

Supplementary Information: Active Learning and Neural Network Potentials

Accelerate Molecular Screening of Ether-based Solvate Ionic Liquids

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I. TRAINING DETAILS

Several neural network (NN) interatomic potentials have demonstrated sub kcal mol⁻¹ accuracy. Here, we implemented a graph convolution model based on SchNet [1], to represent the highly complex potential energy surface (PES). This graph convolution model has been shown to achieve state-of-the-art prediction for chemical properties and graph classification tasks[2, 3]. The model consists of iterative message and update steps that systematically gather information from neighboring atoms to produce atomic feature vectors. A fixed cutoff distance is used to determine molecular geometrical connectivity given a 3D configuration of atoms. We define v as the atomic index and $N(v)$ as its neighbors. The graph convolutions iteratively update the atomic embeddings h_v by aggregating “messages” (msg) from their connected atoms v and their edge features (e_{uv}). By performing this operation several times, a many-body correlation function can be parameterized to represent the PES of the ether-ion complex. The atomic fingerprint vector after each convolution t is represented as:

$$h_v^t = h_v^{t-1} + \sum_{u \in N(v)} msg^t(h_u, e_{uv}) \quad (1)$$

In the case of SchNet, the update function is simply a sum over atomic embeddings. The edge feature is parameterized by Gaussian smearing of distances between pairs of atoms. The message function is parameterized by:

$$msg^t(e_{uv}, h_v) = MLP_3(MLP_2(e_{uv}) \circ MLP_1(h_v)) \quad (2)$$

where MLP_i are independent Multi Layer Perceptrons (MLPs) that parameterize the embeddings into a certain dimension size. For each convolution t , a separate message function is applied to characterize atom correlations at different scales. After an element-wise product of atom fingerprints h_v and pair interaction fingerprints e_{uv} , the joint fingerprint is determined by an additional MLP that incorporates more non-linearity in the model. e_{uv} is parameterized from a Gaussian smearing operations. MLP_2 and MLP_3 output parameterized edge and atom fingerprints of the same dimension. The message is constructed by the elementwise product between parameterized edge and atom fingerprints followed by another MLP_3 . The message update and update procedures is a convolution on 3D graphs. After several convolutions procedures described above. The atomic embeddings are then used to parameterize atom-wise energies which sum to give the total energy of the system (refer to Ref.[1] for more details on the network structure).

dimension of atomic embeddings	256
dimension of filter layer	256
dimension of Gaussian smeared kernels	32
number of convolutions	5
k	10
cutoff distance (\AA)	4.5

Table I. Parameters used for SchNet Graph convolution models

To improve the efficiency of running MD using neural network potentials, we also include classical harmonic bond energy terms that constrain the configurations to those that maintain the molecular graph of the ether molecules in 3D.

$$E_{tot} = \sum_v MLP(h_v) + \frac{1}{2} \sum_{i,j}^{bonds} k(|x_i - x_j| - r_o)^2 \quad (3)$$

where r_o is the equilibrium bond lengths obtained from converged ether molecule geometries. The bond energy is summed over chemical bonds of a molecule or complex. We use parameters described in Table. I for the training of Graph Neural Networks of all the models used (following the parameter definition in Ref. [1])

II. ACTIVE LEARNING

All the DFT calculations were performed using ORCA 4.0.1.2 [4]. We first selected a random set of 44 ether-lithium clusters that are representative of the ether chemical species in terms of the number of carbon spacers and the molecular size. We perform conformer optimization starting from geometry generated by RDKit [5] using MMFF94 force fields [6]. The ion-ether complexes are made by randomly placing ions near oxygens in the ether molecules. These initial geometries are further optimized at the BP86d3/def2-SVP level of theory [7–9]. The initial training set is obtained by generating normal-mode-sampled data using Hessians of converged geometries. The neural networks are first trained on the normal-mode-sampled data and subsequently undergo sampling according to a constant energy ensemble (NVE). The newly-sampled geometries are sent for DFT calculations and included in the next training round. Due to the poor coverage of phase space by the initial data points, the neural sampling steps produce nonphysical geometries that involve bond formation and breaking. These geometries are labeled as “reacted” and are excluded from the training data because they are not representative configurations. The “reacted” geometries are

removed for further DFT validations because they are unlikely to converge in the self-consistent cycle and are not expected to occur near room temperature. We dynamically modify the sampling time by scaling with the fraction of “reacted” geometries. Short 10ps simulations are done for the first round of neural MD. Such sampling time is dynamically changed based on the rejection rate. If the rejection rate is higher than 70 %, the simulation time is reduced by 25 % to ensure more valid conformers are sampled within a shorter simulations. If the rejection rate is lower than 70 %, the simulation time is increased by 50 % for the next round of sampling to better explore the configuration space given initial good performances.

Active Learning has been explored by several works to learn transferable inter-atomic potentials. [10–12] To quantify uncertainties, we also perform uncertainty analysis by training 10 neural networks with different initial random weight initialization and computing the standard deviation of their predictions (Fig. S1) on the trained data. Such ensemble methods can be used as an efficient method to estimate the uncertainty of the trained model and to test the convergence of active learning results.

The same approach with oligoether complexes with with Na^+ and Mg^{2+} ions yield similar results during the active learning process. The resulting interaction energy and HOMO (Highest Occupied Molecular orbitals) follow similar trends as a function of N_{oxygen} and C:O ratio (Fig. S5). Additionally, we include selected optimized geometries in Fig. S4 for ethers with side alkyl group modifications. This provides a potential pathway for tuning physicochemical properties like melting temperature of Mg^{2+} based SILs which show high melting point.

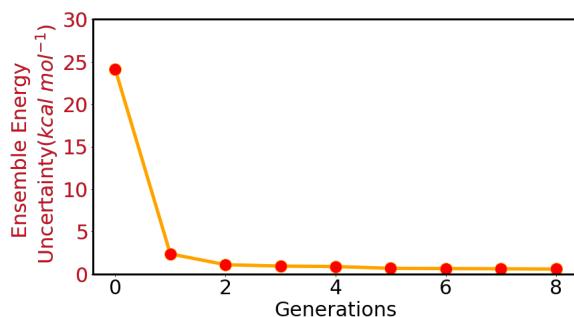


Figure S1. Uncertainty in neural network predictions at each generation of active learning. The uncertainty is estimated by computing the standard deviation of the predictions of 10 neural networks trained on the same set of data (random train/test splitting) to test the robustness of the prediction.

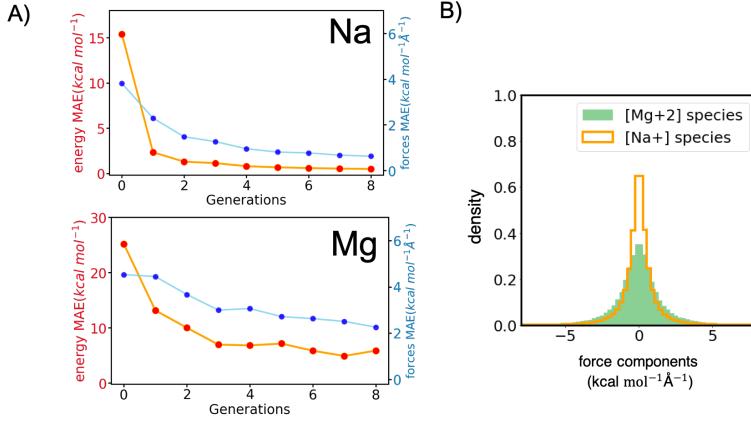


Figure S2. A) The results from active learning of Na^+ and Mg^{2+} ion interactions. B) Force validation for the neural-network optimized structures of ether species with Na^+ and Mg^{2+} ions

III. SOAP ANALYSIS AND DIMENSIONALITY REDUCTION OF SAMPLED CONFIGURATIONAL SPACE

We apply SOAP (Smooth Overlap of Atomic Positions) [13] to convert the coordination structure of lithium into a vector representation. (We choose a cutoff radius of 4.5 \AA , $n_{max}=3$, $l_{max}=5$) The learned vector embeddings from an ensemble of structures are analyzed with t-distributed stochastic neighbor embedding (T-SNE) [14] in a 2-dimensional space for easy visualization. In Fig. 1B in the main text, the plot is produced from T-SNE studies of all data points sampled by the different generations of trained NN.

IV. ENERGY DECOMPOSITION VIA LINEAR REGRESSION

The ether groups and metal ions form n-membered ring structure. For example, two carbon-spacers and two oxygens from a 5-membered ring with a metal ion; 3 carbon spacers form 6-membered rings with oxygens and metal ion upon chelating. We count the number of each n-membered rings in our complex and use this molecular metric as inputs for analysis to correlate with binding energy. We perform linear energy decomposition via a least-square fit of the equation $E_{\text{bind}} \approx \sum_n E_n * N_n + C$ where N_n , E_n and C are the count of n membered rings, the energy of the n-membered ring and a constant energy reference, respectively. We fitted E_n which represents the individual energy contribution from each ring size. We observe that larger n-membered rings contribute more to the interaction energies (Fig. S3) for all the ion clusters.

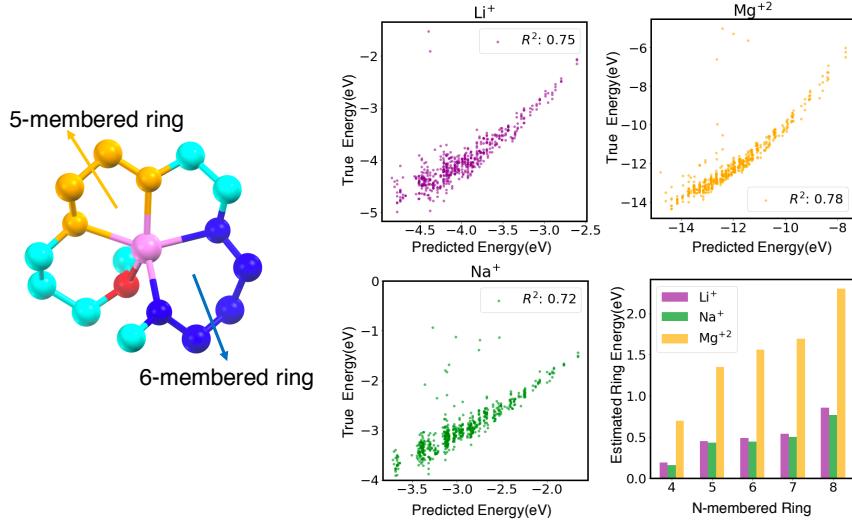


Figure S3. Description of n-membered ring structures in a ether-ion complex and Linear regression analysis to decompose the energy into explicit n-membered ring contributions for the interaction energy between ether and ions.

V. GEOMETRY OPTIMIZATION

We perform neural network molecular dynamics followed by geometry optimizations to bypass expensive DFT calculations. We first run long MD trajectories to sample a handful of starting points for optimization. We then perform the Broyden–Fletcher–Goldfarb–Shannon algorithm (BFGS) [15] to find converged geometries, which subsequently receive further DFT validation. The resulting geometries are close to being truly converged. This was determined by comparing the distribution of DFT atomic forces and atom-wise RSMD (Root Mean Square Distances) to that of NN-optimized geometries. After further DFT refinement with DFT at the theory level of BP86-D3/def2-SVP [7–9]. For better description of non-covalent interactions, we promote the calculations to the theory level of ω b97xD/def2-TZVP [9, 16] for further geometry optimizations using ORCA[4], to optimize the geometries obtained from the NN/DFT pipelines described.

