Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information

Occurence of Polyoxouranium Motif in Uranyl Organic Networks Constructed by Silicon-Centered Carboxylate Linkers: Structures, Spectroscopy and Computation

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Characterization. Fluorescence was recorded on a Hitachi F-7000 luminescence spectrometer. 450 W Xenon lamp was used as excitation light source. Solid-state optical diffuse reflectance spectra of the crystal samples were collected using a Hitachi U-4100 spectrophotometer. Fourier transform infrared (FT-IR) spectra of the materials were recorded in the 4000−500 cm^{-1} region using a Perkin−Elmer Spectrum One FT-IR spectrometer. The powder X-ray diffraction pattern was recorded at a scan rate of 1°/min on a Rigaku-DMAX 2500 diffractometer with CuKα radiation (λ = 1.5406), ranging from 5° to 45°. Simulated PXRD patterns were calculated using Mercury from corresponding single-crystal structural models. Single-crystal data of **1-4** were recorded on a Bruker Apex II CCD diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The sample was kept at 150 K during data collection. The initial structures were obtained by direct methods and further refined by full-matrix least-squares on F^2 with anisotropic displacement using the SHELXTL software package. For the compound **1** and **4**, OMIT command has been applied to omit some bad reflections. For **2** and **3**, ISOR and RIGU commands have been applied to achieve convergence. A global RIGU restraint has been applied for 4 to optimized the ADP values. In addition, for 2 and 4, the diffraction data were treated by the "SQUEEZE" method as implemented in PLATON, 763 and 391 electrons have been masked during the refinement. Five additional bpi molecules for **2** were estimated from PLATON SQUEEZE and thermogravimetric analysis. For 4, 20 waters were estimated from PLATON SQUEEZE. The details for data collection and refinement are listed in Table 1. Crystallographic data for the structures reported herein have been deposited in the Cambridge CCDC Number: 1943775 for **1**；1946628 for **2**；1943776-1943777 for **3-4.**

Computational Approaches. Model compounds $[(UO_2)(OOCH)_3(H_2L^1)]$ (**1a**), $[(UO_2)_3(OOCH)_7(H_6L^2)]$ (**2a**) and $[(UO_2)(OOCH)_3(H_2L^3)]$ (**3a**) were exploited to simulate experimental compounds **1**, **2** and **3**, respectively. Considering effects of polyuranium motifs of experimental real compounds, $[(UO_2)_2(OOCH)_6(H_2L^3)]$ (**3b**) and $[(UO_2)_3(OOCH)_8(HL^3)]$ (**3c**) were further computed and compared, which include two and three uranyl coordination units, respectively. Structural optimizations and frequency calculations were accomplished using the Priroda code.[1] A scalar all-electron relativistic Hamiltonian was used, along with the GGA-PBE functional and all-electron Gaussian basis sets. Building on these calculations, we obtained Mayer bond orders and Mulliken charges. At the optimized geometries, electronic structures in environmental media were calculated with the ADF 2014 code,[2] aiming to understand spectroscopic transition nature. The solvent effects of tetrahydrofuran (THF) were taken into account, which is simulated with the Conductor-Like Screening Model, COSMO. Klamt radius (Å) of each atom was taken as H (1.30), C (2.00), O (1.72), Si (2.40) and U (1.70).[3-4] We utilized the ZORA scalar relativistic approach, the PBE functional and the Slater-type TZP basis sets in the ADF calculations.

References：

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Table S1. X-ray Crystal Data for Compounds **1-4**

compound	**1**	**2**	**3**	**4**
Empirical formula	$C_{22}H_{23}O_{16}SiU_2$	$C_{171}H_{98}O_{92}N_{14}Si_3U_{12}$	$C_{54}H_{34}O_{27}Si_2U_5$	$C_{32}H_{52}O_{54}SiU_6$
Fw	1047.55	7145.76	2361.14	2756.98
Crystal system	Triclinic	Monoclinic	Triclinic	tetragonal
Space group	*P*-1	*C2/c*	*P*-1	$I4_1/acd$
a/Å	9.184(5)	27.1551(16)	14.2639(13)	21.9739(6)
b/Å	10.534(5)	20.3001(12)	16.2562(15)	21.9739(6)
c/Å	16.288(8)	50.380(3)	17.8214(16)	37.455(2)
α/° □□	98.949(9)	90	76.477(2)	90
β/°	90.855(9)	100.579(10)	81.425(2)	90
γ/°	100.674(10)	90	73.681(2)	90
V/ Å^3	1528.1(13)	27300(3)	3840.5(6)	18085.3(14)
Z	2	4	2	8
F(000)	962.0	14132.0	2124.0	8336
ρ_{calcd} (g cm^{-3})	2.277	1.843	2.040	1.760
μ (Mo Kα)/ mm^{-1}	10.692	7.188	10.605	10.775
R_1/wR_2 ($I > 2\sigma(I)$)[a]	0.0452/0.1061	0.0890/0.2009	0.0430/0.1053	0.0271/0.0711
R_1, wR_2 (all data)	0.0679/0.1169	0.1199/0.2141	0.0732/0.1188	0.0357/0.0734

[a] $R_1=\sum(\Delta F/\sum(F_o))$; $wR_2=(\sum[w(F_o^2-F_c^2)])/\sum[w(F_o^2)^2]^{1/2}$, $w=1/\sigma^2(F_o^2)$

Table S2. Selected bond lengths (Å) for compound **1**

U(1)-O(1)	1.775(10)	U(2)-O(3)#1	2.224(8)
U(1)-O(2)	1.739(9)	U(2)-O(4)	2.349(9)
U(1)-O(4)	2.427(8)	U(2)-O(6)	1.738(9)
U(1)-O(10)	2.452(6)	U(2)-O(5)	1.797(7)
U(1)-O(12)#3	2.489(8)	U(2)-O(8)	2.459(6)
		U(2)-O(7)#3	2.477(8)
		U(2)-O(11)#4	2.342(10)

Symmetry code: #1 x+1,y-1,z; #2 x+1,y,z-1; #3 x,y+1,z

Table S3. Selected bond lengths (Å) for compound **2**

U(1)-O(2)	1.845(2)	U(2)-O(6)	1.746(3)	U(3)-O(10)	1.715(3)
U(1)-O(1)	1.732(3)	U(2)-O(7)	1.740(3)	U(3)-O(11)	1.762(3)
U(1)-O(3)	2.296(2)	U(2)-O(5)	2.282(2)	U(3)-O(12)	2.230(2)
U(1)-O(3)#1	2.3748(18)	U(2)-O(8)	2.471(2)	U(3)-O(16)#1	2.348(2)
U(1)-O(4)	2.245(2)	U(2)-O(9)	2.426(2)	U(3)- O(18)	2.267(2)
U(1)-O(5)	2.314(2)	U(2)-O(35)#2	2.295(3)	U(3)-O(41)#3	2.441(2)
U(1)-O(36)#2	2.4565(19)	U(2)-O(45)#2	2.247(3)	U(3)-O(42)#3	2.440(2)
U(4)-O(19)	1.806(4)	U(5)-O(23)	2.263(3)	U(6)-O(28)#5	2.305(2)
U(4)-O(20)	1.734(2)	U(5)-O(24)	2.431(4)	U(6)-O(30)#5	2.311(3)
U(4)-O(17)	2.336(3)	U(5)-O(25)	1.681(3)	U(6)-O(37)	1.744(3)
U(4)-O(18)	2.321(2)	U(5)-O(26)	1.740(4)	U(6)-O(38)	1.691(3)
U(4)-O(21)	2.352(4)	U(5)-O(27)	2.224(3)	U(6)-O(39)	2.436(2)
U(4)-O(22)	2.276(3)	U(5)-O(28)	2.256(2)	U(6)-O(28)	2.256(2)

U(4)-O(23)	2.328(3)	U(5)-O(29)	2.438(3)	U(6)-O(29)	2.444(2)

Symmetry code: #11-X, 1-Y, -Z; #2 1-X, +Y, 1/2-Z; #3 1/2-X, -1/2+Y, 1/2-Z; #4 -1/2+X, -1/2+Y, +Z; #5 1/2+X,1/2+Y,+Z; #6 1-X,2-Y,1-Z; #7 1/2-X,1/2+Y,1/2-Z

Table S4. Selected bond lengths (Å) for compound **3**

U(1)-O(2)	1.643(10)	U(2)-O(6)	1.727(8)	U(3)-O(8)	1.754(15)
U(1)-O(1)	1.703(9)	U(2)-O(5)	1.760(9)	U(3)-O(7)	1.812(14)
U(1)-O(4)	2.307(7)	U(2)-O(9)	2.207(6)	U(3)-O(9)	2.212(7)
U(1)-O(1AA)	2.394(6)	U(2)-O(23)^{5}	2.334(7)	U(3)- O(1AA)	2.339(6)
U(1)-O(21) #1	2.476(7)	U(2)-O(18)^{6}	2.509(5)	U(3)- O(5AA)	2.386(6)
U(1)-O(W)	2.388(11)	U(2)-O(1AA)	2.459(6)	U(3)-O(12)^{3}	2.743(12)
U(1)-O(3)	2.352(8)	U(2)-O(3)	2.358(8)	U(3)-O(27A)^{3}	2.300(14)
U(4)-O(11)	1.763(15)	U(5)-O(22)^{2}	2.306(7)		
U(4)-O(10)	1.73(2)	U(5)-O(16)	1.764(6)		
U(4)-O(12)	2.379(11)	U(5)-O(15)	1.746(7)		
U(4)-O(9)	2.221(6)	U(5)-O(24)^{3}	2.342(7)		
U(4)-O(18)	2.447(5)	U(5)-O(19)^{4}	2.409(6)		
U(4)-O(13)	2.462(7)	U(5)-O(20)^{4}	2.489(6)		
		U(5)-O(17)	2.345(6)		

Symmetry code: #1 3-X, 1-Y, -Z; #2 3-X,-Y,1-Z; #3 2-X, -Y, 1-Z; #4 1+X, +Y, +Z; #5 +X,+Y,1+Z; #6 2-X,-Y,2-Z; #7 +X,+Y,-1+Z; #7 -1+X,+Y,+Z

Table S5. Selected bond lengths (Å) for compound **4**

U(1)-O(5)	1.756(3)	U(2)-O(3)AA	1.778(5)
U(1)-O(6)	1.772(3)	U(2)-O(2)	1.788(4)
U(1)-O(4)	2.364(3)	U(2)-O(4)#1	2.262(3)
U(1)-O(10)	2.441(3)	U(2)-O(3)	2.382(3)
U(1)-O(8)	2.313(2)		
U(1)-O(7)	2.335(3)		
U(1)-O(9)	2.437(3)		

Symmetry code: #1 -3/4+Y, 3/4+X, 7/4-Z; #2 1/2-X, +Y, 2-Z; #3 3/4-Y,5/4-X,1/4+Z; #4 -X,3/2-Y,+Z; #5 -3/4+Y,3/4-X,9/4-Z; #6 3/4-Y,3/4+X,9/4-Z; #7 5/4-Y,3/4-X,-1/4+Z

Table S6. Optimized geometry parameters of the model compounds, compared with experimental values of analogues. (Bond lengths in Å and angles in degree)

		U=O	U-O_{eq}	O=U=O
1a	Calc.	1.822	2.430	175.8
1	Expt.	1.734~1.795	2.229(3)~2.511(3)	176.1
2a	Calc.	1.824	2.309	176.4
3a	Calc.	1.822	2.432	177.2
3b	Calc.	1.821	2.324	179.6
3c	Calc.	1.821	2.365	178.5
3	Expt.	1.723(3)~1.865(3)	2.209 (3)~2.546 (3)	178.6

Table S7. Bond orders for the model compounds.

	ADF		Priroda	
	U=O	U-O_{eq}	U=O	U-O_{eq}
1a	1.85	0.45	2.36	0.60
2a	1.86	0.49	2.34	0.70
3a	1.86	0.44	2.36	0.60
3b	1.88	0.49	2.36	0.72
3c	1.87	0.48	2.36	0.68

Table S8. Atomic charges for the model compounds.

