-Y3	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y5-M1-Y1	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y5-M1-Y2	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y5-M1-Y3	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y5-M1-Y4	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y6-M1-Y1	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y6-M1-Y2	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y6-M1-Y3	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y6-M1-Y4	3	0.00	0.00	3.0	Treat as zero by MCPB.py
no-Y6-M1-Y5	3	0.00	0.00	3.0	Treat as zero by MCPB.py
IMPR					
Y3-Y4-no-o	1.1	180.0	2.0	Using the default value	
Y5-Y6-no-o	1.1	180.0	2.0	Using the default value	
NONB					
M1	1.6840	0.1275827400	IOD set for U4+ ion in TIP3P water from Li et al.		
JPCB, 2015, 119, 883					
Y1	1.6837	0.1700	OPLS ether		
Y2	1.6837	0.1700	OPLS ether		
Y3	1.6612	0.2100	OPLS		
Y4	1.6612	0.2100	OPLS		
Y5	1.6612	0.2100	OPLS		
Y6	1.6612	0.2100	OPLS		

Note: M and Y represent uranium and oxygen atoms respectively.

2. Simulation systems

Table S2. The simulation systems

Simulation systems	Number of molecules	Cubic length/ Å
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	Uranyl nitrate	TBP	CO ₂	H ₂ O	
I	100	200	10000	0	98
II	100	600	10000	0	98
III	100	200	40000	0	155
IV	100	600	40000	0	155
V	100	200	10000	600	98
VI	100	600	10000	600	98
VII	100	200	40000	600	155
VIII	100	600	40000	600	155

3. The RDF of uranyl nitrate and water

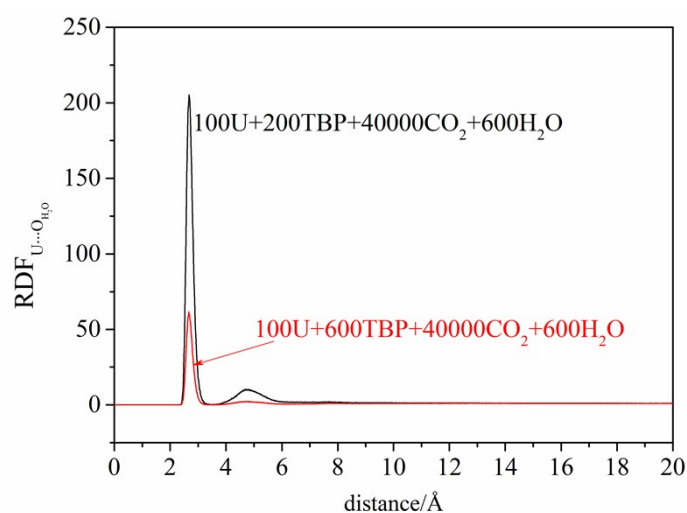


Figure S1. The RDF of O and uranium atom when water present.

4. Simulation at the interface with H₂O

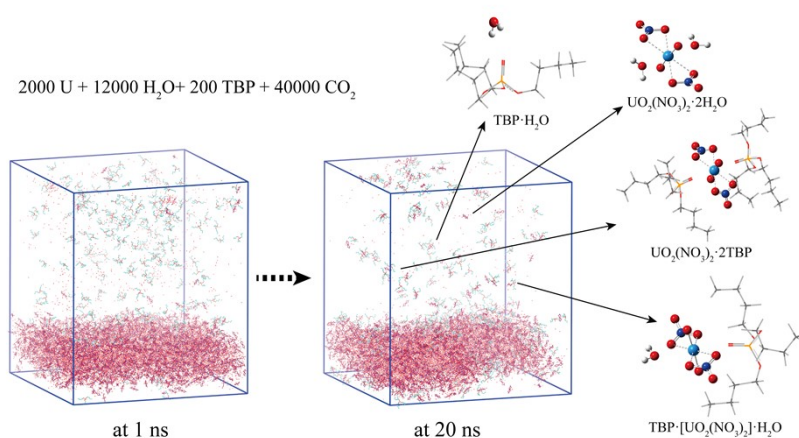


Figure S2 Complexation at the interface of anhydrate uranyl nitrate/ supercritical CO₂