VI. COMPUTATIONAL DATA

The DFT results of all computed geometries at ω -B97xD3/def2-TZVP level of theory are available in `esi_dft.pdf`. We also include approximate volumes of the complexes. The volume estimation is done using the 3D-voxel-based flood-hill algorithm as described in ref. [17]. We treat the ether-ion complexes as a solute and use methane molecules to approximate the solvent using a

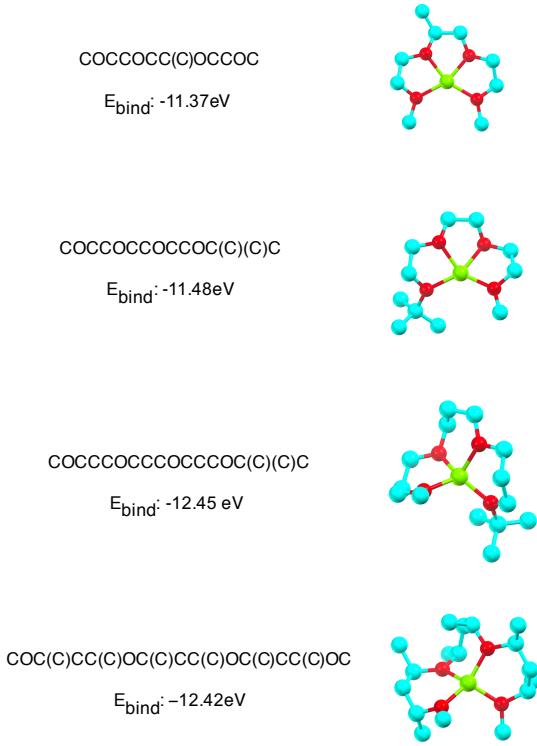


Figure S4. Selected asymmetric ether species binding with Mg^{2+} . These species show stronger binding than G3 baselines.

kinetic radii of 1.9 \AA . We use the Van Der Waal radius described in table VI to approximate the size of the complexes. The atomic Van Der Waal radii is taken from the ElementData function of the Mathematica software [18]. We show the correlation between the volumes of the complex and E_{bind} in Figure. S6. We also show the correlation between the computed ionization energy and HOMO of the optimized complex in Fig. S7.

atom type radius (\AA)	
C	1.7
H	1.1
O	1.52
Li	1.82
Mg	1.73
Na	2.27

VII. COMPARING WITH EXPERIMENTAL BINDING RESULTS

We compare DFT calculations and experimental data on crown-ether and ion binding in Table II. We find our binding energy to be in good agreement with gas-phase Collision Induced Dissociation (CID) experiments for sodium crown-ether binding. The binding affinity between ion and crown ether in solution depends on many factors including the effects of anions and concentration. We perform DFT with Solvent Model based on Density (SMD) [19] at the ω -B97xD3/def2-TZVP level of theory on the gas-phase optimized geometries to incorporate additional solvents effect. These solvents are included in ORCA SMD calculations. We compare our calculations with experimentally obtained binding affinity from literature and focus on the relative trend in ion-selectivity. The selectivity predicted by the solvent-corrected calculations agrees well with most of the available data found in literature. We find that the solvent tends to decrease the binding energy compared with gas-phase DFT, but as discussed in the main text and poor predictors of SIL-forming ability, because of the challenge in representing the solvation environment of SILs in a continuum model.

	gas phase		MeCN		MeOH		DMSO		MeNO ₂	
	DFT (eV)	CID [20]	DFT (eV)	logK[21]	DFT (eV)	logK	DFT (eV)	logK [21]	DFT (eV)	logK
Na	2.61	2.63(0.14)	1.48	2.3(0.03)	1.39	N/A	1.47	<0.5	1.49	N/A
	3.19	3.05(0.19)	1.84	4.96(0.05)	1.72	N/A	1.56	1.17(0.01)	1.85	N/A
	3.5	3.07(0.20)	1.93	4.29(0.12)	1.81	N/A	1.93	1.24(0.02)	1.96	N/A
Li	DFT (eV)	CID[22]	DFT (eV)	logK[23]	DFT (eV)	logK[24]	DFT (eV)	logK	DFT (eV)	logK[25]
	3.52	3.92(0.53)	1.69	3.25(0.06)	1.61	0	1.69	N/A	1.701	3.65(0.04)
	4.14	N/A	2.08	4.73(0.42)	1.96	3.59	2.07	N/A	2.087	>5
	4.34	N/A	2.07	3.07(0.09)	1.94	0	2.06	N/A	2.092	>5

Table II. DFT and experimental data comparison. The numbers in the bracket indicate experimental uncertainty directly transcribed from the corresponding references.

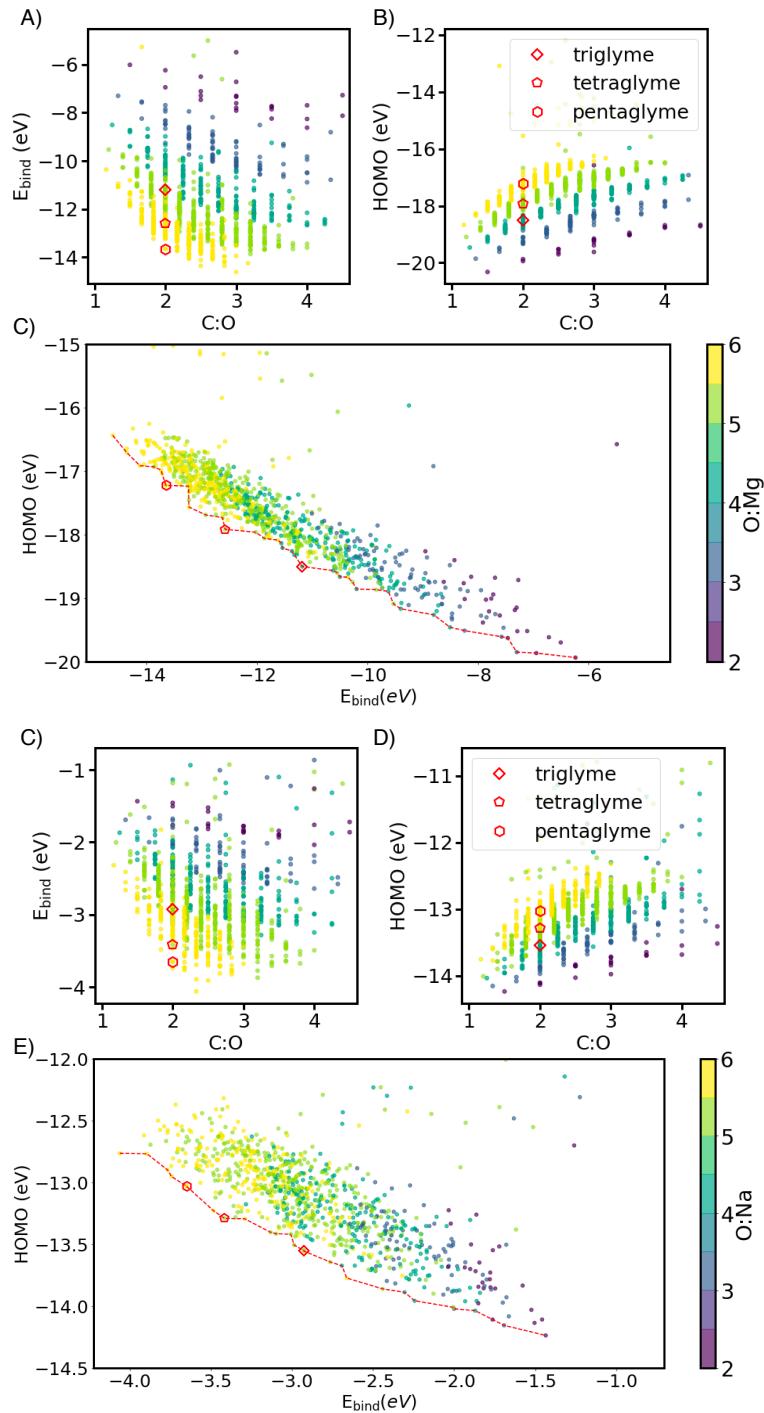


Figure S5. A-C) the chemical space of binding with HOMO and E_{bind} for Mg-ether complexes. D-E) the chemical space of binding with HOMO and E_{bind} for Na-ether complexes.

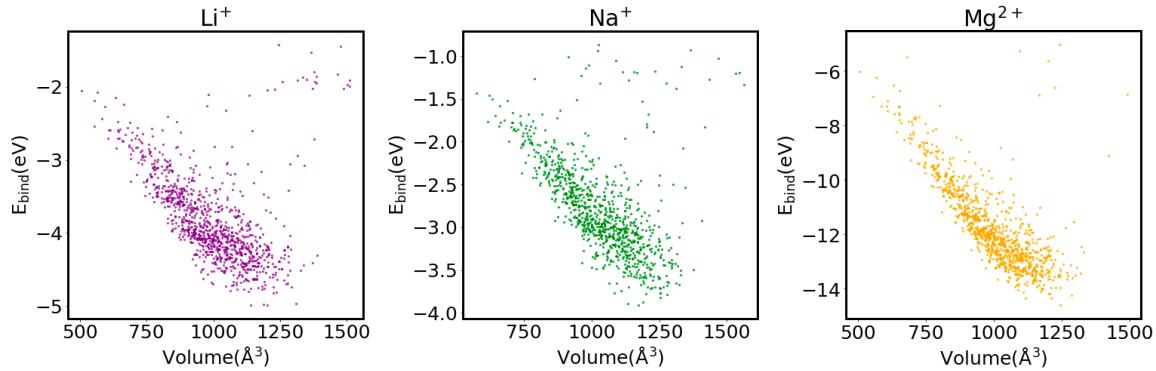


Figure S6. Correlation between molecule sizes and E_{bind}

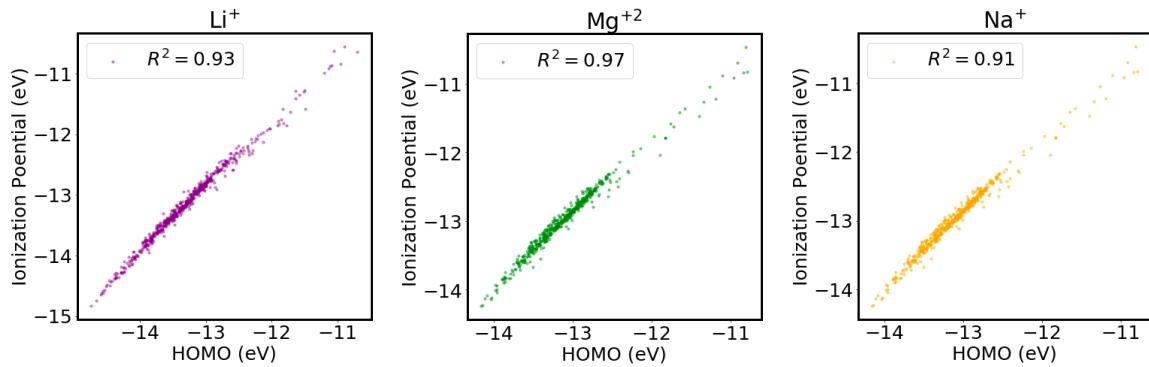


Figure S7. Correlation between HOMO and Ionization energy of ion-ether complexes with R^2 score.

