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Supporting Information

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Table S1: The CHARMM force field is used for the CO₂ molecule. The detailed parameters are:

CO ₂	x	y	z	q (e)	ϵ_0 (kJ/mol ⁻¹)	σ (Å)
C	0.00000000	0.00000000	0.00000000	+0.60	0.2427	2.7849
O	0.00000000	0.00000000	1.16912100	-0.30	0.6904	3.0148
O	0.00000000	0.00000000	-1.16912100	-0.30	0.6904	3.0148

The form of potential energy used in the ABCluster program is:

$$U(\mathbf{Q}) = \sum_{I=1}^N \sum_{I < J}^N \sum_{i_I \in I} \sum_{j_J \in J} \left(\frac{e^2}{4\pi\epsilon_0} \frac{q_{i_I} q_{j_J}}{r_{i_I j_J}} + 4\epsilon_{i_I j_J} \left(\left(\frac{\sigma_{i_I j_J}}{r_{i_I j_J}} \right)^{12} - \left(\frac{\sigma_{i_I j_J}}{r_{i_I j_J}} \right)^6 \right) \right)$$

Table S2: The structural characteristics for the most stable isomers of $(\text{CO}_2)_n$ ($n = 1-4$) from B3LYP, B2PLYP-D, and M06-2X functionals (see Figure S1 and Table S3).

$n = 1$

	C=O (Å)	ν_3 (cm^{-1})
B3LYP	1.169	2410
B2PLYPD	1.174	2393
M06-2X	1.163	2468

$n = 2$

	C=O (Å)	C-C (Å)	ν_3 (cm^{-1})
B3LYP	1.168; 1.170	3.948	2411
B2PLYPD	1.172; 1.175	3.561	2396
M06-2X	1.165; 1.161	3.406	2475

$n = 3$

	C=O (Å)	C-C _{ave} (Å)	ν_3 (cm^{-1})
B3LYP	1.168; 1.170	4.242	2413
B2PLYPD	1.172; 1.175	4.003	2398
M06-2X	1.165; 1.161	3.820	2468; 2475

$n = 4$

	C=O (Å)	C-C _{ave} (Å)	ν_3 (cm^{-1})
B3LYP	1.168; 1.171	4.127	2410-2414
B2PLYPD	1.171; 1.173; 1.176	3.797	2395-2400
M06-2X	1.160; 1.162; 1.166	3.609	2459; 2468-2471

Figure S1: The optimized isomers of $(\text{CO}_2)_n$ for $n = 2-4$ at the M06-2X/6-31+G(d) level of theory. Indicated are the relative energies. The global minimum of $(\text{CO}_2)_2$ is found to have C_{2h} symmetry with C=O and C \cdots C distances of 1.165/1.161 Å and 3.406 Å, respectively, and a \angle C \cdots C–O angle of 58.1°, in good agreement with experiments.^{1,2} For $(\text{CO}_2)_3$, two near energetically degenerate C_{3h} planar cyclic and a C_2 twisted “barrel-shaped” structure are found, again in good agreement with experimental findings.³⁻⁶ Similarly, the trigonal pyramid structure of the global minimum of $(\text{CO}_2)_4$ has also been identified by experiment.^{6,7} Two isomeric trigonal pyramid structures have also been found for $(\text{CO}_2)_4$ with the same stability and almost identical infrared features (see Fig. S2).

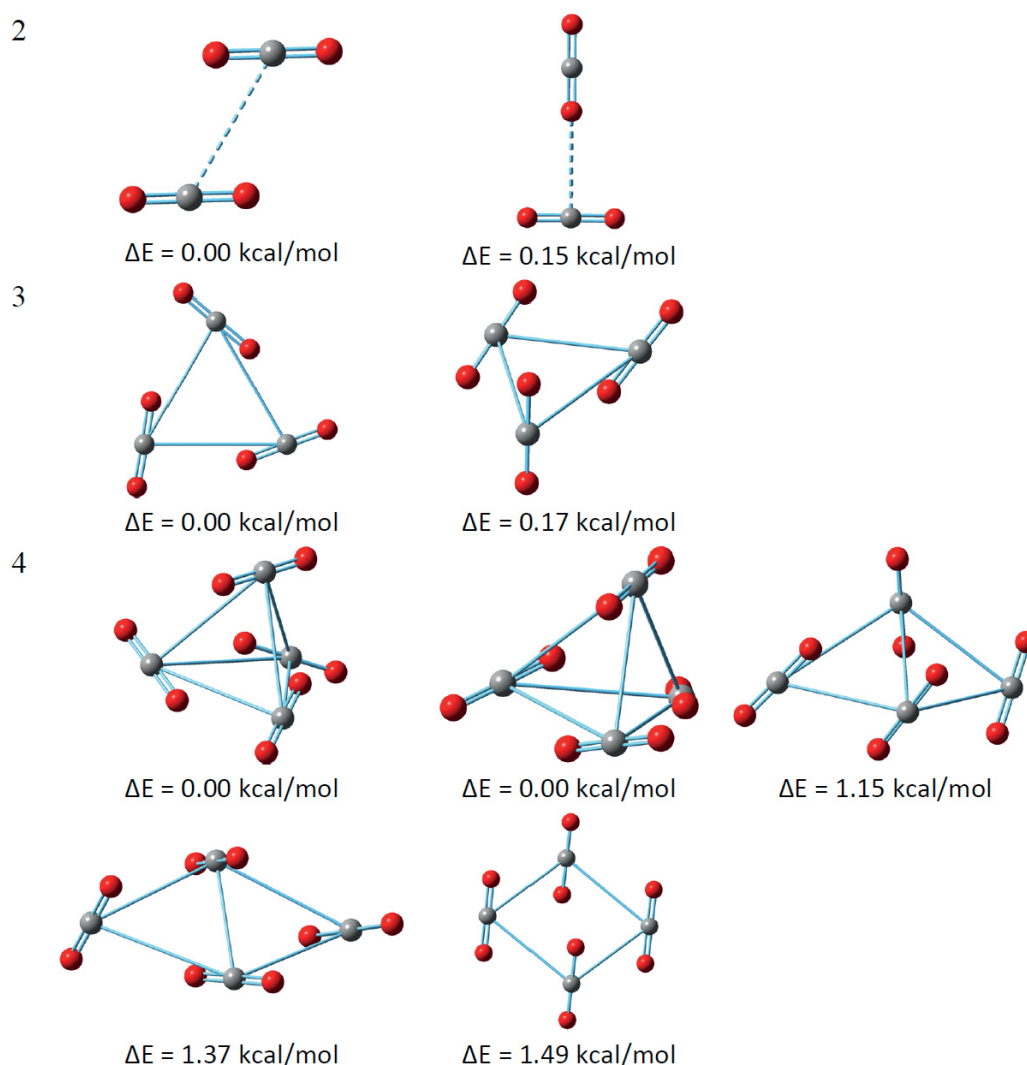


Figure S2: Infrared spectra of all calculated isomers of $(\text{CO}_2)_n$ for $n = 2-4$ calculated with Gaussian09 at the M06-2X/6-31+G(d) level of theory.

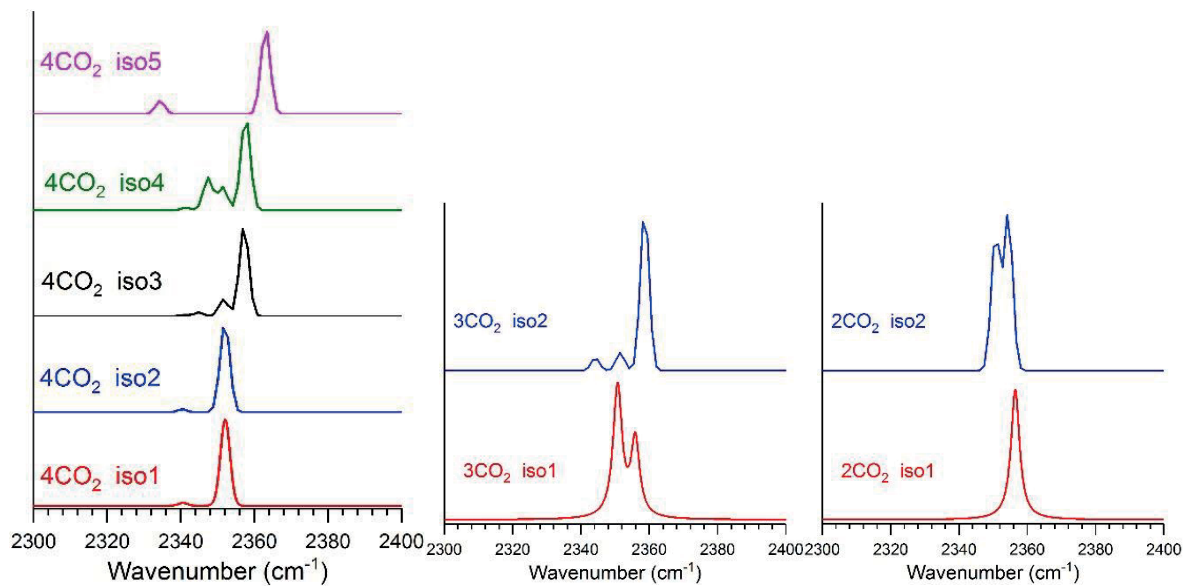
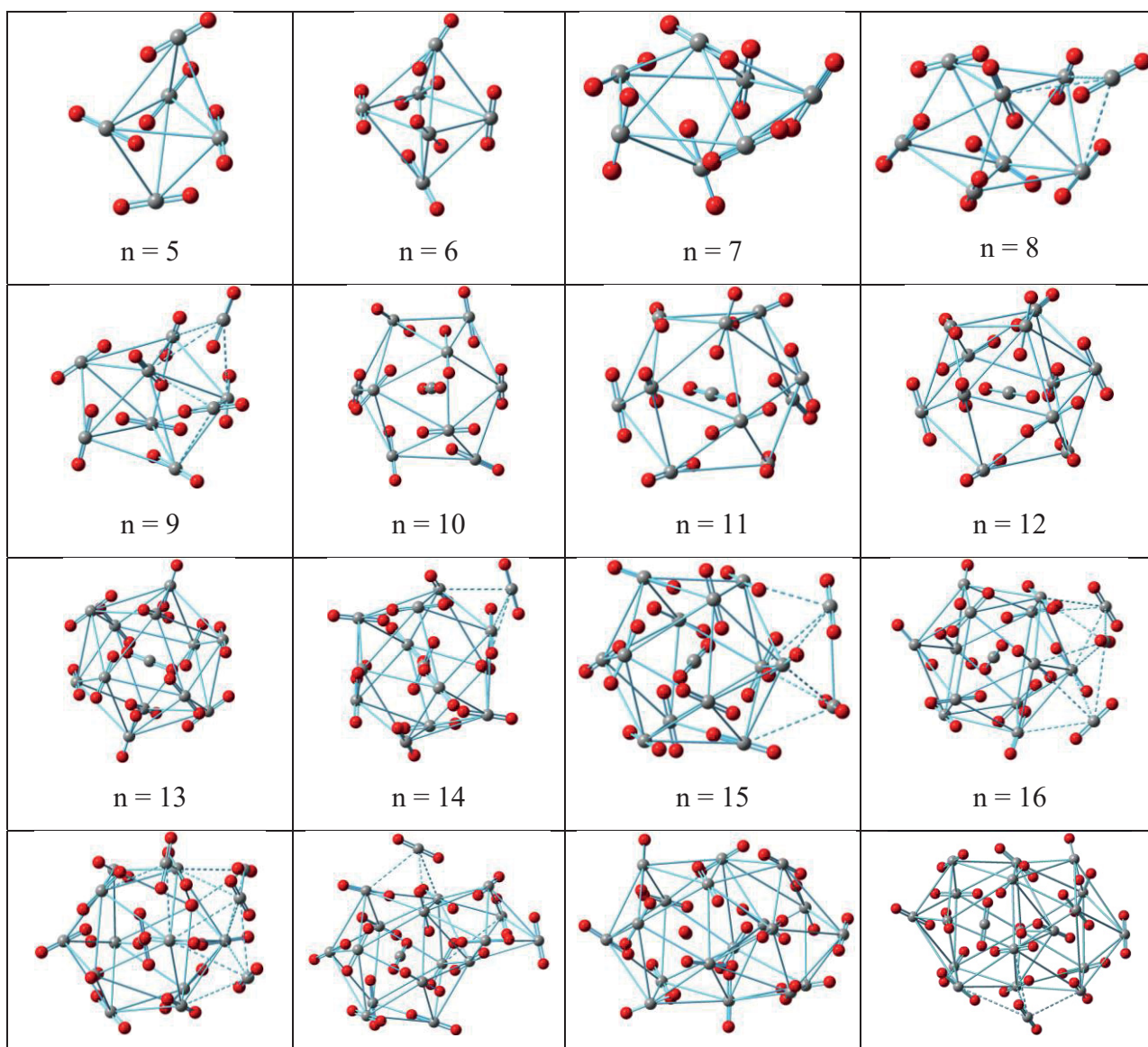


Figure S3: The most stable structures of $(\text{CO}_2)_n$ optimized at the M06-2X/6-31+G(d) level of theory for $n = 2-25$ and at the M06-2X/6-31G(d) level of theory for $n = 26-38$. The most stable isomer of the CO_2 pentamer is a trigonal bipyramid, and that of the hexamer a tetragonal bipyramid. The CO_2 heptamer is pentagonal bipyramid. To form larger clusters CO_2 molecules attach to the edges of the heptamer up to $n = 13$, which forms a symmetric icosahedron. This icosahedral motif is preserved (with some distortion) up to $n = 19$, for which a double icosahedron was found to be the most stable structure. The (distorted) icosahedral motif continues to be preserved up to the largest cluster size studied by DFT, i.e. $n = 38$ in the current study.



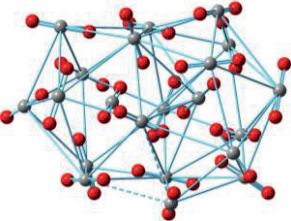
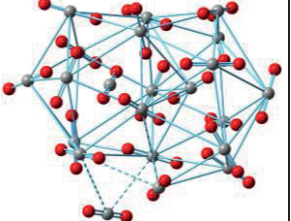
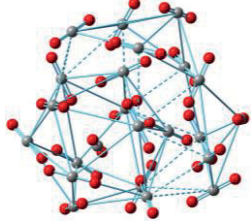
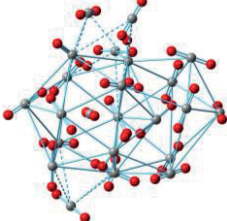
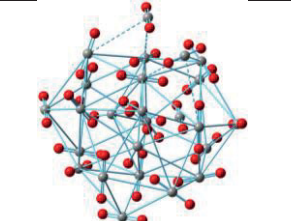
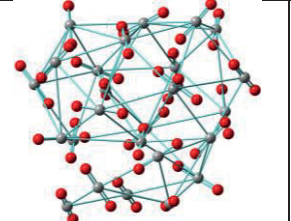
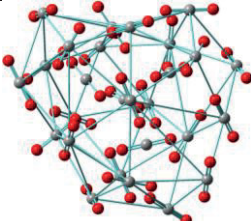
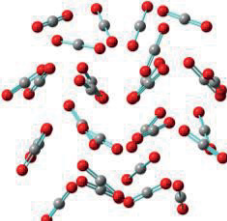
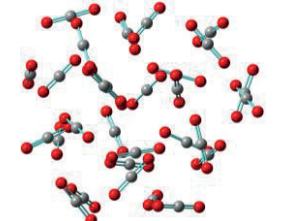
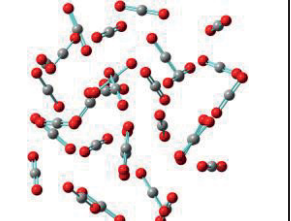
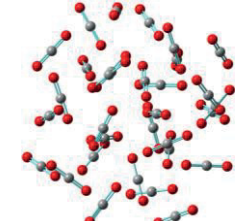
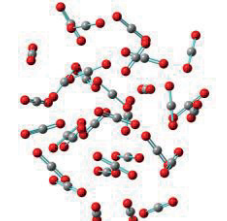
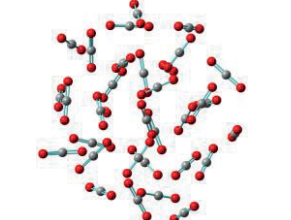
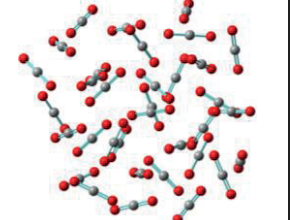
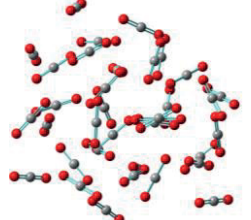
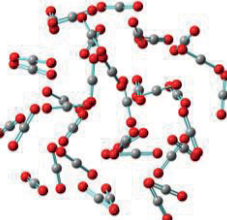
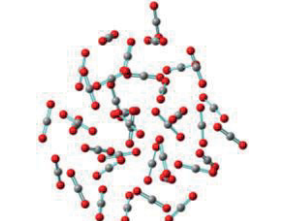
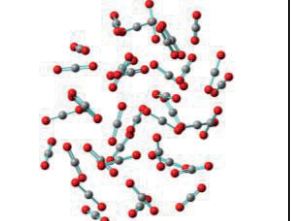
n = 17	n = 18	n = 19	n = 20
			
n = 21	n = 22	n = 23	n = 24
			
n = 25	n = 26	n = 27	n = 28
			
n = 29	n = 30	n = 31	n = 32
			
n = 33	n = 34	n = 35	n = 36
			
n = 37	n = 38		

Figure S4: The most stable structures of $(\text{CO}_2)_n$ for $n \geq 40$ from FF calculations.