APPENDIX

Optimized structure of 1:1 complex

C	0.594395	0.676166	4.171913
C	0.224749	2.148816	3.981871
C	0.089395	2.578240	2.515233
C	1.408454	2.483445	1.776035
O	1.337875	3.034597	0.414940
P	0.437258	2.393127	-0.719156
O	-0.888303	3.246735	-0.820193
C	-2.160239	2.653816	-1.264766
C	-2.967301	2.164451	-0.082846
C	-4.331061	1.622852	-0.516166
C	-5.087964	0.985212	0.646843
O	0.148777	0.917977	-0.480738
O	1.209050	2.686301	-2.071913
C	2.623509	2.338591	-2.247123
C	2.929860	0.882340	-1.959047
C	4.371577	0.520958	-2.318591
C	4.698221	-0.925375	-1.949608
H	1.764753	1.459079	1.700033
H	2.173654	3.092595	2.253095
H	2.816860	2.588781	-3.288122
H	3.203820	3.005519	-1.608281
H	-2.658868	3.464543	-1.792037
H	-1.958458	1.844710	-1.965995
H	2.771535	0.667424	-0.900150
H	2.237279	0.246822	-2.514918
H	-2.414385	1.374637	0.427838
H	-3.093429	2.985026	0.629006
H	-0.272079	3.607720	2.458560
H	-0.652659	1.943301	2.025814
H	0.963523	2.786215	4.479101
H	-0.728459	2.346621	4.477925
H	4.532844	0.676992	-3.389947
H	5.059976	1.196009	-1.799496
H	-4.927724	2.432888	-0.947846
H	-4.188170	0.880231	-1.304364
H	-0.124107	0.028216	3.667146
H	1.584939	0.445407	3.775716
H	0.599284	0.413812	5.231073
H	4.027859	-1.619819	-2.460424
H	5.723164	-1.182170	-2.222103
H	4.584650	-1.087696	-0.875512
H	-4.521706	0.150452	1.066334
H	-5.261577	1.705772	1.450134
H	-6.057379	0.602249	0.324375
U	-0.197905	-1.298529	-0.011929
O	0.715226	-1.802920	-1.431923
O	-1.118703	-0.827843	1.419456
N	2.088212	-1.955109	1.683108
N	-2.710488	-1.920491	-1.345756
O	1.159096	-2.791956	1.391320
O	1.932258	-0.791581	1.149746
O	3.018435	-2.226019	2.389404
O	-2.046917	-2.778648	-0.655953
O	-2.145680	-0.765761	-1.428800
O	-3.763909	-2.167814	-1.862360