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Column name

SMILES(q): X.XX-X:X where X indicates lengths of carbon spacers

n: number of oxygen donors from ether molecules

Eabs: absolute energy (eV) of ether molecules

Ebind: binding energy (eV) of ether-ion complex

paro(T/F): T when the species is on the paro front

size(Å): size of the chelated complex

E^{HOMO}: HOMO level of molecules/complex

DFT Energies for Ion-Ether Complex (o-B97xD3/def2-TZVP)

SMILES	SMILES(s)	n	Ether					[Li(Ether)] ⁺					[Mg(Ether)] ²⁺					[Na(Ether)] ⁺				
			E ^{B88}	E ^{HOMO}	E ^{bind}	E ^{HOMO}	size	paro	E ^{bind}	E ^{HOMO}	size	paro	E ^{bind}	E ^{HOMO}	size	paro	E ^{bind}	E ^{HOMO}	size	paro		
COCOCOC		12:1	2	-308.89	-9.63	-2.54	-14.66	553.67	T	-6.95	-19.87	555.26	T	-1.76	-14.11	616.38	T					
COCCOCOCOC		12:2:1	3	-462.75	-9.61	-3.30	-14.28	690.40	T	-9.26	-19.11	692.77	F	-2.36	-13.82	740.84	F					
COCCOCOCOCOC		12:2:2:1	4	-616.60	-9.27	-3.86	-13.64	829.68	F	-11.18	-18.51	808.28	T	-2.93	-13.55	862.73	T					
COCCOCOCOCOCOC		12:2:2:2:1	5	-770.45	-9.17	-4.36	-13.41	922.67	F	-12.58	-17.92	915.14	T	-3.42	-13.29	964.36	T					
COCCOCOCOCOCOCOC		12:2:2:2:2:1	6	-924.30	-9.08	-4.68	-13.13	992.21	T	-13.65	-17.23	1011.96	T	-3.65	-13.03	1063.17	T					
COOC		1:1:1	2	-269.59	-10.08	-2.06	-14.90	506.34	T	-6.02	-20.32	504.71	T	-1.43	-14.24	573.36	T					
COCCOCOC		1:2:1:1	3	-423.44	-9.72	-2.84	-14.56	635.41	T	-8.25	-19.52	640.64	T	-2.00	-14.02	692.87	T					
COOCOCOC		1:1:1:1	3	-384.13	-10.06	-2.43	-14.74	583.46	T	-7.30	-19.86	586.55	T	-1.69	-14.16	642.40	T					
COCCOCOCOC		1:2:2:1:1	4	-577.29	-9.64	-3.51	-14.09	770.72	F	-10.25	-18.53	776.15	F	-2.50	-13.70	806.70	F					
COCCOCOCOCOC		1:2:1:2:1	4	-577.29	-9.72	-3.45	-14.06	761.79	F	-10.20	-18.86	767.70	T	-2.48	-13.72	811.78	F					
COCCOCOCOCOC		1:2:1:1:1	4	-537.98	-9.74	-3.20	-14.36	712.91	F	-9.39	-19.08	720.13	F	-2.24	-13.96	755.39	T					
COCCOCOCOCOC		1:1:2:1:1	4	-537.98	-9.83	-3.04	-14.24	718.58	F	-9.40	-19.17	723.72	T	-2.15	-13.75	766.65	F					
COCCOCOCOC		1:1:1:1:1	4	-498.68	-10.19	-2.73	-14.59	658.48	T	-8.51	-19.46	667.89	T	-1.87	-14.04	717.58	T					
COCCOCOCOCOC		1:2:2:2:1:1	5	-731.14	-9.13	-3.98	-13.69	878.36	F	-11.87	-18.06	884.46	T	-2.88	-13.42	931.83	F					
COCCOCOCOCOC		1:2:2:1:2:1	5	-731.14	-9.63	-3.94	-13.75	882.71	F	-11.76	-17.95	883.51	F	-2.87	-13.31	936.77	F					
COCCOCOCOCOC		1:2:2:1:1:1	5	-691.83	-9.39	-3.80	-13.95	828.32	F	-10.99	-18.29	837.27	F	-2.76	-13.65	876.80	T					
COCCOCOCOCOCOC		1:2:1:2:1:1	5	-691.84	-9.65	-3.53	-13.82	829.22	F	-10.93	-18.37	840.25	F	-2.32	-13.43	870.31	F					
COCCOCOCOCOCOC		1:2:1:1:2:1	5	-691.83	-9.52	-3.83	-13.80	841.97	F	-11.05	-18.44	848.68	F	-2.66	-13.47	851.52	F					
COCCOCOCOCOCOC		1:2:1:1:1:1	5	-652.53	-9.82	-3.33	-14.03	776.56	F	-10.28	-18.58	801.05	F	-2.26	-13.66	833.23	F					
COCCOCOCOCOCOC		1:2:1:2:1:1	5	-691.83	-9.78	-3.64	-13.85	829.19	F	-11.05	-18.29	858.09	F	-2.67	-13.51	892.90	F					
COCCOCOCOCOCOC		1:2:1:2:1:1:1	5	-652.53	-9.96	-3.37	-14.18	787.26	T	-10.27	-18.75	791.65	T	-2.28	-13.79	829.59	F					
COCCOCOCOCOC		1:1:1:1:1:1:1	5	-613.22	-10.19	-3.01	-14.32	742.14	F	-9.53	-19.09	743.54	T	-2.00	-14.01	776.06	T					
COCCOCOC		1:3:1:2	2	-348.22	-9.40	-2.70	-14.46	603.83	F	-7.47	-19.63	607.87	T	-1.82	-13.86	658.40	F					
COCCOCOCOC		1:1:3:1:1	4	-577.31	-9.94	-3.11	-13.89	772.65	F	-9.87	-18.65	778.64	F	-2.23	-13.51	829.80	F					
COCCOCOCOCOCOC		1:2:3:2:1:1	4	-655.92	-9.28	-3.97	-13.55	844.45	F	-11.56	-18.14	858.72	T	-2.88	-13.28	873.48	F					
COCCOCOCOCOC		1:3:1:2:1:1	4	-616.61	-9.56	-3.57	-13.80	841.97	F	-11.05	-18.44	848.68	F	-2.66	-13.47	851.52	F					
COCCOCOCOCOCOC		1:2:1:3:1:1	4	-652.53	-9.82	-3.33	-14.03	776.56	F	-10.28	-18.58	801.05	F	-2.26	-13.66	833.23	F					
COCCOCOCOCOCOC		1:2:1:2:1:1:1	5	-691.83	-9.78	-3.64	-13.85	829.19	F	-11.05	-18.29	858.09	F	-2.67	-13.51	892.90	F					
COCCOCOCOCOCOC		1:1:1:1:1:1:1:1	5	-613.22	-10.19	-3.01	-14.32	742.14	F	-9.53	-19.09	743.54	T	-2.00	-14.01	776.06	T					
COCCOCOC		1:3:1:1	2	-348.22	-9.40	-2.70	-14.46	603.83	F	-7.47	-19.63	607.87	T	-1.82	-13.86	658.40	F					
COCCOCOCOC		1:1:3:1:1	4	-577.31	-9.94	-3.11	-13.89	772.65	F	-9.87	-18.65	778.64	F	-2.23	-13.51	829.80	F					
COCCOCOCOCOCOC		1:2:3:2:1:1	4	-655.92	-9.28	-3.97	-13.55	844.45	F	-11.56	-18.14	858.72	T	-2.88	-13.28	873.48	F					
COCCOCOCOCOCOC		1:3:1:2:1:1	4	-616.61	-9.56	-3.57	-13.80	841.97	F	-11.05	-18.44	848.68	F	-2.66	-13.47	851.52	F					
COCCOCOCOCOCOC		1:2:1:3:1:1:1	5	-652.53	-9.82	-3.33	-14.03	776.56	F	-10.28	-18.58	801.05	F	-2.26	-13.66	833.23	F					
COCCOCOCOCOCOC		1:1:1:1:1:1:1:1	5	-691.83	-9.78	-3.64	-13.85	829.19	F	-11.05	-18.29	858.09	F	-2.67	-13.51	892.90	F					
COCCOCOCOCOCOC		1:2:2:3:1:1:1:1	5	-613.22	-10.19	-3.01	-14.32	742.14	F	-9.53	-19.09	743.54	T	-2.00	-14.01	776.06	T					
COCCOCOCOCOCOC		1:3:3:3:1:1:1:1	5	-541.39	-9.23	-3.47	-13.69	902.06	F	-11.68	-17.97	902.51	F	-2.84	-13.24	954.50	F					
COCCOCOCOCOCOC		1:2:3:2:1:1:1:1	5	-655.93	-9.47	-3.55	-13.69	846.65	F	-10.92	-18.15	873.05	F	-2.45	-13.43	902.76	F					
COCCOCOCOCOCOCOC		1:3:2:2:2:1:1:1	5	-809.77	-8.82	-4.50	-13.25	956.80	F	-9.97	-14.48	1060.51	F	-3.47	-13.12	999.19	F					
COCCOCOCOCOCOCOC		1:3:1:2:2:1:1:1	5	-770.46	-9.22	-4.08	-13.33	912.65	F	-12.17	-17.80	935.24	F	-3.05	-13.36	966.42	F					
COCCOCOCOCOCOCOC		1:2:3:1:2:1:1:1	5	-731.16	-9.48	-3.67	-13.66	871.56	F	-11.37	-17.95	900.97	F	-2.65	-13.35	920.75	F					
COCCOCOCOCOCOCOC		1:3:2:3:1:1:1:1	5	-809.78	-9.38	-4.16	-13.42	951.18	F	-12.32	-17.45	976.79	F	-3.03	-13.18	1010.60	F					
COCCOCOCOCOCOCOC		1:2:3:2:1:1:1:1	5	-770.46	-9.19	-4.00	-13.44	931.47	F	-12.15	-17.78	938.25	F									
COCCOCOCOCOCOCOC		1:3:2:3:2:1:1:1	5	-849.09	-9.22	-4.42	-13.09	1004.20	F	-12.92	-17.40	1006.91	F	-3.06	-12.86	1046.02	F					
COCCOCOCOCOCOCOC		1:2:3:2:1:2:1:1	5	-706.40	-9.30	-3.98	-13.21	926.54	F	-11.96	-17.63	923.12	F	-2.91	-13.18	948.65	F					
COCCOCOCOCOCOCOC		1:3:1:2:1:2:1:1	5	-731.15	-9.57	-4.02	-13.76	870.40	T	-11.42	-18.15	887.84	F	-2.65	-13.38	914.81	F					
COCCOCOCOCOCOCOC		1:2:3:1:2:1:2:1:1	5	-770.46	-9.22	-4.08	-13.33	912.65	F	-12.17	-17.80	935.24	F	-3.05	-13.36	966.42	F					
COCCOCOCOCOCOCOC		1:3:1:3:1:2:1:1:1	5	-731.16	-9.48	-3.67	-13.66	871.56	F	-11.37	-17.95	900.97	F	-2.65	-13.35	920.75	F					
COCCOCOCOCOCOCOC		1:2:2:2:1:2:1:1:1	5	-770.46	-9.27	-3.98	-13.49	909.57	F	-12.17	-17.73	931.07	F	-3.04	-13.07	976.41	F					
COCCOCOCOCOCOCOC		1:1:3:2:1:2:1:1:1	5	-731.16	-9.41	-3.57	-13.62	862.56	F	-11.50	-18.03	900.50	F	-2.65	-13.18	939.83	F					
COCCOCOCOCOCOCOC		1:3:2:2:1:2:1:1:1	5	-809.78	-9.37	-4.10	-12.84	1004.07	F	-12.59	-17.54	973.76	F	-1.72	-12.39	1040.51	F					
COCCOCOCOCOCOCOC		1:3:2:1:2:1:2:1:1	5	-731.16	-9.39	-3.85	-13.73	882.41	F	-11.30	-17.96	890.23	F	-2.55	-13.12	943.47	F					
COCCOCOCOCOCOCOC		1:3:1:3:1:2:1:1:1	5	-691.85	-9.68	-3.51	-13.06	992.92	F	-13.14	-17.40	1012.94	F	-3.45	-13.09	1046.73	F					
COCCOCOCOCOCOCOC		1:3:1:3:1:1:2:1:1	5	-691.85	-9.94	-3.41	-13.68	848.85	F													