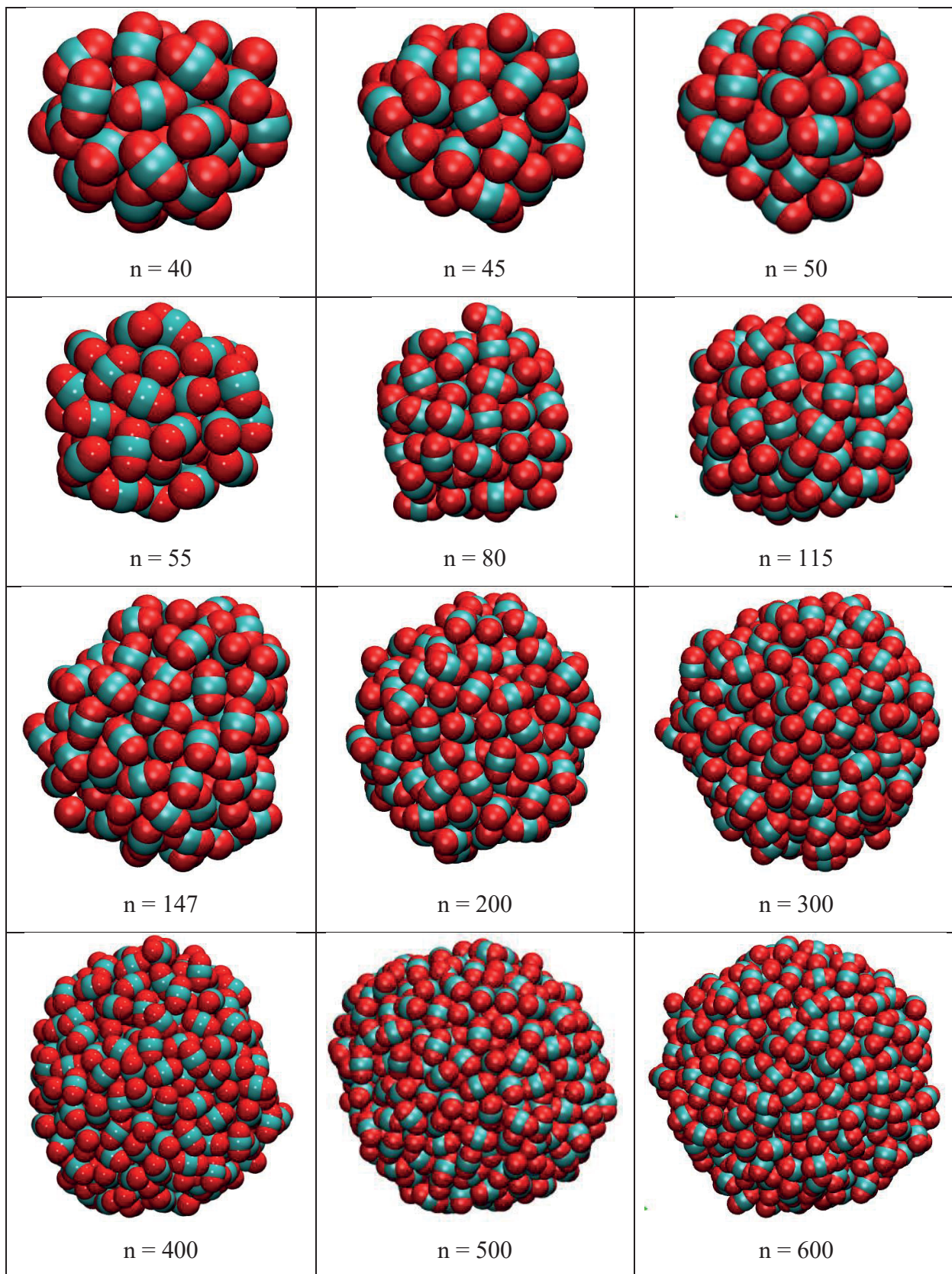
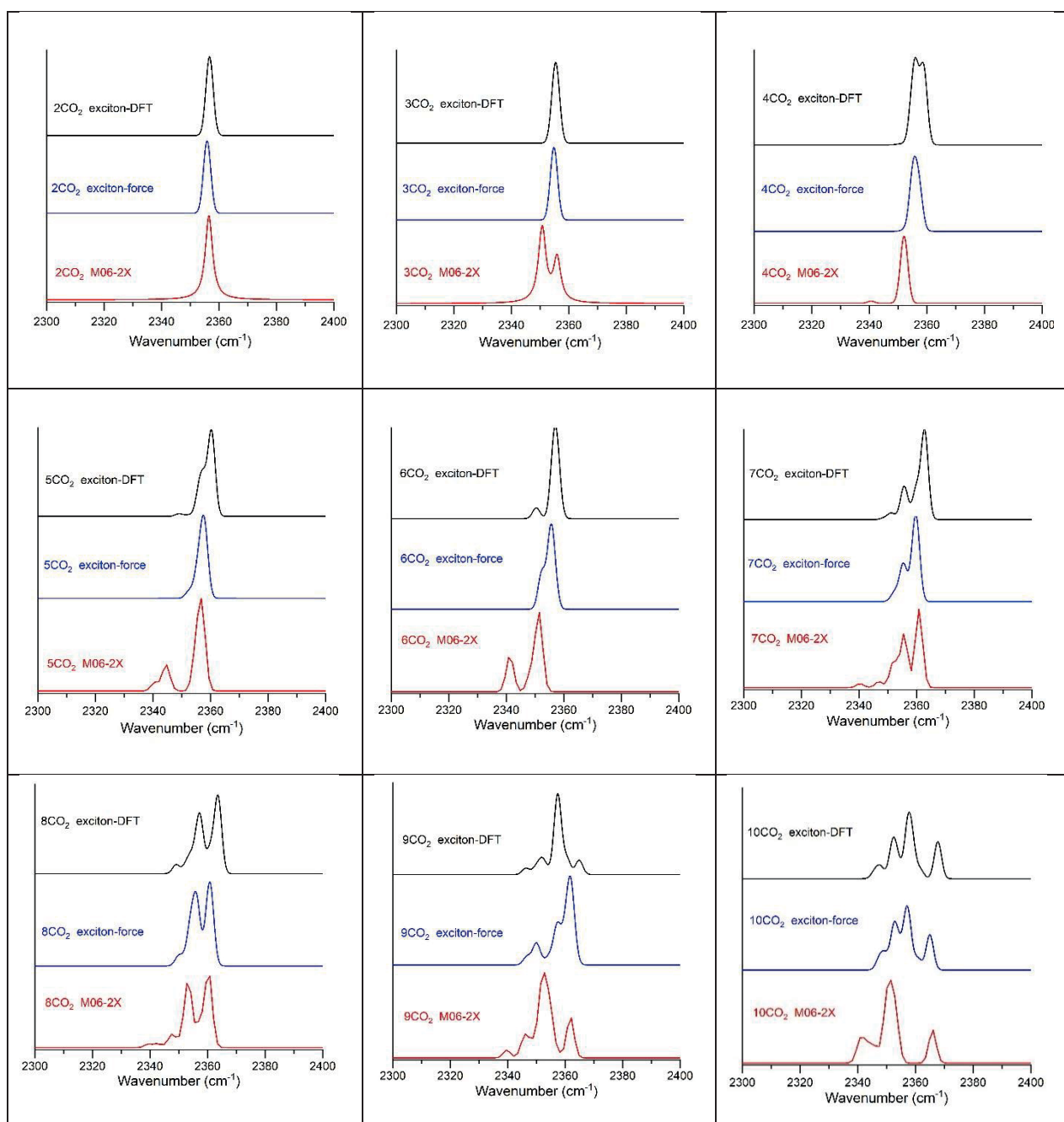
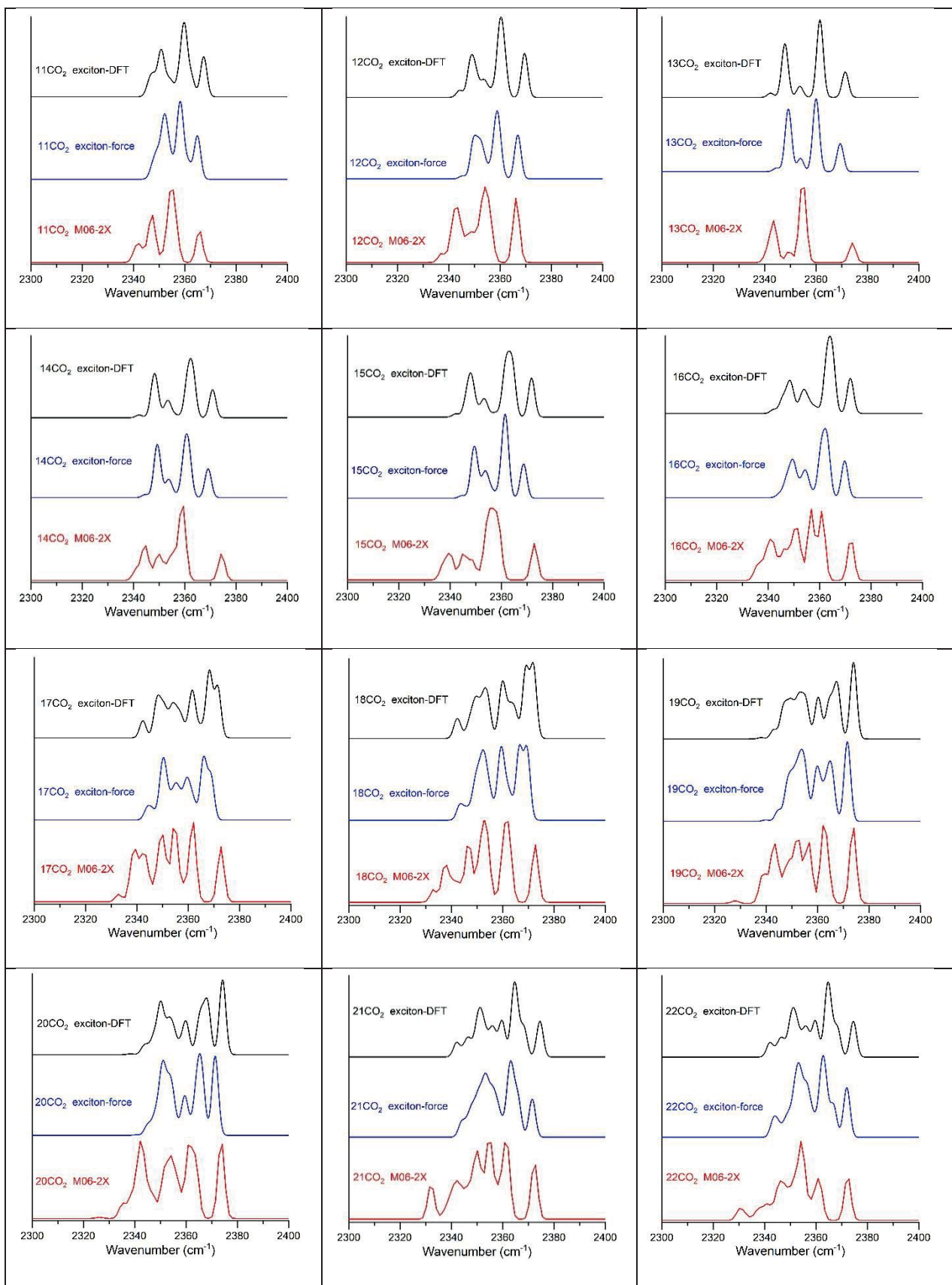
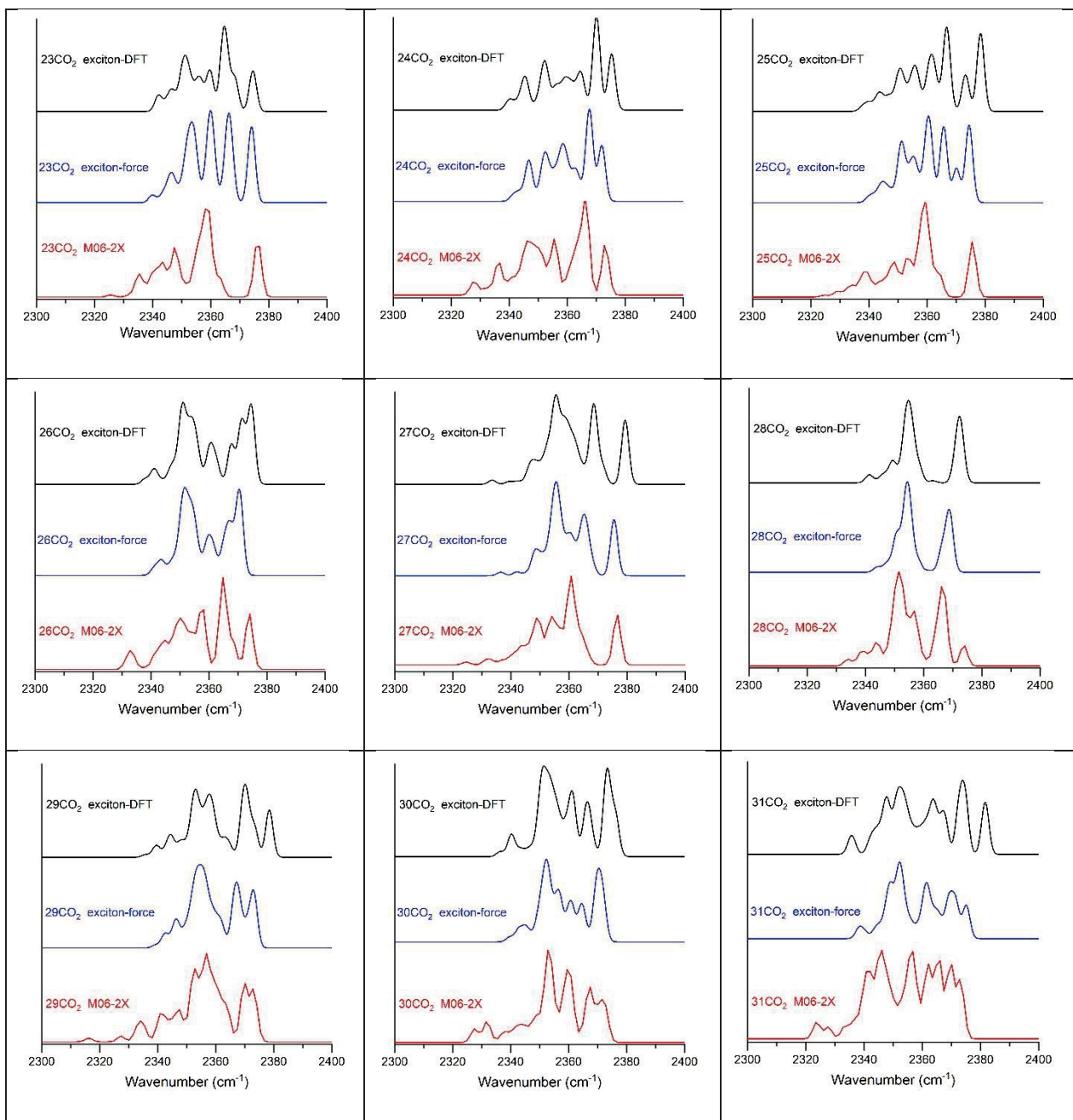


Figure S5: Calculated infrared spectra of the most stable $(\text{CO}_2)_n$ clusters for $n = 2-38$. The top (black) and the bottom (red) trace are infrared spectra calculated with the exciton approach and with Gaussian09 (harmonic vibrational calculations), respectively. Identical cluster structures obtained from optimization with DFT at the M06-2X (M06-2X/6-31+G(d) for $n = 5-25$ and M06-2X/6-31G(d) for $n = 26-38$) level of theory are used for both vibrational calculations. The middle (blue) trace shows infrared spectra calculated with the exciton model, but this time for FF structures without further optimization by DFT.







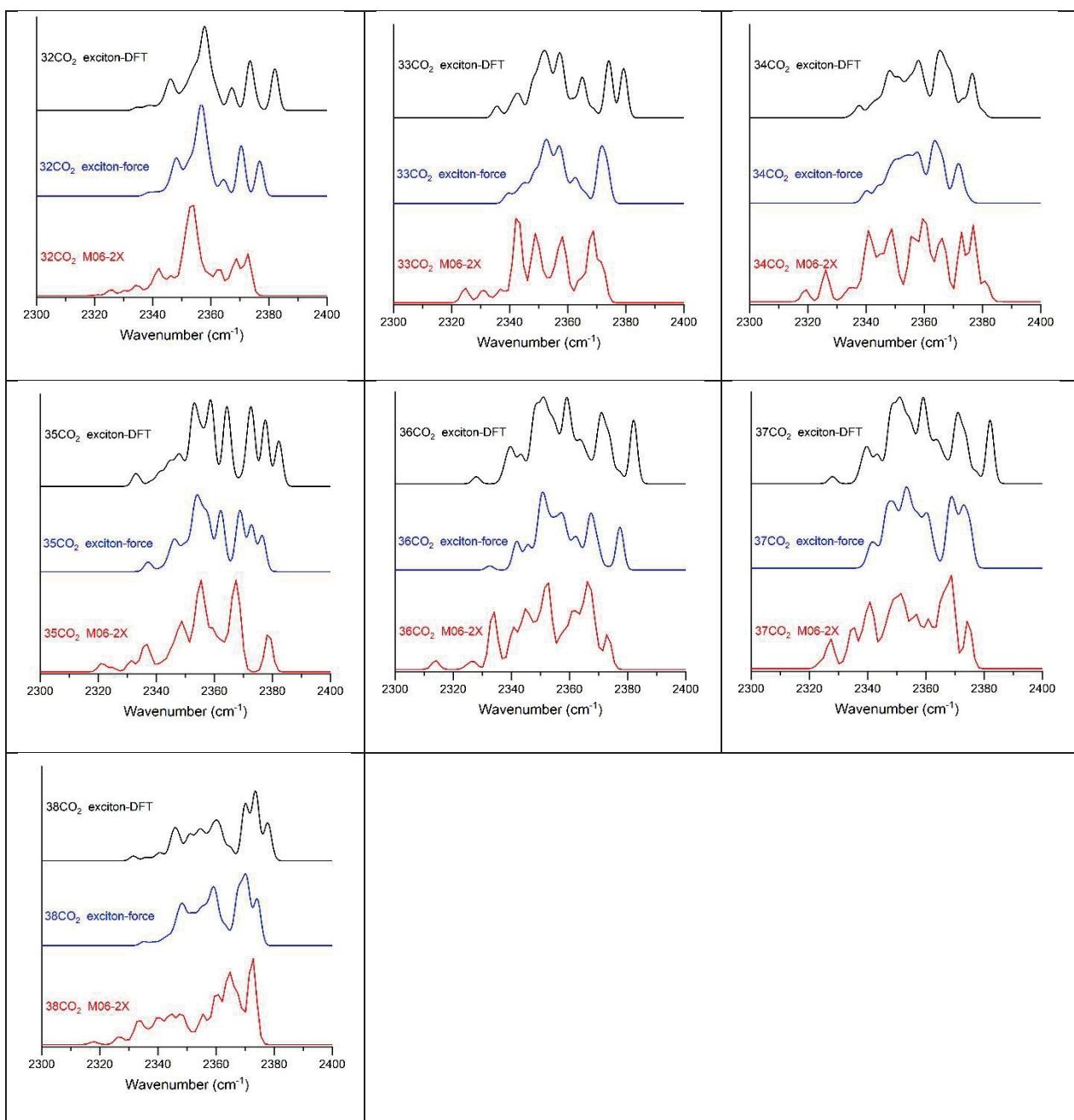


Table S3: Cartesian Coordinates of (CO₂)_n (n = 2-38, 40, 45 and 50)

n = 2	C	-1.67849400	0.28801800	-0.00001000	n = 3	C	0.07088000	2.20351100	0.00035100
	O	-0.90494300	1.15920600	0.00000500		O	0.95169300	1.44115100	-0.00054600
	O	-2.45500600	-0.57498500	0.00000200		O	-0.79096600	2.98071500	0.00149300
	C	1.67849400	-0.28801800	-0.00003000		C	1.87434900	-1.16353500	0.00070500
	O	0.90493300	-1.15919800	0.00001300		O	2.97800800	-0.80485800	-0.00250800
	O	2.45501500	0.57497600	0.00001000		O	0.77397000	-1.54571400	0.00376200
						C	-1.94523100	-1.04012800	-0.00102800
						O	-1.72444600	0.10368300	-0.00239800
						O	-2.18825800	-2.17486300	0.00017700
n = 4	C	0.82229300	2.14260300	0.22422400	n = 5	C	0.04483200	2.15259300	-0.42146200
	O	-0.20327800	1.59535200	0.32460100		O	-0.61647900	2.80552900	-1.11358600
	O	1.82924100	2.70877500	0.13185100		O	0.73431300	1.51400600	0.27028400
	C	-0.75410900	-0.74673800	1.74098800		C	-0.71151500	-1.39023900	-1.46249800
	O	-1.89438300	-0.52200800	1.74309500		O	-0.87533600	-0.23459500	-1.48752600
	O	0.38678600	-0.97588900	1.74848100		O	-0.55905900	-2.53883100	-1.45594600
	C	-1.79895200	-0.05924200	-1.27326900		C	0.58747000	-0.79024300	1.79991400
	O	-2.59949700	0.75557000	-1.47039800		O	-0.42888100	-1.09575400	1.31985600
	O	-0.99859900	-0.88773600	-1.08889200		O	1.59903200	-0.50129800	2.29091400
	C	1.72948900	-1.33742700	-0.68883800		C	-2.73432400	0.23954900	0.57852200
	O	1.56652100	-2.48551400	-0.64908800		O	-2.23044600	1.24490400	0.87915300
	O	1.91416700	-0.18794700	-0.74197900		O	-3.24980900	-0.758864300	0.28217500
						C	2.81214700	-0.21130300	-0.48878900
						O	3.65510000	0.57418100	-0.36268400
						O	1.97260800	-1.00976500	-0.62690700
n = 6	C	-0.84280700	2.51519700	0.10009800	n = 7	C	-2.85925900	1.06617700	-0.06101100
	O	0.03413500	1.99595100	-0.46859500		O	-2.23268100	0.70383000	0.85649400
	O	-1.71035300	3.05232300	0.64879900		O	-3.49173700	1.43712000	-0.95693500
	C	2.52225700	0.84264300	-0.09065300		C	1.59590400	-2.47273400	-0.15506500
	O	2.00451600	-0.03182900	0.48309700		O	1.26955300	-2.28512700	-1.25630500
	O	3.05786300	1.70781700	-0.64460600		O	1.91721000	-2.66954600	0.94431600
	C	-0.00328500	-0.00750400	2.37441200		C	0.05418400	2.74600300	0.50164600
	O	0.00089600	-1.17047500	2.38287000		O	-0.33466700	2.56735900	-0.58227200
	O	-0.00764400	1.15536900	2.38841900		O	0.41450800	2.92919000	1.58999300
	C	-2.51921700	-0.84326800	-0.09883600		C	-2.13224100	-2.09085900	0.08294000
	O	-2.00309000	0.03239100	0.47457800		O	-1.09824900	-2.29651400	0.57841600
	O	-3.05292900	-1.71044300	-0.65150700		O	-3.17039700	-1.89578800	-0.39813000
	C	-0.00001400	0.00643000	-2.37540100		C	3.04472700	0.87862800	-0.31399000
	O	1.16294800	0.00519800	-2.38605300		O	3.39320600	-0.22655600	-0.40950300
	O	-1.16297300	0.00784500	-2.38691800		O	2.71009100	1.98726900	-0.20440200
	C	0.84301400	-2.51333700	0.09012400		C	0.04219300	0.12339300	-1.92971100
	O	1.70903200	-3.05599300	0.63577400		O	1.09853600	0.50639400	-2.21928800
	O	-0.03236400	-1.98827600	-0.47566600		O	-1.02471000	-0.25628800	-1.65469000
						C	0.26462300	-0.25586000	1.86368500
						O	0.68911100	0.05172500	0.81762800
						O	-0.14737300	-0.54912800	2.90330700
n = 8	C	-1.02359400	2.65612400	-0.61342400	n = 9	C	0.04886400	-0.40443100	-1.31809600
	O	-1.64520000	2.44154100	0.34878200		O	-0.01379700	-0.26459400	-0.16008800
	O	-0.42697600	2.86889700	-1.58620000		O	0.12209100	-0.55801000	-2.46296400
	C	3.93995500	-0.21867300	-1.02121800		C	3.29636100	-1.82404000	-0.81108700
	O	3.04066700	0.41487100	-1.40873100		O	3.85477600	-2.83831100	-0.79737400
	O	4.84800300	-0.83385500	-0.64487100		O	2.74886400	-0.79273700	-0.83154900
	C	-3.50001800	0.34878900	-0.69256600		C	-3.08857500	-1.94253700	-0.85128100
	O	-4.43375000	0.57342300	-0.04577300		O	-4.20373700	-1.62683100	-0.79273700
	O	-2.56761900	0.13120600	-1.36235800		O	-1.97493300	-2.27849100	-0.92172400
	C	-1.12975300	0.21499300	1.97906900		C	-0.07449200	3.18070600	0.49825200
	O	-1.95393400	-0.43483900	1.47315700		O	-0.93372400	2.40036000	0.39663400
	O	-0.31819600	0.86264400	2.49744100		O	0.76444800	3.97612200	0.59881700
	C	1.44519800	-1.93212300	1.02584800		C	-1.66753100	0.12067200	1.93163800
	O	2.14721400	-2.03722900	0.10378300		O	-2.58245500	-0.12203000	1.25443100