Optimized structure of 1:2 complex

C	3.448718	4.942271	-0.687027
C	3.578331	3.793725	-1.684830
C	4.020947	2.494188	-1.010845
C	4.144771	1.368863	-2.017796
O	4.597214	0.106096	-1.423975
P	3.798352	-0.588892	-0.240965
O	4.167048	-2.132680	-0.338943
C	3.425874	-2.982820	-1.273130
C	2.423245	-3.832156	-0.523002
C	1.523098	-4.624733	-1.470387
C	0.414698	-5.363674	-0.724259
O	2.309730	-0.323138	-0.296555
O	4.514195	-0.088533	1.082577
C	3.878134	-0.277748	2.391599
C	3.048689	0.936497	2.753373
C	2.308189	0.753424	4.078253
C	1.408894	1.946429	4.396280
H	4.907188	1.584276	-2.763735
H	3.192375	1.186616	-2.510310
H	3.266692	-1.178527	2.373101
H	4.710231	-0.424982	3.077701
H	2.924057	-2.358592	-2.014699
H	4.183696	-3.580381	-1.777647
H	3.697876	1.815565	2.800995
H	2.319377	1.116672	1.963663
H	2.953839	-4.505667	0.155544
H	1.811481	-3.176464	0.095805
H	3.281048	2.225262	-0.253527
H	4.975636	2.634905	-0.496873
H	4.294298	4.065951	-2.467210
H	2.619839	3.627259	-2.183588
H	1.705675	-0.157900	4.027991
H	3.027319	0.603569	4.890219
H	1.072355	-3.936034	-2.190085
H	2.121984	-5.337075	-2.047462
H	4.407005	5.158362	-0.208236
H	3.104975	5.855586	-1.175882
H	2.732158	4.694814	0.099037
H	1.990591	2.869119	4.465954
H	0.660037	2.082954	3.613044
H	0.885291	1.808947	5.343663
H	-0.230010	-4.657341	-0.196411
H	-0.211129	-5.937876	-1.409735
H	0.826601	-6.056133	0.013808
C	-1.965675	-3.785566	-3.559885
C	-2.631956	-2.413709	-3.626848
C	-3.442783	-2.107145	-2.367383
C	-4.078497	-0.733367	-2.431783
O	-4.696962	-0.386152	-1.144130
P	-3.827497	0.445698	-0.108643
O	-3.928120	1.943727	-0.624173
C	-3.034998	2.965785	-0.082389
C	-2.798643	4.005035	-1.156341
C	-1.788397	5.069959	-0.712687
C	-0.346135	4.565005	-0.633714
O	-2.412883	-0.071639	0.032516
O	-4.632598	0.400262	1.258577
C	-4.236779	-0.516309	2.332924
C	-3.265296	0.158691	3.276741
C	-2.868014	-0.762221	4.431595
C	-1.759658	-0.160762	5.291705

H	-4.896543	-0.691163	-3.148317
H	-3.343267	0.028508	-2.693538
H	-5.172239	-0.776547	2.825062
H	-3.794714	-1.414028	1.902074
H	-3.525910	3.394564	0.793151
H	-2.104201	2.496211	0.228182
H	-2.372274	0.439468	2.715698
H	-3.716644	1.078109	3.661030
H	-2.438500	3.500212	-2.054814
H	-3.753682	4.473413	-1.406091
H	-2.780308	-2.150525	-1.502206
H	-4.220423	-2.861867	-2.220241
H	-3.276200	-2.354858	-4.510510
H	-1.864070	-1.644052	-3.747129
H	-3.745379	-0.974135	5.051467
H	-2.526045	-1.717832	4.028001
H	-1.835813	5.901617	-1.419800
H	-2.091216	5.481142	0.256628
H	-1.375912	-3.985356	-4.456621
H	-1.299011	-3.842642	-2.698470
H	-2.708348	-4.581620	-3.463774
H	-0.860215	0.009305	4.697320
H	-2.061834	0.799634	5.717480
H	-1.491648	-0.825653	6.114340
H	-0.006476	4.215403	-1.610930
H	0.326783	5.364054	-0.318977
H	-0.229654	3.742489	0.073871
U	-0.056945	-0.231843	-0.159744
O	0.040572	1.197460	0.884156
O	-0.160760	-1.654709	-1.205363
N	-0.026266	-1.999066	2.254539
N	-0.144438	1.537946	-2.572879
O	1.037840	-1.578136	1.676054
O	-1.105258	-1.619839	1.689892
O	-0.002790	-2.685994	3.246489
O	0.944685	1.137133	-2.039770
O	-1.197706	1.101437	-1.993075
O	-0.178734	2.272288	-3.530529

Optimized structure of 2:3 complex Type I

C	6.842905	2.222382	-2.029478
C	6.169781	2.766089	-0.770650
C	4.825180	3.427520	-1.078431
C	4.127424	3.885275	0.186430
O	2.805684	4.459755	-0.073875
P	1.627825	3.558368	-0.648935
O	0.268439	4.132868	-0.069289
C	-0.280410	3.680998	1.213543
C	0.317065	4.437751	2.377780
C	0.101642	5.947735	2.314031
C	0.713639	6.674139	3.509476
O	1.835734	2.088690	-0.343331
O	1.573952	3.929154	-2.186751
C	0.467652	3.498142	-3.050647
C	0.737561	2.152500	-3.685131
C	1.958383	2.117113	-4.600652
C	2.097166	0.775426	-5.314670
H	4.666487	4.693652	0.676367
H	4.009163	3.063867	0.892236
H	-0.446947	3.486676	-2.461384