CCCCCCCCCCCCCCCCCOC	1:4:2:3:1	5	-888.41	-9.11	-4.44	-13.09	1036.71	F	-13.06	-17.31	1041.36	F	-3.06	-12.73	1125.29	F
CCCCCCCCCCCCCCCCCOC	1:3:4:2:1	5	-888.41	-9.29	-4.48	-13.13	1025.02	F	-13.21	-17.31	1039.42	F	-3.28	-12.79	1091.30	F
CCCCCCCCCCCCCCCCCOC	1:3:2:4:1	5	-888.40	-9.29	-4.54	-12.96	1039.28	F	-12.84	-17.05	1037.02	F	-3.40	-12.99	1068.58	F
CCCCCCCCCCCCCCCCCOC	1:2:4:3:1	5	-888.41	-9.31	-4.52	-12.99	1030.43	F	-13.25	-17.24	1043.48	T	-3.38	-12.95	1098.22	F
CCCCCCCCCCCCCCCCCOC	1:4:4:2:1	5	-927.72	-8.97	-4.66	-13.02	1074.38	F	-13.22	-17.06	1074.88	F	-2.08	-10.79	1337.81	F
CCCCCCCCCCCCCCCCCOC	1:4:3:3:1	5	-927.73	-9.23	-4.29	-12.72	1088.91	F	-13.16	-17.13	1074.10	F	-3.33	-12.68	1135.50	F
CCCCCCCCCCCCCCCCCOC	1:4:3:2:1	5	-927.72	-8.87	-4.71	-13.00	1069.13	T	-13.35	-17.08	1077.65	F	-3.29	-12.75	1123.14	F
CCCCCCCCCCCCCCCCCOC	1:4:2:4:1	5	-927.73	-8.85	-4.46	-13.03	1063.77	F	-13.24	-17.09	1081.76	F	-3.22	-13.02	1101.01	F
CCCCCCCCCCCCCCCCCOC	1:4:2:3:1	5	-927.73	-9.06	-4.57	-12.93	1073.62	F	-13.37	-16.96	1068.90	F	-3.53	-12.84	1123.54	F
CCCCCCCCCCCCCCCCCOC	1:4:2:2:1	5	-927.73	-9.17	-4.40	-13.09	1068.49	F	-11.83	-15.15	1134.99	F	-3.28	-12.97	1121.96	F
CCCCCCCCCCCCCCCCCOC	1:3:4:3:1	5	-927.72	-9.32	-4.51	-12.87	1064.97	F	-13.47	-16.96	1077.69	F	-3.08	-12.73	1137.81	F
CCCCCCCCCCCCCCCCCOC	1:3:4:2:1	5	-927.73	-9.10	-4.36	-12.98	1060.57	F	-12.97	-17.14	1086.19	F	-3.17	-12.76	1155.21	F
CCCCCCCCCCCCCCCCCOC	1:3:4:2:1	5	-927.72	-9.44	-4.91	-11.48	1315.40	F	-13.46	-16.98	1081.13	F	-3.37	-12.60	1130.88	F
CCCCCCCCCCCCCCCCCOC	1:2:4:4:1	5	-927.72	-8.97	-4.53	-10.69	1365.41	F	-13.23	-16.92	1083.92	F	-3.48	-12.92	1127.61	F
CCCCCCCCCCCCCCCCCOC	1:4:4:3:1	5	-967.04	-9.21	-4.49	-12.76	1101.91	F	-12.11	-14.23	1207.20	F	-3.46	-12.77	1157.82	F
CCCCCCCCCCCCCCCCCOC	1:4:4:2:1	5	-967.05	-9.24	-4.47	-12.87	1105.08	F	-13.34	-17.01	1105.61	F	-3.29	-12.77	1173.01	F
CCCCCCCCCCCCCCCCCOC	1:4:4:2:1	5	-967.04	-9.30	-4.58	-12.92	1106.47	F	-13.23	-16.77	1129.42	F	-3.42	-12.75	1158.97	F
CCCCCCCCCCCCCCCCCOC	1:4:3:3:1	5	-967.06	-9.23	-4.42	-12.82	1113.82	F	-13.23	-16.87	1107.38	F	-3.11	-12.73	1187.03	F
CCCCCCCCCCCCCCCCCOC	1:4:3:2:1	5	-967.04	-9.23	-4.37	-12.98	1103.06	F	-13.33	-17.01	1115.65	F	-3.19	-12.66	1189.86	F
CCCCCCCCCCCCCCCCCOC	1:4:2:4:1	5	-967.05	-9.16	-4.37	-12.81	1122.94	F	-13.47	-16.86	1120.49	F	-3.39	-12.68	1184.62	F
CCCCCCCCCCCCCCCCCOC	1:4:3:3:1	5	-967.05	-9.17	-4.67	-12.84	1102.63	F	-13.51	-17.05	1103.75	F	-3.36	-12.71	1138.25	F
CCCCCCCCCCCCCCCCCOC	1:4:4:2:1	5	-1006.36	-9.27	-4.63	-12.86	1152.31	F	-13.32	-16.77	1153.30	F	-3.08	-12.72	1199.62	F
CCCCCCCCCCCCCCCCCOC	1:4:4:3:1	5	-1006.37	-9.13	-4.30	-12.26	1204.68	F	-13.48	-16.81	1141.04	F	-3.36	-12.66	1193.03	F
CCCCCCCCCCCCCCCCCOC	1:4:4:2:1	5	-1006.36	-8.95	-4.54	-12.79	1173.29	F	-13.35	-16.86	1154.24	F	-3.58	-12.66	1195.75	F
CCCCCCCCCCCCCCCCCOC	1:4:4:3:1	5	-1006.36	-9.32	-4.45	-12.71	1144.65	F	-13.44	-16.81	1153.92	F	-3.37	-12.78	1195.75	F
CCCCCCCCCCCCCCCCCOC	1:4:3:3:1	5	-1006.37	-9.07	-4.33	-12.84	1149.99	F	-13.30	-16.72	1148.86	F	-3.11	-12.73	1187.03	F
CCCCCCCCCCCCCCCCCOC	1:4:4:2:1	5	-1006.37	-9.22	-4.38	-12.69	1153.61	F	-13.18	-16.83	1156.21	F	-3.42	-12.69	1219.92	F
CCCCCCCCCCCCCCCCCOC	1:4:4:3:1	5	-1045.68	-9.17	-4.53	-12.54	1184.54	F	-12.08	-14.53	1217.84	F	-3.03	-12.60	1200.17	F
CCCCCCCCCCCCCCCCCOC	1:4:4:3:1	5	-1045.68	-9.25	-4.30	-12.43	1219.11	F	-12.72	-14.87	1252.01	F	-3.31	-12.70	1230.62	F
CCCCCCCCCCCCCCCCCOC	1:4:4:4:1	5	-1085.00	-9.38	-4.05	-12.81	1182.22	F	-12.72	-14.87	1252.01	F	-3.44	-12.62	1264.12	F
COCOCOCOCOCOCOC	1:1:1:1:1:1	6	-727.76	-10.11	-3.35	-14.13	812.22	F	-10.36	-18.67	811.01	T	-2.32	-13.76	847.92	F
COCOCOCOCOCOCOC	1:2:1:1:1:1	6	-767.07	-9.80	-3.58	-14.02	841.36	F	-10.95	-18.28	873.19	F	-2.56	-13.58	894.06	F
COCOCOCOCOCOCOC	1:3:1:1:1:1	6	-806.38	-9.70	-3.85	-13.60	887.85	F	-11.31	-17.93	902.80	F	-2.77	-13.25	916.57	F
COCOCOCOCOCOCOC	1:1:2:1:1:1	6	-767.07	-9.75	-3.52	-13.90	858.18	F	-11.08	-18.28	856.69	F	-2.41	-13.60	883.98	F
COCOCOCOCOCOCOC	1:2:2:1:1:1	6	-806.37	-9.53	-4.06	-13.70	872.17	T	-11.82	-18.03	904.99	F	-2.96	-13.43	925.89	F
COCOCOCOCOCOCOC	1:3:2:1:1:1	6	-845.70	-9.39	-4.08	-13.43	949.28	F	-5.28	-13.09	1094.50	F	-2.96	-13.32	970.42	F
COCOCOCOCOCOCOC	1:1:3:1:1:1	6	-806.39	-9.90	-3.65	-13.79	902.42	F	-11.33	-17.86	916.12	F	-2.62	-13.54	933.34	F
COCOCOCOCOCOCOC	1:2:3:1:1:1	6	-845.69	-9.32	-4.23	-13.55	937.97	F	-12.28	-17.90	938.10	F	-3.13	-13.08	989.52	F
COCOCOCOCOCOCOC	1:3:3:1:1:1	6	-885.02	-9.27	-3.97	-13.35	982.89	F	-12.09	-17.52	999.34	F	-2.81	-12.99	1033.17	F
COCOCOCOCOCOCOC	1:1:2:1:1:1	6	-767.07	-9.89	-3.75	-14.07	839.51	T	-11.07	-18.35	857.71	F	-2.66	-13.78	867.02	T
COCOCOCOCOCOCOC	1:2:2:1:1:1	6	-806.37	-9.44	-3.95	-13.70	887.11	F	-11.89	-17.96	911.23	F	-2.93	-13.56	921.11	T
COCOCOCOCOCOCOC	1:3:1:1:1:1	6	-845.70	-9.29	-3.79	-13.35	928.05	F	-11.80	-17.73	938.47	F	-2.64	-13.29	970.64	F
COCOCOCOCOCOCOC	1:2:1:1:1:1	6	-806.38	-9.62	-3.84	-13.70	898.81	F	-11.76	-18.05	913.52	F	-2.79	-13.40	939.42	F
COCOCOCOCOCOCOC	1:2:2:1:1:1	6	-845.68	-9.23	-4.44	-13.58	933.47	T	-12.48	-17.67	938.28	F	-3.07	-12.87	1005.10	F
COCOCOCOCOCOCOC	1:3:2:1:1:1	6	-885.00	-9.53	-4.62	-13.37	962.32	T	-11.46	-17.46	1061.55	F	-3.33	-13.08	1020.50	F
COCOCOCOCOCOCOC	1:2:3:1:1:1	6	-845.70	-9.36	-4.26	-13.34	970.01	F	-12.02	-17.76	961.53	F	-2.76	-13.40	991.47	F
COCOCOCOCOCOCOC	1:3:3:1:1:1	6	-924.33	-9.15	-4.40	-13.20	1003.87	F	-12.87	-17.34	1018.93	F	-2.90	-13.12	1028.96	F
COCOCOCOCOCOCOC	1:1:1:1:1:1	6	-806.38	-9.84	-3.78	-13.86	887.48	F	-11.41	-18.13	898.95	F	-2.77	-13.51	948.61	F
COCOCOCOCOCOCOC	1:2:1:1:1:1	6	-845.70	-9.73	-3.99	-13.47	928.71	F	-12.02	-17.84	950.46	F	-2.87	-13.27	979.98	F
COCOCOCOCOCOCOC	1:3:1:1:1:1	6	-885.01	-9.63	-3.99	-13.24	1003.03	F	-12.54	-17.54	993.97	F	-2.91	-13.22	998.13	F
COCOCOCOCOCOCOC	1:1:2:1:1:1	6	-845.69	-9.40	-4.04	-13.39	929.03	F	-12.35	-17.73	955.06	F	-3.08	-13.38	985.12	F
COCOCOCOCOCOCOC	1:2:2:1:1:1	6	-885.01	-9.19	-4.12	-13.27	957.30	F	-12.73	-17.49	986.27	F	-3.09	-13.16	1024.53	F
COCOCOCOCOCOCOC	1:3:2:1:1:1	6	-924.33	-9.24	-4.39	-13.05	1026.61	F	-13.05	-17.31	1023.81	F	-3.17	-13.05	1049.40	F
COCOCOCOCOCOCOC	1:2:3:1:1:1	6	-924.33	-9.51	-4.43	-13.15	1009.71	F	-13.00	-17.17	1032.72	F	-3.34	-12.76	1056.75	F
COCOCOCOCOCOCOC	1:3:3:1:1:1	6	-963.65	-9.45	-4.25	-12.95	1050.19	F	-13.14	-17.13	1060.00	F	-3.20	-13.20	1074.50	F
COCOCOCOCOCOCOC	1:2:1:1:1:1	6	-806.38	-9.38	-3.95	-13.66	898.88	F	-11.80	-18.00	913.23	F	-2.71	-13.32	924.54	F
COCOCOCOCOCOCOC	1:3:1:1:1:1	6	-845.70	-9.50	-4.07	-13.47	938.06	F	-11.99	-17.67	948.12	F	-2.89	-13.27	974.55	F
COCOCOCOCOCOCOC	1:1:2:1:1:1	6	-806.37	-9.50	-3.68	-13.43	914.65	F	-11.79	-17.88	915.76	F	-3.22	-13.21	988.13	F
COCOCOCOCOCOCOC	1:2:2:1:1:1	6	-845.67	-8.94	-4.29	-13.55	933.29	F	-12.63	-17.67	947.77	F	-3.22	-13.14	993.23	F
COCOCOCOCOCOCOC	1:3:1:1:1:1	6	-885.01	-9.42	-3.91	-13.34	1006.04	F	-12.37	-17.33	971.58	F	-2.80	-13.13	1025.39	F
COCOCOCOCOCOCOC	1:2:3:1:1:1	6	-845.70	-9.73	-4.29	-13.29	989.08	F	-12.52	-17.39	989.74	F	-2.92	-13.05	1013.05	F
COCOCOCOCOCOCOC	1:3:2:1:1:1	6	-924.33	-9.22	-3.89	-12.99	1030.53	F	-12.78	-17.27	1020.47	F	-2.78	-12.88	1080.16	F
COCOCOCOCOCOCOC	1:2:2:1:1:1	6	-924.32	-9.41	-4.07	-12.91	1031.34	F	-12.86	-17.10	1032.38	F	-3.21	-12.72	1114.57	F
COCOCOCOCOCOCOC	1:1:2:1:1:1	6	-885.00	-9.15	-4.17	-13.23	971.37	F	-12.66	-17.38	995.49	F	-3.21	-13.21	1040.80	F
COCOCOCOCOCOCOC	1:2:2:1:1:1	6	-924.33	-9.45	-4.37	-12.95	1022.66	F	-13.23	-17.33	1008.17	F	-3.23	-13.18	1063.72	F
COCOCOCOCOCOCOC	1:3:1:1:1:1	6	-924.33	-9.48	-4.05	-13.08	1008.95	F	-12.76	-17.40	1013.76	F	-2.92	-12.87	1051.55	F
COCOCOCOCOCOCOC	1:2:1:1:1:1	6	-845.70	-9.26	-4.29	-13.10	1086.56	F	-13.54	-17.67	1095.84	F	-3.74</			