	ADF			Priroda		
	U	O	O_{eq}	U	O	O_{eq}
1a	2.247	-0.715	-0.678	0.833	-0.326	-0.403
2a	2.319	-0.690	-0.666	0.948	-0.321	-0.418
3a	2.255	-0.712	-0.687	0.823	-0.327	-0.397
3b	2.310	-0.689	-0.683	0.880	-0.321	-0.414
3c	2.290	-0.699	-0.679	0.852	-0.325	-0.409

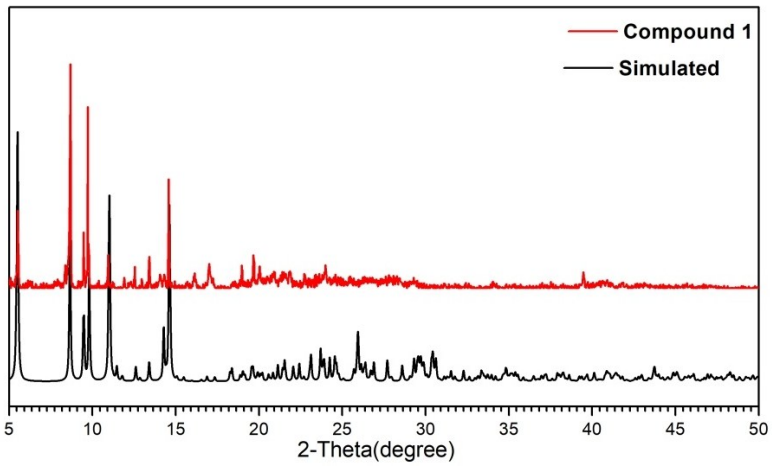


Figure S1. Simulated and experimental XRD patterns of compound **1**.

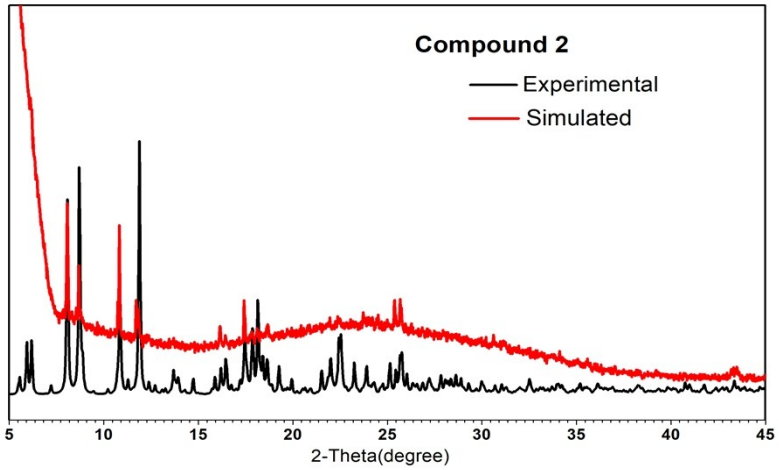


Figure S2. Simulated and experimental XRD patterns of compound **2**.

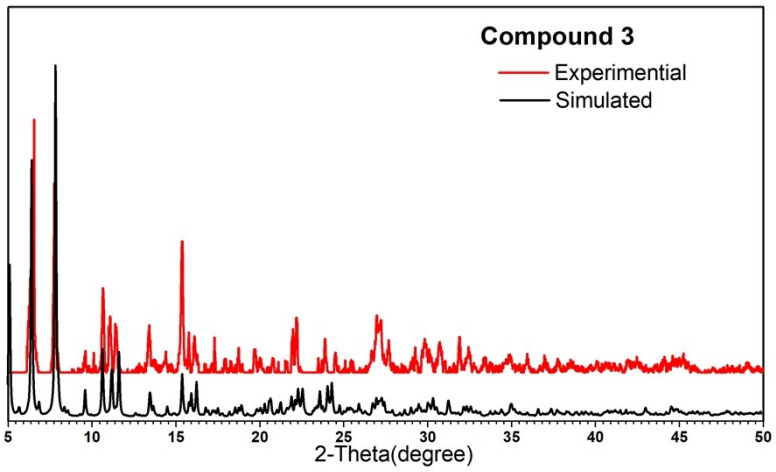


Figure S 3. Simulated and experimental XRD patterns of compound **3**.

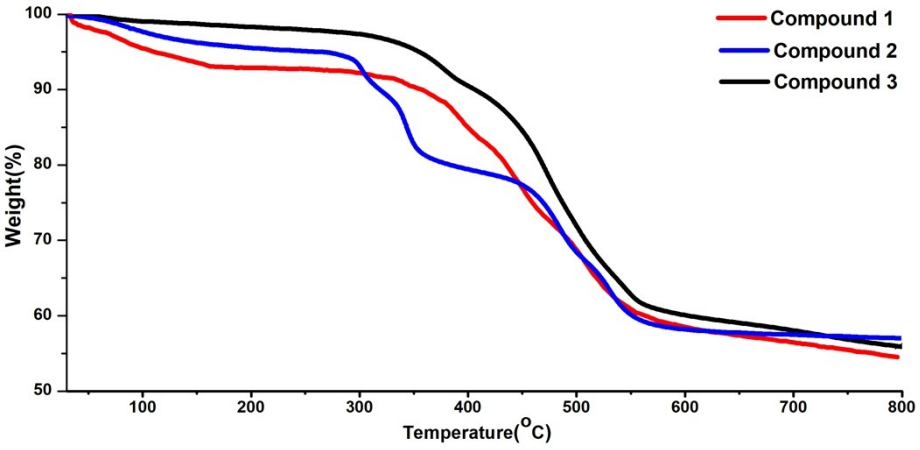


Figure S4. TG curve for compounds 1-3.

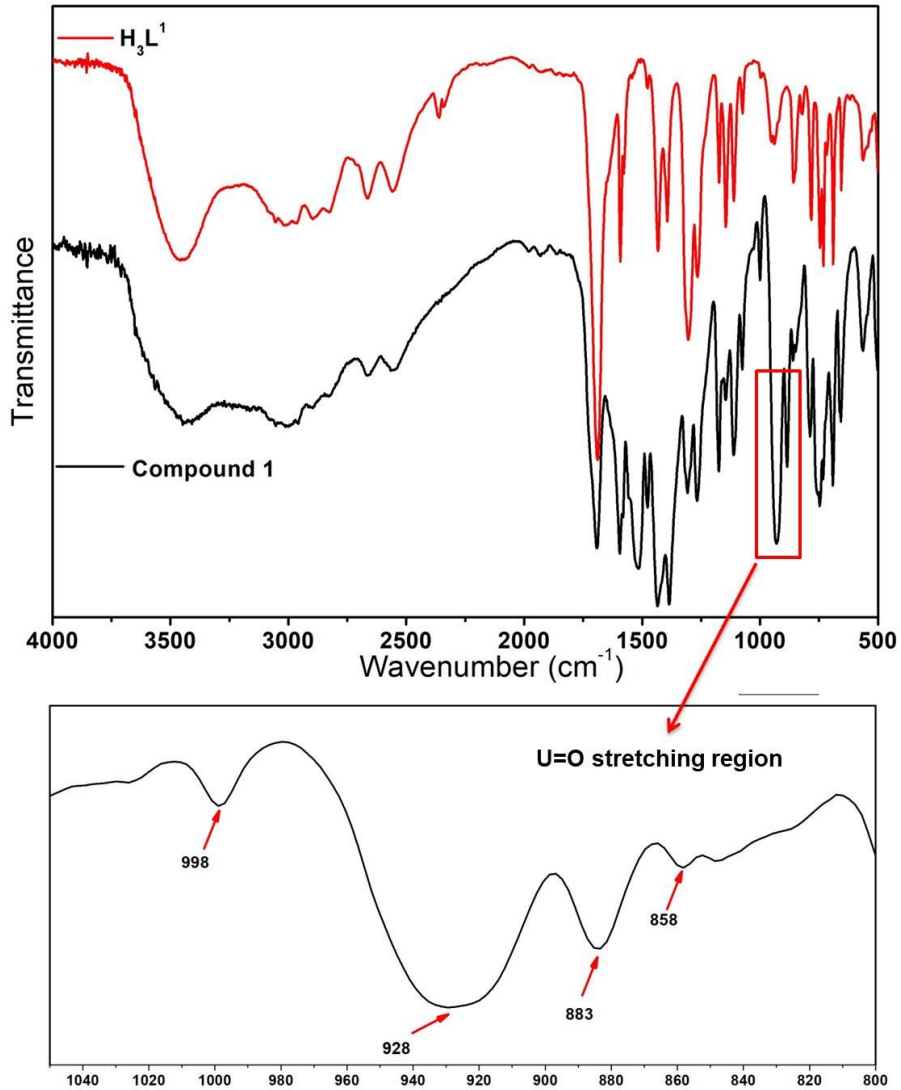


Figure S5. FT-IR spectra of Compound **1**.

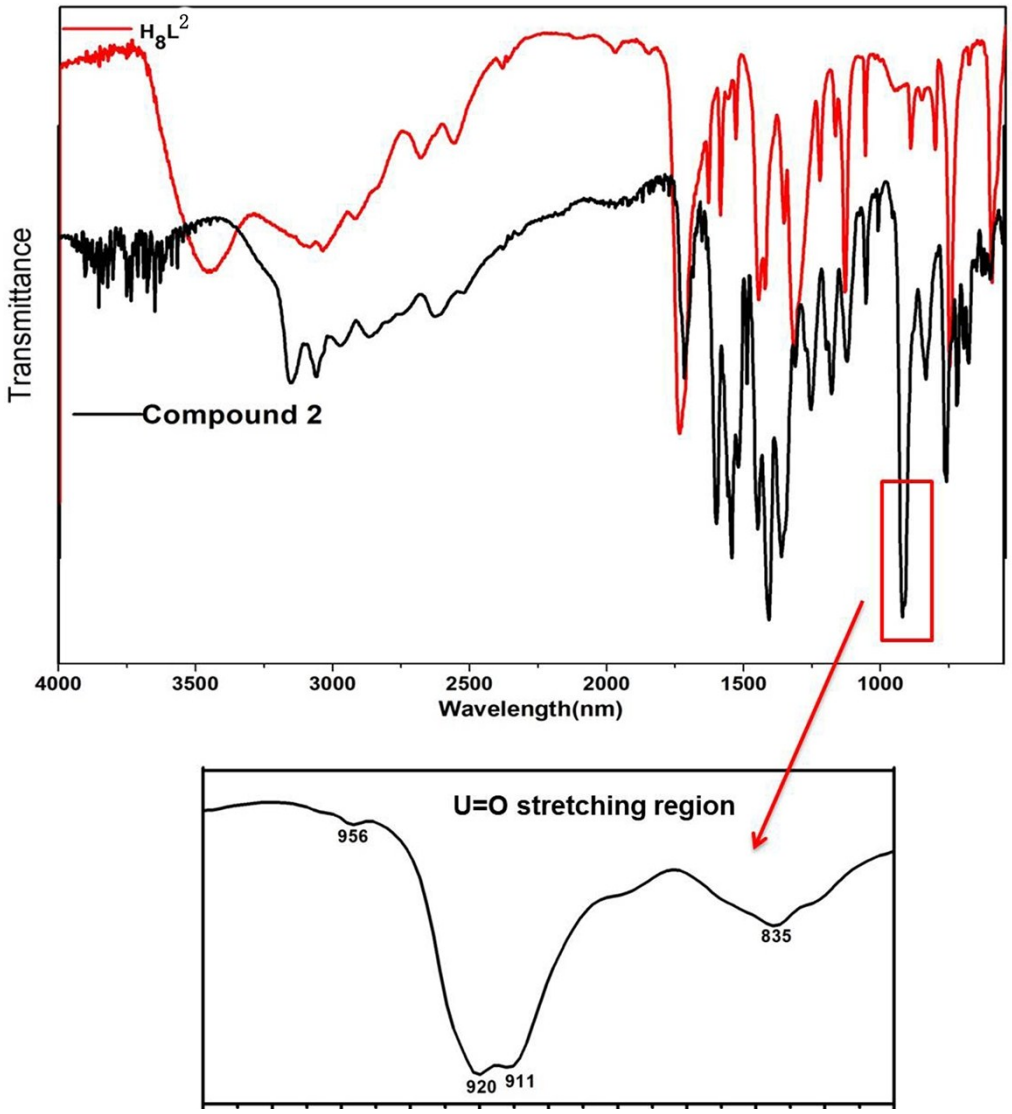


Figure S6. FT-IR spectra of compound **2**.