H	0.403328	4.287648	-3.798161
H	-1.348237	3.861082	1.114054
H	-0.097015	2.615646	1.307390
H	0.838510	1.394387	-2.908641
H	-0.162599	1.895247	-4.256004
H	-0.136988	4.023840	3.284088
H	1.382800	4.207634	2.447212
H	4.196485	2.704682	-1.601298
H	4.960883	4.280744	-1.748355
H	6.832333	3.484102	-0.275805
H	6.009080	1.948831	-0.062557
H	1.883971	2.924854	-5.337629
H	2.853840	2.311320	-4.007826
H	0.534723	6.333026	1.387901
H	-0.972556	6.157326	2.264457
H	6.210509	1.480177	-2.521275
H	7.037063	3.021259	-2.749641
H	7.796460	1.746317	-1.793662
H	2.993403	0.747159	-5.936446
H	2.168873	-0.041697	-4.597242
H	1.232684	0.575189	-5.952527
H	0.549513	7.751822	3.448332
H	0.281289	6.322310	4.449639
H	1.792066	6.503850	3.558712
C	6.800945	-1.222954	2.269118
C	5.960479	-2.496130	2.337856
C	4.855485	-2.406529	3.389415
C	4.104513	-3.704610	3.617406
O	3.572102	-4.293116	2.386217
P	2.366090	-3.646850	1.587271
O	1.979087	-4.728116	0.496244
C	2.219118	-4.538745	-0.939894
C	0.953679	-4.053552	-1.617064
C	1.038888	-4.129881	-3.145608
C	2.084963	-3.206802	-3.767324
O	2.695050	-2.305062	0.965810
O	1.182076	-3.620336	2.643700
C	-0.143029	-3.133793	2.255720
C	-0.876131	-2.705289	3.506500
C	-2.373307	-2.511940	3.253925
C	-3.100799	-1.974696	4.484367
H	3.276992	-3.572033	4.314829
H	4.766672	-4.482299	3.994131
H	-0.032223	-2.303488	1.563853
H	-0.649822	-3.954257	1.745857
H	3.045353	-3.845352	-1.077089
H	2.509300	-5.526407	-1.295581
H	-0.733132	-3.470945	4.274429
H	-0.428950	-1.782131	3.879900
H	0.122332	-4.671002	-1.266309
H	0.746756	-3.026681	-1.310771
H	4.153568	-1.612430	3.131758
H	5.286181	-2.132420	4.359344
H	6.603764	-3.354867	2.558819
H	5.511382	-2.687978	1.361401
H	-2.526704	-1.839659	2.407955
H	-2.812855	-3.468489	2.952756
H	1.231500	-5.167429	-3.441361
H	0.059306	-3.875189	-3.553402
H	7.300026	-1.027157	3.222065
H	7.570862	-1.301211	1.499085