COCOCOCOCOCOC(C)OC	5	-770.47	-9.42	-3.95	-13.31	925.19	F	-11.91	-17.85	926.98	F	-2.92	-13.43	953.33	F
COCOCOCOC(C)OCOC	5	-731.16	-9.11	-3.50	-13.77	866.06	F	-11.04	-18.11	881.09	F	-2.48	-13.36	935.50	F
COCOCOCOC(C)COOC	5	-731.16	-9.73	-3.49	-13.62	874.71	F	-11.01	-17.91	891.03	F	-2.55	-13.52	923.61	F
COCOCOCOC(C)COC	5	-731.16	-9.69	-3.60	-13.79	874.20	F	-10.93	-18.12	892.61	F	-2.53	-13.40	927.48	F
COCOCOCOC(C)OC	5	-731.16	-9.67	-3.63	-13.64	873.55	F	-11.20	-18.16	880.87	F	-2.56	-13.33	940.19	F
COCOCOCOC(C)OCOC	5	-731.16	-9.29	-3.57	-13.82	865.42	F	-11.13	-18.11	890.34	F	-2.60	-13.33	929.12	F
COCOCOCOC(C)OCOC	5	-731.16	-9.62	-3.47	-13.79	904.20	F	-11.04	-18.27	900.67	F	-2.66	-13.57	940.43	F
COCOC(C)OC	2	-348.22	-9.30	-2.59	-14.44	607.94	F	-7.11	-19.52	608.45	F	-1.78	-13.85	662.41	F
COCOC(C)OCOC	4	-538.00	-10.07	-2.75	-14.29	727.14	F	-8.75	-19.21	724.44	F	-1.93	-13.96	763.76	F
COCOCOC(C)OC	4	-538.00	-10.02	-2.83	-14.52	708.87	F	-8.80	-19.27	723.69	T	-1.97	-13.87	767.10	F
COCOC(C)OCOC	4	-577.31	-9.94	-3.09	-14.12	778.59	F	-9.54	-18.85	776.13	F	-2.25	-13.72	826.85	F
COCOCOC(C)OC	4	-577.31	-9.80	-3.06	-14.10	769.54	F	-9.46	-18.74	776.17	F	-2.16	-13.76	809.25	F
COCOCOCOC(C)OC	5	-731.15	-9.58	-3.89	-13.83	882.64	F	-11.23	-18.16	899.72	F	-2.72	-13.47	905.19	F
COCOCOCOC(C)OC	5	-731.16	-9.41	-3.78	-13.74	870.06	F	-11.19	-18.18	891.23	F	-2.14	-12.45	935.99	F
COCOCOCOC(C)OC	5	-731.16	-9.63	-3.93	-13.73	884.83	F	-11.28	-18.18	893.28	F	-2.70	-13.44	901.83	F
COCOCOC(C)OCOC	4	-773.88	-9.35	-4.11	-13.21	968.55	F	-12.16	-17.46	985.24	F	-2.94	-12.92	1023.81	F
COCOCOCOC(C)OCOC	4	-773.87	-9.20	-4.32	-13.31	970.41	F	-12.38	-17.46	996.69	F	-3.09	-12.89	1037.39	F
COCOCOCOC(C)OCOC	4	-773.88	-9.39	-4.30	-13.13	982.28	F	-12.21	-17.69	1000.63	F	-2.99	-13.06	1019.20	F
COCOC(C)OC	3	-423.45	-9.90	-2.59	-14.54	640.61	F	-7.58	-19.61	633.26	T	-2.46	-13.68	841.76	F
COCOCOC(C)OC	4	-616.61	-9.62	-3.56	-14.00	829.95	F	-10.41	-18.48	825.13	F	-2.57	-13.61	868.23	F
COCOCOC(C)OCOC	4	-616.61	-9.39	-3.56	-13.82	828.75	F	-10.50	-18.67	830.69	T	-2.46	-13.68	841.76	F
COCOCOC(C)OCOC	4	-616.61	-9.43	-3.56	-14.01	825.84	F	-10.33	-18.42	815.09	F	-2.57	-13.63	867.09	F
COCOCOC(C)OCOC	4	-616.61	-9.54	-2.59	-13.65	807.87	F	-10.39	-18.33	818.26	F	-2.59	-13.61	862.59	F
COCOCOC(C)OCOC	4	-616.61	-9.36	-3.64	-14.04	818.17	F	-10.63	-18.57	835.62	T	-2.69	-13.67	862.99	T
COCOCOC(C)OCOC	5	-731.15	-9.65	-3.81	-13.75	890.09	F	-11.32	-17.94	908.74	F	-2.70	-13.50	890.66	F
COCOCOC(C)OCOC	5	-731.16	-9.50	-2.10	-11.77	981.61	F	-11.37	-18.06	900.82	F	-2.74	-13.36	929.81	F
COCOCOCOC(C)OC	5	-731.16	-9.56	-3.82	-13.99	849.05	T	-11.26	-18.20	882.25	F	-2.59	-13.33	923.78	F
COCOC(C)OCOC	5	-731.16	-9.61	-3.82	-13.89	881.84	F	-11.30	-18.12	890.03	F	-2.74	-13.52	936.14	F
COCOCOCOC(C)OC	5	-731.16	-9.66	-3.84	-13.76	881.83	F	-11.23	-17.99	885.25	F	-2.61	-13.37	896.87	F
COCOCOCOC(C)OC	5	-731.16	-9.59	-3.77	-13.87	856.07	F	-10.35	-18.62	820.23	F	-2.51	-13.70	843.26	F
COCOC(C)OCOC	4	-616.61	-9.66	-3.52	-13.98	806.16	F	-10.35	-18.71	943.73	F	-3.01	-13.25	971.23	F
COCOCOC(C)OCOC	4	-616.61	-9.70	-3.43	-13.82	832.75	F	-10.16	-18.51	822.87	F	-2.36	-13.55	841.58	F
COCOCOC(C)OCOC	4	-616.61	-9.52	-3.44	-13.90	804.69	F	-10.27	-18.45	823.13	F	-2.24	-13.38	873.70	F
COCOCOCOC(C)OCOC	5	-770.47	-9.23	-3.99	-13.45	920.22	F	-12.00	-17.77	931.09	F	-3.13	-13.40	970.62	T
COCOCOCOC(C)OCOC	5	-770.47	-9.47	-3.97	-13.46	926.59	F	-11.83	-17.84	941.37	F	-2.86	-13.26	953.29	F
COCOCOCOC(C)OCOC	5	-770.47	-9.17	-3.94	-13.59	930.90	F	-11.97	-17.75	939.24	F	-2.98	-13.33	975.23	F
COCOCOCOC(C)OCOC	5	-770.47	-9.11	-4.04	-13.56	905.84	F	-10.97	-17.75	908.05	F	-3.05	-13.31	973.76	F
COCOCOCOC(C)OCOC	5	-770.47	-9.22	-3.99	-13.51	929.62	F	-12.00	-17.71	943.73	F	-3.01	-13.25	971.23	F
COCOCOCOC(C)OCOC	5	-770.47	-9.36	-3.95	-13.60	928.78	F	-11.87	-17.85	946.10	F	-3.08	-13.36	971.29	F
COCOCOC(C)OCOCOC	5	-770.46	-9.61	-4.06	-13.54	915.62	F	-12.00	-17.71	938.42	F	-2.97	-13.15	964.10	F
COCOCOCOC(C)OCOC	3	-462.76	-9.72	-2.87	-14.30	699.39	F	-8.48	-19.31	697.09	F	-2.01	-13.88	745.13	F
COCOCOCOC(C)OCOC	3	-462.76	-9.64	-2.80	-14.45	685.09	F	-8.33	-19.14	692.06	F	-1.80	-13.79	738.65	F
COCOCOCOC(C)OCOC	3	-462.76	-9.34	-2.98	-14.36	691.03	F	-8.47	-19.34	694.00	F	-2.07	-13.91	738.83	F
COCOCOCOC(C)OCOC	5	-691.85	-9.95	-3.41	-13.83	841.54	F	-10.58	-18.52	848.29	F	-2.41	-13.63	892.06	F
COCOCOCOC(C)OCOC	5	-691.85	-10.03	-3.44	-14.14	842.69	T	-10.55	-18.60	847.02	T	-2.31	-13.63	891.71	F
COCOCOCOC(C)OCOC	5	-691.85	-9.98	-3.37	-13.83	847.81	F	-10.50	-18.49	848.88	F	-2.47	-13.64	879.37	F
COCOCOCOC(C)OCOC	5	-691.85	-9.61	-4.06	-13.54	915.62	F	-12.00	-17.71	938.42	F	-2.97	-13.15	964.10	F
COCOCOCOC(C)OCOC	5	-691.85	-9.92	-3.36	-14.04	832.10	F	-10.50	-18.46	843.81	F	-2.33	-13.68	877.67	F
COCOCOCOC(C)OCOC	4	-695.24	-9.47	-4.02	-13.54	889.49	F	-11.64	-17.89	908.05	F	-2.92	-13.35	953.01	F
COCOCOCOC(C)OCOC	4	-695.24	-9.27	-3.95	-13.41	885.62	F	-11.59	-17.91	915.24	F	-2.83	-13.14	922.84	F
COCOCOCOC(C)OCOC	2	-387.54	-9.39	-2.70	-14.35	647.21	F	-5.49	-16.58	680.31	F	-1.78	-13.73	703.63	F
COCOCOCOC(C)OCOC	3	-580.71	-9.39	-3.56	-13.78	836.22	F	-10.17	-18.37	848.20	F	-2.42	-13.36	875.27	F
COCOCOCOC(C)OCOC	3	-580.71	-9.24	-3.54	-13.69	825.16	F	-10.21	-18.35	848.92	F	-2.32	-13.39	870.56	F
COCOCOCOC(C)OCOC	4	-691.85	-9.71	-3.51	-14.12	825.54	T	-10.49	-18.30	843.39	F	-2.52	-13.61	884.64	F
COCOCOCOC(C)OCOC	5	-691.85	-9.66	-3.17	-13.89	831.88	F	-10.46	-18.36	839.05	F	-2.92	-13.35	953.01	F
COCOCOCOC(C)OCOC	5	-691.85	-9.73	-3.44	-14.07	948.78	F	-10.32	-18.55	951.85	F	-2.35	-13.54	878.14	F
COCOCOCOC(C)OCOC	5	-691.85	-9.75	-3.15	-13.77	846.40	F	-10.49	-18.50	848.69	F	-2.40	-13.54	863.68	F
COCOCOCOC(C)OCOC	4	-734.56	-9.16	-4.07	-13.50	926.32	F	-11.79	-17.75	954.98	F	-3.03	-13.26	967.69	F
COCOCOCOC(C)OCOC	4	-734.56	-9.11	-4.04	-13.48	963.62	F	-11.73	-17.78	960.44	F	-2.92	-13.24	983.26	F
COCOCOCOC(C)OCOC	4	-655.92	-9.40	-4.02	-13.45	947.57	F	-11.81	-17.70	951.16	F	-2.90	-13.19	1002.28	F
COCOCOCOC(C)OCOC	4	-655.92	-9.40	-3.93	-13.76	858.06	F	-11.28	-18.31	870.89	F	-2.65	-13.34	907.50	F
COCOCOCOC(C)OCOC	4	-655.92	-9.30	-3.97	-13.87	843.87	T	-11.37	-18.26	866.46	T	-2.72	-13.29	909.43	F
COCOCOCOC(C)OCOC	4	-577.30	-9.62	-3.23	-14.11	765.06	F	-9.48	-18.77	771.19	F	-2.17	-13.62	788.18	F
COCOCOCOC(C)OCOC	4	-577.31	-9.54	-3.19	-14.17	764.16	F	-9.61	-18.84	777.23	F	-2.24	-13.74	811.29	F
COCOCOCOC(C)OCOC	4	-577.31	-9.73	-3.23	-14.25	769.28	F	-9.49	-18.79	774.66	F	-2.42	-13.77	804.33	F
COCOCOCOC(C)OCOC	4	-502.07	-9.56	-3.29	-14.37	753.25	T	-9.52	-18.80	769.39	F	-2.29	-13.77	804.33	F
COCOCOCOC(C)OCOC	3	-502.07	-9.43	-3.30	-14.25	750.15	F	-9.34	-18.87	745.91	F	-2.41	-13.80	792.59	F
COCOCOCOC(C)OCOC	5	-809.77	-9.14	-4.33	-13.47	948.37	F	-12.47	-17.56	972.18	F	-3.33	-13.24	1015.09	F
COCOCOCOC(C)OCOC	5	-809.77	-9.03	-4.38	-13.32	963.90	F	-12.59	-17.47	972.40	F	-3.35	-13.28	1001.50	F
COCOCOCOC(C)OCOC	5	-809.78	-9.13	-4.17	-13.27	959.20	F	-12.57	-17.68	979.21	F	-3.13	-13.10	1025.76	F
COCOCOCOC(C)OCOC	5	-809.77	-9.49	-4.25	-12.87	989.49	F	-12.75	-17.69	973.94	F	-3.36	-13.19	1010.02	F
COCOCOCOC(C)OCOC	3	-541.39	-9.20	-3.49	-13.95	788.75	F	-9.85	-18.61	789.71	F	-2.28	-13.53	827.07	F
COCOCOCOC(C)OCOC	3	-541.39	-9.37	-3.50	-13.88	791.53	F	-9.75	-18.53	785.47	F	-2.40	-13.47	834.74	F
COCOCOCOC(C)OCOC	3	-541.39	-9.02	-3.46	-13.91	790.06	F	-9.88	-18.58	798.45	F	-2.43	-13.41	828.84	F
COCOCOCOC(C)OCOC	3	-541.39													