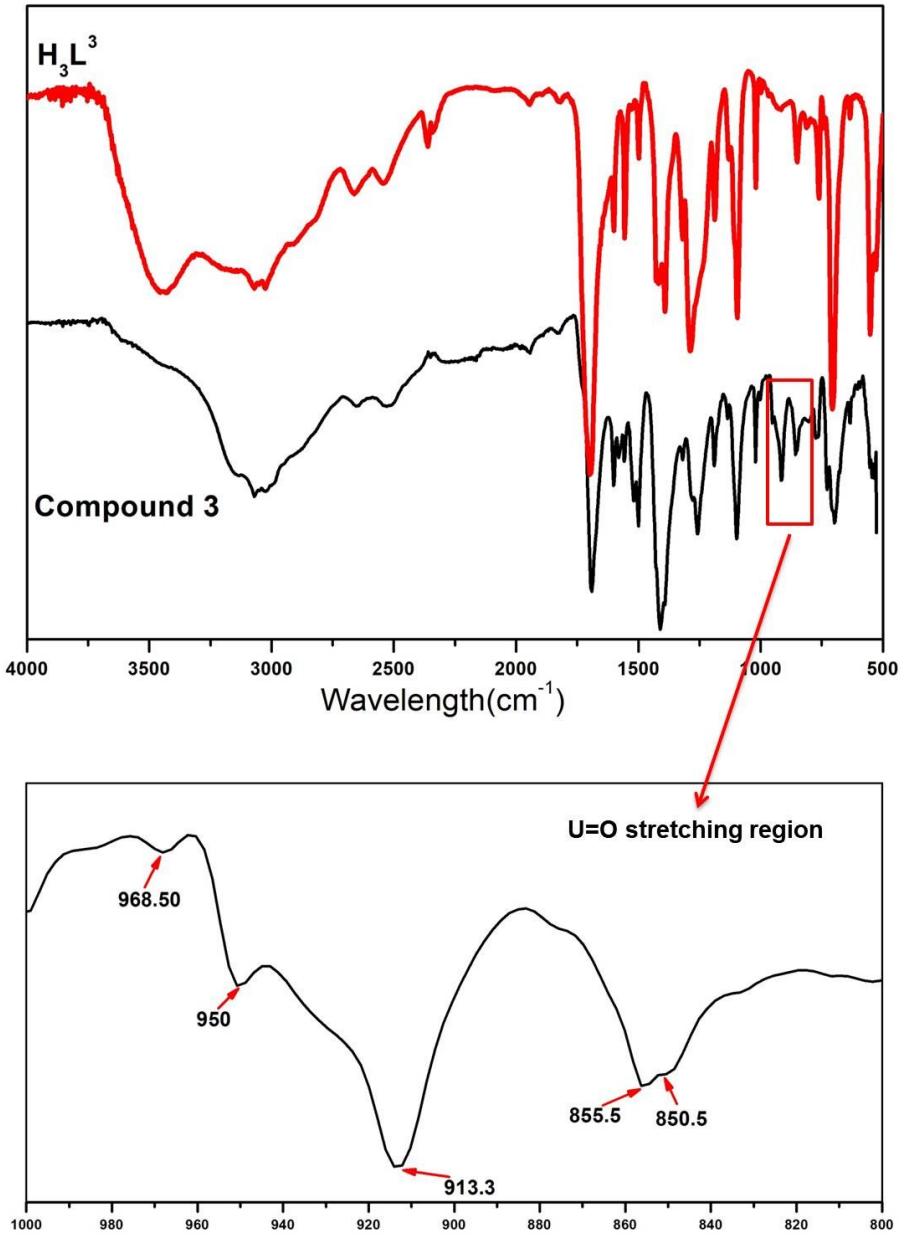


Figure S7. FT-IR spectra of compound **3**. The peaks in the range of 1400 to 1600 cm^{-1} are attributed to benzene skeleton vibrations. The absorption bands located at 1094 and 727 cm^{-1} in **1**, 1052 and 760 cm^{-1} in **2**, and 1092 and 696 cm^{-1} in **3** are related to the Si-C characteristic stretching modes.

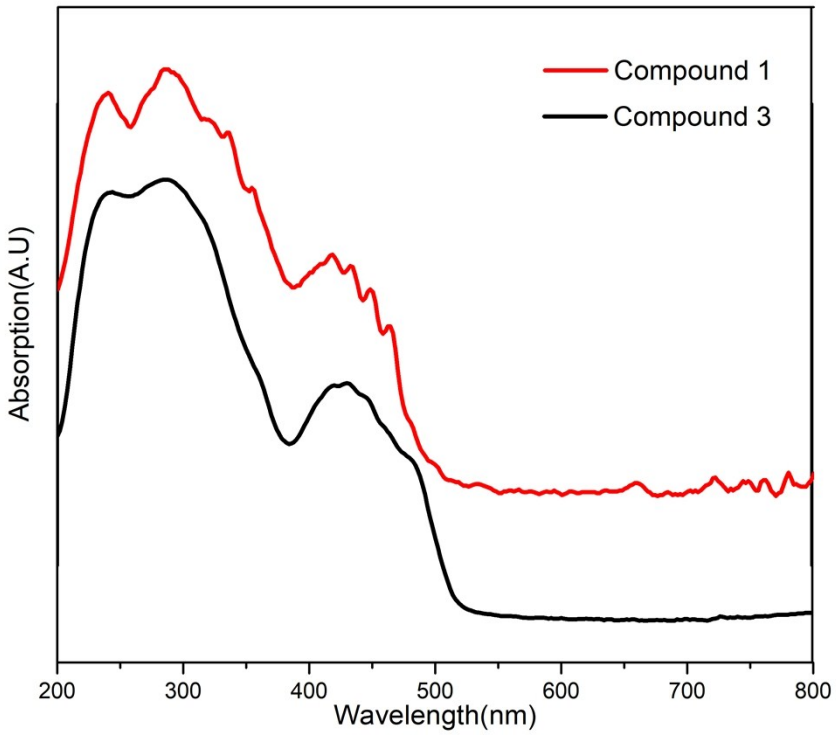


Figure S8. Solid state absorption spectra of compounds **1** and **3**

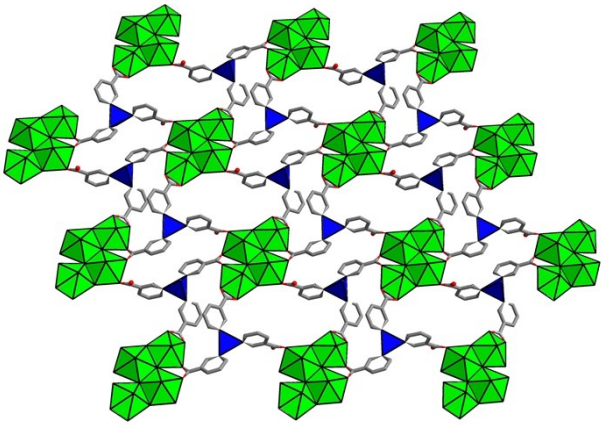


Figure S9. The layered structure of **1** formed by uranyl tetramer and tripodal linker.

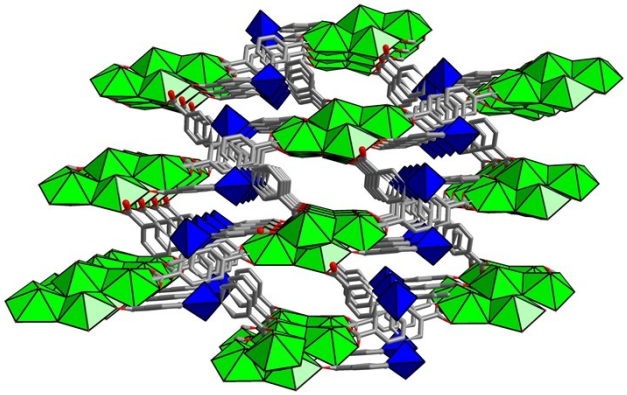


Figure S10. Packing model of alternate layers in **1**. All hydrogen atoms and solvents molecules

were removed for the sake of clarity.

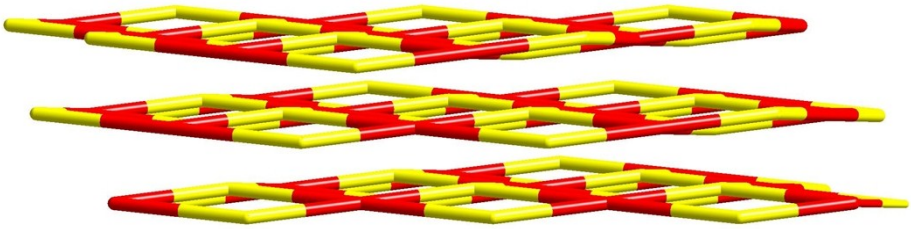


Figure S11. Simplified network showing the connectivity for **1**.

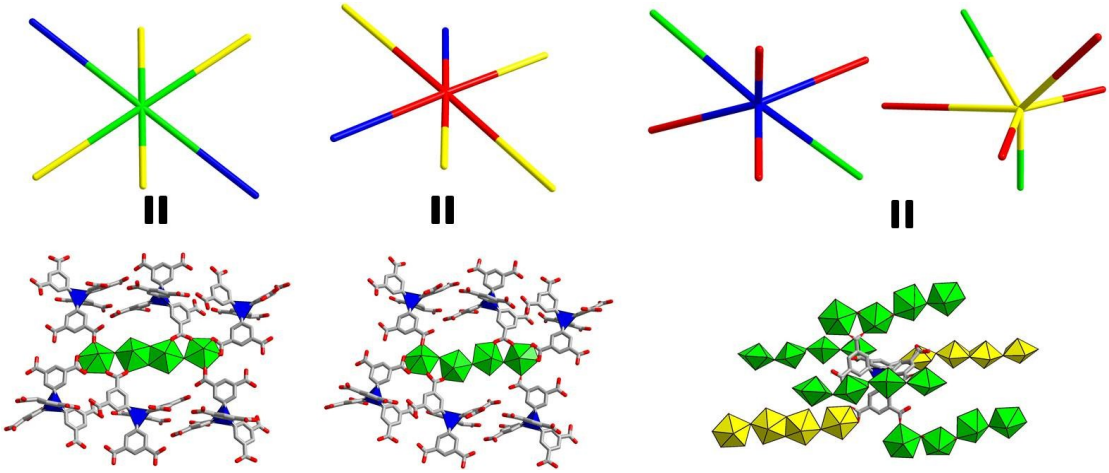


Figure S12. Schematic representation of structural nodes in **2**.

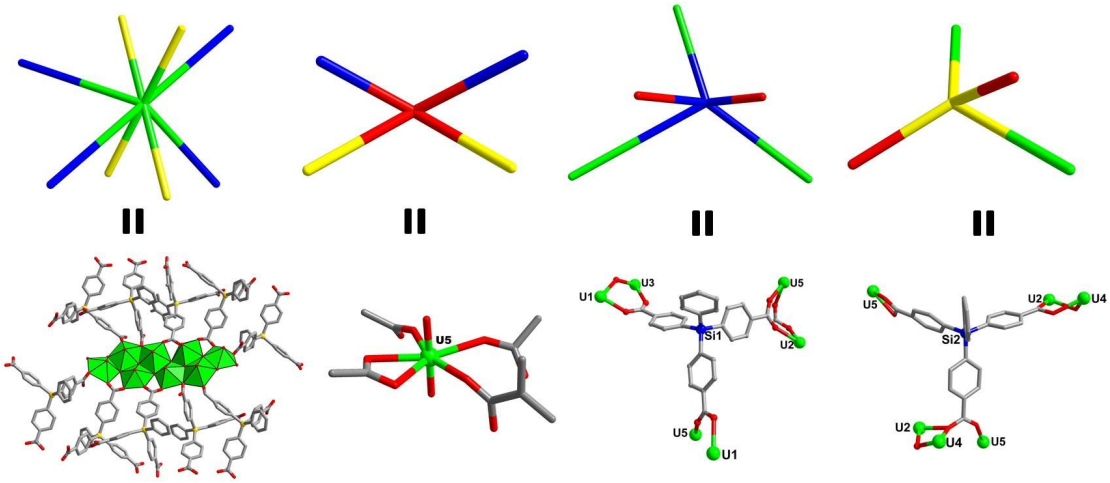


Figure S13. Schematic representation of structural nodes in **3.**

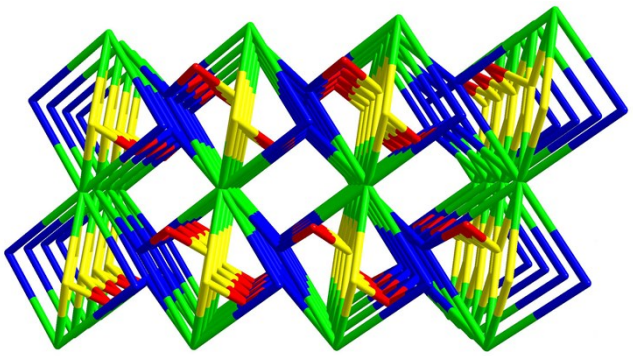


Figure S14. Simplified network showing the connectivity for **3**. The Sc atom represents the octanuclear motif, Ti and V sites represent the two silicon-centered ligands respectively, and the Cr atom represents the UO_7 monomers.