H	6.177410	-0.360626	2.030039
H	-4.174180	-1.888362	4.305018
H	-2.961113	-2.636250	5.342935
H	-2.726879	-0.986570	4.759078
H	1.871454	-2.171663	-3.505691
H	3.097898	-3.438479	-3.435404
H	2.066593	-3.280138	-4.855770
C	-3.513442	4.349449	-0.863243
C	-4.724043	3.489992	-0.506534
C	-5.313677	2.792634	-1.732080
C	-6.531502	1.936850	-1.435670
O	-6.285163	0.930745	-0.399513
P	-5.317964	-0.305021	-0.636078
O	-5.290355	-1.067267	0.748946
C	-6.222694	-0.882344	1.856851
C	-5.769324	0.236787	2.769088
C	-6.627265	0.324250	4.030920
C	-6.159209	1.440094	4.963225
O	-3.923602	0.038190	-1.106664
O	-6.070293	-1.196889	-1.725584
C	-5.311005	-2.182511	-2.506761
C	-4.889796	-3.365763	-1.655342
C	-4.188073	-4.457651	-2.471211
C	-2.824234	-4.041452	-3.023912
H	-6.893163	1.422537	-2.327111
H	-7.342247	2.531116	-1.017947
H	-6.004680	-2.482973	-3.289899
H	-4.459283	-1.673210	-2.953545
H	-7.222421	-0.704375	1.459149
H	-6.213850	-1.843046	2.369599
H	-4.217077	-3.026387	-0.863755
H	-5.778815	-3.776274	-1.169623
H	-4.727441	0.070069	3.041154
H	-5.802154	1.182624	2.225402
H	-4.545423	2.188056	-2.217340
H	-5.635477	3.539427	-2.466637
H	-5.496524	4.107845	-0.035808
H	-4.427809	2.741782	0.230785
H	-4.061146	-5.329166	-1.824072
H	-4.839937	-4.780929	-3.289867
H	-7.675388	0.486653	3.757719
H	-6.592257	-0.632742	4.562391
H	-3.763226	5.095584	-1.622130
H	-3.137320	4.883763	0.010760
H	-2.700588	3.731976	-1.248547
H	-2.326785	-4.884567	-3.505849
H	-2.905657	-3.245166	-3.764714
H	-2.178057	-3.684188	-2.219979
H	-6.768701	1.484217	5.867616
H	-5.120131	1.286935	5.261803
H	-6.219381	2.412921	4.469764
U	2.461310	-0.052083	0.365943
O	4.087938	0.394789	0.884599
O	0.781853	-0.510370	-0.167126
N	1.625522	0.616608	3.131688
N	3.817568	-0.589289	-2.201824
O	1.888384	-0.575926	2.740600
O	1.763304	1.494742	2.212743
O	1.284159	0.880355	4.252983
O	3.638265	-1.490841	-1.312580
O	3.213748	0.512754	-1.942265

O	4.494043	-0.751331	-3.183221
U	-1.614294	-0.155806	-0.684941
O	-1.922055	-1.834311	-0.219650
O	-1.283435	1.519054	-1.138550
N	-1.103537	-0.981832	-3.478769
N	-2.005336	0.821876	2.105726
O	-0.196756	-0.958603	-2.574695
O	-2.257458	-0.607926	-3.065345
O	-0.891749	-1.327994	-4.612173
O	-0.916089	0.284508	1.697471
O	-2.926150	0.860110	1.223840
O	-2.143355	1.254115	3.223076

Optimized structure of 2:3 complex Type II

C	-8.381963	-3.862805	0.246037
C	-7.247514	-3.386779	1.152300
C	-5.888263	-3.285507	0.456548
C	-5.854884	-2.357046	-0.740123
O	-6.346918	-1.012937	-0.413974
P	-5.466393	0.058163	0.352287
O	-6.254617	1.427952	0.205830
C	-5.971797	2.373481	-0.883262
C	-6.336537	1.824253	-2.248203
C	-7.791913	1.374389	-2.404523
C	-8.815277	2.481282	-2.155273
O	-4.039486	0.152077	-0.141885
O	-5.599970	-0.328279	1.886285
C	-4.811416	0.383068	2.895090
C	-3.762822	-0.543478	3.471606
C	-3.016903	0.078017	4.657851
C	-2.281324	1.377533	4.327078
H	-6.525943	-2.681788	-1.531429
H	-4.845951	-2.268413	-1.137861
H	-4.362835	1.268462	2.444934
H	-5.530697	0.702554	3.648833
H	-6.572654	3.240128	-0.619611
H	-4.917482	2.636385	-0.839318
H	-4.255186	-1.466534	3.787210
H	-3.056080	-0.809293	2.685547
H	-6.111808	2.620529	-2.966332
H	-5.662373	0.999195	-2.493723
H	-5.576644	-4.269346	0.088816
H	-5.123740	-2.974269	1.168858
H	-7.142929	-4.074532	1.995758
H	-7.501521	-2.415039	1.581341
H	-3.720278	0.247598	5.480345
H	-2.293463	-0.655725	5.018685
H	-7.916919	0.986040	-3.419029
H	-7.982595	0.536709	-1.730989
H	-8.595125	-3.142663	-0.546758
H	-8.138063	-4.818348	-0.226641
H	-9.304162	-3.999914	0.813708
H	-1.678007	1.705957	5.174786
H	-1.612456	1.236569	3.479283
H	-2.972786	2.188649	4.084464
H	-8.626101	3.348865	-2.793514
H	-9.827306	2.130150	-2.364724
H	-8.799602	2.819939	-1.117392
C	0.487558	3.059667	-4.844914
C	1.832163	3.554955	-4.313951