O	0.74444700	-1.84022100	1.94845500	O	-0.76982500	0.37056000	2.62553800
C	0.32749500	-0.18272900	-1.49774100	C	-3.14743100	1.43001100	-1.00549400
O	0.36983700	-0.56459200	-2.58781000	O	-3.84128900	2.16908600	-0.44285400
O	0.27524400	0.20656600	-0.39522500	O	-2.45780600	0.69347300	-1.59092400
C	-2.02901500	-2.52821700	-0.34255000	O	0.11797200	-2.78792700	0.94618900
O	-0.87741300	-2.47795900	-0.51079800	O	-0.67573400	-2.54637200	1.75996500
O	-3.17770000	-2.59135200	-0.18770800	O	0.91035200	-3.04738600	0.13393600
C	1.97528300	1.63814100	1.17474400	C	2.67258600	2.02015400	-1.14064100
O	2.52931800	0.66921500	1.50789300	O	3.79388400	2.11241400	-0.85882300
O	1.44189500	2.61445500	0.84084100	O	1.54833100	1.93322800	-1.43774900
				C	1.84125300	0.20800900	1.75855300
				O	1.83863500	1.33281100	1.46036900
				O	1.87266400	-0.91375600	2.06107100
n = 10				n = 11			
C	3.26663500	1.17941700	-0.14106700	C	1.48598700	-3.03959400	-0.38538200
O	2.67575300	0.59983800	-0.96296600	O	1.12726100	-3.44231600	0.64400100
O	3.87078100	1.76148400	0.65906000	O	1.85119400	-2.65181800	-1.42008800
C	0.00284500	-0.02467700	-1.13071900	C	-3.30301100	0.23207200	-2.26580800
O	0.00503800	0.45025300	-2.18832800	O	-3.38520100	1.37894900	-2.08948900
O	-0.01185600	-0.50580700	-0.06807700	O	-3.24112900	-0.91369300	-2.45234600
C	0.34688600	3.35740800	-1.71164700	C	-1.53849300	3.09213700	-0.87468800
O	1.02666000	3.06509200	-0.81022100	O	-1.30018900	3.57522900	-1.90140100
O	-0.32027700	3.66482600	-2.60868400	O	-1.77522100	2.62556600	0.16794700
C	-0.32714000	-3.23368700	-0.15181200	C	0.09637700	2.05753800	2.36163400
O	-1.10687200	-3.07728000	-1.00130300	O	-0.42837000	1.02296600	2.25735500
O	0.45119500	-3.40717500	0.69369700	O	0.61344600	3.08952800	2.48239500
C	-3.42926900	-1.53074200	-1.23162800	C	-0.05844500	-0.05698500	-0.82727900
O	-2.83153500	-0.57865200	-0.91487000	O	-0.58707600	0.40347400	-1.75286000
O	-4.03951100	-2.46211500	-1.54838000	O	0.48021400	-0.51602800	0.09715700
C	1.57064400	-1.21651600	2.04399000	C	-2.92709500	0.18633000	1.37149500
O	2.50524900	-1.20042900	1.35096000	O	-3.33290500	0.56621400	2.38727600
O	0.65063000	-1.23715400	2.75368800	O	-2.54170800	-0.20088700	0.34004200
C	-2.75552800	2.03545700	0.01826000	C	3.38560000	-0.45037600	-2.22154400
O	-3.85256400	2.02376700	0.39218200	O	2.68104400	0.26547400	-1.62515800
O	-1.65505100	2.05711100	-0.36694500	O	4.09506500	-1.14244400	-2.81964300
C	2.93192000	-2.09580400	-1.39439500	C	-2.24187000	-2.80445100	-0.51134600
O	4.07175700	-2.05746200	-1.18268000	O	-3.27494900	-3.06226500	-0.05170300
O	1.79081500	-2.15285900	-1.62697800	O	-1.20174300	-2.56514000	-0.98097000
C	-1.92459800	-0.78650000	1.85030200	C	2.93291900	-0.23493400	1.25050800
O	-1.85240300	0.35608800	2.05896000	O	2.61990100	0.82461400	1.61636200
O	-2.02837300	-1.92575000	1.64318800	O	3.27346300	-1.28126500	0.87548600
C	0.31829000	2.31253600	1.85478900	C	2.20300200	2.71606000	-0.40163000
O	1.08089900	1.45785900	1.64447100	O	3.31630900	3.03479900	-0.44448600
O	-0.43084900	3.17069500	2.07867000	O	1.07953800	2.40478900	-0.36553500
				C	-0.03226900	-1.70292300	2.50696800
				O	1.04593100	-1.46480200	2.87022400
				O	-1.11690200	-1.94709800	2.16323700
n = 12				n = 13			
C	2.83176100	-0.83686000	1.49771600	C	-2.34629400	-2.48906900	-1.00788100
O	1.87256900	-0.17067000	1.49162300	O	-1.19943200	-2.29878800	-1.10706300
O	3.78589500	-1.49171300	1.51746400	O	-3.48295300	-2.69585600	-0.92041800
C	-3.02935800	0.92539100	-1.97758900	C	0.72475100	-1.62099500	-3.07107100
O	-3.97532500	1.55068200	-1.73466400	O	-0.14079800	-1.22555900	-3.73782400
O	-2.08578200	0.29221300	-2.23854400	O	1.59163300	-2.03462700	-2.41262300
C	-1.26512900	-2.38399800	-2.35522600	C	2.33898500	2.51225100	0.98519800
O	-2.29128300	-2.66403500	-1.88745900	O	3.47085000	2.73435900	0.87565700
O	-0.24266700	-2.10541900	-2.83750700	O	1.19712800	2.30542600	1.10634200
C	-2.86335900	-1.77549400	0.84589200	C	-0.71781800	1.61963300	3.07482500
O	-2.35185700	-2.75546600	1.20348200	O	0.14871200	1.22519100	3.74077000
O	-3.39070700	-0.79763500	0.49744900	O	-1.58579600	2.03231100	2.41706100
C	0.03802200	0.04481700	-0.50635700	C	-1.03932800	3.41766400	-0.14960500
O	0.60418000	1.00414700	-0.84241300	O	-0.64729200	4.45491600	0.18606200

O	-0.51833200	-0.92117200	-0.18157400	O	-1.44891400	2.38164000	-0.49658900
C	-2.43611500	1.78804000	1.43839600	C	-3.48192700	0.71999800	0.40516100
O	-1.89781000	1.72719900	0.40386100	O	-4.20928900	1.61596900	0.30056900
O	-2.97934900	1.86892300	2.45746400	O	-2.76548400	-0.19430400	0.51558100
C	-0.52656000	3.50242600	-1.20706000	C	1.02958800	-3.42023800	0.14784400
O	-1.15295800	3.13399600	-2.11412600	O	1.43903800	-2.38447600	0.49665600
O	0.09120700	3.89054600	-0.30099900	O	0.63856200	-4.45704600	-0.19026800
C	1.39070900	2.48940300	1.68071000	C	3.48225100	-0.71885400	-0.38786300
O	0.38694400	2.25496900	2.22183000	O	2.76691400	0.19559800	-0.50384500
O	2.40394700	2.72035900	1.16114600	O	4.20914700	-1.61447500	-0.27732100
C	0.36037900	-3.35333300	0.67620300	C	-1.66827000	-1.83157100	2.53872100
O	0.74288000	-2.86664800	1.66255800	O	-1.91403700	-0.99049100	3.30167700
O	-0.00561900	-3.85406400	-0.30598500	O	-1.43835200	-2.68440600	1.77955300
C	2.55466900	-1.65447300	-2.03715600	C	0.00338700	-0.00068200	0.00224100
O	2.97818700	-1.47820900	-3.10076900	O	-0.06263500	-0.15250500	1.15179300
O	2.12942900	-1.82824300	-0.96433200	O	0.06833400	0.15208700	-1.14732400
C	-0.21852900	-0.54021300	3.28371700	C	1.66849800	1.83349800	-2.53440000
O	0.59708200	-0.70441200	4.09220000	O	1.43464200	2.68551200	-1.77542200
O	-1.05061900	-0.37276600	2.48547400	O	1.91810700	0.99283400	-3.29648500
C	3.16770200	1.79085100	-1.33564200	C	1.82464300	-0.94606100	2.90491800
O	2.79469100	2.78457700	-1.80283800	O	2.60160500	-0.24283100	2.39787300
O	3.55215400	0.78542400	-0.88604000	O	1.06254300	-1.65898300	3.41548000
				C	-1.81837700	0.92428300	-2.90828300
				O	-2.58857700	0.21229400	-2.40311300
				O	-1.06372300	1.64660200	-3.41663000
n = 14				n = 15			
C	-3.21531000	-1.86041100	-1.05098300	C	-0.66627700	-0.02839300	0.02568300
O	-3.86174500	-1.99755000	-2.00254000	O	-0.02931400	0.61016000	-0.70634700
O	-2.57637900	-1.73455000	-0.08247900	O	-1.30268200	-0.66857700	0.75669900
C	-0.36784000	-0.01679700	0.00140600	C	2.17387600	-0.10578200	-2.08119500
O	-1.16700800	0.55144600	0.62435100	O	1.68295500	-1.12249800	-2.36110700
O	0.42943400	-0.58612400	-0.62250900	O	2.66482600	0.91244300	-1.80803500
C	-1.80534700	0.71872500	-3.21549000	C	2.37244400	-0.33326900	1.85173800
O	-2.06947000	1.62479100	-3.88727500	O	1.99532300	-0.62351300	0.78343400
O	-1.54384100	-0.20591400	-2.55347300	O	2.74986400	-0.05003900	2.90811100
C	-0.90072200	2.49830900	2.46862800	C	1.28245400	2.94845000	-0.36204400
O	-0.18191100	3.07758100	1.75889800	O	0.85203900	3.35572000	-1.36012500
O	-1.61001800	1.92933100	3.19165400	O	1.71721400	2.55479700	0.64534000
C	-0.80944100	-3.33068700	1.35434700	C	1.18637900	-3.05699200	-0.36649600
O	-1.63560600	-4.14158000	1.40479300	O	2.27875700	-3.41293100	-0.20666600
O	0.03428600	-2.52594900	1.31275900	O	0.08377000	-2.71622800	-0.52901500
C	0.00307700	3.31894000	-1.27353500	C	-1.17899300	-2.02040200	-2.91596400
O	0.80194200	4.15753200	-1.23823400	O	-1.44206800	-0.95113400	-2.53029500
O	-0.81422300	2.48749500	-1.32053500	O	-0.92400200	-3.07844400	-3.31364500
C	-3.34387600	1.95382900	-0.13711200	C	-2.48873000	3.08272200	0.16331800
O	-3.58866900	1.15477800	-0.94804300	O	-3.52585400	3.49262400	-0.15148900
O	-3.11107400	2.76463400	0.66149600	O	-1.44021700	2.68654700	0.48724700
C	-2.88055200	-0.51746200	2.42466100	C	-0.63119000	-1.77955000	3.12450300
O	-3.74356200	0.12189600	1.98152000	O	0.36315200	-2.17359800	2.66517000
O	-2.02958900	-1.17125600	2.87644100	O	-1.61536000	-1.38480400	3.59970000
C	5.11967300	0.01489500	-0.15077500	C	-0.74951100	1.75667900	-3.06648000
O	5.48024300	-1.04804800	-0.45098000	O	0.22512500	1.36389200	-3.56200400
O	4.77408900	1.08379200	0.15386000	O	-1.73530500	2.15106600	-2.58864600
C	0.99860400	-0.73902500	3.22077200	C	-3.55030500	0.06431100	2.08603200
O	0.80993400	0.18974500	2.54042900	O	-3.07683700	1.09325500	2.35619500
O	1.19377100	-1.64952100	3.91048100	O	-4.04270700	-0.95363800	1.81946200
C	0.11802500	-2.46800200	-2.52209000	C	-0.30546500	2.04086100	2.92471000
O	-0.63867500	-3.04621500	-1.85258000	O	-0.62330000	3.07756400	3.33359000
O	0.86667100	-1.90000400	-3.20588500	O	0.02493000	0.99521100	2.52724000
C	2.17821500	0.49705100	-2.36521200	C	-2.61963700	-2.98083400	0.34269200
O	3.01634300	-0.18056400	-1.92714000	O	-2.23214600	-3.38703900	1.35958700
O	1.35459300	1.18231400	-2.81637100	O	-3.01065100	-2.59135600	-0.68273700

C	2.55248800	-2.07604200	0.13157900	C	-3.81500000	0.20237600	-1.67139700
O	2.82632700	-1.28599500	0.94411000	O	-4.31517400	-0.15530800	-2.65336400
O	2.28970900	-2.87317800	-0.67005200	O	-3.32722100	0.57050500	-0.67740800
C	2.35203400	2.00698500	1.11334300	C	4.45974900	1.95845200	-0.00510700
O	2.86772800	2.31166000	2.10437900	O	4.44654300	2.96122300	-0.58913700
O	1.82743000	1.70921900	0.11327000	O	4.48990100	0.95847800	0.59238700
				C	4.53029300	-1.75570800	-0.05406300
				O	4.67648600	-2.02702200	1.06608400
				O	4.39188900	-1.48204400	-1.17717600
n = 16				n = 17			
C	-1.59011500	1.54713400	2.04257600	C	-2.05834200	-3.01946200	1.51702200
O	-2.11075100	1.62782200	1.00170600	O	-2.98605100	-2.70438500	2.14110600
O	-1.07932300	1.48170200	3.08140100	O	-1.13638400	-3.35228200	0.88865100
C	2.33054600	-3.03731300	1.21844000	C	3.81977900	-0.90971500	3.23998300
O	2.35939200	-4.16917400	0.97444300	O	4.87489800	-0.42582800	3.25023500
O	2.30983700	-1.90020400	1.48045900	O	2.76567600	-1.40612600	3.24793200
C	-2.31491600	-0.09995200	-1.42652000	C	1.89041500	1.64632100	1.29219400
O	-2.95476700	0.67315000	-2.00469400	O	2.89464300	1.21128200	1.68102300
O	-1.67292400	-0.88220500	-0.84302300	O	0.88348100	2.09017800	0.91310700
C	0.61230300	0.34975300	-3.51681600	C	-1.87129400	0.62155100	-3.32374000
O	1.40998200	1.17442300	-3.70168500	O	-1.62853200	1.75388200	-3.42304700
O	-0.19734900	-0.46886400	-3.34539600	O	-2.12954400	-0.51004600	-3.23762000
C	-3.85925100	2.97108700	-0.68108100	C	3.55715400	3.02944100	-1.50503100
O	-2.98962800	3.57256100	-1.16503300	O	3.31310700	3.28288100	-0.39510500
O	-4.73815600	2.38916000	-0.19069300	O	3.80062500	2.79161700	-2.61546000
C	4.14744200	0.16102900	1.50556900	C	4.59400600	-0.20859100	-0.05626300
O	4.85405100	-0.48148000	2.16119500	O	4.12110700	-1.16108400	0.41972100
O	3.44750800	0.81980900	0.84393500	O	5.08301900	0.72987200	-0.53356000
C	-4.49803900	0.05254400	1.33801500	C	2.35112600	-3.08345900	-2.50954700
O	-4.40584500	-0.50426500	0.31866500	O	1.79230300	-4.06417800	-2.78204800
O	-4.59817800	0.60104700	2.35571800	O	2.91231100	-2.09728500	-2.24606000
C	-1.40125700	-2.01897900	1.73562400	C	-1.44328900	3.09377800	2.03090500
O	-0.65300600	-2.82075100	1.34858800	O	-0.82987800	3.97382100	2.46808300
O	-2.14797600	-1.21899700	2.12931300	O	-2.07669100	2.21337000	1.60008200
C	-0.15273400	-3.13898300	-1.45757200	C	-4.23788600	-1.38661000	-1.07198100
O	-1.15813300	-3.61448500	-1.78669500	O	-5.28818500	-1.02451100	-1.40347800
O	0.86639000	-2.67477500	-1.13506700	O	-3.18569900	-1.76731900	-0.74396700
C	3.30127600	-1.68129000	-2.09163000	C	-3.63687400	0.03787300	2.52821900
O	2.81411200	-1.50601300	-3.13185100	O	-4.31798700	0.07445500	1.58406600
O	3.79659400	-1.87268100	-1.05570000	O	-2.96998000	0.01260500	3.47883700
C	-0.24586500	3.13528600	-1.30353500	C	1.65337200	0.36956400	-2.26834000
O	-0.41898400	1.98754500	-1.43240500	O	1.04709400	0.15448600	-3.23383200
O	-0.07352900	4.27413700	-1.18526400	O	2.27087600	0.58284600	-1.30271300
C	1.18087800	-0.26775600	3.53350300	C	1.56672300	-2.14209100	0.62638400
O	1.95066900	0.58816800	3.35779200	O	1.93070400	-3.22128000	0.40784500
O	0.42290500	-1.12722600	3.72426400	O	1.19930500	-1.05628400	0.83969800
C	-3.69351900	-2.94188000	-0.78105000	C	-0.88985600	-2.92960100	-1.91269300
O	-4.02155200	-2.55414000	-1.82595300	O	-0.13194600	-2.11556100	-1.55250800
O	-3.36993600	-3.33126000	0.26728400	O	-1.62710300	-3.74044200	-2.28407800
C	1.94392700	3.05915900	1.59962500	C	-0.24939100	3.24657300	-1.43842100
O	0.95125100	2.65168300	1.14152900	O	-1.22060900	3.52457600	-0.86172100
O	2.92076900	3.47918800	2.06038800	O	0.72539900	2.98788600	-2.01723200
C	3.32820600	1.90766200	-1.71472700	C	-1.07941700	0.09460300	0.03766300
O	2.63234900	2.74928200	-1.31058800	O	-0.65947800	0.61907200	-0.91061000
O	4.03724400	1.07963700	-2.11615200	C	-1.49378700	-0.42927900	0.98758500
C	0.90987900	-0.00622700	-0.00598200	O	-0.05543500	-0.61930100	3.30878700
O	1.52230400	0.02211500	-0.99201000	O	-0.34745600	-1.74303800	3.35044700
O	0.29561200	-0.03836200	0.97970300	O	0.23922200	0.50672200	3.27638200
				C	-3.90907000	2.15803300	-0.48898500
				O	-3.39502200	1.23705600	-0.98920100
				O	-4.43072900	3.07314000	-0.00717500
n = 18				n = 19			

C	-0.42448100	-1.69710100	-3.00869600	C	-2.69084100	2.35745100	2.49908600
O	0.45802800	-1.02025900	-3.34724600	O	-1.94615700	3.25018600	2.55283400
O	-1.29963000	-2.39005400	-2.68069400	O	-3.43764700	1.46858400	2.43543300
C	-1.40702700	-0.17838700	0.00158300	C	2.91734000	-2.45234300	2.43545600
O	-1.12062600	0.15333500	-1.07485300	O	2.01186200	-3.17752400	2.50213100
O	-1.68962000	-0.50979400	1.07783400	O	3.82892400	-1.72993000	2.38390500
C	-4.60607900	1.32669200	-0.06387600	C	2.86086500	-3.16582500	-1.13243500
O	-5.63429400	1.20832300	-0.58410300	O	2.34119100	-2.75105600	-2.08863500
O	-3.57707100	1.45826300	0.47039700	O	3.39185200	-3.58660700	-0.18880000
C	-1.25435600	-3.86370400	-0.17935100	C	0.24092100	0.33985000	3.44105400
O	-0.45066700	-4.66166100	-0.42598600	O	-0.70546300	0.83311600	3.89619800
O	-2.07354500	-3.07278100	0.07334400	O	1.19417700	-0.15964500	2.99357800
C	1.12922500	1.64859700	1.76307200	C	-3.61421000	-2.76087600	-1.16948100
O	0.82620800	0.60431600	1.34412600	O	-4.70996000	-2.37957300	-1.11570200
O	1.42243600	2.69194200	2.17730500	O	-2.52016800	-3.15457100	-1.23531300
C	-0.05964000	-1.37504800	3.09282500	C	-3.35717000	0.57538200	-2.88747100
O	-0.47469200	-0.54088800	3.78693300	O	-3.66388300	1.68626900	-3.03206700
O	0.36272000	-2.21607000	2.40720800	O	-3.03692100	-0.53760700	-2.76684800
C	1.63897500	4.40520400	-0.13476100	C	-0.38810900	-1.62838100	-2.52940100
O	2.25498800	3.54074800	-0.61554300	O	-0.34684300	-1.21906600	-1.43675800
O	1.02447200	5.27334000	0.32982100	O	-0.42993200	-2.03116100	-3.61409600
C	-1.56940700	3.49837500	0.23539900	C	-1.82557700	0.05012000	0.51570100
O	-2.45503000	4.20540700	0.47190200	O	-0.90006100	0.60649500	0.95205900
O	-0.66582400	2.80024800	-0.01308800	O	-2.75426500	-0.49885800	0.08891500
C	-2.58764800	1.19552500	-3.06710400	C	3.63177600	1.20924600	2.62423100
O	-2.17757700	0.38083700	-3.78739400	O	3.63071300	1.09175700	1.46294000
O	-3.01150800	2.01428400	-2.35672700	O	3.64779600	1.34018300	3.77495300
C	0.97994000	1.47168100	-2.10266200	C	-3.35544900	-2.20720000	2.31731900
O	0.29858100	2.10447300	-2.79611200	O	-3.73014400	-3.07187900	1.63421900
O	1.66687500	0.83779300	-1.40616400	O	-2.97027500	-1.34998500	3.00141100
C	-2.42761400	1.29875400	2.99484200	C	-5.39631000	-0.00976900	0.22008500
O	-1.59610600	2.03296400	2.63881900	O	-5.47032100	-0.59367100	1.22230500
O	-3.26638400	0.58179700	3.35608300	C	-5.33449300	0.58425400	-0.77891200
C	4.11099300	1.34885700	-0.24550700	O	1.63324200	-0.10281200	0.00996200
O	4.49386700	1.44317700	-1.33748900	O	1.71723500	-1.18850500	0.41299600
O	3.72757400	1.27228800	0.85227400	O	1.54620600	0.98456300	-0.39088900
C	5.38844200	-2.05514600	0.04573500	C	0.18332600	2.22357400	-2.36350600
O	5.62724300	-0.93086700	-0.14067100	O	-0.75595900	1.56165500	-2.16226900
O	5.17000200	-3.18213700	0.22079300	O	1.10994700	2.88717400	-2.57784900
C	3.33172800	-0.63812600	-3.03739300	C	2.92725100	-0.21317300	-3.41152400
O	3.23853000	0.15323400	-3.88060500	O	1.85380100	-0.00396800	-3.00558000
O	3.42736000	-1.44388800	-2.20009900	O	3.98821500	-0.41603500	-3.83214300
C	3.71132800	-0.67687500	3.01280200	C	-2.60365500	3.29603500	-1.00084700
O	4.74439700	-1.10362200	2.69831400	O	-2.29830500	4.13193100	-1.74333200
O	2.68039100	-0.25549700	3.35326400	O	-2.91711400	2.46017300	-0.24938400
C	1.73413700	-1.70822000	0.06060400	C	0.46716000	3.02315400	1.11155300
O	0.72752300	-1.91305800	-0.48838100	O	1.01951200	2.63746300	2.05972100
O	2.73853700	-1.51821100	0.60889500	O	-0.08613700	3.41190100	0.16522100
C	-4.07220500	-2.00146000	-1.53574800	C	-0.22518800	-3.09959800	0.60773700
O	-4.47469400	-3.07941400	-1.66874800	O	-0.81736000	-2.38861000	1.31560700
O	-3.68026100	-0.90840700	-1.41742300	O	0.36253700	-3.81421500	-0.09266400
C	-3.61559800	-1.99949700	2.17390300	C	5.14121800	-0.26799800	-0.42569500
O	-4.39073600	-1.60200700	1.40137300	O	4.17580800	-0.75411600	-0.86524800
O	-2.85200100	-2.40824700	2.94839100	O	6.10861300	0.20323300	0.00358100
				C	3.44631600	2.83119900	-0.84695300
				O	2.90098000	3.58900200	-0.15539100
				O	4.00735900	2.08011800	-1.53727800
n = 20				n = 21			
C	5.22924400	-0.09925800	-0.60003900	C	-0.55881400	-1.90872000	-1.94205500
O	4.24996700	-0.09442100	-1.23439200	O	-1.11816600	-1.66940100	-0.94913500
O	6.20995300	-0.09892700	0.01674500	O	0.00470400	-2.15407500	-2.92728700
C	-3.61716200	0.56353800	-2.85112500	C	1.06141700	1.47414100	2.95031100