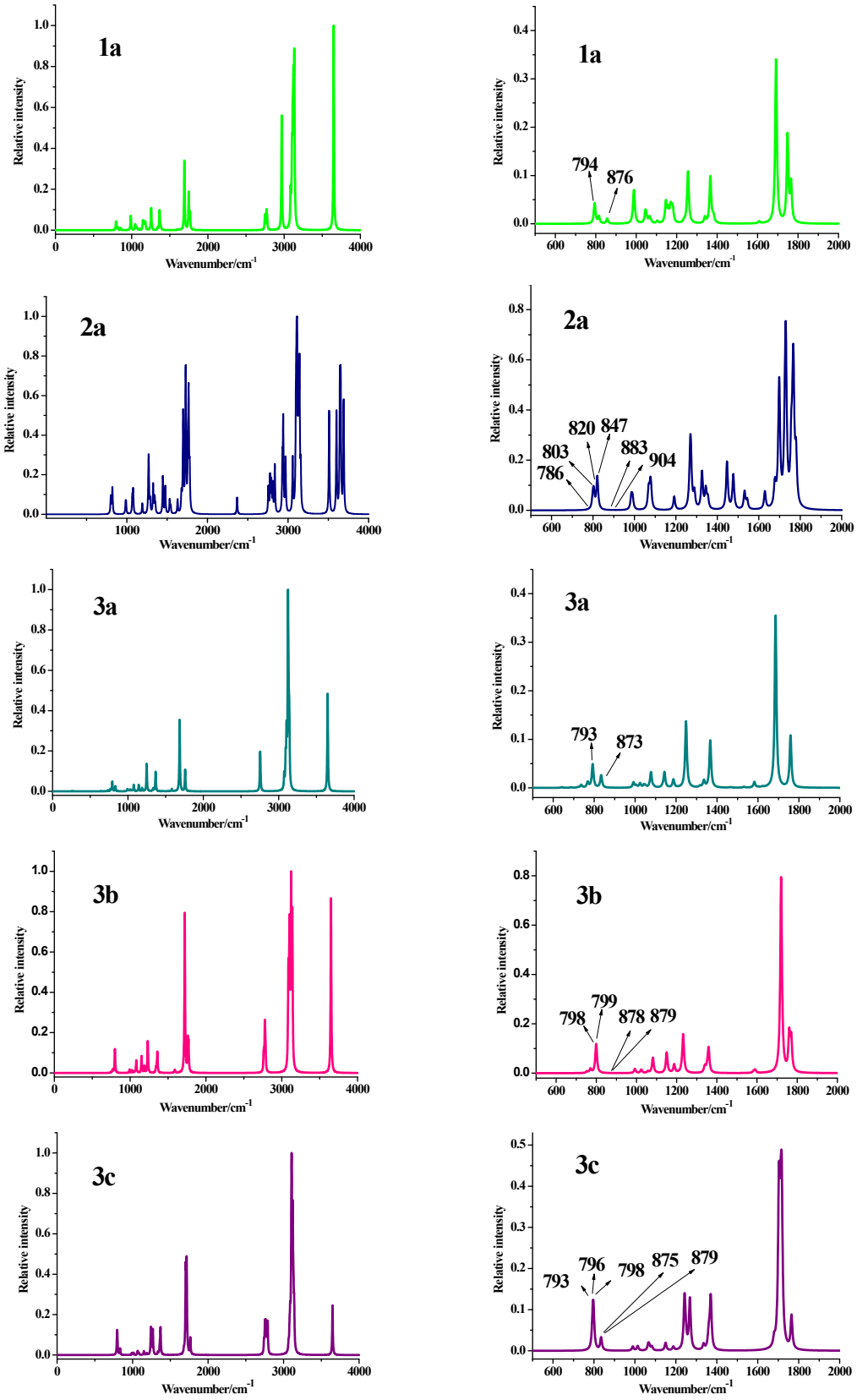
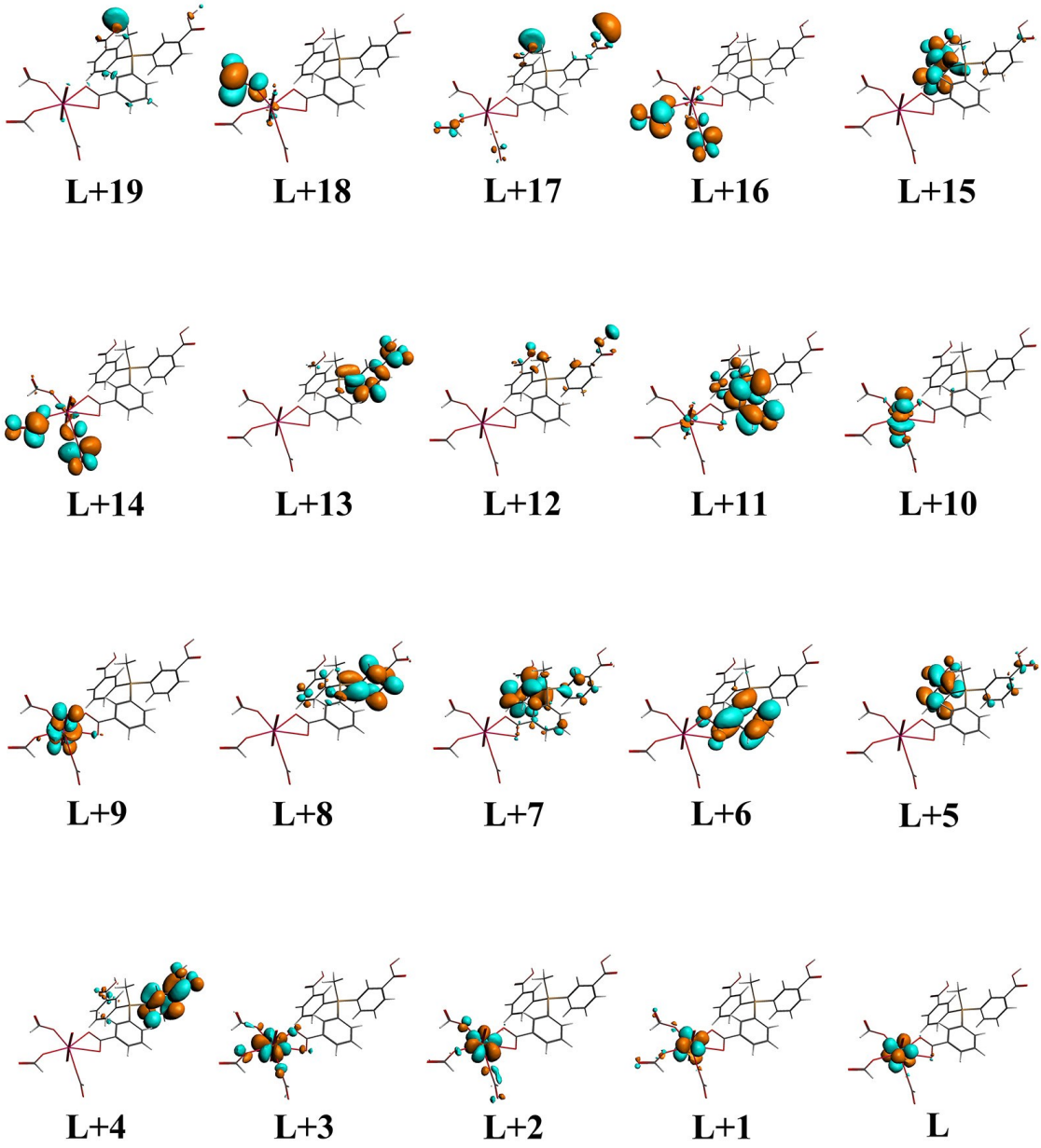


Figure S15. Simulated vibrational spectra of the model compounds, where the one ranging from 0 and 4000 cm^{-1} was placed on the left side, and the one between 500 and 2000 cm^{-1} on the right side with the marked U=O stretches. The peaks at 794/876 cm^{-1} of 1a and 793/873 cm^{-1} of 3a are

attributed to symmetric/asymmetric U=O stretching vibrational modes. They fall well within the range of experimental IR spectra. The computed U=O vibrations of 2a, 3b and 3c are a little more complicated because of the involvement of multiple uranyl units.

Unoccupied orbitals of **1a**



Occupied orbitals of **1a**

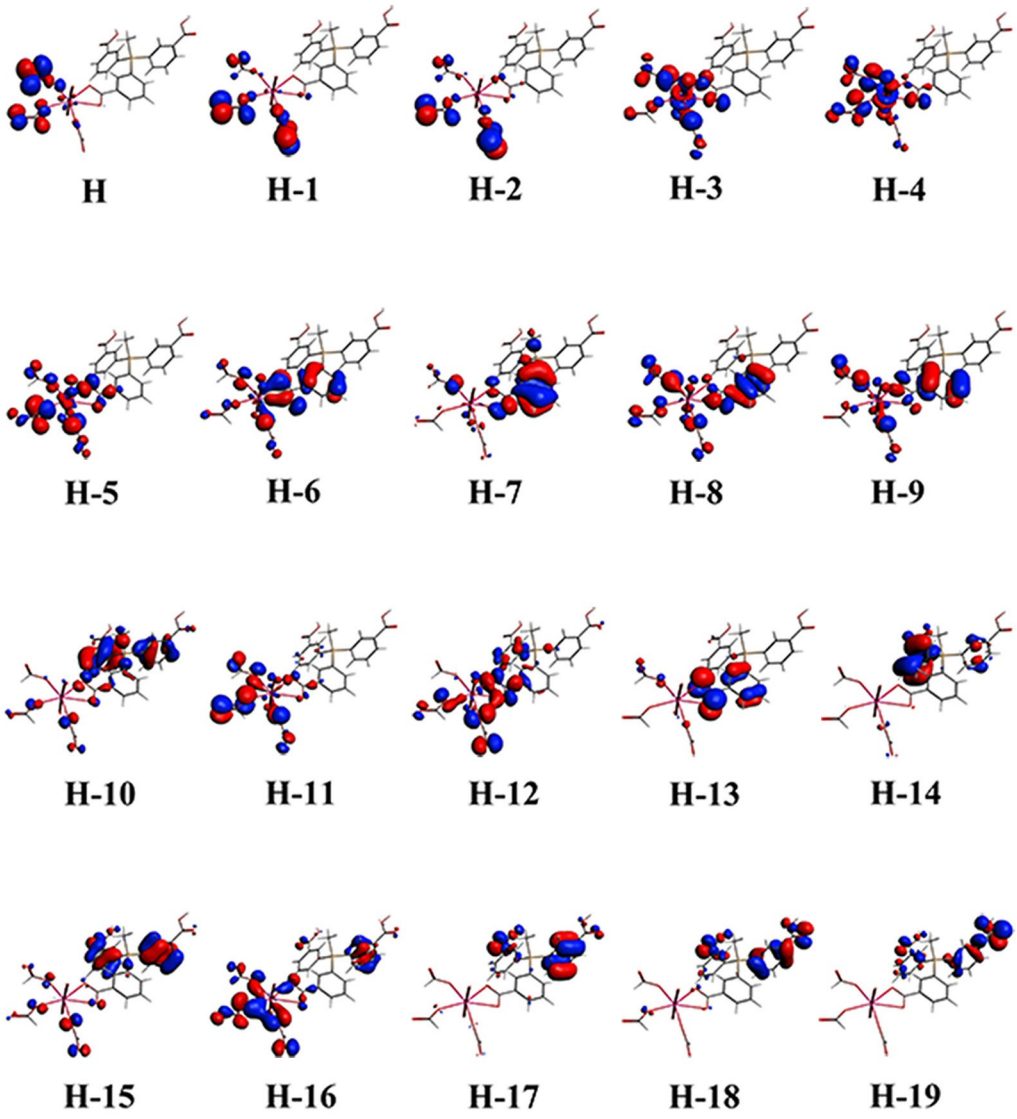
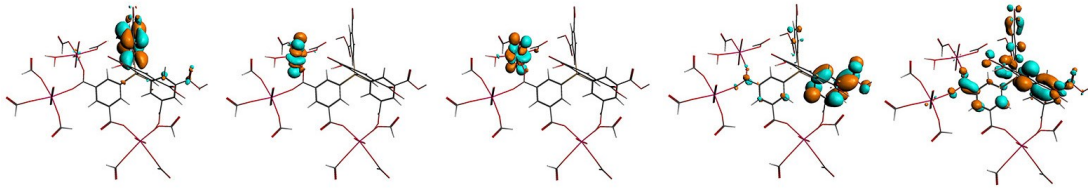
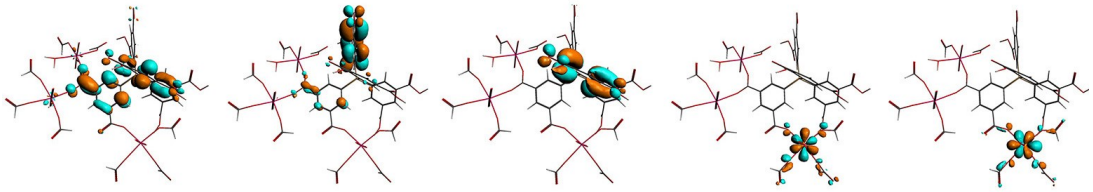