COCCOC(C)(C)OCOC	4	-655.93	-9.50	-3.60	-13.84	865.63	F	-10.54	-18.13	878.76	F	-2.43	-13.40	899.47	F
COCCOCOC(C)(C)OC	4	-655.93	-9.58	-3.42	-13.86	853.33	F	-10.58	-18.21	871.92	F	-2.49	-13.21	905.64	F
COCCOCOC(C)(C)OC	4	-655.93	-9.09	-3.54	-13.81	845.43	F	-10.51	-18.23	863.13	F	-2.60	-13.39	904.33	F
COCCOCOC(C)(C)OC	4	-655.94	-9.36	-3.59	-13.75	867.84	F	-10.75	-18.22	871.64	F	-2.61	-13.44	905.27	F
COCCOCOC(C)(C)OC	5	-770.48	-9.31	-3.72	-13.74	935.64	F	-11.50	-18.01	942.72	F	-2.75	-13.37	971.13	F
COCCOCOC(C)(C)OC	5	-770.48	-9.42	-3.85	-13.64	922.60	F	-11.33	-17.83	931.84	F	-2.74	-13.42	940.75	F
COCCOCOC(C)(C)OC	5	-770.48	-9.20	-3.84	-13.63	916.43	F	-11.30	-17.81	923.90	F	-2.68	-13.22	989.26	F
COCCOCOC(C)(C)OC	5	-770.48	-9.25	-3.70	-13.63	920.31	F	-11.43	-18.07	930.24	F	-2.75	-13.32	955.48	F
COCCOC(C)(C)OCOC	5	-770.48	-9.56	-3.75	-13.66	910.26	F	-11.45	-17.76	925.11	F	-2.78	-13.35	976.18	F
COCCOC(C)(C)OCOC	5	-770.47	-9.30	-3.87	-13.75	908.75	F	-11.49	-17.87	940.71	F	-2.80	-13.33	951.90	F
COCCOCOC(C)(C)OC	4	-655.93	-9.42	-3.26	-13.75	864.19	F	-10.39	-18.22	863.70	F	-0.94	-11.14	1021.58	F
COCCOCOC(C)(C)OC	4	-655.93	-9.54	-3.52	-13.97	849.55	F	-10.40	-18.28	866.64	F	-2.54	-13.47	894.35	F
COCOC(C)(C)OCOC	4	-655.94	-9.37	-3.44	-13.74	859.07	F	-10.40	-18.28	866.64	F	-2.42	-13.42	900.45	F
COCCOCOCOC(C)(C)OC	5	-809.79	-8.99	-4.08	-13.59	942.80	F	-12.18	-17.80	968.74	F	-3.18	-13.28	1012.57	F
COCCOCOCOC(C)(C)OC	5	-809.78	-9.20	-4.09	-13.45	950.45	F	-12.12	-17.55	978.76	F	-2.95	-13.26	986.59	F
COCCOC(C)(C)OCOCOC	5	-809.79	-9.53	-4.09	-13.53	958.31	F	-12.10	-17.65	986.68	F	-3.06	-13.20	1025.04	F
COCCOCOC(C)(C)OCOC	5	-809.78	-9.44	-3.70	-13.28	1019.05	F	-12.13	-17.70	970.35	F	-3.05	-13.18	1032.84	F
COCCOCOC(C)(C)OCOC	5	-809.78	-9.09	-4.18	-13.54	978.68	F	-12.14	-17.62	998.79	F	-3.05	-13.22	990.46	F
COCCOC(C)(C)OCOCOC	5	-809.78	-9.15	-4.09	-13.57	952.77	F	-11.94	-17.73	976.42	F	-3.05	-13.19	1017.18	F
COCCOCOCOC(C)(C)OC	5	-809.78	-9.18	-3.90	-13.34	974.83	F	-11.93	-17.69	958.99	F	-3.09	-13.19	1017.18	F
COCCOC(C)(C)OC	3	-502.08	-9.45	-2.56	-13.83	715.37	F	-8.59	-18.84	735.66	F	-2.03	-13.63	780.16	F
COOCOC(C)(C)OC	3	-502.08	-9.61	-2.93	-14.29	735.43	F	-8.66	-19.10	739.99	F	-1.98	-13.68	772.87	F
COCCOC(C)(C)OC	3	-502.09	-9.52	-2.99	-14.19	728.94	F	-8.76	-18.95	737.61	F	-2.01	-13.75	776.59	F
COCOCOC(C)(C)OCOC	5	-731.17	-9.86	-3.36	-13.83	898.19	F	-10.50	-18.20	898.84	F	-2.40	-13.69	931.04	F
COCCOCOC(C)(C)OCOC	5	-731.17	-9.72	-3.44	-13.79	882.09	F	-10.76	-18.08	885.95	F	-2.44	-13.46	919.76	F
COCCOCOC(C)(C)OCOC	5	-731.17	-9.95	-3.25	-13.81	890.32	F	-10.61	-18.21	901.80	F	-2.44	-13.43	918.84	F
COCCOCOC(C)(C)OCOC	5	-731.17	-9.87	-3.38	-13.79	887.93	F	-10.75	-18.25	884.16	F	-2.33	-13.55	896.75	F
COCCOCOC(C)(C)OC	4	-734.56	-9.31	-4.14	-13.49	944.04	F	-11.79	-17.71	951.42	F	-2.99	-13.25	986.34	F
COCCOCOC(C)(C)OC	4	-734.56	-9.27	-3.91	-13.50	934.88	F	-10.75	-17.69	958.10	F	-2.83	-13.19	966.01	F
COCCC(C)(C)OC	2	-426.85	-9.43	-2.73	-14.13	693.37	F	-7.86	-19.03	697.26	F	-1.90	-13.50	747.29	F
COCCOCOC(C)(C)OC	3	-620.03	-9.31	-3.62	-13.60	884.68	F	-10.37	-18.11	885.23	F	-2.38	-13.05	902.71	F
COCCOCOC(C)(C)OC	3	-620.03	-9.35	-3.62	-13.60	865.43	F	-10.34	-18.24	885.08	F	-2.48	-13.28	922.82	F
COCCOCOC(C)(C)OC	5	-620.03	-9.35	-3.60	-13.76	865.43	F	-10.71	-18.38	885.10	F	-2.33	-13.32	939.64	F
COCCOCOC(C)(C)OC	5	-731.17	-9.82	-3.46	-13.70	873.89	F	-10.77	-18.25	884.16	F	-2.33	-13.55	896.75	F
COCCOCOC(C)(C)OC	4	-734.56	-9.31	-4.14	-13.49	944.04	F	-11.79	-17.71	951.42	F	-2.99	-13.25	986.34	F
COCCOCOC(C)(C)OC	4	-734.56	-9.27	-3.91	-13.50	934.88	F	-10.75	-17.69	958.10	F	-2.83	-13.19	966.01	F
COCCOC(C)(C)OC	2	-426.85	-9.43	-2.73	-14.13	693.37	F	-7.86	-19.03	697.26	F	-1.90	-13.50	747.29	F
COCCOCOC(C)(C)OC	3	-620.03	-9.31	-3.62	-13.60	884.68	F	-10.37	-18.11	885.23	F	-2.38	-13.05	902.71	F
COCCOCOC(C)(C)OC	3	-620.03	-9.35	-3.62	-13.60	865.43	F	-10.34	-18.24	885.08	F	-2.48	-13.28	922.82	F
COCCOCOC(C)(C)OC	5	-620.03	-9.35	-3.60	-13.76	865.43	F	-10.71	-18.38	885.10	F	-2.33	-13.32	939.64	F
COCCOCOC(C)(C)OC	5	-731.17	-9.82	-3.46	-13.70	873.89	F	-10.77	-18.25	884.16	F	-2.33	-13.55	896.75	F
COCCOCOC(C)(C)OC	4	-734.56	-9.31	-4.14	-13.49	944.04	F	-11.79	-17.71	951.42	F	-2.99	-13.25	986.34	F
COCCOCOC(C)(C)OC	4	-734.56	-9.27	-3.91	-13.50	934.88	F	-10.75	-17.69	958.10	F	-2.83	-13.19	966.01	F
COCCOC(C)(C)OC	2	-426.85	-9.43	-2.73	-14.13	693.37	F	-7.86	-19.03	697.26	F	-1.90	-13.50	747.29	F
COCCOCOC(C)(C)OC	3	-620.03	-9.31	-3.62	-13.60	884.68	F	-10.37	-18.11	885.23	F	-2.38	-13.05	902.71	F
COCCOCOC(C)(C)OC	3	-620.03	-9.35	-3.62	-13.60	865.43	F	-10.34	-18.24	885.08	F	-2.48	-13.28	922.82	F
COCCOCOC(C)(C)OC	5	-620.03	-9.35	-3.60	-13.76	865.43	F	-10.71	-18.38	885.10	F	-2.33	-13.32	939.64	F
COCCOCOC(C)(C)OC	5	-731.17	-9.82	-3.46	-13.70	873.89	F	-10.77	-18.25	884.16	F	-2.33	-13.55	896.75	F
COCCOCOC(C)(C)OC	4	-734.56	-9.31	-4.14	-13.49	944.04	F	-11.79	-17.71	951.42	F	-2.99	-13.25	986.34	F
COCCOCOC(C)(C)OC	4	-734.56	-9.27	-3.91	-13.50	934.88	F	-10.75	-17.69	958.10	F	-2.83	-13.19	966.01	F
COCCOC(C)(C)OC	2	-426.85	-9.43	-2.73	-14.13	693.37	F	-7.86	-19.03	697.26	F	-1.90	-13.50	747.29	F
COCCOCOC(C)(C)OC	3	-620.03	-9.31	-3.62	-13.60	884.68	F	-10.37	-18.11	885.23	F	-2.38	-13.05	902.71	F
COCCOCOC(C)(C)OC	3	-620.03	-9.35	-3.62	-13.60	865.43	F	-10.34	-18.24	885.08	F	-2.48	-13.28	922.82	F
COCCOCOC(C)(C)OC	5	-620.03	-9.35	-3.60	-13.76	865.43	F	-10.71	-18.38	885.10	F	-2.33	-13.32	939.64	F
COCCOCOC(C)(C)OC	5	-731.17	-9.82	-3.46	-13.70	873.89	F	-10.77	-18.25	884.16	F	-2.33	-13.55	896.75	F
COCCOCOC(C)(C)OC	4	-734.56	-9.31	-4.14	-13.49	944.04	F	-11.79	-17.71	951.42	F	-2.99	-13.25	986.34	F
COCCOCOC(C)(C)OC	4	-734.56	-9.27	-3.91	-13.50	934.88	F	-10.75	-17.69	958.10	F	-2.83	-13.19	966.01	F
COCCOC(C)(C)OC	2	-426.85	-9.43	-2.73	-14.13	693.37	F	-7.86	-19.03	697.26	F	-1.90	-13.50	747.29	F
COCCOCOC(C)(C)OC	3	-620.03	-9.31	-3.62	-13.60	884.68	F	-10.37	-18.11	885.23	F	-2.38	-13.05	902.71	F
COCCOCOC(C)(C)OC	3	-620.03	-9.35	-3.62	-13.60	865.43	F	-10.34	-18.24	885.08	F	-2.48	-13.28	922.82	F
COCCOCOC(C)(C)OC	5	-620.03	-9.35	-3.60	-13.76	865.43	F	-10.71	-18.38	885.10	F	-2.33	-13.32	939.64	F
COCCOCOC(C)(C)OC	5	-731.17	-9.82	-3.46	-13.70	873.89	F	-10.77	-18.25	884.16	F	-2.33	-13.55	896.75	F
COCCOCOC(C)(C)OC	4	-734.56	-9.31	-4.14	-13.49	944.04	F	-11.79	-17.71	951.42	F	-2.99	-13.25	986.34	F
COCCOCOC(C)(C)OC	4	-734.56	-9.27	-3.91	-13.50	934.88	F	-10.75	-17.69	958.10	F	-2.83	-13.19	966.01	F
COCCOC(C)(C)OC	2	-426.85	-9.43	-2.73	-14.13	693.37	F	-7.86	-19.03	697.26	F	-1.90	-13.50	747.29	F
COCCOCOC(C)(C)OC	3	-620.03	-9.31	-3.62	-13.60	884.68	F	-10.37	-18.11	885.23	F	-2.38	-13.05	902.71	F
COCCOCOC(C)(C)OC	3	-620.03	-9.35	-3.62	-13.60	865.43	F	-10.34	-18.24	885.08	F	-2.48	-13.28	922.82	F
COCCOCOC(C)(C)OC	5	-620.03	-9.35	-3.60	-13.76	865.43	F	-10.71	-18.38	885.10	F	-2.33	-13.32	939.64	F
COCCOCOC(C)(C)OC	5	-731.17	-9.82	-3.46	-13.70	873.89	F	-10.77	-18.25	884.16	F	-2.33	-13.55	896.75	F
COCCOCOC(C)(C)OC	4	-734.56	-9.31	-4.14	-13.49	944.04	F	-11.79	-17.71	951.42	F	-2.99	-13.25	986.34	F
COCCOCOC(C)(C)OC	4	-734.56	-9.27	-3.91	-13.50	934.88	F	-10.75	-17.69	958.10	F	-2.83	-13.19	966.01	F
COCCOC(C)(C)OC	2	-426.85	-9.43	-2.73	-14.13	693.37	F	-7.86	-19.03	697.26	F	-1.90	-13.50	747.29	F
COCCOCOC(C)(C)OC	3	-620.03	-9.31	-3.62	-13.60	884.68	F	-10.37	-18.11	885.23	F	-2.38	-13.05	902.71	F
COCCOCOC(C)(C)OC	3	-620.03	-9.35	-3.62	-13.60	865.43									