O	-4.69270100	0.24235300	-2.55254900	O	0.84196400	2.55219200	2.57242400
O	-2.54318800	0.88415500	-3.16671100	O	1.28024500	0.39811100	3.33339600
C	-1.01861000	4.73781400	0.75754000	C	2.79705600	-1.89233900	-2.98717400
O	-1.58657800	5.07423600	-0.20003500	O	2.67966900	-0.80509600	-3.38748900
O	-0.45427300	4.41607200	1.72195300	O	2.92716800	-2.97910200	-2.59742400
C	1.68722600	-0.06030200	-0.08882700	C	4.09412600	1.60458300	-2.32732500
O	1.72745900	0.97198600	-0.61930300	O	5.17938800	1.45571700	-2.70709100
O	1.64151400	-1.09255800	0.44331800	O	3.00228000	1.77205800	-1.95274800
C	0.61318300	-1.59290700	2.90183900	C	1.80924300	-3.83380500	0.00971200
O	1.10966600	-0.63017000	3.32359900	O	2.82006400	-3.67638300	0.56143900
O	0.11575800	-2.55764200	2.48275900	O	0.79799500	-4.00970400	-0.53933400
C	-5.36411100	-0.43835800	0.07679000	C	-1.30684100	4.05597300	1.61711400
O	-5.52898200	0.68154900	0.34094700	O	-0.68545000	5.03488100	1.61760500
O	-5.21050100	-1.56363700	-0.17739100	O	-1.93830000	3.07584800	1.62649400
C	0.48078500	-3.47851000	-0.12506900	C	-3.95658700	-1.69674100	1.75984400
O	-0.51022100	-2.95917700	-0.45494800	O	-4.77577600	-1.81244700	2.56956500
O	1.46108100	-4.01012800	0.19353700	O	-3.12597900	-1.59927000	0.94342500
C	0.20124600	1.91794600	2.62823300	C	-1.98685900	3.61797400	-1.84485900
O	-0.74639400	1.88341500	3.29556200	O	-1.70873500	2.90783200	-2.72534400
O	1.15630200	1.94751400	1.95972400	O	-2.25503600	4.34300800	-0.97870200
C	-0.34294100	2.34485000	-1.75229900	C	-3.09318600	0.51069400	-3.13893300
O	0.21053200	2.41906100	-2.76806100	O	-2.09100900	0.00894700	-3.44973200
O	-0.90101900	2.27798800	-0.73012400	O	-4.09814800	1.01831200	-2.84810700
C	-2.35200100	-3.44440900	1.62037800	C	4.33566500	1.73787200	1.56789400
O	-2.74511700	-2.34762000	1.55137200	O	4.89970300	1.53288200	0.57010900
O	-1.97006100	-4.53590700	1.69535900	O	3.79014300	1.94032100	2.57338200
C	-3.08944100	-2.94091000	-1.62996300	C	0.49001900	1.18126600	-3.05112300
O	-3.36912700	-3.84672500	-0.95938800	O	0.26567600	0.71938800	-2.00273900
O	-2.79518900	-2.04798000	-2.31693700	O	0.71415600	1.64367600	-4.08870800
C	-1.81160900	-0.02473800	0.39249000	C	-2.39084800	1.05175600	3.36570800
O	-2.74469500	0.01696300	-0.29602300	O	-3.27934300	0.75233400	2.67549400
O	-0.88191200	-0.06250900	1.09248400	O	-1.50681100	1.35565900	4.05497600
C	2.80179200	1.41925500	-3.06512700	C	-1.51802000	0.72176200	0.25052100
O	2.35859400	0.42673400	-3.48284600	O	-2.30966700	1.04180500	-0.53526800
O	3.25394200	2.40965800	-2.65989800	O	-0.72852100	0.41650100	1.05091000
C	-2.62981600	-0.30703000	3.40814200	C	1.50015500	3.38722300	-0.01762900
O	-1.84670500	-0.86336000	4.06477700	O	0.42918900	3.11053600	-0.38816200
O	-3.41381500	0.23992800	2.74577300	O	2.56327800	3.67739200	0.34407900
C	3.68076500	0.99718200	2.63943100	C	1.87194600	-0.21080600	-0.05413300
O	3.73375500	0.29069300	1.71156000	O	1.71727000	-1.22181700	-0.60280500
O	3.64750200	1.68862800	3.56779100	O	2.02339200	0.80033100	0.49933100
C	-3.52037400	2.74593000	-0.07102900	C	-4.99848100	1.36872300	-0.19676700
O	-3.14611000	2.73280900	1.03131300	O	-4.84856800	2.51190800	-0.32977400
O	-3.88221100	2.76366500	-1.17543900	O	-5.16391700	0.22436000	-0.05082500
C	2.57453800	3.44258500	0.01489600	C	-4.57473400	-2.37197300	-1.32272900
O	3.55135200	3.02104600	0.48262000	O	-3.89486100	-1.87989700	-2.12761000
O	1.60290800	3.88256600	-0.45133200	O	-5.26236500	-2.87378600	-0.53051100
C	-0.29953400	-0.92486500	-2.93878800	C	3.30196500	-1.73411000	2.77185700
O	-0.30200800	-1.43684400	-3.97737800	O	3.62024200	-1.06548000	1.86925000
O	-0.29525600	-0.41061400	-1.89079400	O	3.00479500	-2.39357700	3.67619400
C	3.67590500	-2.61383100	1.35250900	C	-0.28262600	-1.82109800	2.52753300
O	4.21651200	-2.53352700	0.32455800	O	-1.19917000	-1.56578600	3.19359800
O	3.15267400	-2.69554100	2.38659200	O	0.64458600	-2.07539400	1.87063900
C	3.09244900	-2.23620200	-2.66106200	C	5.35689100	-1.10737700	-0.28799800
O	2.05428700	-2.16018400	-2.13409500	O	4.46084700	-0.88008400	-0.99943900
O	4.11865400	-2.32938700	-3.19139100	O	6.25385200	-1.33995200	0.40802200
				C	-1.95583400	-4.13576500	0.34907900
				O	-1.50442100	-4.04472300	1.41795600
				O	-2.42310100	-4.24745100	-0.70919200
n = 22				n = 23			
C	-1.14196700	-3.57706500	1.01890000	C	-0.19101700	5.15482800	0.30543200
O	-0.09007100	-3.34173400	0.57262400	O	0.64768900	5.04640500	-0.49675200

O	-2.18487500	-3.82844300	1.45981600	O	-1.02009500	5.26121900	1.11027200
C	-4.14616000	-1.79418600	2.02134600	C	-1.74216100	-3.38360700	-1.39043900
O	-4.69127400	-1.97169800	1.00761500	O	-0.87093100	-2.87967600	-1.97745300
O	-3.61937000	-1.61366300	3.04064400	O	-2.61213100	-3.88444600	-0.80757000
C	2.47625200	0.00858000	3.41117000	C	-3.31151600	-0.22149900	3.55077800
O	3.30906400	0.17695100	2.61454700	O	-2.47844100	-0.97900700	3.84511700
O	1.64853700	-0.16467200	4.20689800	O	-4.14260900	0.54097400	3.26821000
C	1.68698700	-3.47657900	2.74520000	C	-1.03322300	-3.14305500	2.32855900
O	2.23318000	-2.49297600	2.43899500	O	-1.00820600	-3.75955800	3.30843500
O	1.15021800	-4.45502500	3.05998700	O	-1.06215400	-2.53442200	1.33288000
C	2.43979100	-4.08871800	-0.66797700	C	1.45174800	3.58896800	-2.72534200
O	2.72535800	-4.48460400	0.38555800	O	2.46175700	4.15826100	-2.74979200
O	2.14859100	-3.71178200	-1.73083100	O	0.43873600	3.01151000	-2.69418000
C	-2.16694800	3.13067700	-1.34566600	C	-4.63880100	-2.15329800	0.45234400
O	-3.19959700	2.99635000	-0.82853500	O	-4.02552600	-2.03934200	1.43699500
O	-1.13475700	3.26561100	-1.86546400	O	-5.25172200	-2.26620600	-0.52669200
C	-5.33937500	0.21271800	-0.68741500	C	-4.04539600	-1.12197900	-2.86500100
O	-6.26455400	0.60612600	-0.11093500	O	-4.49345800	-0.06351600	-2.68693500
O	-4.41481900	-0.18207900	-1.27910500	O	-3.60499100	-2.18157300	-3.05151800
C	-0.22103000	-2.39928900	-2.55645500	C	4.40780200	3.15991900	-0.64570300
O	-0.05516200	-1.60176800	-1.72019000	O	4.63764600	2.44296200	-1.53139300
O	-0.38613900	-3.19418800	-3.38189200	O	4.17911200	3.88145000	0.23762200
C	-2.80111900	0.27046200	-3.51302300	C	2.61686800	-2.91405300	2.88883600
O	-3.03420500	1.40854200	-3.50584400	O	3.44694900	-2.67942400	3.66209500
O	-2.58049200	-0.87269900	-3.53010200	O	1.77822300	-3.16743100	2.11774700
C	5.13452300	-1.01470000	0.26350400	C	2.95551800	0.37392200	-2.30905800
O	5.13500000	-2.13994900	0.54669100	O	2.71766000	1.03029900	-3.23514000
O	5.14821600	0.11834600	-0.00969200	O	3.19584700	-0.28380200	-1.37654700
C	0.51699600	0.96723600	-2.52469500	C	1.07035600	-1.44151300	-0.00997300
O	1.06735000	1.12317900	-1.51049500	O	0.63681400	-0.50568200	0.52699000
O	-0.03722900	0.81790200	-3.53428300	O	1.50229500	-2.37220000	-0.55286300
C	-1.24756900	5.08882000	1.41818400	C	0.79242100	2.15419400	0.01357300
O	-0.69401700	4.91564100	2.42588700	O	1.93105800	2.00103400	-0.18436600
O	-1.79784100	5.26628600	0.40881700	O	-0.33808800	2.33323400	0.20499600
C	1.62268600	-0.74653500	0.37689000	C	0.61553100	0.19066800	3.11932300
O	0.76987700	-0.28963200	1.02517300	O	0.55450000	-0.91377500	3.47450000
O	2.47959400	-1.21234900	-0.25207000	O	0.67572300	1.30204800	2.77934200
C	-3.48675100	2.14881900	1.82761800	C	-2.56302500	2.89285600	1.97560600
O	-3.29358800	3.19718300	2.28418100	O	-3.16812800	3.01327300	0.98601500
O	-3.69439400	1.09160700	1.38187800	O	-1.96763300	2.77800800	2.96445500
C	3.79924100	2.34320500	1.04753700	C	-2.13386500	-0.23720300	0.30596900
O	4.61936900	2.71258200	1.77653400	O	-2.30226600	-0.81558000	-0.69143300
O	2.96518100	1.98962300	0.30925900	O	-1.96504600	0.33667900	1.29991400
C	3.34270900	-1.40865600	-2.85239400	C	-5.01613800	1.50723600	-0.44788300
O	4.37991200	-1.66655000	-2.39375500	O	-5.32264500	2.43107900	-1.07764100
O	2.30998100	-1.16221800	-3.32678100	O	-4.72060400	0.58431000	0.20088000
C	-0.92120000	-0.81803600	3.23647200	C	1.59798900	-3.13134800	-3.16279700
O	-0.61928400	-1.94097300	3.19673700	O	1.55372000	-4.25375900	-2.86896200
O	-1.21969400	0.30453800	3.28053600	O	1.64186900	-2.00981500	-3.47523200
C	0.11395200	2.23101800	1.78995000	C	-0.64013700	-0.04308700	-2.87179900
O	1.03885200	2.25207100	2.48929100	O	0.17120000	0.18329500	-2.06517500
O	-0.82055100	2.21112200	1.09198300	O	-1.44528300	-0.25992400	-3.67653800
C	-1.82273200	-0.24417300	-0.16134800	C	-2.23626900	3.03222300	-1.62548800
O	-1.72701400	0.51210600	-1.03664000	O	-2.40501500	1.88307400	-1.72672500
O	-1.91668900	-0.99792900	0.71861100	O	-2.06710800	4.17634700	-1.53330100
C	-3.76727400	-2.88536800	-1.74406000	C	1.39423200	-5.00159800	-0.01923600
O	-4.84375800	-2.98313100	-2.16247900	O	2.55161600	-5.07739600	-0.09103000
O	-2.68139000	-2.80667500	-1.32486700	O	0.23463300	-4.94124000	0.06303000
C	4.40806700	2.06814200	-2.10895200	C	4.20205800	-2.82941700	-0.70172500
O	5.02721400	2.86052500	-1.52527900	O	4.31319300	-2.54334000	0.42191300
O	3.79761200	1.28027800	-2.70846600	O	4.11014200	-3.10982500	-1.82496700
C	1.51721500	3.98873900	-0.99578000	C	2.51093700	3.30605300	2.44494200

O	2.03064900	3.82545200	-2.02421600	O	1.66438400	4.01497200	2.07776500
O	1.01978800	4.17888100	0.04040400	O	3.34907600	2.59210400	2.81702700
				C	3.93915900	0.26096500	1.38300700
				O	3.04739600	-0.31389400	1.86537100
				O	4.82853400	0.83216300	0.90519200
n = 24				n = 25			
C	-1.42137500	1.04839600	-3.46132400	C	-0.06185500	5.29701400	0.83786700
O	-0.33846900	1.06918400	-3.88207200	O	-1.10476500	4.88765800	1.15541900
O	-2.50477200	1.02655600	-3.03451400	O	0.97960000	5.71432400	0.53570800
C	4.73558700	1.65277600	-0.27459300	C	1.62373200	-3.14751300	3.75732100
O	4.45901400	0.55473700	-0.54457100	O	0.78301300	-2.57375800	4.32254700
O	5.01973200	2.74638300	-0.00540500	O	2.47302000	-3.71574400	3.20420900
C	2.39528500	-1.00634500	0.84905100	C	-1.17939000	-3.77839100	1.11995500
O	1.46920100	-0.29739700	0.82446000	O	-0.24625900	-3.80693500	1.80874700
O	3.31703400	-1.70818700	0.88309800	O	-2.11400400	-3.76290200	0.42413100
C	3.16937400	-4.25152800	1.80781200	C	4.33410400	-1.44440500	-2.68691800
O	3.02546800	-4.59019600	0.70349000	O	4.14952400	-0.56148800	-3.42015800
O	3.31805500	-3.93124000	2.91491900	O	4.51745700	-2.33166900	-1.95693400
C	1.88370900	-1.77078500	4.24589800	C	-4.63881500	-2.69208400	0.03647400
O	1.28234900	-2.52965800	4.88487300	O	-4.37314500	-1.86878200	0.81877700
O	2.48917800	-1.00162800	3.61279900	O	-4.90926000	-3.52283500	-0.72558900
C	-0.83580400	4.29293400	-2.19627400	C	0.86344000	-4.69485000	-1.63361500
O	-0.25835400	4.82752400	-1.34114600	O	1.39122100	-4.07625900	-2.46923700
O	-1.41590400	3.75893500	-3.05172400	O	0.34402400	-5.30764800	-0.79674700
C	-5.89185000	0.98757300	0.50385100	C	3.83973400	0.71834200	0.07839500
O	-5.87358300	1.96501400	-0.12362500	O	3.02960300	0.89330900	0.89990000
O	-5.91286600	0.01080300	1.13703500	O	4.64374500	0.53771800	-0.73620200
C	-2.47940500	-4.30117200	-0.91168200	C	-1.70922000	0.68905900	-2.85241900
O	-1.51132100	-3.89173400	-0.40517700	O	-2.75606800	0.76658000	-3.34320700
O	-3.43774200	-4.72500800	-1.40719400	O	-0.65211500	0.60778000	-2.36661900
C	2.56392600	1.67594200	2.64138500	C	-2.06621300	-1.59969900	3.92729200
O	1.51718500	1.94347600	3.07352400	O	-1.68034400	-0.55507800	4.26058200
O	3.60655500	1.39189700	2.21337800	O	-2.45547900	-2.64617300	3.59796700
C	2.72913400	2.93373500	-2.83805400	C	0.91041300	-1.54222100	-1.15271600
O	3.85387700	2.66968100	-2.71931200	O	-0.07070600	-2.05291300	-0.80006500
O	1.59981000	3.18529100	-2.96767800	O	1.90084300	-1.04645900	-1.51351600
C	-2.87285400	1.88687400	-0.18657100	C	-5.15930900	0.54251700	-1.68403100
O	-2.64850200	3.02451900	-0.19687700	O	-5.32027600	-0.60918100	-1.70535700
O	-3.09250400	0.74083600	-0.17250500	O	-5.00760900	1.69530200	-1.67006300
C	-3.54964900	1.88928200	3.27026100	C	3.34319900	-2.76104500	0.60543500
O	-4.10975700	2.13236600	2.27761200	O	2.57500700	-3.50840900	0.15604100
O	-2.99718100	1.64746700	4.26176400	O	4.10871400	-2.00415600	1.04677300
C	-4.26508900	-1.16595200	-1.88635800	C	1.02898600	-2.06833500	-4.33001100
O	-5.23322300	-0.53945600	-1.76135700	O	2.05135000	-2.30789100	-4.82054300
O	-3.30005300	-1.80565600	-2.01974800	O	0.00108200	-1.82685900	-3.83259400
C	-0.73074600	0.36650700	2.61890600	C	-2.15845300	-2.98812300	-2.28802900
O	-1.08835000	1.25717900	1.95815300	O	-1.66880900	-4.00276000	-2.57009600
O	-0.37955000	-0.52162000	3.27807200	O	-2.65113200	-1.96918100	-2.01261800
C	-0.85062300	3.96474300	2.01419100	C	1.94653500	1.21327700	-3.23069400
O	0.07275300	3.92485300	1.30877700	O	1.61428700	0.72433500	-4.22836400
O	-1.76881900	4.01458400	2.72527800	O	2.28229700	1.70568200	-2.22812900
C	-3.62412900	-1.47719500	1.63441100	C	1.04469100	-0.42880900	2.35078200
O	-3.30746200	-0.76685600	2.49986800	O	1.29801500	-1.36369500	1.70370200
O	-3.93646200	-2.19210800	0.77231400	O	0.79366200	0.49805200	3.00197400
C	1.71356600	-0.66365800	-2.90064100	C	-0.38384400	4.33339900	-2.69440700
O	2.02098000	0.18993700	-2.16917600	O	-0.15680400	3.39092300	-3.34024700
O	1.41677300	-1.51512700	-3.63201000	O	-0.61785800	5.27970100	-2.06298500
C	1.30909600	-3.77409000	-1.38568100	C	2.85264100	4.17566100	-1.07877400
O	1.18686600	-2.73613900	-0.86464700	O	3.33538000	3.63799100	-0.16538300
O	1.42913600	-4.80334000	-1.90140300	O	2.38558400	4.71215800	-1.99708900
C	0.87457300	2.02630200	-0.48552700	C	4.35861000	-0.28931300	3.22444500
O	-0.20146500	1.75404200	-0.83152100	O	5.32123900	0.15896000	2.75596700