Figure S16. Diagrams of partial frontier molecular orbitals of **1a.**

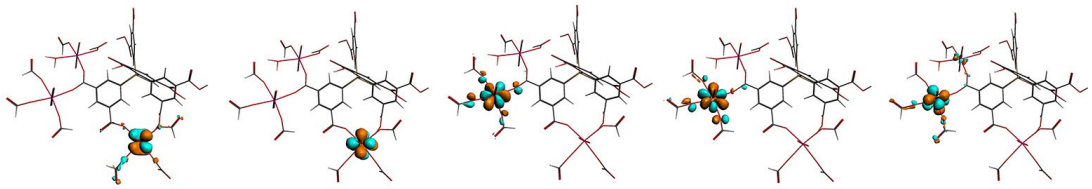
Unoccupied orbitals of **2a**



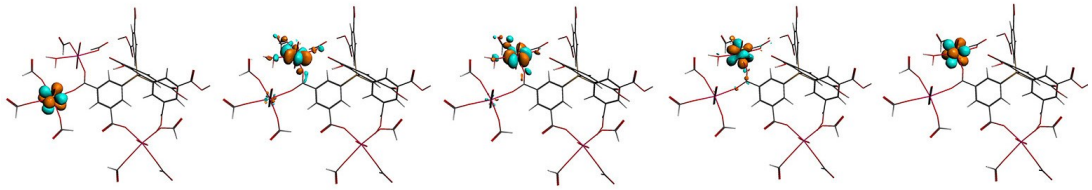
L+19 **L+18** **L+17** **L+16** **L+15**



L+14 **L+13** **L+12** **L+11** **L+10**



L+9 **L+8** **L+7** **L+6** **L+5**



L+4 **L+3** **L+2** **L+1** **L**

Occupied orbitals of **2a**

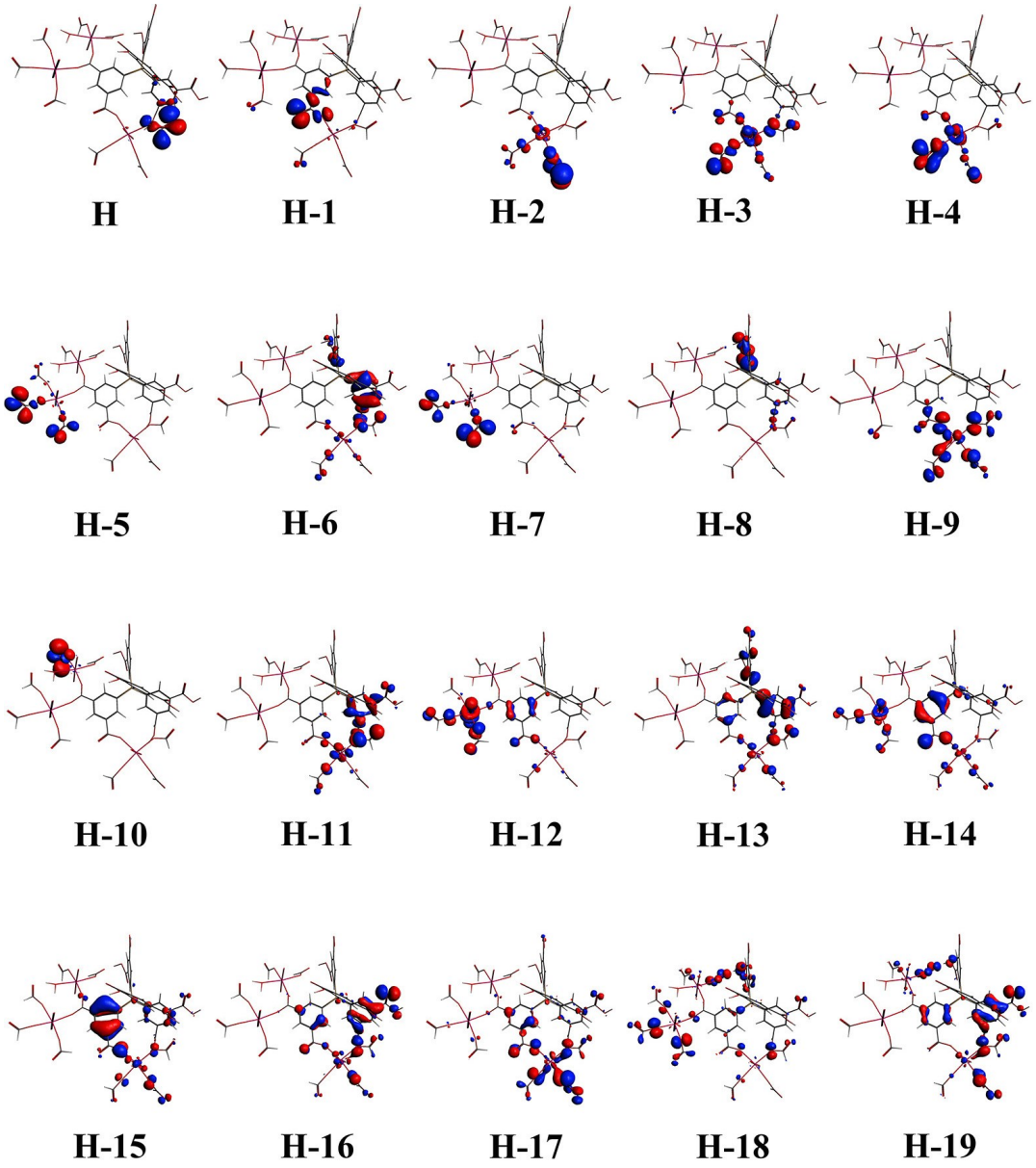
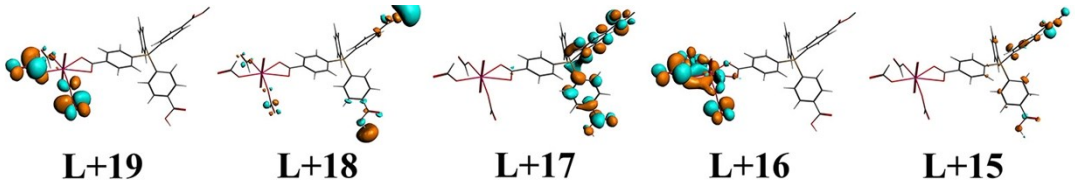
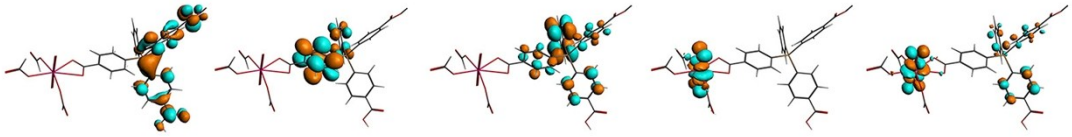


Figure S17 Diagrams of partial frontier molecular orbitals of **2a.**

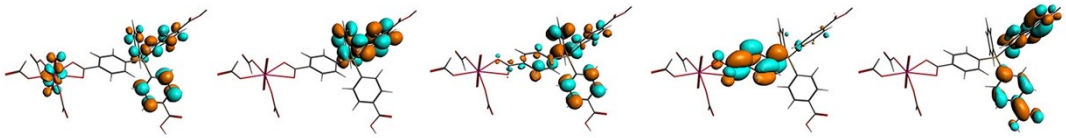
Unoccupied orbitals of **3a**



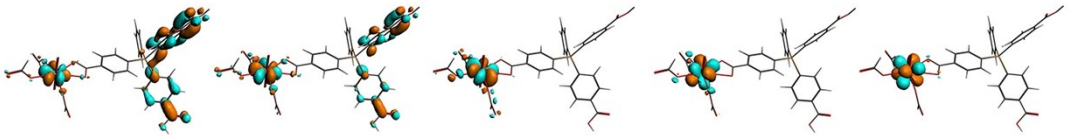
L+19 **L+18** **L+17** **L+16** **L+15**



L+14 **L+13** **L+12** **L+11** **L+10**



L+9 **L+8** **L+7** **L+6** **L+5**



L+4 **L+3** **L+2** **L+1** **L**

Occupied orbitals of **3a**

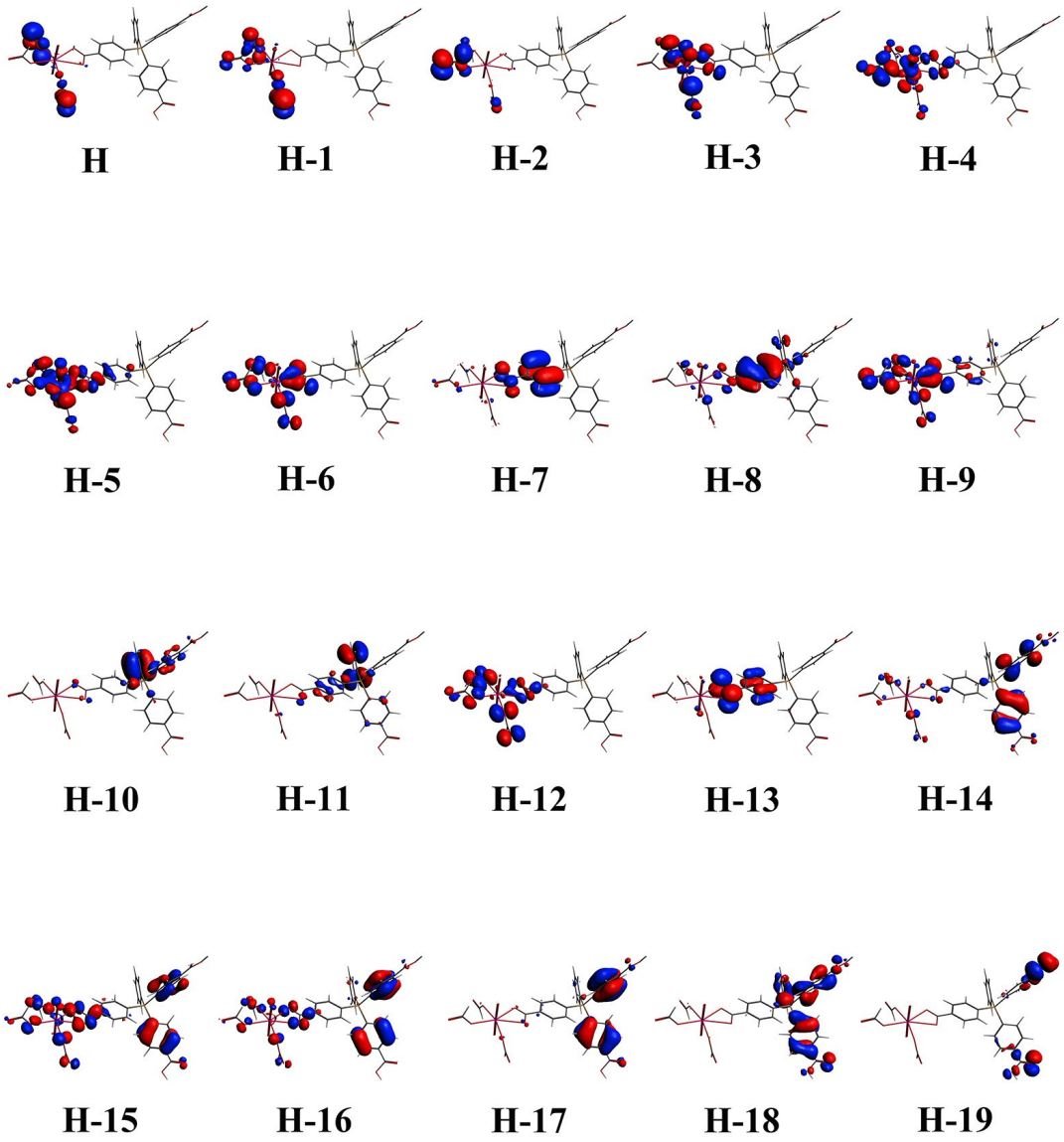
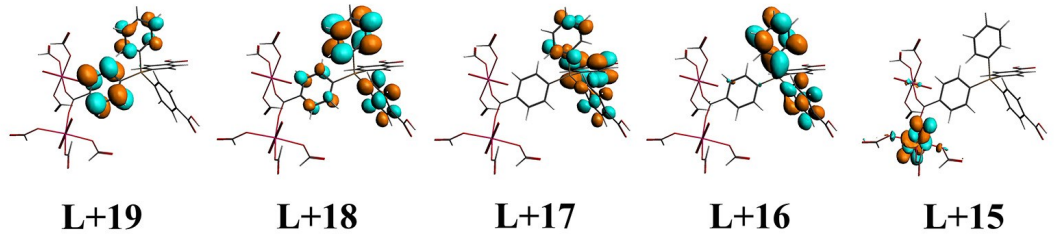
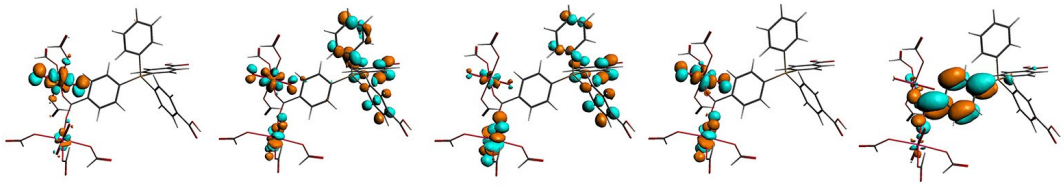