CCCCCCCCCCCC(C)C	4	-852.52	-9.21	-4.20	-13.02	1049.67	F	-12.45	-17.30	1075.92	F	-3.02	-12.96	1133.39
COOCOC(C)C(C)	3	-502.09	-9.85	-2.64	-14.23	736.28	F	-7.95	-18.88	746.76	F	-1.82	-13.75	773.67
COCOCOCOC(C)C	4	-695.25	-9.49	-3.64	-13.65	917.75	F	-10.86	-17.97	909.26	F			F
COCCOCOCOC(C)C	4	-695.25	-9.63	-3.62	-13.80	905.16	F	-10.76	-18.04	922.57	F	-2.62	-13.42	954.23
COCCOCOCOC(C)C	5	-809.80	-8.99	-3.75	-13.42	961.99	F	-11.48	-17.56	977.58	F	-2.72	-13.06	973.15
COCCOCOCOC(C)C	5	-809.80	-9.25	-3.86	-13.61	985.02	F	-11.68	-17.81	979.57	F	-2.99	-13.51	1001.25
COCCOCOCOC(C)C	4	-695.25	-9.23	-3.57	-13.63	899.07	F	-10.72	-18.06	913.78	F	-2.55	-13.37	952.53
COCCOCOCOC(C)C	5	-849.10	-9.67	-4.26	-13.39	984.42	F	-12.30	-17.52	1020.49	F	-3.06	-13.03	1104.38
COCCOCOCOC(C)C	5	-849.11	-9.04	-4.11	-13.23	996.48	F	-12.11	-17.34	1020.30	F	-2.85	-13.00	1091.34
COCOCOC(C)C(C)	3	-541.40	-9.69	-2.89	-13.92	797.28	F	-8.78	-18.75	789.07	F	-2.05	-13.56	849.61
COCOCOC(C)C(C)	3	-541.40	-9.53	-3.00	-13.96	791.59	F	-8.96	-18.61	792.24	F	-1.63	-12.48	883.81
COCOCOCOCOC(C)C	5	-770.49	-9.80	-3.13	-13.80	924.85	F	-10.67	-17.93	931.43	F	-2.21	-13.42	934.34
COCOCOCOCOC(C)C	5	-770.49	-9.91	-3.53	-13.70	944.53	F	-10.74	-17.88	929.53	F	-2.42	-13.25	963.27
COCCOCOCOCOC(C)C	4	-773.88	-9.38	-4.08	-13.33	996.93	F	-11.96	-17.65	997.31	F	-3.05	-13.17	1044.80
COCCOC(C)C(C)	2	-466.18	-9.29	-2.79	-13.99	757.72	F	-8.26	-18.77	755.73	F	-1.76	-13.55	783.96
COCCOCOCOC(C)C	3	-659.35	-9.22	-3.54	-13.45	941.54	F	-10.66	-17.90	935.20	F	-2.43	-13.24	962.89
COCCOCOCOC(C)C	5	-770.49	-9.54	-3.46	-13.72	915.85	F	-10.83	-17.84	939.67	F	-2.23	-13.29	999.61
COCCOCOCOC(C)C	5	-770.49	-9.73	-3.58	-13.64	930.28	F	-10.75	-18.01	939.55	F	-2.32	-13.37	975.56
COCCOCOCOCOC(C)C	4	-813.20	-9.28	-4.01	-13.26	1041.11	F	-12.10	-17.42	1048.92	F	-2.93	-12.98	1055.37
COCCOCOCOCOC(C)C	4	-734.56	-9.14	-4.02	-13.37	928.58	F	-11.48	-17.72	962.24	F	-3.03	-13.26	991.02
COCCOCOCOC(C)C	4	-655.94	-9.67	-3.38	-13.92	862.31	F	-9.87	-18.39	867.51	F	-2.17	-13.55	874.71
COCCOCOCOC(C)C	4	-655.95	-9.51	-3.33	-13.86	853.25	F	-10.02	-18.26	862.24	F	-2.35	-13.37	912.47
COCCOCOCOC(C)C	3	-580.71	-9.42	-3.43	-13.77	827.64	F	-9.89	-18.26	844.37	F	-2.51	-13.50	877.75
COCCOCOCOCOC(C)C	5	-888.41	-9.13	-4.53	-13.13	1035.80	F	-13.00	-17.27	1056.20	F			F
COCCOCOCOCOC(C)C	2	-387.55	-9.88	-2.24	-14.46	665.27	F	-6.72	-19.62	650.88	F			F
COCCOCOCOCOC(C)C	4	-852.52	-9.13	-4.01	-13.11	1087.93	F	-12.15	-17.41	1081.63	F	-2.50	-12.23	1170.90
COCCOCOCOC(C)C	3	-620.03	-8.96	-3.53	-13.75	889.05	F	-10.19	-18.06	893.27	F	-2.54	-13.43	925.22
COCCOCOCOC(C)C	3	-620.03	-9.29	-3.50	-13.59	886.04	F	-10.34	-18.20	883.62	F	-2.48	-13.27	930.57
COCCOCOCOC(C)C	4	-734.59	-9.61	-3.43	-13.49	972.40	F	-10.67	-17.97	976.45	F	-2.31	-13.32	998.62
COCCOCOCOC(C)C	5	-927.77	-9.01	-3.49	-13.24	1108.77	F	-11.88	-18.18	971.41	F	-2.66	-12.89	1129.52
COCCOCOCOC(C)C	5	-770.51	-9.86	-3.29	-13.96	918.57	F	-10.40	-18.18	971.41	F	-2.20	-13.47	1002.12
COCCOCOCOC(C)C	3	-580.73	-9.41	-3.06	-13.90	838.01	F	-9.19	-18.55	850.54	F	-2.15	-13.35	878.56
COCCOCOCOC(C)C	5	-927.76	-9.32	-3.42	-10.96	1243.28	F	-11.02	-15.49	1168.01	F	-2.88	-12.87	1133.63
COCCOCOCOC(C)C	5	-927.77	-9.36	-3.86	-13.15	1126.93	F	-11.85	-17.45	1130.09	F			F
COCCOCOCOC(C)C	4	-616.65	-9.79	-2.99	-14.42	817.10	F	-9.34	-18.78	834.05	F	-1.98	-13.70	861.21
COCCOCOCOC(C)C	4	-695.27	-9.50	-3.24	-13.68	920.96	F	-10.15	-18.23	926.19	F	-2.11	-13.28	962.52
COCCOCOCOC(C)C	5	-927.77	-9.25	-3.82	-13.38	1105.65	F	-11.63	-17.37	1128.30	F	-2.71	-12.89	1125.96
COCCOCOCOC(C)C	4	-970.49	-9.13	-4.28	-12.94	1206.38	F	-12.42	-16.94	1200.54	F	-2.50	-11.88	1299.98
COCCOCOCOC(C)C	3	-462.78	-9.88	-2.62	-14.37	696.12	F	-7.95	-19.28	699.47	F	-1.70	-13.97	734.73
COCCOCOCOC(C)C	4	-734.58	-9.44	-3.57	-13.59	966.67	F	-10.92	-17.90	968.22	F	-2.62	-13.33	992.90
COCCOCOCOC(C)C	5	-927.77	-9.27	-3.32	-12.54	1151.30	F					-2.45	-12.23	1181.30
COCCOCOCOC(C)C	4	-734.58	-9.15	-3.63	-13.58	969.39	F	-10.77	-18.13	968.50	F	-2.63	-13.36	999.12
COCCOCOCOC(C)C	3	-541.41	-9.47	-3.11	-14.13	789.73	F	-8.90	-18.74	796.91	F	-2.11	-13.62	839.72
COCCOCOCOC(C)C	5	-849.14	-9.64	-3.52	-13.43	1050.53	F	-11.17	-17.52	1043.24	F			F
COCCOCOCOC(C)C	4	-813.21	-9.22	-4.05	-13.34	1040.07	F	-11.85	-17.59	1059.69	F	-2.82	-13.12	1065.96
COCCOCOCOC(C)C	2	-426.86	-9.36	-2.70	-14.16	706.89	F	-7.76	-19.01	710.89	F	-1.84	-13.65	753.45
COCCOCOCOC(C)C	3	-696.87	-9.21	-3.47	-13.55	949.99	F	-10.51	-17.84	990.48	F	-2.27	-13.03	1004.95
COCCOCOCOC(C)C	5	-849.14	-9.50	-3.40	-13.49	1024.33	F	-10.87	-17.61	1013.11	F	-2.54	-13.18	1049.50
COCCOCOCOC(C)C	4	-852.52	-8.91	-4.16	-13.25	1075.16	F	-11.95	-17.34	1091.57	F	-2.81	-12.91	1123.50
COCCOCOCOC(C)C	4	-724.56	-9.08	-3.90	-13.53	929.63	F	-11.45	-17.89	965.49	F	-1.32	-12.14	1029.82
COCCOCOCOC(C)C	4	-695.27	-9.50	-3.40	-13.81	915.46	F	-9.85	-18.09	912.13	F	-2.20	-13.48	947.01
COCCOCOCOC(C)C	5	-927.74	-9.01	-4.30	-13.10	1105.84	F	-12.75	-16.95	1108.49	F	-2.32	-12.95	1159.96
COCCOCOCOC(C)C	3	-620.03	-9.36	-3.46	-13.70	882.84	F	-10.08	-18.23	900.40	F	-2.37	-13.24	929.48
COCCOCOCOC(C)C	2	-387.54	-9.44	-2.58	-14.28	650.70	F	-7.34	-19.19	651.57	F	-1.87	-13.72	710.51
COCCOCOCOC(C)C	3	-659.36	-9.32	-3.29	-13.73	928.73	F	-10.14	-18.10	938.26	F	-2.30	-13.23	962.62
COCCOCOCOC(C)C	5	-1006.39	-9.25	-3.51	-12.80	1205.59	F	-12.74	-16.94	1198.49	F			F
COCCOCOCOC(C)C	4	-931.17	-9.26	-4.17	-12.99	1174.73	F	-12.16	-17.21	1169.20	F			F
COCCOCOCOC(C)C	5	-1006.40	-9.20	-3.90	-12.80	1159.18	F	-12.16	-17.01	1195.46	F			F
COCCOCOCOC(C)C	4	-970.48	-9.25	-4.33	-13.06	1198.00	F	-12.48	-17.08	1190.82	F	-2.69	-12.43	1257.21
COCCOCOCOC(C)C	4	-773.90	-9.25	-3.60	-13.59	1009.83	F	-10.68	-17.93	1007.18	F	-2.50	-13.20	1058.56
COCCOCOCOC(C)C	3	-620.03	-9.37	-3.38	-13.75	880.07	F					-1.11	-11.83	988.50
COCCOCOCOC(C)C	4	-891.85	-9.27	-3.89	-13.18	1122.76	F	-9.82	-17.86	958.84	F	-3.02	-12.91	1168.39
COCCOCOCOC(C)C	4	-852.53	-9.35	-2.60	-11.71	1146.65	F	-11.78	-17.36	1096.18	F	-2.93	-12.93	1114.56
COCCOCOCOC(C)C	5	-1085.02	-8.95	-4.19	-12.47	1279.28	F							F
COCCOCOCOC(C)C	4	-773.90	-9.18	-3.42	-13.45	1010.13	F	-11.15	-17.79	1025.98	F	-2.64	-13.21	1029.03
COCCOCOCOC(C)C	4	-891.86	-9.56	-3.43	-13.27	1099.04	F	-11.26	-17.37	1116.10	F	-1.53	-11.98	1185.85
COCCOCOCOC(C)C	5	-1163.67	-9.23	-1.86	-11.09	1384.73	F					-1.03	-10.91	1468.17
COCCOCOCOC(C)C	5	-927.79	-9.58	-3.33	-13.33	1074.98	F	-10.98	-17.39	1105.50	F	-1.96	-12.88	1121.34
COCCOCOCOC(C)C	3	-696.88	-9.26	-3.21	-13.51	947.23	F	-9.82	-17.86	958.84	F	-0.87	-11.76	1026.42
COCCOCOCOC(C)C	5	-1124.34	-9.18	-1.95	-11.20	1385.81	F	-11.55	-15.58	1293.04	F			F
COCCOCOCOC(C)C	4	-1163.66	-9.25	-2.02	-11.31	1370.86	F							F
COCCOCOCOC(C)C	3	-659.36	-9.39	-2.62	-13.51	876.35	F	-9.30	-18.26	895.07	F	-1.22	-12.31	960.45
COCCOCOCOC(C)C	5	-1045.73	-9.52	-1.93	-11.64	1257.39	F							F
COCCOCOCOC(C)C	4	-970.47	-9.22	-3.47	-12.44	1186.45	F					-1.88	-11.66	1228.56
COCCOCOCOC(C)C	4	-1206.37	-8.99	-1.97	-11.05	1502.71	F	-6.85	-12.97	1490.79	F	-1.34	-11.32	1562.97
COCCOCOCOC(C)C	3	-541.42	-9.63	-2.57	-14.14	769.33	F	-8.19	-18.89	774.75	F	-1.68	-13.51	815.15
COCCOCOCOC(C)C	5	-1163.67	-9.16	-1.93	-11.12	1380.14	F							F
COCCOCOCOC(C)C	4	-891.85	-9.42	-3.06	-12.25	1128.61	F							F
COCCOCOCOC(C)C	5	-1124.35	-9.27	-2.72	-11.63	1375.67	F							F
COCCOCOCOC(C)C	3	-659.36	-9.39	-2.62	-13.51	876.35	F	-9.30	-18.26	895.07	F	-1.22	-12.31	960.45
COCCOCOCOC(C)C	5	-1045.73	-9.52	-1.93	-11.64	1257.39	F					-1.88	-11.66	1228.56
COCCOCOCOC(C)C	2	-505.49	-9.26	-2.83	-13.94	780.98	F	-8.13	-18.67	785.45	F	-1.86	-13.26	828.28
COCCOCOCOC(C)C	3	-855.93	-9.11	-3.73	-12.98	1112.68	F	-6.87	-14.12	1165.30	F	-1.18	-11.18	1234.70
COCCOCOCOC(C)C	5	-1045.72	-9.35	-2.02	-11.47	1486.25	F							F
COCCOCOCOC(C)C	4	-852.52	-9.33	-3.04	-13.26	1051.18	F	-9.25	-15.97	1068.25	F	-2.27	-12.44	1105.29
COCCOCOCOC(C)C	5	-1242.28	-8.96	-1.99	-10.90	1509.21	F					-1.10	-11.32	1158.98
COCCOCOCOC(C)C	4	-1088.43	-9.14	-1.87	-11.09	1333.91</								