C	1.744652	3.972982	-2.844750
C	3.109990	4.283433	-2.276543
O	3.072513	4.672582	-0.858835
P	2.411145	3.783604	0.273703
O	3.235902	4.140475	1.591333
C	4.551656	3.533714	1.781624
C	4.486079	2.481831	2.868283
C	5.790421	1.693721	2.985322
C	5.666912	0.521515	3.956128
O	2.415571	2.301219	-0.039353
O	0.975952	4.399710	0.510289
C	-0.036202	3.740363	1.344010
C	0.177380	4.009955	2.818906
C	0.279418	5.490569	3.190513
C	-0.949991	6.313661	2.807934
H	3.570893	5.144025	-2.757747
H	3.767936	3.421354	-2.362397
H	-0.970480	4.162261	0.982420
H	-0.018736	2.673817	1.139637
H	4.891324	3.092733	0.842481
H	5.218532	4.356135	2.037494
H	-0.668487	3.548778	3.338066
H	1.068130	3.476254	3.152518
H	4.238541	2.957813	3.821157
H	3.669512	1.800222	2.633777
H	1.297726	3.155652	-2.281114
H	1.085327	4.836198	-2.729087
H	2.184709	4.395716	-4.920942
H	2.575649	2.759789	-4.416792
H	0.442046	5.558187	4.269761
H	1.168290	5.916543	2.719874
H	6.064161	1.311196	1.998121
H	6.601795	2.356812	3.302934
H	0.556976	2.777572	-5.897304
H	0.151962	2.185306	-4.283447
H	-0.282603	3.828343	-4.748863
H	-0.863096	7.339297	3.171549
H	-1.080544	6.363957	1.725182
H	-1.861349	5.885665	3.235351
H	4.902444	-0.179755	3.613705
H	6.607893	-0.025286	4.041360
H	5.385199	0.861264	4.955782
C	0.507672	-1.338784	-4.624219
C	0.254318	-2.741100	-4.070769
C	1.064403	-2.987607	-2.799032
C	0.847602	-4.370594	-2.224732
O	1.421183	-4.568952	-0.894069
P	2.708324	-3.881753	-0.294592
O	2.946951	-4.653538	1.072734
C	2.362672	-4.206733	2.338614
C	0.852337	-4.129172	2.298539
C	0.276581	-3.729087	3.658476
C	-1.191218	-3.320118	3.557444
O	2.639875	-2.377022	-0.106275
O	3.902433	-4.337978	-1.241942
C	5.151710	-3.583219	-1.340498
C	5.855759	-3.406387	-0.008033
C	7.213249	-2.711202	-0.168838
C	7.119912	-1.273258	-0.684352
H	1.276735	-5.144263	-2.863109
H	-0.209636	-4.578559	-2.073408