Figure S18. Diagrams of partial frontier molecular orbitals of **3a.**

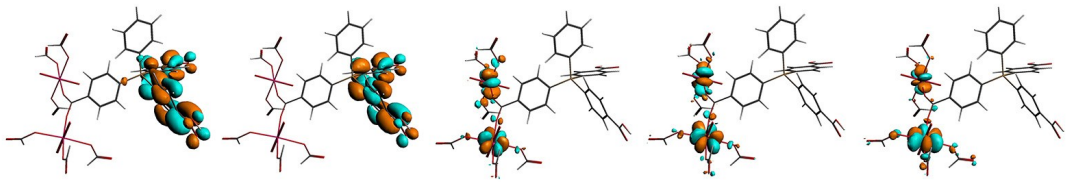
Unoccupied orbitals of **3b**



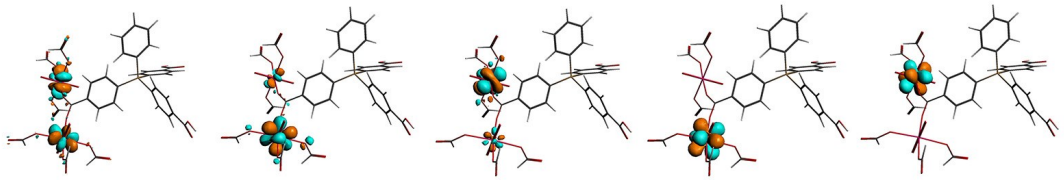
L+19 **L+18** **L+17** **L+16** **L+15**



L+14 **L+13** **L+12** **L+11** **L+10**



L+9 **L+8** **L+7** **L+6** **L+5**



L+4 **L+3** **L+2** **L+1** **L**

Occupied orbitals of **3b**

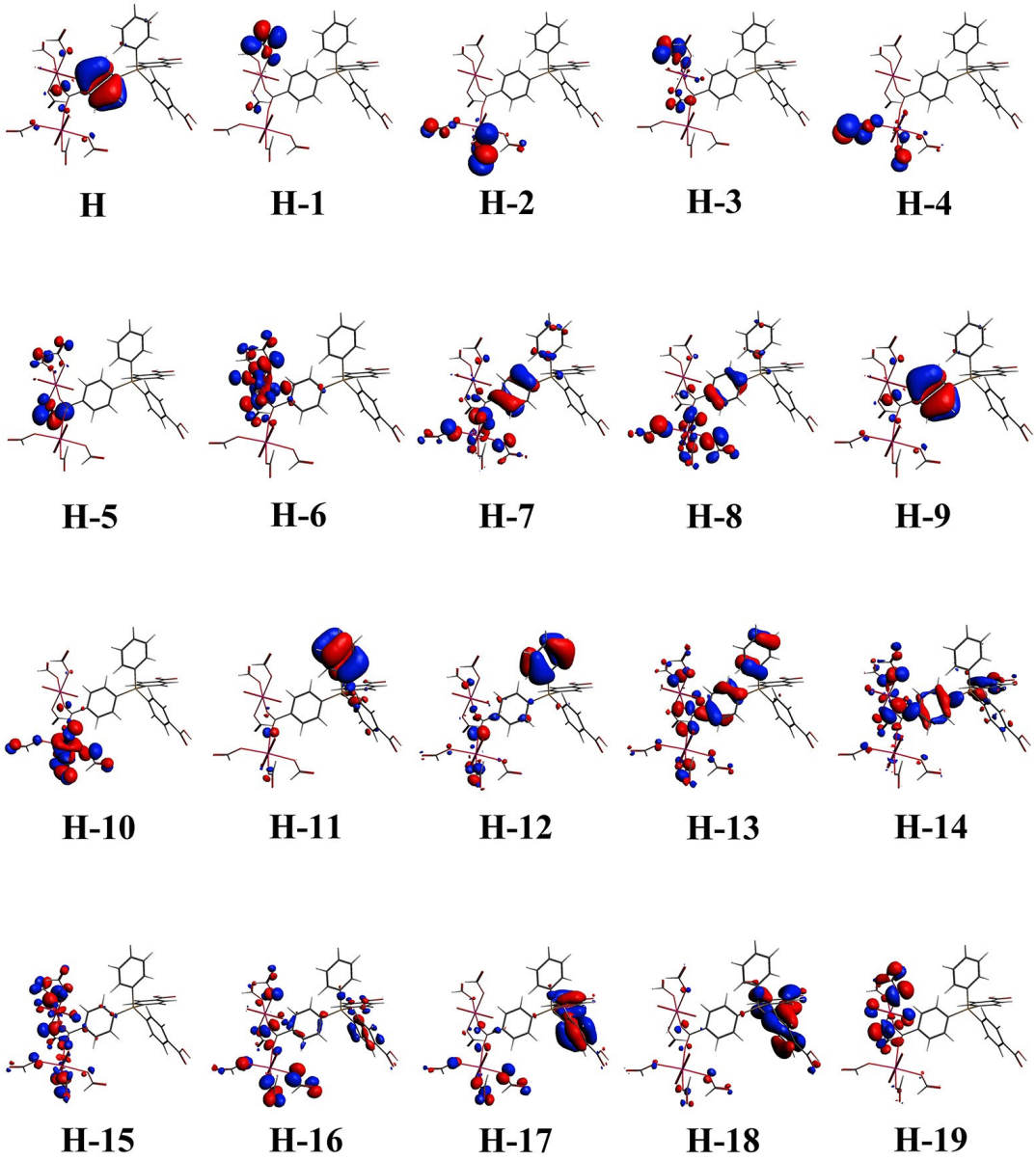
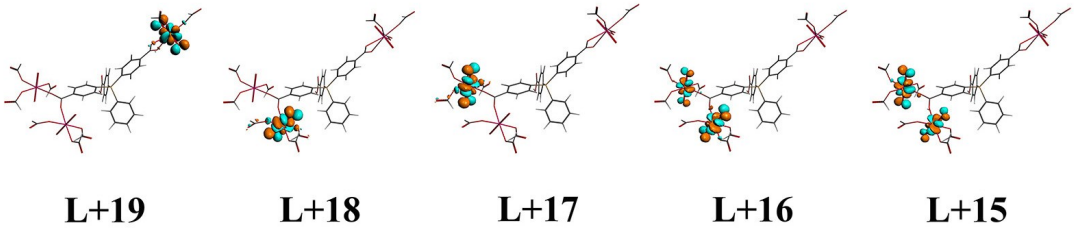
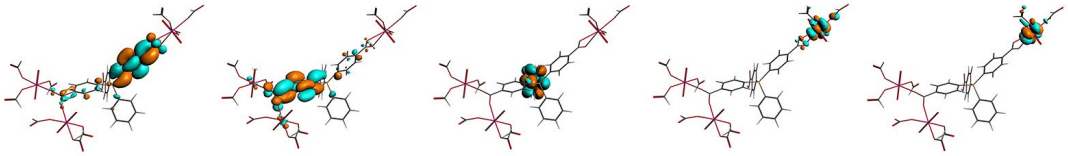


Figure S19. Diagrams of partial frontier molecular orbitals of **3b.**

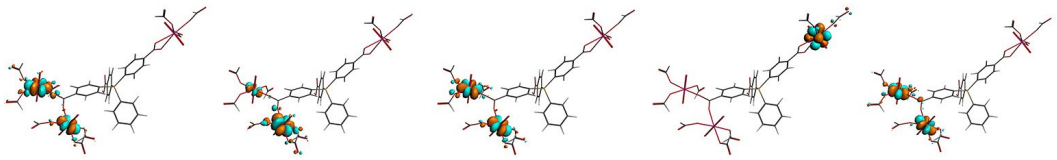
Unoccupied orbitals of **3c**



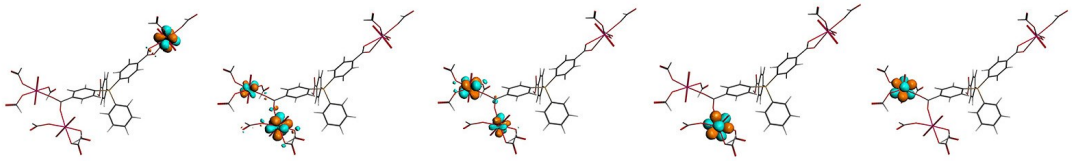
L+19 **L+18** **L+17** **L+16** **L+15**