O	1.95529400	2.29369500	-0.14995300	O	3.39559500	-0.74137900	3.70031100
C	-0.46849300	-3.16816500	2.28439700	C	0.40278100	1.91876600	-0.18035500
O	0.65447000	-3.06148400	1.98798500	O	0.35422100	0.80021800	0.13155100
O	-1.58155900	-3.28703600	2.58729400	O	0.45471400	3.03397500	-0.49619400
C	4.82231700	-2.24238300	-1.34789800	C	-1.33398600	2.37510700	2.92142100
O	5.79063900	-2.31668400	-0.71401400	O	-1.18316300	2.75957600	4.00305300
O	3.85772300	-2.18497200	-2.00044400	O	-1.48902900	1.99983100	1.82679400
C	3.03811000	4.67270900	0.45923600	C	-4.91687500	0.65346800	1.80063400
O	2.99903000	4.94142200	-0.67181700	O	-5.81752500	0.76510400	1.07605300
O	3.07498700	4.41504600	1.59274900	O	-4.01512900	0.53739300	2.52913100
C	-1.31721800	-2.47897000	-3.85621300	C	2.27004800	2.80083700	2.78820700
O	-1.59601100	-1.55394400	-4.50106800	O	3.19523800	2.43027000	3.38202600
O	-1.04489400	-3.41528500	-3.22015700	O	1.34044300	3.18284100	2.19777800
C	-0.93509400	-1.07142600	-0.60375000	C	-2.13025000	-0.33917000	0.58399000
O	-0.70345600	-0.87260200	-1.72380000	O	-1.54683700	-0.98316700	1.35417600
O	-1.16811000	-1.25764600	0.51934600	O	-2.71139800	0.30681100	-0.19130000
				C	-3.08456800	3.05780800	-0.21964200
				O	-3.86082000	3.13072300	0.64046000
				O	-2.30744700	2.98713300	-1.08499200
n = 26				n = 27			
C	3.11288300	-2.63154200	-2.77879400	C	0.53894600	2.35835400	3.47266400
O	3.91816800	-1.79164100	-2.74818500	O	1.18781500	3.30889500	3.31720500
O	2.31644300	-3.47510500	-2.83393300	O	-0.10899900	1.40379100	3.62671800
C	-1.32590000	3.76700300	2.95940100	C	0.21706100	-0.66823400	1.83125200
O	-0.49065700	3.49682600	3.72176700	O	-0.56637300	-0.24554900	1.08323800
O	-2.16367300	4.05460200	2.20598300	O	1.00196300	-1.07520900	2.58353300
C	-2.45691900	2.41655300	-2.92478700	C	-0.60541500	2.35844000	0.06603400
O	-1.58000500	3.04613200	-3.35737200	O	-0.33934600	2.04410700	-1.02146700
O	-3.35149400	1.79878900	-2.51262800	O	-0.86652600	2.69151500	1.14786800
C	1.01118900	3.64859200	-2.56666900	C	-2.06169000	-4.23820200	-1.59882300
O	0.59157800	4.55948000	-1.97695000	O	-2.63927200	-4.10610700	-2.59780200
O	1.44610500	2.75365200	-3.16818500	O	-1.48996600	-4.39644300	-0.59752600
C	-1.37384500	-1.31146700	0.21821700	C	-5.42323500	0.37350100	-1.81835900
O	-0.57988400	-0.76923300	-0.43339100	O	-5.84255400	-0.51494300	-1.19696700
O	-2.15973000	-1.85479700	0.87917600	O	-5.01791900	1.27184300	-2.43627300
C	-5.63347500	0.12456300	-1.79282300	C	5.58996700	0.49578600	-0.98699000
O	-5.59294000	0.39618300	-0.66146500	O	5.85475200	-0.18352800	-0.08191200
O	-5.69765700	-0.14808100	-2.91993000	O	5.33586300	1.18128700	-1.89205900
C	0.67130100	-4.06271100	0.74016500	C	0.45605500	-2.38259100	-3.56883300
O	1.55878000	-4.36108100	1.42457000	O	0.72439100	-1.51203400	-4.29046900
O	-0.21962700	-3.77866400	0.04482600	O	0.19950500	-3.26319300	-2.85222600
C	-4.75792200	-1.47316300	1.25996800	C	-2.50798100	4.03272500	2.81734500
O	-4.96019800	-2.32732600	0.49698000	O	-1.72093000	3.90137800	3.66249100
O	-4.56792500	-0.61830300	2.02591400	O	-3.30487200	4.17579300	1.98298400
C	1.22466100	5.16052100	0.65456900	C	-2.05589000	-3.52516200	1.96005900
O	2.03762400	5.93990100	0.38664500	O	-0.98991500	-3.05710400	1.91664800
O	0.40379700	4.38284900	0.94542300	O	-3.11022800	-4.00632000	2.01651500
C	5.63429500	-0.28231400	-0.61620700	C	3.98342100	-1.91362500	1.15441200
O	4.78562000	-0.87488100	-0.07664400	O	4.13043100	-2.78687200	0.40079700
O	6.48969800	0.28809800	-1.14837400	O	3.83832500	-1.03723900	1.90478400
C	3.57042500	2.48940100	0.21302900	C	-0.55651100	-0.92990900	4.90749100
O	2.70171300	3.09631800	-0.26717900	O	-1.45153900	-1.14652800	4.19286200
O	4.45312600	1.90398100	0.69117700	O	0.32728700	-0.70856100	5.62592400
C	2.08063600	-0.79671700	-0.08715800	C	4.08879400	-2.34360600	-2.40494500
O	2.02141700	0.33048700	0.18322400	O	5.17941800	-1.94923500	-2.38022800
O	2.13093500	-1.92740500	-0.35944000	O	2.99384200	-2.74260000	-2.43906500
C	-2.23205000	-3.38751000	3.09000500	C	-1.12499300	4.44575200	-2.18041400
O	-3.34755100	-3.10955600	3.24996400	O	-0.88194400	4.96559900	-1.16589200
O	-1.11201300	-3.67544300	2.94748000	O	-1.36767600	3.92451300	-3.18837700
C	0.96741700	-1.78937200	3.15660600	C	-2.16634400	-0.67549600	-1.02278500
O	1.23456700	-2.03155500	4.25495400	O	-1.52346700	-1.56780800	-1.39211300
O	0.69817900	-1.55690400	2.04256500	O	-2.80584800	0.22342400	-0.64654800

C	-0.42595600	-3.79054600	-2.67224800	C	3.45607700	1.06879100	-3.96769600
O	-0.32611500	-4.94496200	-2.70086700	O	3.64232000	2.16200200	-4.30833700
O	-0.53316000	-2.62982200	-2.64833500	O	3.26136100	-0.03278800	-3.64092600
C	-0.25149800	1.81959000	0.22072500	C	2.90397600	-0.33268500	4.32946500
O	-0.15153400	1.96717000	-0.92641600	O	2.77100000	0.77883400	4.00721200
O	-0.35912900	1.65765400	1.36812800	O	3.04799100	-1.43619000	4.66066100
C	-1.96134800	4.95652000	-0.42077600	C	1.51863600	-3.51825100	3.48435300
O	-1.65982000	6.05785700	-0.21832300	O	2.27440200	-3.65601700	2.60941700
O	-2.27701400	3.85588600	-0.63972600	O	0.75878700	-3.40419400	4.35579700
C	-3.12547200	-1.50153200	-2.83293000	C	-2.95514400	-1.71577400	-3.91556200
O	-3.08893300	-1.92515400	-3.91091100	O	-2.11521200	-2.08228200	-4.62847000
O	-3.18332600	-1.07510600	-1.74768700	O	-3.80203500	-1.34057700	-3.21008100
C	-2.10078500	0.32525500	3.38756900	C	1.31621500	-3.62392900	-0.16042500
O	-2.59452700	1.37392200	3.29727600	O	1.48596500	-4.75366400	-0.34293100
O	-1.61087200	-0.72377700	3.49170600	O	1.15194800	-2.48296900	0.03231500
C	1.54103900	1.68512100	3.18741800	C	-4.88795800	-2.61521000	0.28650900
O	0.92451200	0.91641600	3.80423700	O	-3.96033700	-2.63565300	-0.42272300
O	2.16874200	2.45652200	2.58323300	O	-5.81022900	-2.60993500	0.98581200
C	4.13737100	-3.41975800	0.75807600	C	-3.10909300	0.05220400	2.23323700
O	4.08184100	-2.93619500	1.81466000	O	-2.88134300	1.15914400	2.49762600
O	4.20514900	-3.91192500	-0.29296800	O	-3.34600500	-1.05697000	1.96921900
C	0.17189600	-0.04267800	-2.94574700	C	1.97746800	-0.32066000	-1.26421700
O	1.26831900	-0.29032000	-2.64301900	O	0.92839800	-0.29207600	-1.75299500
O	-0.91781700	0.19776200	-3.26451800	O	3.02981000	-0.35239300	-0.76299900
C	-3.66111900	1.77900700	0.66764900	C	2.90960700	1.67791600	1.12995500
O	-4.46761100	2.53062200	1.01955700	O	1.77670600	1.39313600	1.18420800
O	-2.84752200	1.02052500	0.30818800	O	4.02891000	1.96251000	1.06800900
C	3.60459500	0.93239400	-3.24389100	C	0.77626200	4.92980600	1.07750900
O	3.80897300	1.09100000	-2.10635400	O	1.53217200	4.28254200	0.46624700
O	3.42003400	0.77962700	-4.37743400	O	0.02455600	5.57221900	1.68086200
C	4.51428500	-0.30447300	2.62906200	C	-0.37889800	1.11879700	-3.61645500
O	5.67383000	-0.31994200	2.62738400	O	0.62482200	1.66408700	-3.83486800
O	3.34879200	-0.27830900	2.64990900	O	-1.38754400	0.58048500	-3.40411200
C	-2.92852200	-4.30147100	-0.25781900	O	2.06167400	3.26001800	-2.06042600
O	-3.00023300	-4.73803700	0.81572600	O	1.59867400	4.20261200	-2.55066200
O	-2.85236000	-3.88568500	-1.34237700	O	2.53348600	2.31466500	-1.56575700
				C	-3.95853500	2.63728900	-0.18299200
				O	-3.09872700	3.15579900	-0.77071700
				O	-4.81794700	2.11026500	0.39453100
n = 28				n = 29			
C	-3.64276900	1.41619300	1.78328500	C	-0.52122000	1.86665700	-0.62546200
O	-3.72609500	1.10637100	2.89988600	O	-0.30236100	0.77823200	-0.28026300
O	-3.58520500	1.73439700	0.66546100	O	-0.73273500	2.95546200	-0.97017900
C	-3.64630300	1.03272100	-2.02489900	C	-4.13170000	-1.78848600	1.96642800
O	-3.64311600	-0.09426200	-1.73463700	O	-4.13837500	-0.64422500	2.17497100
O	-3.67608300	2.15560400	-2.32156100	O	-4.13662600	-2.93399500	1.77093700
C	-0.18905300	-2.31163600	4.89949400	C	3.08376600	-0.12897300	3.44869300
O	-0.08406300	-1.24092200	5.34215300	O	2.91843200	-0.74911600	4.41664600
O	-0.30043200	-3.38731300	4.47293600	O	3.25528900	0.49415900	2.48007100
C	-0.64229200	-0.52881500	1.96143400	C	-1.49305200	3.43050700	2.46800000
O	-0.07342700	-1.49591900	2.26628900	O	-2.09861100	3.28173200	1.48499300
O	-1.20527500	0.43797300	1.64857500	O	-0.88814500	3.58909600	3.44600700
C	2.27582900	-0.08368100	0.00888000	C	0.35780000	5.37467700	-0.34576600
O	1.11541000	-0.05410500	0.00314200	O	0.39240300	5.04616800	0.77063200
O	3.43648700	-0.11186600	0.01287000	O	0.33708500	5.71776300	-1.45537700
C	-3.66369900	-2.30217900	-3.32944000	C	-2.85934600	-4.63573100	-1.30672000
O	-2.51340900	-2.41369400	-3.16748100	O	-2.38435900	-5.65117200	-1.60548300
O	-4.80259900	-2.19488700	-3.50914000	O	-3.34573100	-3.62391100	-0.99660200
C	-3.76386600	-2.05941600	0.21740600	C	2.01430500	-3.01465500	1.65897200
O	-3.69706800	-1.24948800	1.05034800	O	2.96454200	-2.42082500	1.97014400
O	-3.85739200	-2.87125300	-0.60829600	O	1.06416800	-3.61028900	1.35964000
C	5.11776500	0.62997000	1.92982900	C	2.16257800	-0.33549800	-0.50419000

O	4.45771800	0.12109100	2.74319000	O	2.67148600	0.70610500	-0.38760800
O	5.78404800	1.14932100	1.13278400	O	1.67009300	-1.38137800	-0.62678700
C	5.14850500	1.07635500	-1.64752800	C	-0.67897800	4.09517700	-3.47226100
O	5.75010000	0.08660100	-1.73421900	O	0.36339600	3.61628400	-3.67022700
O	4.55263300	2.07464800	-1.58024900	O	-1.72275100	4.57381900	-3.30043300
C	0.11739100	5.35706200	-0.44781200	C	0.25027200	-4.58780500	-1.02655200
O	0.03964600	5.55047300	0.69569200	O	0.80175500	-5.58278700	-0.81863300
O	0.18979100	5.17958800	-1.59544900	O	-0.31312000	-3.58879800	-1.25938200
C	2.03035400	2.50185600	-2.94723000	C	-1.83402900	-1.36609300	-0.61450500
O	1.62969300	1.97613500	-1.98509300	O	-1.69679600	-1.63764700	0.50782800
O	2.43663000	3.02402100	-3.89734000	O	-1.97993300	-1.08551900	-1.73289700
C	-0.86694700	-3.92701600	1.63507200	C	-2.99500800	4.46888100	-0.87387600
O	-1.98983300	-3.62535500	1.70041300	O	-2.41572300	5.40458600	-0.50370000
O	0.24846600	-4.24574600	1.57310200	O	-3.59248200	3.53879200	-1.23962000
C	-0.65786300	-1.39555600	-1.46082900	C	-2.32414100	-2.21386700	-4.12548100
O	-1.26578600	-1.59794100	-0.49182900	O	-2.46713900	-1.14147600	-4.54938100
O	-0.04246900	-1.18721100	-2.42529500	O	-2.17672500	-3.29444900	-3.71782000
C	-3.43679000	4.21931400	-0.44140300	C	4.39164700	-0.07990000	-2.65876800
O	-4.57457600	4.38046600	-0.29888500	O	5.36107100	0.48420900	-2.36255600
O	-2.28695700	4.07392000	-0.57822800	O	3.41535200	-0.64750700	-2.95037100
C	-0.71353700	0.59940800	-4.25386600	C	2.61605700	2.93802900	-2.13206100
O	-1.84988300	0.43719200	-4.05724400	O	2.04691200	3.36822200	-1.21190400
O	0.41630600	0.76669700	-4.46575400	O	3.18642400	2.50786500	-3.04773500
C	1.77470600	-3.92665200	-0.76415000	C	-3.04862200	1.21085500	-2.92483500
O	2.09789500	-5.03853400	-0.76256000	O	-1.95320300	1.56831500	-3.09531600
O	1.45877500	-2.80281400	-0.76982200	O	-4.14382700	0.86447900	-2.76027400
C	-1.93406800	-4.81497200	-1.75457700	C	-3.26188200	0.83717200	4.33548100
O	-1.09851200	-4.43305300	-1.03747700	O	-3.41152700	1.86854200	3.81560600
O	-2.76875300	-5.21212000	-2.45567400	O	-3.12124300	-0.19056500	4.85781300
C	5.00498000	-2.24955600	-0.24503300	C	-4.86690300	-1.56895200	-1.75348800
O	5.64675500	-1.86616100	0.64384900	O	-4.87409900	-1.97090500	-2.84234800
O	4.36878000	-2.65424900	-1.13249100	O	-4.86619200	-1.17391400	-0.65729900
C	2.64922800	-1.47358700	-3.17857600	C	5.23983900	2.21017800	0.00098000
O	2.90635100	-0.42766500	-2.73722400	O	4.92953100	3.03117100	-0.76106400
O	2.40337100	-2.51457600	-3.63148400	O	5.56744800	1.39582400	0.76304800
C	-3.66794600	-1.54136800	3.75808000	C	5.19674100	-1.26149200	1.01437600
O	-4.81773800	-1.67673000	3.78585900	O	5.67913200	-1.24513000	2.06699300
O	-2.50722800	-1.42133800	3.74144200	O	4.72060600	-1.30472100	-0.05110100
C	-0.62348000	3.41337700	2.61842600	C	0.07714300	1.56564400	5.00999800
O	0.50248400	3.46341100	2.89962600	O	-0.88389700	1.63853000	5.65479300
O	-1.75584600	3.37583100	2.34904500	O	1.04550800	1.48959100	4.36520000
C	-1.74643300	0.97175100	5.08408800	C	0.58806800	0.87969000	-3.88579300
O	-2.58480500	0.61818600	5.80391700	O	0.86644800	0.90959800	-2.75205800
O	-0.90551800	1.34621400	4.36902000	O	0.32132100	0.84865700	-5.01159200
C	-0.17496700	-3.06571500	-4.42646500	C	1.16624100	-2.59111800	-3.34559600
O	-0.22811600	-2.16441000	-5.15845000	O	1.94792700	-3.41337000	-3.09229500
O	-0.12889600	-3.97905900	-3.70698700	O	0.38019900	-1.78172700	-3.62417500
C	-1.63726500	4.02833000	-3.34529300	C	2.07336900	2.79901100	1.56505300
O	-2.41682100	4.88764000	-3.35806000	O	1.01193800	2.31607200	1.56069000
O	-0.85679700	3.16302600	-3.35302600	O	3.12577900	3.28481600	1.57614000
C	2.02882800	1.25398900	3.64780000	C	-3.95465500	1.49368500	0.53893700
O	1.58426300	0.65358500	2.75083400	O	-3.03495800	0.98785000	0.02590600
O	2.47805400	1.84412200	4.53691300	O	-4.86819500	1.99667700	1.04017300
C	2.57988300	-2.15914800	2.80225900	C	-1.53262600	-3.82163500	2.07836600
O	2.37128400	-2.02178600	3.93646800	O	-1.42475800	-3.04616100	2.94019800
O	2.80005700	-2.30834700	1.66910700	O	-1.64782600	-4.60767200	1.23074800
C	-0.53909400	1.98564400	-0.49777200	C	0.53267700	-2.13816800	4.62045200
O	-1.15988200	1.28518100	-1.18562000	O	-0.07081800	-1.18524500	4.90974800
O	0.08730600	2.68083000	0.19278700	O	1.12830100	-3.09297900	4.33310200
C	2.81590800	3.35535700	0.42135800	C	-0.29841700	-0.05886800	2.29542100
O	2.62941900	4.26383600	-0.27766400	O	-1.23321500	0.59165500	2.52299900
O	3.01310400	2.45292000	1.12962600	O	0.64444000	-0.70910100	2.08717700

				C	4.04886200	-3.56709600	-1.40423300
				O	3.31971600	-3.89393500	-0.55697600
				O	4.78958500	-3.25461900	-2.24192500
n = 30				n = 31			
C	-4.23854600	1.26216900	2.33885400	C	4.59783600	1.99980700	2.36825000
O	-4.07534100	0.39452300	3.09578700	O	4.15610100	2.09313800	3.43666600
O	-4.40699300	2.12623000	1.57841300	O	5.06084700	1.92388800	1.30095800
C	1.09470300	-4.77689200	-1.20144000	C	-3.88489900	-0.80231800	1.21593700
O	0.31515700	-4.71413200	-0.33732200	O	-2.84079400	-0.31189000	1.37630200
O	1.87252800	-4.85368400	-2.05851600	O	-4.92385000	-1.29090400	1.05210600
C	-2.05195300	2.79382400	-3.12393800	C	2.61752000	1.47950600	-3.55595900
O	-2.07998100	3.94677800	-2.97835200	O	3.61091000	0.87628300	-3.60892700
O	-2.02775600	1.64126300	-3.28107000	O	1.64049300	2.10688700	-3.52158600
C	-5.57786200	-1.77623200	0.24116600	C	4.12596800	-3.92471600	-0.49396800
O	-5.11498600	-2.38594600	-0.63867000	O	4.51098400	-3.37854800	0.45649500
O	-6.04217800	-1.18000900	1.12118200	O	3.76368200	-4.48417500	-1.44837300
C	2.92577200	2.08214500	3.75858000	C	1.32220200	-4.18906900	-2.68440900
O	3.36704200	1.05097200	4.06948700	O	1.76665000	-3.52074800	-3.52763700
O	2.49274700	3.12136600	3.47192500	O	0.85737300	-4.86464200	-1.86199900
C	3.57927500	-3.46913200	1.23028700	C	0.92908100	3.02948900	4.01656600
O	2.80120400	-3.41310200	0.36482200	O	0.34049400	2.78825800	4.98868800
O	4.35249800	-3.55350600	2.09113300	O	1.52145200	3.27811100	3.04705600
C	2.60582400	-2.41396900	-3.20384500	C	0.71053500	-3.59080600	4.11197200
O	1.72891200	-2.51109600	-3.96374300	O	0.18664200	-4.37425100	3.42982300
O	3.48358500	-2.31053400	-2.45018800	O	1.25406900	-2.81931700	4.79117600
C	-2.88140100	-2.12378300	2.22730400	C	-3.29912200	-1.79216700	-3.85616400
O	-3.80552000	-2.79797500	2.02573900	O	-3.03963800	-2.85148900	-3.45115400
O	-1.95063400	-1.45216300	2.41946500	O	-3.56067700	-0.73219700	-4.25628000
C	1.48510600	-1.66369300	3.54567700	C	-0.28826700	-1.13648500	1.70500500
O	2.49289500	-1.58891700	2.97094500	O	-0.47471500	-1.59098800	2.75605100
O	0.47857200	-1.75013200	4.12129000	O	-0.09622100	-0.67421900	0.65405000
C	-1.83578600	3.20058500	3.95730700	C	0.66389100	-0.10319800	4.75856000
O	-0.68718700	3.36717000	3.87175100	O	1.60000700	0.12670400	4.10409200
O	-2.98176000	3.03116900	4.05289900	O	-0.27388900	-0.31070000	5.41134600
C	-0.10966900	-4.23832500	2.29003000	C	0.26737500	-1.27635200	-4.52650200
O	-1.24614600	-4.27816900	2.04811000	O	-0.70704000	-1.78805300	-4.89963500
O	1.02387900	-4.21261900	2.54827800	O	1.24863200	-0.77111800	-4.16107100
C	-2.18071800	3.47826300	0.51173000	C	-4.92238100	0.70863500	-1.78002700
O	-2.28589100	4.23383400	1.38701600	O	-3.95563500	0.18388100	-1.38565500
O	-2.07617300	2.71470900	-0.36156000	O	-5.88434600	1.21520000	-2.17716800
C	-5.28382500	1.36917900	-1.42483400	C	0.89121500	-4.18596100	0.77325800
O	-6.09039100	0.57998300	-1.14549100	O	1.88886000	-4.75465900	0.92581300
O	-4.48752000	2.16679600	-1.70969300	O	-0.11424300	-3.61060200	0.63026900
C	-2.42118000	-3.85025400	-0.60946300	C	4.00547300	-1.83537200	-3.84630200
O	-2.06990800	-2.74271700	-0.46494300	O	4.11533100	-1.79007900	-2.68494800
O	-2.77263400	-4.94257600	-0.74654600	O	3.91638700	-1.89119000	-4.99985200
C	0.60902400	1.83386500	-1.02265200	C	-1.90264000	1.56504100	3.02957200
O	0.33619200	2.63063500	-1.82300400	O	-0.80350800	1.24494300	2.79287300
O	0.87550200	1.02576600	-0.23143600	O	-2.98533300	1.89475600	3.27043600
C	5.53047700	-1.39257700	-0.86107100	C	-4.48240500	2.82915700	1.14438600
O	5.51667600	-0.36194800	-1.40222400	O	-4.06018300	3.87236600	1.43231300
O	5.57047800	-2.41893400	-0.31924400	O	-4.92310000	1.78886500	0.86391800
C	-0.26802100	1.00739100	2.26834000	C	5.02051500	0.05228200	-0.74938600
O	-1.33894100	1.23806700	1.87190100	O	4.27466000	-0.55081400	-0.09041700
O	0.79740500	0.77549200	2.66596700	C	5.77472400	0.64946800	-1.40023500
C	-2.43015500	-0.06268200	-0.42541400	O	-4.98700800	-3.18695800	-0.94507700
O	-3.42632300	-0.10853700	0.17575900	O	-5.34778800	-2.37961300	-1.70177800
O	-1.43833700	-0.04126300	-1.02584700	O	-4.63930300	-4.00874200	-0.20066000
C	5.16118200	-1.09231600	3.29434500	C	1.50114900	1.70759200	0.80319500
O	5.10699100	-1.52782300	4.36729200	O	2.23884100	0.98100500	1.32749800
O	5.23939000	-0.64690000	2.21916500	O	0.75229400	2.43879400	0.29128100
C	3.25921300	0.43250700	0.71351600	C	-2.38967600	-1.89940700	4.60105600