H	5.755569	-4.177267	-2.024627
H	4.917340	-2.630555	-1.806259
H	2.716393	-4.945617	3.055512
H	2.789523	-3.234367	2.581387
H	5.229472	-2.809792	0.660253
H	5.987779	-4.385439	0.458054
H	0.561450	-3.383245	1.560256
H	0.439249	-5.085253	1.970104
H	0.772013	-2.253003	-2.054537
H	2.123392	-2.832073	-3.009208
H	0.503958	-3.490387	-4.829411
H	-0.811144	-2.857403	-3.849974
H	7.709675	-2.711332	0.804869
H	7.850016	-3.304187	-0.833903
H	0.387535	-4.557630	4.365424
H	0.846626	-2.888538	4.061480
H	1.560558	-1.201061	-4.880715
H	-0.083691	-1.152125	-5.522232
H	0.237506	-0.579856	-3.887692
H	6.455494	-0.678107	-0.055780
H	8.102733	-0.798180	-0.687727
H	6.733386	-1.227703	-1.704332
H	-1.796784	-4.108709	3.105416
H	-1.609201	-3.091931	4.539654
H	-1.292392	-2.424121	2.942018
U	-1.729469	-0.029865	-0.543967
O	-1.392207	0.441064	1.126901
O	-2.019549	-0.524736	-2.211697
N	-1.794520	-2.924489	0.080357
N	-1.603925	2.787304	-1.459413
O	-0.715311	-2.299176	-0.200378
O	-2.810957	-2.161138	0.230003
O	-1.853103	-4.123734	0.184594
O	-0.588989	2.007527	-1.443085
O	-2.673806	2.250246	-1.002311
O	-1.558574	3.921730	-1.859897
U	2.478326	-0.042197	-0.085784
O	0.796827	-0.138609	-0.756754
O	4.106647	0.037700	0.591817
N	1.271511	-0.093062	2.635669
N	3.590433	0.094875	-2.849369
O	1.527103	0.991563	2.009369
O	1.622945	-1.144037	1.998318
O	0.753435	-0.122520	3.722750
O	3.211806	1.123501	-2.194706
O	3.460686	-0.999489	-2.197725
O	4.025331	0.145169	-3.971912

Optimized structure of 3:3 complex

C	-4.425032	1.604749	5.541073
C	-4.085625	0.464563	4.585270
C	-5.040676	0.402926	3.390563
C	-4.590912	-0.649399	2.403319
O	-5.509346	-0.788210	1.266556
P	-5.603229	0.232546	0.065511
O	-6.255296	-0.582583	-1.124401
C	-5.492825	-1.507012	-1.980040
C	-4.712429	-2.548130	-1.200219
C	-4.077525	-3.598565	-2.118804
C	-5.077864	-4.552273	-2.771017

O	-4.295052	0.913529	-0.315045
O	-6.708274	1.295410	0.478479
C	-6.755668	2.586702	-0.209485
C	-6.023311	3.637665	0.600918
C	-6.009153	5.007901	-0.085618
C	-5.185199	5.046880	-1.374560
H	-4.584861	-1.644295	2.843270
H	-3.597229	-0.435594	2.022089
H	-6.333224	2.476750	-1.207802
H	-7.816464	2.813893	-0.304048
H	-6.266742	-1.956333	-2.596180
H	-4.830430	-0.908365	-2.601947
H	-6.503330	3.713190	1.579647
H	-4.999056	3.303401	0.773165
H	-3.918815	-2.055525	-0.637574
H	-5.368784	-3.032278	-0.473267
H	-5.060180	1.376160	2.897829
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C	0.392756	-6.875392	-0.687598
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O	2.493606	-6.028909	0.296833
P	2.312970	-4.585147	0.930671
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C	3.755563	-1.430573	4.116338
C	4.614826	-0.193600	3.864463
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C	4.279940	-3.415575	-2.041933
C	5.612259	-2.913250	-2.610801
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H	5.675454	-0.453177	3.831414
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C	2.771514	6.731696	2.063328
C	2.208644	5.308664	2.048579
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P	3.214114	4.193181	-1.022255
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O	-0.842501	2.332323	1.480429
O	-2.968557	2.128348	1.663148
O	-1.836512	3.049189	3.289653
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O	-1.285061	-2.119371	-1.615131
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O	0.084687	-2.487286	3.137468
O	-1.239144	-0.889229	2.599718
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