L+14 **L+13** **L+12** **L+11** **L+10**



L+9 **L+8** **L+7** **L+6** **L+5**



L+4 **L+3** **L+2** **L+1** **L**

Occupied orbitals of **3c**

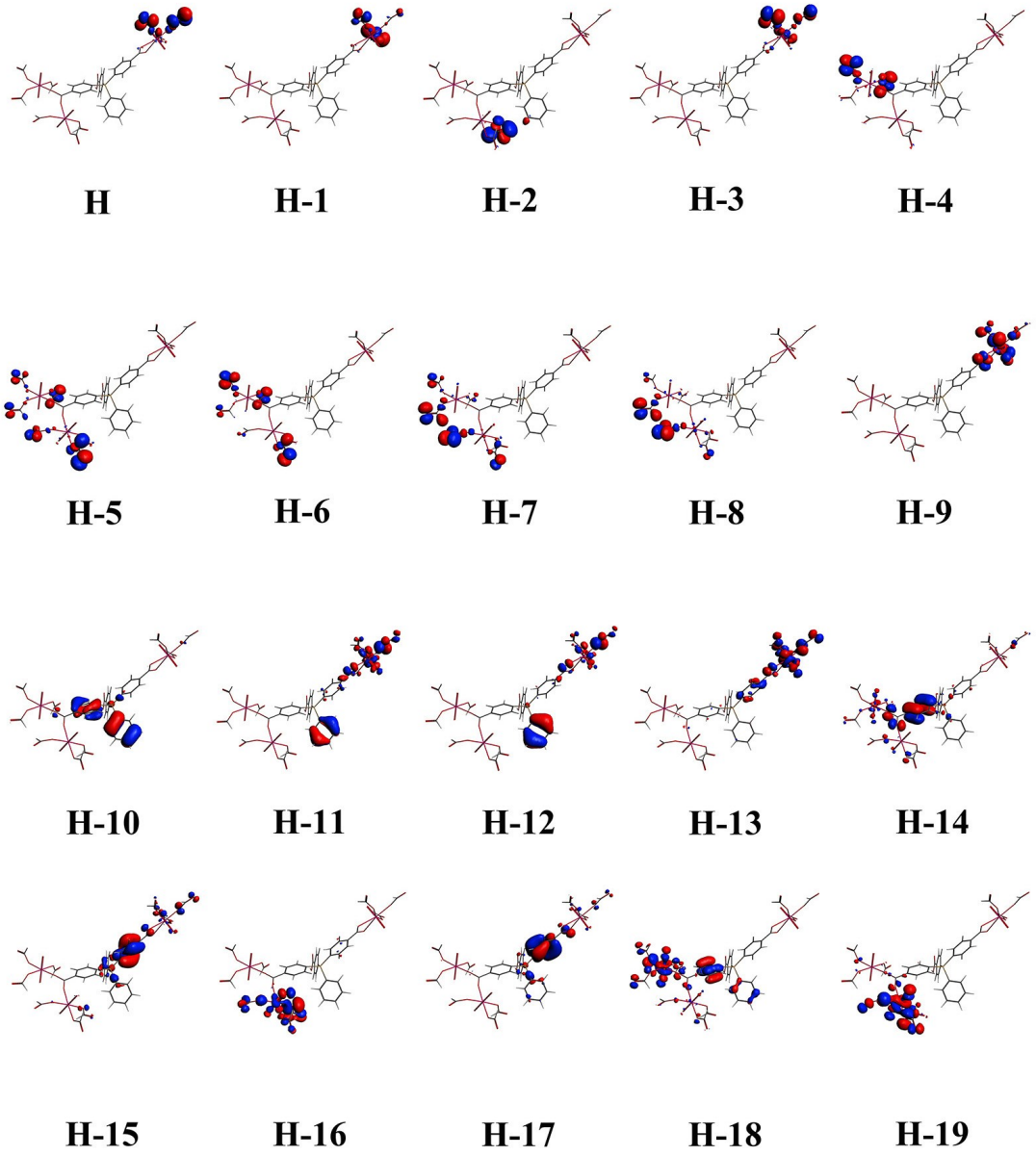


Figure S20. Diagrams of partial frontier molecular orbitals of **3c.**

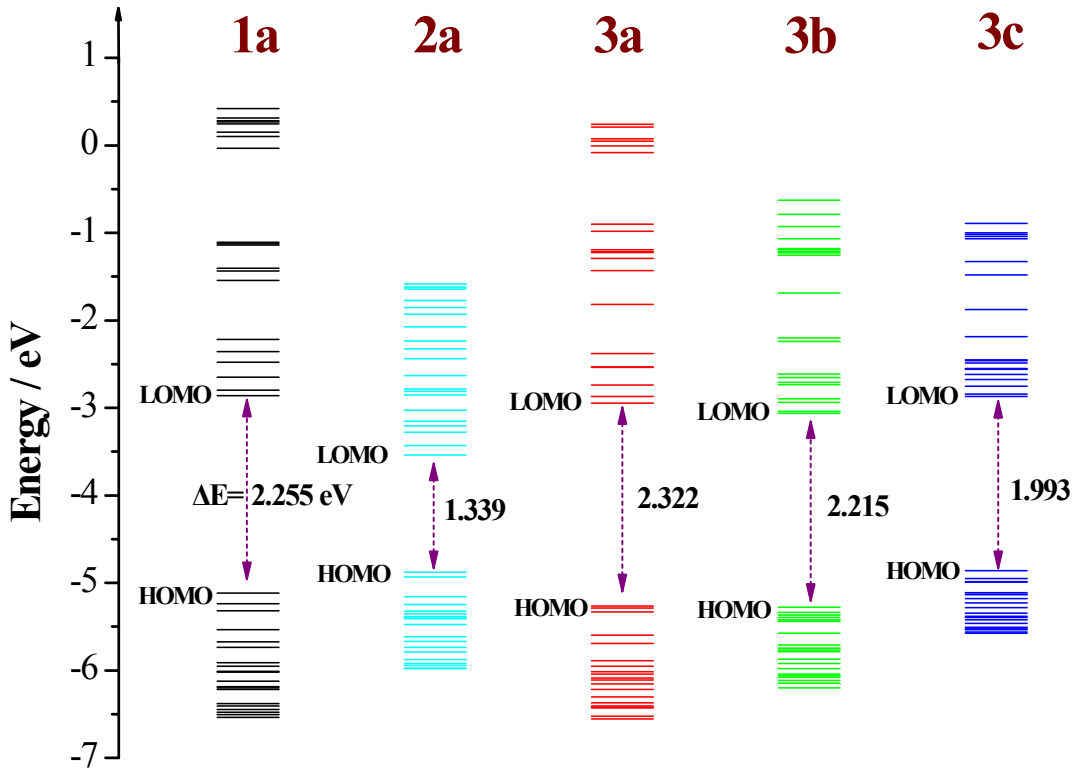


Figure S21. Energy levels of orbitals of the model compounds in solution.

Cartesian coordinates of optimized model compounds

1a

O	6.46484245	4.58348425	18.45838109
C	6.37027961	5.38433837	19.36741989
C	5.13765261	6.11357111	19.75834729
C	2.77400022	7.45102602	20.40294539
H	1.84052604	7.97275240	20.63481118
C	2.79496497	6.54002083	19.34020041
H	3.49506553	6.32225767	23.86309327
C	4.79654620	6.13827792	25.57414944
H	4.42327740	5.14491963	25.83877193
C	3.97030444	5.87208049	19.01597919
H	4.01807916	5.15968223	18.18913993
Si	3.95935681	8.98422421	22.59071429
O	-0.12083784	11.44369450	20.04513588
O	-1.75614489	11.88987448	21.49801843
O	7.73978681	9.83553644	26.41255432
O	7.83528681	8.06880154	27.82301403
C	-0.62991692	11.40452109	21.20364244
C	0.17007886	10.71340550	22.29833318
C	1.46145082	10.24870880	22.03036180
H	1.83870310	10.43977956	21.01822280
C	2.21973314	9.57931019	23.00967135
C	1.64550659	9.39447966	24.28300604
H	2.21309090	8.88255719	25.06706123
C	4.72876195	8.08998067	24.09580068
C	5.73126139	8.67642003	24.88132967
H	6.11164547	9.67039874	24.63376528
C	3.92932662	7.71380526	21.16063901
C	5.10782834	7.02773545	20.82147494
H	6.02705216	7.19784473	21.38937489
C	7.33636640	8.59444093	26.84414916
C	5.07263588	10.42983778	22.07411497
H	5.17094718	11.16431180	22.89046141
H	6.07690603	10.08437763	21.77799162
H	4.61974733	10.94901857	21.21290557
C	4.27252102	6.80727473	24.46272367
C	5.79193207	6.73461168	26.34134325
H	6.22379637	6.23804258	27.21337278
C	6.26990718	8.01031372	25.99784245
C	0.35954584	9.86847004	24.55996391
H	-0.06894294	9.72210107	25.55677940

C	-0.37633284	10.52506257	23.57233713
H	-1.38440799	10.91056163	23.75038461
O	7.44857131	5.70263116	20.15671637
H	8.17948396	5.16088695	19.79012736
U	-2.13769944	12.64944354	18.99603543
O	-1.30321322	14.22716675	19.35802462
O	-2.93780570	11.02960659	18.75791778
C	-0.70216693	12.44701562	15.90010908
O	0.19106348	12.08351562	15.13670482
O	-0.75246853	12.26214931	17.18406908
C	-4.95515415	12.64259386	20.78471166
O	-5.96610168	13.09611389	21.30988442
O	-4.00108107	13.32146634	20.20994603
C	-4.41261808	14.35529353	17.06457582
O	-3.37575977	13.60962891	17.31144372
O	-4.77317965	14.78256962	15.97231302
H	-4.99892874	14.59217639	17.99491786
H	-1.59845638	13.00184337	15.50896098
H	-4.77165894	11.53125805	20.76739472
H	1.88046089	6.35860942	18.76791731
H	8.43079467	10.09878117	27.05684677

2a

O	12.43012170	23.34840367	19.71476745
U	15.24967184	29.96855840	17.78231445
O	12.24553553	32.69186900	18.08076590
O	13.60283172	31.10543837	18.95640895
O	13.94537215	29.01424917	16.94011751
O	16.56467471	30.91343341	18.72184648
C	11.31137451	30.39869738	22.24690268
C	11.65223629	31.62549586	20.15385260
C	12.52875342	31.85115158	18.92992574
C	11.98460363	30.57774423	21.02330480
H	12.83289427	30.01231587	20.60968521
C	10.58173769	32.47280097	20.45209956
H	10.31115333	33.25354705	19.73866774
O	7.09115791	26.85468617	20.78875303
C	11.13093345	27.36394955	22.10144088
C	9.38495711	26.10844382	20.91758574
C	7.97647155	26.10727097	20.44371516
C	9.78970723	27.17303545	21.74855151
H	9.00489638	27.85972399	22.08399642
C	10.33377572	25.17078468	20.49427713
H	10.05427850	24.32162195	19.87033727

O	7.82697695	27.03285328	28.29546961
O	17.33211924	31.01538971	23.04380980
C	16.78965865	30.16066482	22.37470714
C	15.83077083	29.10168905	22.96585010
C	14.49493858	29.50082360	23.14150852
H	14.20314335	30.52351567	22.88292382
C	8.25703734	27.05217890	27.15776496
C	9.27963585	27.98512633	26.63172827
C	9.81643875	27.86524009	25.33549861
H	9.47504873	27.05576373	24.68684663
U	7.10467358	35.13795059	19.50535266
O	8.44772777	34.14731464	21.14602460
O	8.00500201	36.69214921	19.77731169
O	6.21726697	33.55704785	19.39085515
O	14.90577255	24.63285867	24.47541255
C	13.52413196	28.57715988	23.56730729
C	15.28065427	26.88588681	23.68419160
C	15.63626789	25.48030769	23.99439421
C	13.96744142	27.30533405	23.94252843
H	13.27616668	26.57274624	24.36940678
C	16.21354641	27.75741884	23.11170913
H	17.09951091	27.34030932	22.61771946
O	12.15769811	31.68742635	27.60586487
C	10.78259019	28.77917082	24.89414747
C	10.69664685	29.89200237	27.08560779
C	11.15821664	31.06294554	27.91858684
C	11.25495692	29.74077591	25.81679074
H	12.05836384	30.43543238	25.55457389
C	9.69023581	29.01201162	27.48692514
O	8.41556924	33.35807754	23.24595566
C	8.84108590	33.33272956	22.03219715
C	9.89595360	32.33164319	21.66998976
C	10.28244636	31.31321327	22.57021607
H	9.73722935	31.22267902	23.51459666
C	12.68622140	24.35009737	20.35767537
C	11.67390266	25.33551156	20.84401182
C	12.06445271	26.44775729	21.59787332
H	13.13108797	26.58421298	21.78568215
Si	11.64837953	28.84106640	23.22027311
H	9.21378385	29.11701051	28.46570729
C	4.29633981	36.03631652	21.30723640
O	5.56376715	35.97459671	21.15252707
O	3.68874992	35.87444548	22.39514715
C	4.77271701	36.78069743	17.42542497

O	3.63709418	37.15247742	17.69808833
O	5.56837787	36.05853738	18.15324444
C	8.92158364	34.31291148	16.61582040
O	8.67993345	34.86206670	15.55880071
O	8.39307873	34.59100625	17.78695769
U	7.40265984	34.26005203	25.13537917
O	6.42459460	32.76422124	25.39061588
O	8.45942358	35.71124907	24.91502981
C	6.36928477	36.64609588	27.15680038
O	5.72416809	37.15550839	28.05382112
O	6.38989955	35.37093179	26.83012634
C	9.19424583	34.08730570	27.79451531
O	9.75053702	33.68800898	28.84877167
O	8.92208463	33.36466203	26.76602025
C	16.67901331	27.66254591	19.71739041
O	16.72343826	26.85450692	20.65268631
O	15.61654619	28.23679862	19.23560326
C	14.89363679	32.18418228	15.08246686
O	15.75150999	32.78925671	14.45897880
O	15.08031147	31.46278519	16.17244275
C	18.08718682	29.35967364	16.13217129
O	18.86423978	28.70230568	15.44303623
O	16.82923615	29.09581638	16.34483261
H	3.71109563	36.26621777	20.39165882
H	7.04369360	37.26295218	26.50177729
H	8.87888125	35.14589226	27.75557593
H	5.25151509	37.06598393	16.45441262
H	9.67589720	33.48529644	16.72156627
H	13.82209243	32.19164868	14.76473031
H	18.44279877	30.29905193	16.64089699
H	17.60467080	27.90617050	19.14289998
O	16.85807484	29.97098475	21.06547710
H	17.01182489	30.74008647	20.40408267
O	16.94926251	25.18482706	23.70286279
H	17.01870692	24.23426487	23.93358372
O	13.94401903	24.70476613	20.72477082
H	14.57720330	24.09774378	20.29113562
O	7.77027285	25.13540901	19.46848594
H	7.16232237	25.57575211	18.83093800
O	7.80685079	26.14808177	26.22379229
H	7.12820603	25.64502503	26.72011369
O	10.37125346	31.34360587	28.94714743
H	10.12482824	32.40673108	28.95148213
O	5.65332348	35.06542071	23.71179330