O	3.12446900	-0.63562000	0.26766800	O	-1.83949200	-2.84510900	4.99509600
O	3.39283000	1.50304300	1.14346500	O	-2.95321900	-0.95680500	4.21819500
C	-3.66357300	-1.77465100	-2.91657200	C	3.22632500	-1.40322300	2.38487900
O	-3.85400600	-0.65416000	-2.66719700	O	2.26973800	-1.96125500	2.01587200
O	-3.47710700	-2.89181900	-3.17563000	O	4.17682500	-0.86058400	2.76433400
C	-0.19970300	-0.45950500	-3.46072100	C	-1.36350100	4.45141000	1.11419500
O	0.70294100	0.25001700	-3.26245000	O	-1.19571300	4.04404600	2.19099000
O	-1.08912500	-1.17325300	-3.67362400	O	-1.52568400	4.87000500	0.04221700
C	-0.92880700	-3.86280800	-4.02432500	C	-1.60678900	1.29202900	-0.75003900
O	-1.05391500	-3.73017600	-5.16830900	O	-1.19374500	0.59572400	-1.58548800
O	-0.80364300	-4.01335600	-2.87438500	O	-2.01243000	1.99230100	0.08553700
C	0.97635600	4.39339000	1.52263800	C	2.13013100	4.94756000	1.03303000
O	1.42106200	5.41823200	1.82333800	O	1.15103400	5.56351700	1.13094300
O	0.52056600	3.36409600	1.21061600	O	3.11917500	4.33931300	0.94632100
C	3.48031200	4.10604300	-1.42120400	C	-1.98083700	1.58131000	-4.07309900
O	2.49365600	4.14488400	-0.79924800	O	-1.05360100	1.11085800	-4.58938500
O	4.46737700	4.08447700	-2.02759200	O	-2.91603700	2.05928200	-3.57121100
C	-2.04263200	-0.38896100	4.95205600	C	1.89758500	-1.15341700	-1.12991500
O	-1.42835400	0.56696900	4.69168100	O	1.76726500	-0.04319900	-1.44526500
O	-2.64875800	-1.33612000	5.23555500	O	2.01401200	-2.26626600	-0.80881900
C	3.46196900	0.85108200	-2.83204100	C	0.34671900	3.92339400	-1.97265100
O	3.69905000	0.30677300	-3.82781300	O	1.31478100	4.50141900	-1.69213400
O	3.20743200	1.39891200	-1.83439600	O	-0.62785500	3.35472100	-2.25764600
C	0.60854900	-1.78024400	-0.15414700	C	4.30041000	3.09073700	-1.11409400
O	0.38697700	-1.66808300	0.98120700	O	5.19412600	3.82415600	-1.16014800
O	0.80825900	-1.90633800	-1.29312700	O	3.39283100	2.35385600	-1.08785500
C	0.09948700	5.29563900	-1.82405100	C	-2.56568900	-4.25002600	1.81797900
O	0.61917000	5.33551300	-2.86286800	O	-2.81162800	-3.15738600	2.14543200
O	-0.41134900	5.27954800	-0.77863600	O	-2.32869700	-5.33997600	1.50418000
C	1.23325300	3.04714200	-4.34495500	C	-3.45854300	4.28551500	-2.07651300
O	2.32317500	3.10946600	-3.94039700	O	-3.97298700	3.48257500	-1.40659100
O	0.15473500	2.97452400	-4.76919900	O	-2.96744200	5.09279800	-2.74892500
				C	-1.42124900	-2.22758400	-1.31840600
				O	-0.49598800	-2.20080600	-2.02287400
				O	-2.35512900	-2.25659700	-0.62861100
n = 32				n = 33			
C	3.72971400	2.88499800	1.45617700	C	5.19629900	-1.31777700	1.26734900
O	4.58057400	2.28397400	1.97165200	O	4.18452900	-1.51739400	1.80635500
O	2.88331200	3.49160600	0.93752800	O	6.20574100	-1.12507700	0.72772900
C	1.72129300	2.74891900	-1.51487800	C	0.46343200	-3.87523900	-2.93270000
O	2.41825500	3.42596700	-2.15026900	O	0.91867300	-2.97590000	-3.51232600
O	1.03953500	2.04942600	-0.87935600	O	0.01699900	-4.79058100	-2.36756000
C	0.67522500	-0.87397600	4.96596800	C	0.87644700	3.98519000	2.35561600
O	1.42342300	-0.02093800	4.69405700	O	1.68620700	3.17947500	2.58131700
O	-0.06633400	-1.72219800	5.24088800	O	0.07036700	4.79043000	2.12876100
C	-1.49532200	2.18571500	0.14248000	C	0.93725100	2.25201600	-0.86120500
O	-1.05696700	2.21203800	1.21892500	O	1.35763900	1.53238000	-1.67322500
O	-1.94348700	2.16100000	-0.92995500	O	0.51111500	2.97666100	-0.06083500
C	-0.82927700	-1.76529500	-4.87206000	C	-1.37076000	-3.72546800	2.87345500
O	-0.11540000	-2.67509900	-4.97671700	O	-0.27172500	-4.10724700	2.93970400
O	-1.55413900	-0.85828300	-4.78314500	O	-2.47541000	-3.37353500	2.81574300
C	0.70231500	-4.22247700	0.06192100	C	6.23430000	0.72183900	-1.38145600
O	1.02272800	-5.32893300	0.18156300	O	6.16760500	1.54842500	-0.56683400
O	0.36738100	-3.10928000	-0.05195100	O	6.30406600	-0.09523700	-2.20579000
C	1.20829100	2.71625600	4.09537600	C	-4.29127000	3.71399100	-1.14088200
O	0.09143000	2.68760300	4.41409000	O	-4.35379200	3.32878000	-0.04351900
O	2.33251700	2.74868400	3.79733900	O	-4.24139900	4.11517300	-2.22886100
C	-1.91231000	-3.94984800	-2.05175100	C	-2.58312600	-1.87554600	-3.09672000
O	-2.12705700	-3.11235600	-2.82959000	O	-3.07827600	-1.02138100	-2.47385200
O	-1.71766900	-4.79514200	-1.27778600	O	-2.08905100	-2.72006700	-3.71723600
C	-2.60297000	-1.22225600	0.56108000	C	2.77909800	-0.74934800	-0.95360900
O	-2.38759500	-2.24959100	0.06482700	O	1.81105600	-1.35337100	-1.18117600

O	-2.80840000	-0.20015900	1.07922700	O	3.74749800	-0.14627200	-0.73214300
C	-4.50449400	-1.55333900	3.04843100	C	-0.56490700	-2.10401600	-0.01119800
O	-4.75287000	-2.24016500	2.13814300	O	-0.33367200	-1.88010500	1.10437100
O	-4.25714000	-0.87450400	3.95422700	O	-0.81755800	-2.33277000	-1.12378800
C	-4.94443800	1.51070700	1.22361000	C	-0.31154700	2.13194300	5.09099500
O	-5.54073200	0.64028400	1.70990000	O	-0.59205800	3.06347300	4.45181100
O	-4.37011300	2.39315000	0.72846800	O	-0.02489700	1.22081500	5.75097400
C	4.26225600	-3.08264800	-0.23976900	C	-0.87781300	5.30386100	-0.51740800
O	4.96205300	-2.44043800	0.43085500	O	0.07660500	5.94104100	-0.69225300
O	3.57128000	-3.73739900	-0.90901600	O	-1.84831700	4.68276500	-0.35017700
C	-1.06459700	-3.18738100	2.88930900	C	-2.70723100	1.50808900	-3.48964700
O	-1.94369100	-2.42849100	2.96399400	O	-3.13113600	1.08935500	-4.48222400
O	-0.18654700	-3.94464300	2.82028400	O	-2.26317700	1.94704400	-2.50123400
C	4.83170000	-0.93808100	-3.25169400	C	-4.22358000	-1.92361500	0.86513100
O	4.88702900	-1.17186300	-2.11106800	O	-3.34201300	-2.28106200	0.18672300
O	4.77831400	-0.72490900	-4.39070600	O	-5.09582700	-1.55491300	1.53138700
C	-6.00137000	-1.74062900	-0.27880400	C	2.22769200	-2.97151000	2.87838300
O	-6.96862700	-2.28805000	0.04602500	O	2.73783500	-3.99807100	2.70479400
O	-5.03952500	-1.17003500	-0.61359600	O	1.71125100	-1.94423200	3.06531500
C	-1.38464500	1.69148000	-3.56539700	C	2.62702800	4.96204500	-0.53958800
O	-0.30772900	1.37582500	-3.25909600	O	2.60773700	4.55790300	-1.63200300
O	-2.45611900	2.00456700	-3.88630100	O	2.64483900	5.35402200	0.55408500
C	-4.35711100	2.76682500	-2.04003700	C	1.12328000	-5.12986100	0.49381900
O	-3.93599000	3.85057600	-1.99670300	O	0.94126300	-6.22445900	0.82029000
O	-4.80450300	1.69474100	-2.08102900	O	1.33062300	-4.02955500	0.15611900
C	3.05601000	-0.11152200	-0.34829400	O	-5.37284900	-3.46549400	-1.91798300
O	3.69692800	0.85642900	-0.31982200	C	-5.69313800	-3.76814900	-0.84159300
O	2.40768600	-1.07782200	-0.36305200	O	-5.06956500	-3.17253500	-3.00198000
C	-3.77334900	-4.47176700	0.74372200	C	-2.24044400	0.61196000	-0.16027900
O	-3.03613800	-4.75300600	1.59693600	O	-1.08270900	0.51966600	-0.23943000
O	-4.51393800	-4.20113600	-0.11245300	O	-3.39715100	0.68251800	-0.08922200
C	0.96147100	-0.13401800	1.95777100	C	3.65048600	-3.80690200	-1.39575100
O	0.61191500	-1.22385100	2.17265100	O	3.11486900	-4.51531900	-2.14506000
O	1.33850500	0.94307500	1.74252900	O	4.19370200	-3.11844200	-0.63102500
C	-1.31087000	5.08473100	-2.19666000	C	-5.46138600	1.39933900	1.51400600
O	-1.86562700	6.01038200	-1.76909800	O	-4.70951500	1.60397600	2.37858500
O	-0.74545800	4.17112700	-2.64686500	O	-6.22924700	1.20099100	0.66586400
C	1.82343000	-3.32225400	-3.04540000	C	-5.45549700	0.18783300	-1.77550500
O	1.08551100	-4.13771400	-2.67098300	O	-5.72243700	-0.83932500	-1.30169300
O	2.56710500	-2.51500700	-3.43206900	O	-5.19811000	1.21313800	-2.26076800
C	2.49937200	-3.10332000	2.95109800	C	-2.25216600	-4.67747600	-0.65528600
O	2.60757300	-3.46123600	1.85131900	O	-1.59184300	-4.73751100	0.30327900
O	2.40810000	-2.76067200	4.05855100	O	-2.91887000	-4.62871300	-1.60262100
C	0.41778400	4.66368900	1.13818900	C	3.32662600	-0.10808800	4.40938700
O	0.35052200	4.68390500	-0.02440900	O	4.08811800	-0.93497800	4.69868500
O	0.48226300	4.66495200	2.29647900	O	2.56684700	0.72903900	4.12933300
C	1.95688700	0.12352200	-3.96940300	C	0.70423400	-0.21661600	-3.61209300
O	1.46778400	-0.18097200	-4.97465700	O	1.80993000	-0.12537300	-3.95961900
O	2.45091500	0.43933000	-2.96027700	O	-0.40130300	-0.27892300	-3.25950800
C	4.05132900	-0.07115700	3.37855700	C	-2.45920000	3.40100500	2.15627600
O	4.51266900	0.40796300	4.32369900	O	-3.02962300	4.33081200	2.54310500
O	3.57849600	-0.58094700	2.43642400	O	-1.87333400	2.46242300	1.77760500
C	-3.57739200	5.05097000	0.56733600	C	-0.11317700	3.20629900	-3.74268900
O	-2.49075900	4.65727600	0.71805500	O	0.02842300	3.96632300	-2.87422400
O	-4.65870900	5.45011600	0.44062500	O	-0.27667700	2.44551900	-4.60692400
C	-0.09355900	-0.79067900	-1.39450900	C	4.38863000	-0.98233400	-3.96657900
O	0.16336800	-1.32354300	-2.39453700	O	4.07709400	-1.80252000	-3.19880000
O	-0.35264500	-0.26102700	-0.39345100	O	4.68455500	-0.17908500	-4.74913700
C	5.20328500	2.47390800	-1.83403500	C	0.84982400	0.49447700	2.02461900
O	5.15740200	1.76165500	-2.75220600	O	1.64429900	0.43895600	1.17434500
O	5.25437700	3.19842400	-0.92635500	O	0.05305800	0.57011800	2.86265500
C	-3.51503200	-0.67496700	-2.81500100	C	-2.55332100	0.19770800	3.31527900

O	-4.35687900	-1.01688500	-3.53124400	O	-2.56236900	0.85694800	4.27077000
O	-2.66353300	-0.33098900	-2.09195300	O	-2.54910300	-0.46579800	2.35945500
C	-2.19954500	1.10182200	3.42851300	C	0.15795500	-1.47901700	5.22458100
O	-3.10599700	1.81483400	3.28984700	O	-0.83893900	-1.56449400	4.62693000
O	-1.30409600	0.37278500	3.57031000	O	1.14579000	-1.42862500	5.83299500
C	6.45771500	0.22835000	0.80224200	C	3.35320700	2.39080900	-3.38322600
O	6.56403700	0.56979300	-0.30462500	O	4.15116400	1.92171800	-2.68041100
O	6.37758000	-0.11641300	1.90936000	O	2.55430600	2.85938100	-4.08530300
				C	3.96706100	1.94334400	1.06217300
				O	3.42813500	2.55066000	0.22829700
				O	4.51187000	1.34850900	1.89702000
n = 34				n = 35			
C	5.96629800	0.32031400	-1.21166600	C	-0.86881800	0.46620400	-4.24643000
O	6.17859900	-0.21721300	-2.21982900	O	-0.38751700	0.11802700	-3.23987400
O	5.77672200	0.85454400	-0.19358300	O	-1.35268000	0.79157400	-5.24593100
C	-0.72060200	2.26736300	4.67118700	C	4.59790000	-1.25839400	-2.08681200
O	-1.71081300	2.32037500	4.06220400	O	4.59607900	-2.40656200	-1.90902200
O	0.26069200	2.21097500	5.28798200	O	4.59897400	-0.11308400	-2.28717600
C	-5.67058100	2.38560500	0.69067300	C	4.04121500	0.35461000	3.85113000
O	-5.46895500	3.09537900	-0.20793500	O	3.76693000	-0.13658200	2.82767200
O	-5.89570900	1.66868700	1.57936200	O	4.33565300	0.83804800	4.86106600
C	4.91793700	-3.14143100	-0.61016000	C	-3.13757100	-3.32041000	1.85916200
O	4.86510100	-4.22478700	-1.02299700	O	-4.06004800	-2.63283800	1.69723400
O	4.98162900	-2.05615000	-0.18741700	O	-2.22459700	-4.02458500	2.01186800
C	-1.10634600	5.75282300	-0.69302800	C	-1.86584500	1.75260800	3.91136300
O	-1.13485900	5.98731000	-1.83039400	O	-2.52020600	0.81638000	3.69129400
O	-1.08623900	5.53651700	0.45117700	O	-1.20979900	2.68656000	4.12722000
C	3.32103100	2.15388300	-2.71217800	C	-6.43163800	1.66234800	-0.23413100
O	2.18208900	2.06875700	-2.95093500	O	-6.87623500	0.67907600	-0.66445900
O	4.45490800	2.24358200	-2.48479200	O	-6.01010000	2.65111100	0.21065400
C	0.12811600	0.45406400	1.98548100	C	-3.54832200	1.92638500	-2.52712500
O	0.84937000	1.23794600	2.45122600	O	-4.65082300	1.66601600	-2.27056900
O	-0.60135500	-0.32455400	1.52778900	O	-2.44788300	2.17397400	-2.81049800
C	-2.24214800	3.18696800	1.48225700	C	6.26305900	-0.11637300	1.05651700
O	-3.29372500	3.61512800	1.72168200	O	6.08444500	-0.98132600	0.30082600
O	-1.18737500	2.75649800	1.24467300	O	6.45127800	0.73192100	1.83145000
C	0.46667100	-0.17590100	-3.29901700	C	-3.34976800	5.32049700	-1.56806500
O	-0.46466300	0.51120900	-3.19601100	O	-2.84973800	5.95735900	-0.73418800
O	1.39607000	-0.86633300	-3.40837300	O	-3.87477900	4.69875900	-2.39906800
C	-0.19303600	-4.72986600	3.07147700	C	-2.38411700	-0.92541800	-0.67170200
O	-1.32917200	-4.89747500	2.90144400	O	-2.22628600	-2.07954300	-0.68557600
O	0.95031400	-4.58440000	3.23397400	O	-2.53025900	0.22514100	-0.66110300
C	0.45127700	2.31780800	-0.85755800	C	-0.33532100	-3.97425900	0.04772800
O	0.29497100	3.43601200	-1.13189100	O	-0.87871400	-4.79502700	-0.56437200
O	0.59643000	1.19662200	-0.59439700	O	0.21406000	-3.14794000	0.66086800
C	-5.56378000	0.14904200	-2.03512600	C	2.77060300	-2.28619300	1.45846000
O	-6.02905100	-0.03705300	-3.07711100	O	2.91460800	-1.61316100	0.51609400
O	-5.10050200	0.34569600	-0.98194300	O	2.62364900	-2.96359700	2.38772400
C	0.92680400	4.26415200	2.27328700	C	0.24662800	-4.11745300	3.35237700
O	1.60446800	4.18780600	1.33259400	O	0.01785900	-3.10486600	3.88118800
O	0.25263200	4.35966300	3.21649700	O	0.45968200	-5.13687200	2.83994000
C	-3.20074800	2.95153500	-2.07953300	C	4.86132000	-4.57514800	-0.29814600
O	-2.72632900	3.65522500	-1.28341100	O	4.89393300	-5.24090600	-1.25064700
O	-3.69234200	2.24821000	-2.87114600	O	4.83431700	-3.92550000	0.66564000
C	3.87611500	2.71367200	0.75757800	C	2.31268000	-4.00030200	-2.31240200
O	3.07426100	2.06143200	0.21840600	O	2.17396600	-4.04729700	-1.15602500
O	4.66869000	3.36941400	1.28829800	O	2.43815500	-3.96590600	-3.46529200
C	-1.21486200	-3.57427600	-4.12191900	C	2.99455600	1.15277300	0.57109900
O	-0.99672600	-2.45340100	-3.88804400	O	1.89589900	1.20280800	0.93796300
O	-1.44558900	-4.68077500	-4.38642500	O	4.09630100	1.11274800	0.20132000
C	-0.88624800	-1.58735300	4.65292400	C	1.09250900	-0.93078800	-1.33211400
O	-1.02201200	-0.45856700	4.41134000	O	1.89658000	-1.24127700	-2.11591400

O	-0.75492400	-2.70848300	4.91867800	O	0.29588600	-0.59673200	-0.55777600
C	-0.86117500	-5.29630100	-0.89222800	C	1.37674900	2.63525300	3.16452400
O	-0.30816900	-4.64903900	-1.69180200	O	1.16841500	3.55114800	2.48092400
O	-1.40605500	-5.93549900	-0.09484000	O	1.59355300	1.72014300	3.84988800
C	-3.97439700	-3.08187100	-1.58511400	O	-5.81724400	-1.81875600	-0.25736200
O	-5.00317200	-2.60948000	-1.32015300	O	-5.01351500	-1.70266400	-1.09606600
O	-2.95360100	-3.56208000	-1.87471000	O	-6.61693400	-1.95225200	0.56969800
C	1.94725600	-3.44619300	-2.55582200	C	-0.53714300	2.07744300	0.34418000
O	1.69730900	-3.80281400	-3.62638100	O	-0.90861200	1.60668500	1.34321900
O	2.19668400	-3.09319200	-1.47099100	O	-0.16976100	2.57509700	-0.63857400
C	-2.98408200	-3.01123600	1.85465700	C	-0.86669800	-2.71215300	-3.67339400
O	-2.59984800	-2.26593500	2.66288700	O	-0.27471100	-2.92652800	-2.69182300
O	-3.36437300	-3.76031100	1.05136200	O	-1.45710100	-2.50123000	-4.64916700
C	2.70352900	-0.56491500	-0.40647900	C	-2.93346400	-1.45854500	5.20010400
O	3.21796000	-0.21009000	-1.38530500	O	-2.75296600	-2.19183600	4.31339500
O	2.19002900	-0.93924100	0.56426200	O	-3.11603100	-0.75036800	6.10121600
C	-2.90619800	-0.37990500	-3.99458100	C	5.70484000	2.29175800	-1.56326600
O	-3.17396900	-0.74892100	-2.92085500	O	4.82291400	2.89094000	-2.03148200
O	-2.66401700	-0.03292300	-5.07163200	O	6.59607400	1.70222400	-1.10809400
C	2.79577000	1.67285100	4.18804200	C	-3.55203100	-4.18809600	-1.62976000
O	2.88216100	2.72916600	3.70484300	O	-3.92663700	-4.50524300	-0.57671800
O	2.72951700	0.62226400	4.68163800	O	-3.19845700	-3.87976400	-2.69509100
C	-2.51560200	-0.13978700	-0.37340400	C	0.85514900	-0.69301200	5.05985600
O	-2.79033000	-1.23141000	-0.08217200	O	-0.26664500	-0.37690400	5.07572300
O	-2.23375100	0.94716600	-0.67360900	O	1.97065200	-1.01059100	5.06616800
C	4.13764200	-1.11121500	-3.79094800	C	2.28456800	1.38822900	-3.06221600
O	4.22593100	-2.17132800	-3.31539800	O	2.41343300	1.13680300	-4.18684800
O	4.06068600	-0.06520700	-4.28884200	O	2.14065700	1.61975600	-1.92877200
C	0.03380900	4.24403100	-3.66251100	C	-0.43976000	-0.96728900	2.12784200
O	-0.95590300	3.64595500	-3.76612200	O	0.67884400	-0.76898800	2.37335900
O	1.03088600	4.83178400	-3.58644000	O	-1.56043700	-1.14550000	1.87400600
C	-0.20190300	-2.31340500	-0.18436100	C	2.41316900	-1.56413400	-4.80765500
O	-0.20411200	-1.59456900	-1.09618000	O	1.26646900	-1.59030700	-5.00723500
O	-0.21170800	-3.04356100	0.72055000	O	3.55992600	-1.54032900	-4.62687000
C	-6.17796600	-1.26384600	0.97295200	C	-0.42819700	5.15279000	0.76757300
O	-7.16319600	-1.14789900	0.37102700	O	0.42590200	5.65188700	0.15899000
O	-5.20027900	-1.38488700	1.59287900	O	-1.27391700	4.64497800	1.38591200
C	2.51216100	-1.86616900	3.36105100	C	-0.33017200	3.85035700	-3.06381400
O	1.38019200	-1.65482100	3.18377700	O	-0.84824400	4.70504800	-2.47194100
O	3.63617100	-2.08533500	3.55039200	O	0.19031500	3.00806400	-3.67487200
C	5.26277200	-0.24915000	2.25934000	C	-4.13482400	-1.37744400	-3.70399800
O	6.23435700	-0.87832800	2.30445400	O	-3.23389100	-0.77965800	-3.26047200
O	4.28989800	0.40048100	2.21773800	O	-5.03228600	-1.95292100	-4.15334800
C	2.31031300	5.35788000	-1.07736400	C	2.50583300	4.17553000	-1.02324500
O	3.07110200	4.50549900	-1.30238700	O	2.16049200	4.54911400	-2.06654500
O	1.57894900	6.22666200	-0.84369800	O	2.85395000	3.81382900	0.02774100
C	2.26910200	-4.57845400	0.84588900	C	-3.44084500	2.99962600	1.06461300
O	2.96366900	-3.74403900	1.25906100	O	-3.72112600	2.98310500	2.18967300
O	1.58983700	-5.42039800	0.43046800	O	-3.14098500	3.02388800	-0.06206600
C	-3.59919000	0.32106800	3.08864500	C	4.91666100	3.22752900	1.77113900
O	-3.17060000	0.70839600	2.07545400	O	5.68028500	3.64023700	1.00256200
O	-4.02466500	-0.04520200	4.10070100	O	4.14532000	2.81930900	2.54527300
n = 36				n = 37			
C	1.88727300	0.76824400	1.58940100	C	3.41386900	-4.78270700	2.39977400
O	0.89750000	1.35387500	1.42526700	O	4.35348600	-4.53646700	1.76067400
O	2.87582600	0.18212700	1.76088300	O	2.49313100	-5.03940100	3.06200900
C	-0.05970200	2.31957200	-0.77116900	C	3.75368200	2.22557300	-3.69727600
O	-0.38383100	3.28802600	-0.21380500	O	3.65212400	2.53141100	-2.57510500
O	0.24959000	1.34208100	-1.31910600	O	3.86668900	1.93349100	-4.81174900

C	-0.60498200	-2.00534300	-4.57563000	C	-4.31369900	3.33542200	0.57651100
O	0.42656800	-2.42387300	-4.91132000	O	-5.35888300	2.83196800	0.66568000
O	-1.65014400	-1.59668600	-4.27098300	O	-3.27759700	3.85664100	0.49839600
C	1.18726300	1.24003600	-3.88315700	C	2.01963600	4.70297400	-1.98830300
O	2.05964100	1.91732700	-3.51617700	O	1.50937500	4.18383500	-1.07659200
O	0.31984700	0.56741200	-4.26488700	O	2.51773600	5.22016000	-2.89817600
C	-2.22010500	-5.20399200	1.73085200	C	-0.00359800	-3.86154300	2.81802400
O	-3.05364100	-4.50117500	2.13868000	O	0.35423000	-2.83063600	3.22347300
O	-1.40298500	-5.91600200	1.31146000	O	-0.38458900	-4.88504800	2.42535300
C	1.72027800	-4.62694600	-3.46032000	C	-5.49645600	-2.60472800	0.37857900
O	2.18945500	-3.76386800	-2.82982000	O	-5.38803300	-2.93804500	1.48636100
O	1.27434200	-5.49308900	-4.08624800	O	-5.62445300	-2.27559800	-0.73076900
C	-1.77516900	3.41654100	-3.59118000	C	-2.73846800	-4.15124000	-3.01811500
O	-0.67580300	3.17583200	-3.28759300	O	-3.80681300	-4.10060300	-3.46882900
O	-2.86178100	3.65901400	-3.91373400	O	-1.66981900	-4.20696800	-2.55893100
C	3.70532300	2.63347300	-1.26445800	C	-0.47314200	-0.99232100	-1.68069600
O	3.03145700	2.05444500	-0.50874500	O	-0.14883700	-1.71643400	-2.52940000
O	4.37042500	3.21513300	-2.01531600	O	-0.78380000	-0.28626800	-0.81144400
C	-2.24937900	-0.12845600	-2.01711400	C	-0.03370700	-0.37872200	1.90716800
O	-2.20069200	-1.17288100	-1.50611300	O	-1.15457000	-0.39372300	2.20761300
O	-2.31971900	0.90726100	-2.53779100	O	1.09256100	-0.36978300	1.60601100
C	1.56001500	3.35548900	4.11078700	C	5.14698700	3.39260900	-0.50522900
O	2.01726600	4.41537700	4.23627400	O	4.25872600	4.09445400	-0.23411600
O	1.09669600	2.29262600	4.00377800	O	6.03990400	2.70720500	-0.78984800
C	-1.64273400	5.63717400	-0.78816600	C	-0.75711000	-0.43774100	5.65678400
O	-1.20133900	5.60485500	-1.86473400	O	-1.27204000	-1.26535900	5.02057600
O	-2.10320100	5.68853500	0.27753500	O	-0.23976900	0.37100400	6.31110800
C	5.28019200	-0.14739300	0.64418500	C	-1.29160700	4.67375500	-3.19055100
O	5.06927200	-1.29090400	0.59517800	O	-1.79968200	3.89536300	-3.88995600
O	5.51487500	0.98975000	0.69331300	O	-0.77833300	5.46320800	-2.50873500
C	-2.36291200	1.46204100	5.03076000	C	0.51347300	-5.96364500	0.06808600
O	-1.84748000	2.47030900	4.76462800	O	1.61743000	-6.09896900	0.40535300
O	-2.88932100	0.46422400	5.31093800	O	-0.59164800	-5.86242800	-0.28331100
C	-3.99084000	2.99311700	-0.36914000	C	-1.96800100	-3.44204000	0.11726000
O	-3.09279400	3.28152100	-1.05232100	O	-3.00754800	-3.93986900	-0.01071900
O	-4.89922700	2.72640000	0.30284800	O	-0.92993600	-2.92296300	0.24000100
C	4.28429100	0.28674900	4.10722400	C	-5.93226500	0.53321100	2.29142000
O	5.28647800	0.16810700	3.53014600	O	-6.10212300	1.05266800	3.31302600
O	3.29290600	0.41739000	4.70179700	O	-5.77409700	0.00205000	1.26483800
C	1.49662000	4.78794100	-2.90186800	C	4.46211800	1.53346800	2.45332200
O	1.66375800	4.36788300	-1.82613600	O	4.94684400	2.55209800	2.17824100
O	1.34004400	5.21089800	-3.96889100	O	3.99148500	0.50696600	2.73554100
C	-5.08631800	0.19780400	2.28651000	C	-3.25719700	-0.02887900	0.08940600
O	-4.30773900	0.94409200	2.72019800	O	-3.23075900	1.03233000	-0.38062100
O	-5.87122000	-0.54241900	1.85061700	O	-3.27253500	-1.09257200	0.55907300
C	3.12318200	-1.88299500	-4.58453300	C	1.34880400	1.95353200	4.06468800
O	3.42471300	-2.76128700	-5.27682000	O	2.38046700	2.33069000	4.44014200
O	2.82399800	-0.98626300	-3.89920500	O	0.30326000	1.59609100	3.69487800
C	1.39326100	5.11853500	0.81447300	C	-3.73992300	2.25614200	-2.74746600
O	2.01324800	4.21496200	1.20486600	O	-4.12284400	3.19247900	-2.17250700
O	0.78574400	6.02862200	0.42455800	O	-3.36390300	1.33025500	-3.33964400
C	1.48359200	-1.24455100	-1.53216700	C	2.19382800	4.10743200	1.55862000
O	2.45028000	-0.99659300	-0.93694500	O	2.30871500	5.26094500	1.55771800
O	0.51175100	-1.48966300	-2.12479500	O	2.06892200	2.94653200	1.56568200
C	-4.62548500	1.51516800	-3.90838100	C	1.97510800	-2.44108500	0.00310300
O	-5.11256900	1.85415500	-2.90452800	O	2.08408700	-1.61114600	-0.80844800
O	-4.15741600	1.17323700	-4.91287900	O	1.84788700	-3.25229200	0.82099300
C	-4.15941400	-2.37475200	-3.09327600	C	-3.98904400	-1.31810700	-3.06451800
O	-4.63129800	-1.31203200	-3.17539900	O	-4.84934200	-1.22447000	-3.83083800
O	-3.69901300	-3.43695900	-3.01945100	O	-3.11789400	-1.43511900	-2.29115800
C	-1.51130700	3.87670600	2.31905200	C	2.54539200	-1.46307600	3.89513900
O	-0.54406100	4.43615800	2.63952500	O	1.86779900	-0.71967000	4.48004300

O	-2.47995000	3.31510300	2.00363800	O	3.23126500	-2.20948700	3.32887800
C	-3.78422500	-2.23030400	0.52160700	C	5.70921600	-0.10080000	-1.37311600
O	-4.53043000	-2.75898100	-0.19132500	O	6.41270100	-0.12284200	-0.45089900
O	-3.04322200	-1.68897400	1.24172200	O	5.01845100	-0.08498900	-2.31250500
C	4.34319000	-3.21828800	-1.25963600	C	-6.73168100	0.31451300	-1.26659800
O	4.73512600	-2.56599900	-2.14141700	O	-5.66848600	0.58511200	-1.65919700
O	3.96790100	-3.89891400	-0.39742100	O	-7.79759400	0.05504700	-0.88960000
C	0.47228100	-0.48519100	4.43822000	C	-3.20995700	-2.01759100	3.10924200
O	0.04697200	-0.05380100	5.42599400	O	-2.57169800	-2.92615600	2.76629300
O	0.89489400	-0.92553500	3.44417000	O	-3.86367500	-1.12364600	3.46447200
C	4.41593200	3.22599100	1.88781000	C	-0.02138800	6.05823700	0.17334000
O	4.94560400	3.83916500	1.05744900	O	-0.58975500	5.17895000	0.68834500
O	3.88374500	2.62710100	2.73433800	O	0.53578600	6.93767000	-0.33608900
C	-1.32863600	-3.86858800	-1.64792700	C	4.85472500	-3.45433700	-1.43139700
O	-0.82919900	-3.98606800	-2.68931900	O	3.87271600	-4.03925400	-1.22344100
O	-1.83103700	-3.76847800	-0.60308700	O	5.84355900	-2.87673200	-1.64085500
C	-5.71840200	0.01817200	-0.97421700	C	0.20547200	1.82410800	-3.55624700
O	-6.82611500	-0.06945400	-1.29474400	O	0.93242200	2.73416300	-3.59154700
O	-4.60059300	0.09885000	-0.63935300	O	-0.52708000	0.92438800	-3.54565200
C	5.30966300	-0.08531500	-3.07484000	C	-0.93177100	2.51401600	-0.16792500
O	5.68071600	-0.50136800	-4.09393300	O	-1.10512600	2.78074300	-1.28773400
O	4.94746200	0.33963000	-2.05430000	O	-0.75463600	2.22267100	0.94347000
C	0.25701400	-4.37543400	4.14444400	C	0.94220200	-4.13571300	-3.07656400
O	-0.69221100	-5.04170100	4.06238900	O	0.71326400	-4.03688500	-4.21129000
O	1.20825300	-3.71367300	4.24677900	O	1.17968400	-4.24507500	-1.94296400
C	-1.80673800	0.68191200	1.60073900	C	2.49599100	1.18412600	-0.50111700
O	-2.07023100	0.97309000	0.50644200	O	1.42874700	1.31570200	-0.93619300
O	-1.53956200	0.38457800	2.69256300	O	3.57051800	1.05256100	-0.07017500
C	-2.89002400	-2.01922800	4.06001700	C	-2.90599700	1.42250200	3.43700700
O	-1.74498800	-2.15505100	4.22099800	O	-2.45612800	1.37074200	4.50471300
O	-4.03492500	-1.89368500	3.90781500	O	-3.37221900	1.48344600	2.37097100
C	1.23604300	-4.99659700	0.70620700	C	-0.70396200	-1.78731700	-5.11857200
O	1.52440300	-5.46624700	1.72704300	O	-1.75969200	-2.23052800	-4.90710900
O	0.95049400	-4.53136300	-0.32442100	O	0.33997400	-1.33414700	-5.35247100
C	-0.31136700	-2.18297700	1.27736000	C	5.24789100	-1.75926500	1.54824700
O	-0.12795300	-1.21794400	0.65456200	O	6.06248600	-1.72419100	2.37033100
O	-0.50019800	-3.15546400	1.88392800	O	4.43646100	-1.78375200	0.70957700
C	2.98361000	-2.45479200	2.43780800	C	2.59322200	-1.11487200	-3.42058900
O	2.28071700	-2.65155700	1.52980600	O	2.23824800	-0.01083300	-3.31415800
O	3.69545800	-2.26384200	3.33322900	O	2.95748200	-2.21309300	-3.51526700
				C	-0.90960200	4.20695400	3.24705000
				O	-2.04102200	3.98276600	3.11738100
				O	0.21855800	4.44749900	3.40945600
n = 38				n = 40			
C	-2.03147600	-1.95906200	0.93720500	C	-2.26774490	-1.17974351	1.45218723
O	-1.23655800	-1.46869800	1.62838500	O	-2.26901235	-1.45036063	2.58955642
O	-2.82412300	-2.44728600	0.24001200	O	-2.26647745	-0.90912640	0.31481804
C	-5.94844800	0.97539700	-3.15389200	C	2.46118937	-2.00072441	-4.46610234
O	-6.38000600	-0.08729700	-3.33549000	O	1.75515621	-2.62471647	-3.77400769
O	-5.51804600	2.04304200	-2.98353700	O	3.16722253	-1.37673235	-5.15819698
C	5.50077500	1.54619200	4.43498600	C	-2.08266502	1.47701060	-1.50535942
O	4.51037800	0.99746000	4.71302000	O	-1.22602758	1.05318474	-2.17870024
O	6.49366800	2.08986400	4.18313000	O	-2.93930245	1.90083645	-0.83201861
C	-3.50876600	0.54328000	4.11003500	C	-1.03635405	-0.19990338	-5.14656584
O	-4.20800400	1.46595100	4.01041900	O	-2.20245620	-0.12530154	-5.18509173
O	-2.82280000	-0.38746200	4.23699500	O	0.12974811	-0.27450522	-5.10803995
C	4.73242700	-0.05999900	1.20824900	C	5.83401654	-1.25829646	-3.19924462
O	5.34499400	0.71734900	1.81058800	O	6.84682730	-1.37646870	-3.77116559
O	4.12939400	-0.84526300	0.59005400	O	4.82120578	-1.14012422	-2.62732365
C	-1.27087100	1.21597700	1.66216100	C	-4.29261570	1.84942188	-4.45493931
O	-0.11375700	1.30247200	1.69222600	O	-3.44470897	2.46890437	-3.94099424
O	-2.43141400	1.12446200	1.63481300	O	-5.14052243	1.22993938	-4.96888437

C	3.38628600	-1.51109600	4.14753300	C	3.46792785	-2.96554144	3.61893142
O	2.55031400	-1.33085900	4.93175000	O	3.32995308	-3.91195584	4.29132020
O	4.22936700	-1.70320200	3.36693900	O	3.60590262	-2.01912704	2.94654265
C	-0.85244200	3.11945800	-2.63699100	C	-5.43326488	-2.14074075	0.40441724
O	-0.47299800	4.15613300	-2.27275000	O	-5.16643723	-1.74134497	1.47031120
O	-1.23330600	2.08268000	-3.00254500	O	-5.70009253	-2.54013653	-0.66147672
C	3.48474200	-4.60015500	-2.83317800	C	2.52600725	3.55321144	1.58279647
O	2.89677400	-4.42895700	-3.82064000	O	3.66910446	3.30793824	1.57908900
O	4.08180500	-4.77813000	-1.85030600	O	1.38291005	3.79848464	1.58650393
C	0.82549900	-2.39659300	-4.20791900	C	-4.26643045	4.42852244	0.04225640
O	1.52028600	-1.622261800	-4.72201600	O	-3.46931108	5.04794269	-0.54745808
O	0.13532100	-3.17772500	-3.68695800	O	-5.06354982	3.80910220	0.63197089
C	-4.40648400	4.37277100	-2.02675700	C	6.41689268	-2.27346283	1.03146532
O	-3.58788200	4.34586400	-2.85346000	O	6.16390467	-2.34732682	-0.10756282
O	-5.22134800	4.40302100	-1.19842100	O	6.66988069	-2.19959884	2.17049345
C	2.87934900	-1.16976300	-2.04588600	C	2.19436683	0.31629841	5.71982693
O	2.55774100	-2.27462200	-1.89215500	O	2.29491823	-0.82062191	5.46655729
O	3.19869900	-0.06239000	-2.20352500	O	2.09381542	1.45321873	5.97309658
C	-4.49169400	2.93465200	1.70445800	C	-5.15568418	1.20020938	2.49882974
O	-5.24672100	2.12251700	1.35599100	O	-4.04578687	1.18614225	2.13171397
O	-3.74220300	3.75592100	2.04779500	O	-6.26558149	1.21427650	2.86594552
C	2.38613100	1.59125500	-4.23754100	C	-0.79995019	-2.76918386	4.89831350
O	3.10780200	1.01114700	-4.93741300	O	0.12766425	-3.00734602	4.22775095
O	1.65984400	2.18104200	-3.54359400	O	-1.72756464	-2.53102170	5.56887605
C	5.08227200	1.80803200	-1.79911900	C	-0.35686748	-1.82178531	-1.86985080
O	5.67995900	1.08419700	-1.11509800	O	0.38686857	-1.74439086	-0.97112353
O	4.48417000	2.53041000	-2.48674800	O	-1.10060353	-1.89917976	-2.76857807
C	-2.40011600	-0.01177800	-4.44093800	C	-1.30911284	6.48697499	2.59182814
O	-1.39867900	-0.35863800	-4.91838200	O	-0.24694942	6.20215960	2.98873238
O	-3.40268400	0.33977500	-3.96828300	O	-2.37127626	6.77179038	2.19492391
C	3.95230600	-3.61819400	0.67260400	C	-3.67014775	4.41775247	4.31015751
O	5.11211000	-3.61367300	0.69945300	O	-2.75061829	4.96160730	4.78505899
O	2.78690600	-3.62501100	0.65789600	O	-4.58967720	3.87389764	3.83525602
C	0.77679000	-4.28125900	2.67849100	C	-2.57993735	-4.84460761	-0.94923561
O	1.63529300	-4.38036500	3.45110900	O	-2.80213789	-3.70845792	-1.11243702
O	-0.08003900	-4.19083200	1.89230200	O	-2.35773680	-5.98075731	-0.78603420
C	0.49545500	-3.85598400	-1.01774900	C	0.13307564	2.99122965	-4.29759353
O	-0.04843000	-2.86567200	-0.71699500	O	-0.58287959	2.75708414	-5.19170086
O	1.03113300	-4.83646000	-1.32063400	O	0.84903086	3.22537515	-3.40348620
C	-0.21422800	-1.20325300	4.25938900	C	-4.57755760	-1.87587974	4.56283473
O	-0.43675700	-2.34011500	4.37944300	O	-4.41821679	-0.73052912	4.73495787
O	0.00888400	-0.06689900	4.14429100	O	-4.73689841	-3.02123036	4.39071159
C	-1.88460100	4.54546900	0.19489700	C	1.35409468	-5.24800896	-2.13234184
O	-1.21015700	3.69167900	0.62113100	O	2.15749895	-5.70466345	-2.84847882
O	-2.55220500	5.38933200	-0.23708600	O	0.55069041	-4.79135448	-1.41620485
C	2.04326900	1.65082000	3.36114600	C	3.21954948	-2.09848493	-0.45406800
O	2.52288100	0.83093900	2.68295400	O	3.19305628	-3.15206383	-0.96014460
O	1.57085200	2.46628200	4.03542100	O	3.24604268	-1.04490603	0.05200861
C	6.27016700	-1.66294100	-0.94962900	C	1.67759721	0.93569502	-1.45241617
O	7.00909000	-1.37186100	-0.10498500	O	1.38723394	1.41093479	-0.42446664
O	5.52610600	-1.95744700	-1.79848700	O	1.96796048	0.46045525	-2.48036571
C	1.17916400	4.87651200	1.07428700	C	-3.09877872	-4.75961467	2.66441074
O	1.66017700	3.87989200	1.43888000	O	-2.39367833	-4.98790697	3.56860097
O	0.70950300	5.87410300	0.71270100	O	-3.80387912	-4.53132237	1.76022051
C	-0.95654500	3.70705200	3.62177400	C	5.00367354	0.69134088	2.93725244
O	-0.47784400	4.72449600	3.32790200	O	4.73103516	0.81373573	4.06753193
O	-1.45188000	2.69665400	3.91843300	O	5.27631192	0.56894603	1.80697295
C	-7.15503900	0.43342400	0.30816400	C	1.33957084	-0.03353904	2.33996755
O	-6.99986100	1.04197600	-0.66921400	O	0.73458309	-0.94972353	1.93817193
O	-7.32879700	-0.16027600	1.29141500	O	1.94455859	0.88264544	2.74176317
C	-5.12932900	-1.83443100	1.90154000	C	3.89347929	-5.48084407	0.79084419
O	-5.68053100	-2.85448200	1.90724100	O	4.62368250	-4.74615146	1.33294561