H	6.13560052	35.38587298	22.91225737
H	4.71069358	35.35224715	23.31102436

3a

C	27.87863046	18.37364439	14.04252955
C	28.65511636	17.72671374	15.02298779
H	29.08274280	18.30915842	15.84601873
H	30.45143352	19.45224611	13.50966104
C	27.34523706	17.59068530	13.00339999
H	26.73758289	18.06765946	12.22789810
C	28.89345922	16.35182086	14.96505329
H	29.50646691	15.87250870	15.73365212
C	27.57887762	16.21436394	12.94293641
H	27.15659952	15.62593741	12.12319271
C	28.35454635	15.59216932	13.92354429
H	28.54299748	14.51587397	13.87473186
O	21.59294044	21.41721944	10.78168833
C	22.75437941	21.48530285	10.42558572
H	22.68819200	20.81610626	12.97693175
Si	27.61852108	20.26246728	14.10870192
O	33.72087316	22.70965464	11.96856667
O	32.53355012	24.59672363	11.90797633
C	29.14453952	21.18614758	13.51348584
C	31.42534570	22.60259578	12.62914290
C	32.64912853	23.35896669	12.13503693
C	31.50098247	21.22957064	12.88692660
H	32.46593100	20.74038099	12.72454995
C	30.20845671	23.26995277	12.81463046
H	30.18406758	24.34200691	12.59796055
C	30.37701181	20.52876188	13.32330224
C	26.12394422	20.68848942	12.99583520
C	24.79568240	20.61298089	13.46237382
H	24.60383378	20.35552136	14.50872527
C	23.93844589	21.22242673	11.27745552
C	23.71978879	20.87241128	12.62051743
C	25.25570573	21.31461084	10.79875488
H	25.43324794	21.59765188	9.75951923
C	29.08191046	22.57258744	13.24843743
H	28.13288011	23.10879115	13.36926113
C	26.32817293	21.05130335	11.64904151
H	27.34951692	21.14019201	11.26558325
C	26.32012927	19.87327709	16.66844548
H	25.95240074	18.93863379	16.23162399
C	25.94927027	20.20125677	17.96972962

H	25.28899135	19.54595329	18.54117817
C	27.29440655	22.21252014	17.82731942
H	27.67157137	23.11969524	18.30576517
C	27.65830898	21.87768062	16.52625189
H	28.34165084	22.53036926	15.97391586
C	27.17320197	20.70528228	15.91287294
C	26.43183542	21.38104040	18.56134952
C	26.07375702	21.78593032	19.94038524
O	35.51165109	25.16587745	12.82574622
U	35.00804865	24.79866531	11.11430505
O	34.43305630	24.38802776	9.43338871
C	36.55769253	22.03149315	10.11317640
O	37.34319248	21.08729704	10.13957224
O	36.46174670	22.98738778	10.98934054
C	33.24116903	27.35949905	9.94171815
O	32.75145541	28.48512983	9.89911942
O	34.02844940	26.89055505	10.86492237
C	37.83930449	26.54056094	11.00599636
O	38.79626089	27.12094704	10.50421267
O	36.87600229	25.93438529	10.37076432
O	26.45123267	22.79085772	20.51041013
H	37.72729717	26.49303417	12.12510667
H	35.82319955	22.12896803	9.26515683
H	33.02113929	26.61708567	9.12426924
O	23.09461277	21.82540783	9.13919110
H	22.23392272	21.97860978	8.69466814
O	25.23293781	20.88504054	20.55675570
H	25.08515355	21.27538803	21.44437963

3b

O	20.68438621	14.02463653	33.09449236
C	22.31708147	16.24145605	32.79742136
C	21.88060212	13.94623519	33.76866173
Si	25.61626964	18.85610235	32.94687866
O	22.15179372	12.98961069	34.46580510
O	31.05015308	18.76310057	28.70551074
O	30.20835593	16.75367084	28.20778705
C	29.06360118	18.07477790	29.84854472
C	28.30138103	16.99974660	30.32808798
H	28.50029390	15.97586849	29.99244350
C	27.27439658	17.21825087	31.24668915
H	26.70176195	16.35522633	31.60176416
C	26.96647532	18.51668692	31.69440045
C	28.77382250	19.37324961	30.29449984

H	29.35669743	20.23092084	29.94135536
C	27.73226643	19.59121821	31.19394448
H	27.51593417	20.62195709	31.49824339
H	24.54845464	18.73998892	35.77896360
C	24.53635015	20.33069134	32.39239997
C	23.83329359	21.13210996	33.31042891
C	30.18640908	17.84497116	28.85049725
C	24.45327572	17.35584720	33.19369772
C	24.86990701	16.22634516	33.92636252
C	23.16366383	17.33562599	32.63118526
C	24.39765467	20.61898392	31.02193874
H	24.95231011	20.02534931	30.28817185
C	23.58170049	21.66579660	30.58508597
H	23.50268507	21.87873067	29.51547896
C	22.88873291	22.44732872	31.51184875
H	22.25867099	23.27411378	31.17062483
C	23.01579717	22.17857181	32.87750068
C	22.74310810	15.13185911	33.54230155
C	24.02914635	15.13134570	34.10311932
U	32.53503116	20.51074499	29.42163145
O	32.29828736	19.93011347	31.13112344
O	32.76505756	21.10310870	27.71562861
C	27.88265700	20.33926503	38.55345046
C	26.07917921	19.48808447	37.09140353
H	25.48676604	19.38689990	38.00438120
C	27.38911089	19.98001762	37.20051303
C	28.17730145	20.10477529	36.04576941
C	27.65478446	19.75340897	34.80153529
H	28.28741802	19.84340041	33.91233170
C	26.33882398	19.27082038	34.67400685
C	25.56632556	19.13852579	35.84600282
H	23.94092425	20.94582769	34.38420949
H	22.48624138	22.79588761	33.60966756
H	20.23843895	13.17803677	33.30991427
C	30.23895769	22.83953762	28.74669747
O	29.20419626	23.47355790	28.89073660
O	30.68052967	21.88910914	29.53843730
C	34.41845623	23.24700265	29.48818134
O	35.01212162	24.19216939	29.98931285
O	33.80349314	22.28584902	30.13242974
C	35.03863338	18.50030616	30.23099623
O	34.42886522	19.24594396	29.33494830
O	36.20170948	18.13165324	30.18808498
O	27.67253446	15.75743976	26.97449198

U	29.25241491	14.85677939	27.06089884
O	30.82902445	13.95283963	27.15976754
C	30.86597889	15.29689858	24.20335288
O	30.90613351	15.38672518	22.98617901
O	29.82164979	15.54526253	24.96303500
C	29.30268114	13.08463552	29.87999082
O	28.99485345	12.78226425	31.02291055
O	28.72210839	14.00380812	29.14070844
C	26.95138626	12.85546519	25.76212216
O	28.18901260	13.03761057	26.15475890
O	26.48188693	11.82418588	25.30093497
H	34.36704393	18.21568123	31.08655266
H	34.35559532	23.12958620	28.37028986
H	30.92601987	23.03537180	27.87874128
H	31.76797972	14.98100830	24.79479256
H	26.31482852	13.77464642	25.88993051
H	30.14831735	12.57071753	29.34821782
O	27.24994633	20.24801425	39.58871107
H	29.20252096	20.47185166	36.12358438
H	24.35155585	14.25181940	34.66490134
H	21.32213661	16.23734543	32.34850423
H	22.81919206	18.19612071	32.04994385
H	25.87286006	16.20336926	34.36397727
O	29.17048832	20.80699448	38.53865715
H	29.37062258	20.99689934	39.47973219

3c

O	20.27625554	14.21614499	31.82194247
C	22.42582056	15.89307791	32.33342263
C	21.16761351	13.74144641	32.76076218
Si	25.94239946	17.56852901	33.95377554
O	21.00122600	12.65360651	33.27836719
O	29.94425189	18.03317712	28.45872320
O	29.63188916	15.81734291	28.34589328
C	28.80391183	16.96601940	30.26910486
C	27.92670349	15.93661170	30.64163126
H	27.80696260	15.06479759	29.98967079
C	27.16431567	16.05035909	31.80762880
H	26.43455107	15.26538780	32.03025960
C	27.27849288	17.16875762	32.65861824
C	28.98202886	18.05159779	31.14083153
H	29.67914386	18.85204508	30.87408192
C	28.24380452	18.14059207	32.32053544
H	28.37213823	19.02852655	32.94955392

H	24.17003297	17.33670455	36.27692442
C	25.36525025	19.35337342	33.57290668
C	24.78838653	20.17625038	34.55952975
C	29.51268507	16.93519738	28.92814178
C	24.45057545	16.40257527	33.60224894
C	24.29016060	15.18092679	34.28554698
C	23.49631466	16.73568078	32.62228490
C	25.50515788	19.88411404	32.27546996
H	25.97852140	19.29568120	31.48463260
C	25.09618825	21.18402023	31.96306364
H	25.27801441	21.55022752	30.94422556
C	24.51811503	21.97680466	32.95768959
H	24.20556219	23.00109769	32.72820160
C	24.36318102	21.47176169	34.25337366
C	22.27940414	14.68115116	33.02723229
C	23.22477917	14.33017803	34.00345220
U	30.28361156	20.36867983	28.03649290
O	29.50056973	20.23287014	26.39997328
O	31.03998383	20.51376843	29.68921662
C	26.75781537	17.29976711	40.16937575
C	25.34089000	17.31622678	38.07916296
H	24.48417743	17.27175450	38.75755175
C	26.61842225	17.33182717	38.65291006
C	27.73230950	17.37682462	37.80412787
C	27.57460640	17.41023916	36.41363830
H	28.46297634	17.44216684	35.77327215
C	26.29523791	17.40296469	35.82290651
C	25.18319312	17.35361799	36.69453708
H	24.69008949	19.80551761	35.58513389
H	23.92725623	22.09671599	35.03998647
H	19.64136965	13.47528262	31.72463808
C	27.06154328	21.10181507	28.28294629
O	26.00921620	21.46021439	28.80399630
O	28.18862274	20.85348422	28.89628990
C	31.19789018	23.53119559	28.48469191
O	31.28906771	24.72771802	28.23855968
O	30.59221390	22.63290475	27.75010134
C	32.86223326	19.59706894	25.98871253
O	32.32247214	19.99038597	27.11722955
O	33.83310365	20.09624044	25.43865953
O	28.60791091	14.48466379	25.83103850
U	29.67540149	13.76274230	27.11666977
O	30.73714530	13.03544954	28.40363281
C	31.70942436	14.97177154	24.76416893

O	32.46894555	14.64318175	23.86453778
O	31.50550527	14.31833636	25.88451750
C	26.51583684	13.07955515	27.77008322
O	25.56052944	12.57888102	28.34397864
O	27.75235450	13.12553188	28.21632432
C	30.20443071	10.56770708	26.33931894
O	29.62368494	11.70592753	26.06522164
O	30.09474497	9.52167567	25.70939714
H	32.34691549	18.70098511	25.54978419
H	31.65563003	23.09809098	29.41699171
H	27.12364073	20.96020393	27.17016902
H	31.11232297	15.92080378	24.69866710
H	30.85525172	10.61930336	27.25693730
H	26.40036030	13.56445025	26.76211310
O	25.69664527	17.18221892	40.85808505
O	27.90398376	17.39277719	40.69555223
O	26.68698062	19.06503198	43.11029143
U	26.89688558	17.25578952	43.11707721
O	27.11125790	15.44819582	43.01762833
C	23.93112843	15.81463660	43.62526786
O	22.76696040	15.70243474	44.00277809
O	24.64000557	16.90517102	43.59474580
C	30.20473858	16.69008352	43.15436658
O	31.34203091	16.78275075	43.60766036
O	29.19844469	17.47944706	43.40025354
C	27.89841669	17.48330891	46.39617318
O	27.67041552	17.47556030	47.60593468
O	27.05869720	17.22961908	45.43900091
H	28.92837726	17.72381113	46.01023665
H	24.49679614	14.91214438	43.25579580
H	29.94400855	15.85845927	42.44123080
H	28.72624130	17.38561261	38.26123615
H	23.10216783	13.37999284	34.52880273
H	21.69993094	16.16407473	31.56462327
H	23.59902153	17.67739821	32.07384459
H	25.01337827	14.89770988	35.05634535