O	-4.56436700	-0.81386200	1.91305200	O	3.16327608	-6.21553668	0.24874276
C	1.44711600	-1.17476800	1.22682900	C	-1.50068703	2.63904226	1.86080486
O	1.50538300	-1.73411900	2.24213300	O	-1.99803671	3.69586442	1.91193354
O	1.39349100	-0.61796600	0.20795500	O	-1.00333736	1.58222011	1.80967619
C	-4.03587400	-4.89718900	0.32471500	C	0.40141824	-3.82658106	1.37435852
O	-3.25768100	-5.28312200	1.09907900	O	1.55967160	-3.89377968	1.51850229
O	-4.81418600	-4.52447000	-0.45361700	O	-0.75683511	-3.75938244	1.23021476
C	5.11291400	-0.77268600	-4.21736600	C	3.75258176	1.63105367	-4.82720797
O	5.78805100	0.14033300	-3.96175400	O	2.75431546	1.89192021	-5.37698697
O	4.44701800	-1.69479700	-4.45749800	O	4.75084806	1.37018713	-4.27742896
C	-0.46465900	-0.16818800	-1.63498200	C	-2.90765486	5.35229049	-3.48088322
O	-1.25466900	0.05374700	-0.81015700	O	-4.05009739	5.54027256	-3.64315376
O	0.32205400	-0.38749200	-2.46043500	O	-1.76521234	5.16430842	-3.31861269
C	2.55265700	4.70428000	-2.40904600	C	-5.92368446	1.47814706	-1.16080293
O	2.52772900	4.43940400	-1.27361900	O	-5.99628520	0.65882840	-0.32996602
O	2.59064800	4.98209200	-3.53227700	O	-5.85108371	2.29746572	-1.99163984
C	-5.58981900	-2.22435800	-1.74427500	C	-4.01092353	-1.60032507	-3.19580462
O	-6.21120800	-1.86050500	-0.82952800	O	-4.03441839	-0.60796795	-2.57813218
O	-4.97586500	-2.59949000	-2.65640200	O	-3.98742867	-2.59268219	-3.81347706
C	-2.45915500	-4.07186700	3.61094800	C	5.03573953	-4.65936461	-2.77494943
O	-3.02853500	-3.18115400	3.11973600	O	4.72277973	-4.01568925	-3.69938553
O	-1.90850900	-4.96070300	4.10881900	O	5.34869933	-5.30303996	-1.85051332
C	1.97559800	1.92750500	-0.39843700	C	-0.40746370	4.96137635	-0.53942122
O	0.90750700	2.04007600	-0.83943600	O	-0.57812612	3.83078865	-0.78332634
O	3.04553900	1.80217300	0.04150900	O	-0.23680128	6.09196405	-0.29551611
C	4.69549500	3.42504400	1.59015700	C	-1.55965288	0.96426118	4.74866371
O	4.22803100	3.25362500	2.64274400	O	-2.47419773	1.69252501	4.75779776
O	5.17091100	3.61964300	0.54841800	O	-0.64510804	0.23599736	4.73952967
C	-2.27885700	-3.09143900	-2.37471200	C	1.11584064	3.88336999	4.49098224
O	-2.31056400	-4.22547000	-2.12772100	O	2.13576935	4.44788784	4.57991439
O	-2.23369700	-1.95233100	-2.60738400	O	0.09591192	3.31885214	4.40205009
C	-3.70694000	1.19328100	-0.92906400	C	3.20834079	4.41327014	-2.17138176
O	-3.24679900	2.26009300	-0.84967800	O	3.80898120	4.21045588	-3.15369606
O	-4.16150300	0.12782300	-1.00697000	O	2.60770038	4.61608440	-1.18906746
				C	-1.27323996	-4.00164855	-4.75647652
				O	-1.19900585	-3.20708801	-5.61088085
				O	-1.34747406	-4.79620908	-3.90207218
				C	5.47505538	1.36780196	-1.08648375
				O	4.42505854	1.88092381	-1.11898808
				O	6.52505221	0.85468012	-1.05397942
n = 45				n = 50			
C	-0.43670565	-2.18923257	2.37010679	C	0.87299600	-2.19895348	2.31752530
O	-0.52453620	-3.34554974	2.51863396	O	0.10604352	-2.27769551	3.19640384
O	-0.34887510	-1.03291541	2.22157961	O	1.63994848	-2.12021144	1.43864675
C	4.87683207	3.29652520	-4.33523632	C	-2.38225035	3.52186091	1.52585966
O	4.88442091	4.29142978	-4.94919984	O	-2.99574911	4.33839907	2.09483121
O	4.86924322	2.30162062	-3.72127280	O	-1.76875160	2.70532275	0.95688811
C	1.15612244	-5.59864301	3.18853678	C	2.73733085	1.63723882	-2.06374257
O	1.87021329	-4.89243346	3.78702341	O	2.89186247	1.03392844	-1.07430815
O	0.44203158	-6.30485256	2.59005016	O	2.58279923	2.24054920	-3.05317700
C	-1.75515513	3.38903195	5.44854404	C	-0.90525996	-5.29035384	2.64550603
O	-0.98129965	3.13021228	6.28580385	O	-2.00475354	-5.27055318	3.04245151
O	-2.52901062	3.64785162	4.61128424	O	0.19423362	-5.31015450	2.24856055
C	1.13717078	3.82892388	-3.69241233	C	-1.98889124	-3.34144862	-0.26386709
O	2.19336222	3.84773790	-3.19146366	O	-2.40162005	-3.59944125	-1.32685281
O	0.08097933	3.81010987	-4.19336101	O	-1.57616243	-3.08345599	0.79911863
C	-3.68595497	1.85368378	-1.25911835	C	1.43081827	-3.82332980	5.37308705
O	-3.98735902	2.40388534	-0.27256995	O	2.25466268	-2.99573269	5.42972019
O	-3.38455091	1.30348222	-2.24566675	O	0.60697386	-4.65092692	5.31645390
C	4.84894500	3.43919009	2.07838143	C	4.90021814	3.45538782	-4.50896710
O	4.72605590	2.38041817	2.55873983	O	4.70511229	4.46488732	-3.95247058
O	4.97183410	4.49796202	1.59802303	O	5.09532398	2.44588832	-5.06546362

C	-5.43478395	2.14936621	2.22340949	C	1.00036633	1.75156302	1.20201924
O	-5.86267220	1.10301284	1.92524816	O	1.42418937	2.83789024	1.11769181
O	-5.00689571	3.19571959	2.52157081	O	0.57654330	0.66523580	1.28634666
C	-1.64354259	-4.08166966	5.25193708	C	-0.97280550	-4.40508156	-3.68258688
O	-2.32421987	-3.13127062	5.26818619	O	-1.03925210	-3.32443108	-4.12374817
O	-0.96286532	-5.03206869	5.23568798	O	-0.90635891	-5.48573205	-3.24142559
C	-0.95795826	-0.09680071	-3.02302730	C	-4.67075731	-4.59538685	-3.08533738
O	-1.54029437	-1.10990699	-3.05969100	O	-3.94841144	-4.82387114	-3.97576159
O	-0.37562214	0.91630557	-2.98636360	O	-5.39310319	-4.36690257	-2.19491316
C	-2.38564416	-5.30513437	1.43893974	C	-0.02667067	2.65084275	4.81028955
O	-1.87732698	-5.34496092	0.38686018	O	-0.25933245	2.74416366	3.66835977
O	-2.89396133	-5.26530783	2.49101930	O	0.20599112	2.55752184	5.95221933
C	4.92176905	0.10604621	4.68008432	C	5.15291162	-5.76230284	-1.44611157
O	5.26542563	-0.63396699	3.84275253	O	4.20100728	-5.62104307	-2.11001497
O	4.57811247	0.84605941	5.51741612	O	6.10481595	-5.90356261	-0.78220817
C	5.21303869	-0.52771583	-2.84955342	C	2.97688197	4.94195334	-0.18370814
O	4.63241441	-1.02935907	-3.73163812	O	3.65707233	4.12778872	-0.67495245
O	5.79366297	-0.02607259	-1.96746873	O	2.29669161	5.75611795	0.30753616
C	7.15269749	2.59596192	-1.13298301	C	-3.02803219	7.25418945	1.69465658
O	7.54261715	2.76317068	-2.22240846	O	-3.08015809	6.99770214	0.55520887
O	6.76277784	2.42875315	-0.04355756	O	-2.97590630	7.51067676	2.83410428
C	-1.62139957	1.46688634	2.77393982	C	1.18364487	-5.89091654	-1.06249584
O	-0.55586171	1.87226167	3.03306107	O	1.32091822	-7.01554778	-1.35094779
O	-2.68693743	1.06151101	2.51481857	O	1.04637153	-4.76628531	-0.77404389
C	-2.46524193	4.99114159	1.84747289	C	-0.89495418	-0.77238196	5.84720890
O	-1.94916142	4.05005231	1.38394750	O	-1.49882876	0.06061342	5.29196293
O	-2.98132244	5.93223087	2.31099828	O	-0.29107960	-1.60537734	6.40245488
C	-1.47974152	-2.52879869	-5.75735276	C	-3.42978275	-2.65864677	3.68010684
O	-0.84050270	-1.65472797	-6.19805449	O	-4.02881630	-2.68836990	2.67655353
O	-2.11898034	-3.40286941	-5.31665104	O	-2.83074920	-2.62892364	4.68366016
C	4.18150994	5.36325934	-1.23579424	C	6.62830454	-3.87446312	1.46888346
O	3.20286553	5.77705286	-0.74807102	O	7.13023746	-3.09969514	0.75149804
O	5.16015436	4.94946581	-1.72351747	O	6.12637161	-4.64923110	2.18626888
C	1.71531425	-3.90338795	-4.10415439	C	0.50353521	5.66046426	2.74502606
O	2.39733515	-3.79680539	-3.16058057	O	-0.37480266	5.87937870	2.00513217
O	1.03329335	-4.00997051	-5.04772821	O	1.38187308	5.44154982	3.48491995
C	-4.06525146	-1.33757874	3.55639718	C	-4.12205567	4.92739454	-1.40524787
O	-4.65753936	-0.74616110	4.37264722	O	-3.73927163	5.63689336	-2.25196608
O	-3.47296357	-1.92899638	2.74014713	O	-4.50483971	4.21789573	-0.55852967
C	5.92488638	-0.37937285	0.96541289	C	-5.88508150	4.79853787	2.44430845
O	7.07986739	-0.54359950	1.04217470	O	-5.72985030	5.90642803	2.10471078
O	4.76990536	-0.21514619	0.88865108	O	-6.04031271	3.69064771	2.78390613
C	-4.91515405	-4.70453840	-4.60604494	C	-2.95127528	-1.04747386	-3.35115325
O	-5.22995625	-3.63877252	-4.96920684	O	-3.88127748	-1.75160428	-3.42951250
O	-4.60035184	-5.77030429	-4.24288305	O	-2.02127307	-0.34334345	-3.27279399
C	0.25486089	6.03631495	-0.65641894	C	-5.13704771	1.92253548	-2.74492752
O	0.23966140	6.03260447	0.51259737	O	-4.83354415	0.92683892	-2.21265141
O	0.27006039	6.04002542	-1.82543524	O	-5.44055127	2.91823204	-3.27720364
C	-1.79725248	-4.00088512	-2.35893724	C	6.32578162	0.94236860	3.57362703
O	-0.63235615	-4.10003898	-2.35355417	O	6.12083350	2.04666533	3.89823279
O	-2.96214880	-3.90173126	-2.36432032	O	6.53072974	-0.16192814	3.24902126
C	-5.47141879	4.93548502	-0.23575936	C	-1.22345844	2.22791385	-1.90112493
O	-4.46286675	5.47765463	-0.47180765	O	-0.16854364	1.82615143	-1.59684603
O	-6.47997083	4.39331540	0.00028893	O	-2.27837323	2.62967626	-2.20540384
C	1.89943043	0.13150800	-4.71749707	C	-2.96004332	1.39953696	-6.21089936
O	2.20702403	1.19306271	-5.09872100	O	-2.21782542	1.78575198	-7.02747420
O	1.59183684	-0.93004672	-4.33627315	O	-3.70226121	1.01332194	-5.39432452
C	1.32837327	-5.33868356	-0.39694197	C	-0.60533930	6.15092711	-1.03741202
O	1.41552375	-4.35909958	0.23524782	O	-0.88522523	5.02539481	-0.89015434
O	1.24122278	-6.31826754	-1.02913177	O	-0.32545337	7.27645941	-1.18466970
C	-2.15438464	2.12478851	-5.38379325	C	3.55536066	3.46480887	3.23744202
O	-2.99088476	2.81135420	-4.94136923	O	4.12434733	4.07236059	2.41647979

O	-1.31788452	1.43822282	-5.82621727	O	2.98637399	2.85725714	4.05840426
C	3.56178529	-2.83003471	1.98021190	C	2.76289872	0.03896688	4.83842185
O	2.57289637	-2.27563259	2.26583564	O	3.87311767	0.00275166	5.20303980
O	4.55067420	-3.38443683	1.69458816	O	1.65267977	0.07518209	4.47380389
C	4.67044679	-6.46526072	1.43280923	C	-2.49286569	-6.68733286	-0.90589310
O	3.51796281	-6.40883137	1.62106519	O	-3.35583761	-6.96084383	-1.64570059
O	5.82293078	-6.52169007	1.24455328	O	-1.62989377	-6.41382188	-0.16608561
C	1.89527997	-1.65696681	-0.95832565	C	1.72774977	4.93949086	-3.92461292
O	3.02737136	-1.92487325	-0.84239832	O	1.78138847	4.62687211	-5.04988458
O	0.76318859	-1.38906037	-1.07425298	O	1.67411108	5.25210961	-2.79934125
C	-5.49587908	-3.93065616	-0.86251868	C	-2.95890900	5.21400388	4.89278299
O	-6.14952026	-4.09964070	-1.81700354	O	-1.79131697	5.16133211	4.86452644
O	-4.84223789	-0.76167162	0.09196617	O	-4.12650104	5.26667565	4.92103955
C	-4.39982717	-0.95504066	-3.94960388	C	4.23220491	-0.42876614	-4.88673559
O	-4.93056699	-1.30284188	-2.96767035	O	4.17647168	-0.53809490	-6.04939846
O	-3.86908734	-0.60723943	-4.93153741	O	4.28793813	-0.31943738	-3.72407273
C	2.07140223	0.63092223	2.19538039	C	5.92313253	2.10811303	-0.75999220
O	1.84470165	0.74654496	1.05429225	O	5.77064480	2.22872442	-1.91283403
O	2.29810282	0.51529950	3.33646853	O	6.07562025	1.98750163	0.39284964
C	-5.70979615	2.65577136	-3.62901570	C	3.46208187	-3.00699021	-0.65945101
O	-5.41963003	3.57469703	-2.96703145	O	3.90981280	-3.67080234	0.19244945
O	-5.99996227	1.73684568	-4.29099995	O	3.01435094	-2.34317808	-1.51135146
C	1.69266755	1.87692719	5.79433298	C	-6.79086448	-1.50884323	2.81735799
O	1.35363878	0.86187298	6.26504346	O	-6.68364812	-0.82939232	1.87200354
O	2.03169633	2.89198140	5.32362250	O	-6.89808084	-2.18829413	3.76271244
C	3.20017886	1.75543701	-1.25914080	C	-5.39016277	-4.53233225	0.85432314
O	2.67801630	0.96380254	-1.94288421	O	-6.42046175	-4.00672446	1.02480592
O	3.72234141	2.54707147	-0.57539739	O	-4.35986380	-5.05794004	0.68384036
C	-1.43462224	-0.43528209	6.36669128	C	0.58241318	-1.15266731	-2.38074897
O	-1.67044607	0.11642960	5.36327450	O	1.08697451	-0.58919504	-3.27224254
O	-1.19879842	-0.98699378	7.37010807	O	0.07785185	-1.71613959	-1.48925541
C	-6.68279365	-0.22566190	-0.76465540	C	-2.08445853	4.67516062	-4.53587317
O	-6.90534433	-1.26986420	-0.28825572	O	-2.97738173	4.12509251	-5.05255213
O	-6.46024297	0.81854041	-1.24105508	O	-1.19153533	5.22522874	-4.01919422
C	5.04980918	-4.05372925	-1.31290865	C	6.48530630	-1.71842840	-1.90671057
O	5.76843417	-3.17411015	-1.58984235	O	6.00229941	-2.76829761	-2.08369331
O	4.33118419	-4.93334835	-1.03597495	O	6.96831320	-0.66855919	-1.72972782
C	-0.28064275	2.17441151	-0.38116902	C	4.22617820	-0.11371579	1.25065008
O	0.47100412	3.02410417	-0.66382302	O	4.79996356	-0.80390769	0.50148426
O	-1.03228961	1.32471885	-0.09851502	O	3.65239284	0.57647610	1.99981589
C	-2.46685734	4.95187500	-2.79732836	C	-5.76276521	-1.61212054	-0.90823601
O	-2.12553896	4.11154211	-2.05963850	O	-6.78645371	-1.42118609	-1.43969608
O	-2.80817571	5.79220788	-3.53501821	O	-4.73907670	-1.80305499	-0.37677595
C	1.05579125	4.31063216	2.85562827	C	3.16551334	-5.75303291	2.21281931
O	1.85697081	3.75933545	2.20676222	O	3.21540355	-6.39396097	1.23631222
O	0.25461168	4.86192887	3.50449432	O	3.11562313	-5.11210485	3.18932641
C	1.85121991	-2.05251708	5.25723111	C	0.64393067	1.77604911	-5.26693859
O	0.69917804	-2.08351163	5.06055171	O	1.52705811	1.29608797	-5.86407103
O	3.00326178	-2.02152252	5.45391052	O	-0.23919676	2.25601025	-4.66980615
C	-2.91952419	-1.46649860	-0.04575656	C	0.27038717	-1.49387420	-6.06125560
O	-3.81475670	-0.71480632	-0.06476687	O	1.24007177	-2.14615683	-6.02834588
O	-2.02429168	-2.21819087	-0.02674625	O	-0.69929743	-0.84159157	-6.09416532
				C	4.87432489	-2.69442320	4.10668099
				O	4.25986710	-2.27100582	3.20667918
				O	5.48878267	-3.11784059	5.00668280
				C	-2.22876412	-0.18905097	0.99817499
				O	-2.21496160	-0.13516421	-0.16962192
				O	-2.24256664	-0.24293773	2.16597190
				C	-4.01878562	1.18920355	4.14492884
				O	-3.40436936	2.18384807	4.14927106
				O	-4.63320188	0.19455904	4.14058662
				C	2.95168015	-3.78366240	-4.14845912

	O	1.92130412	-4.17727155	-3.76084979
	O	3.98205618	-3.39005326	-4.53606845
	C	-5.66467097	1.68746813	0.61080203
	O	-6.68405893	1.91554926	0.08575813
	O	-4.64528301	1.45938701	1.13584594

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