CCOCOCOCOCOCOCOCOC	2:2:2:1:2	5	-809.79	-9.34	-3.91	-13.48	975.37	F	-11.98	-17.63	971.77	F	-3.00	-13.21	1026.70	F
CCOCOCOCOC	2:2:1:2	3	-502.08	-9.65	-2.91	-14.21	760.85	F	-8.64	-18.99	752.77	F	-1.81	-13.84	756.22	F
CCOCOCOCOCOCOC	2:1:2:1:2	5	-731.17	-9.95	-3.42	-13.83	878.88	F	-10.71	-18.38	900.03	F	-2.53	-13.71	929.23	F
CCOCOCOCOCOCOCOC	2:2:3:2:2	4	-734.57	-8.92	-4.01	-13.48	945.05	F	-11.75	-17.81	962.02	F	-2.84	-13.20	979.63	F
CCOCOCOCOC	2:3:2	2	-426.86	-9.36	-2.83	-14.23	714.62	F	-8.25	-19.02	700.97	F	-1.93	-13.69	743.04	F
CCOCOCOCOCOC	2:3:3:2	3	-620.03	-9.38	-3.58	-13.72	867.89	F	-10.55	-18.27	903.95	F	-2.56	-13.33	924.04	F
CCOCOCOCOCOCOC	2:2:1:1:2	5	-731.17	-9.45	-3.42	-13.97	890.22	F	-10.53	-18.33	884.83	F	-2.44	-13.42	915.43	F
CCOCOCOCOCOCOC	2:2:4:2:2	4	-773.88	-8.97	-4.09	-13.50	1000.32	F	-12.06	-17.70	995.54	F	-2.96	-13.10	1047.60	F
CCOCOCOCOCOCOC	2:2:2:2	4	-695.24	-9.12	-3.96	-13.69	907.76	F	-11.33	-18.04	905.73	F	-2.89	-13.46	942.18	F
CCOCOCOCOCOC	2:2:1:1:2	4	-616.63	-9.63	-3.28	-14.05	828.64	F	-9.81	-18.67	823.10	F	-2.33	-13.66	856.76	F
CCOCOCOCOC	2:2:2:2	3	-541.39	-9.19	-3.39	-13.86	794.36	F	-9.81	-18.68	791.64	F	-2.48	-13.68	840.18	F
CCOCOCOCOCOCOC	2:2:2:2:2	5	-849.09	-9.24	-4.41	-13.18	996.32	F	-12.86	-17.50	1023.03	F	-3.44	-13.08	1064.14	F
CCOCOC	2:1:2	2	-348.23	-9.98	-2.15	-14.58	632.32	F	-6.51	-19.70	628.66	F	-1.52	-14.03	686.75	F
CCOCOCOCOCOCOC	2:2:5:2:2	4	-813.19	-9.50	-4.28	-13.17	1041.00	F	-12.23	-17.51	1052.47	F	-3.28	-13.18	1060.69	F
CCOCOCOCOCOC	2:3:2:2	3	-580.71	-9.24	-3.52	-13.89	847.56	F	-10.14	-18.34	846.47	F	-2.48	-13.49	883.52	F
CC(C)CJOCCOCOC(C)(C)C	4	-813.23	-9.60	-3.19	-13.49	1081.30	F	-10.83	-17.80	1070.15	F	-2.43	-13.10	1127.11	F	
CC(C)CJOCCOCOCOC(C)(C)C	5	-927.76	-9.34	-3.96	-13.35	1108.13	F	-12.02	-17.46	1129.21	F	-2.74	-13.12	1139.30	F	
CC(C)CJOCCOCOC(C)(C)C	5	-849.14	-9.95	-3.41	-13.73	1003.92	F	-10.48	-17.95	1019.89	F	-2.46	-13.42	1079.97	F	
CC(C)CJOCCOCOC(C)(C)C	3	-698.69	-9.39	-3.25	-13.61	994.30	F	-9.95	-18.01	991.34	F	-2.19	-13.19	1024.94	F	
CC(C)CJOCCOCOCOC(C)(C)C	5	-967.08	-9.13	-3.13	-13.13	994.30	F	-12.31	-17.11	1120.59	F	-2.95	-12.94	1182.13	F	
CC(C)CJOCCOCOCOCOC(C)(C)C	5	-927.76	-9.36	-3.78	-13.25	1085.71	F	-11.69	-17.46	1097.02	F	-2.74	-13.12	1139.30	F	
CC(C)CJOCCOC(C)(C)C	2	-544.82	-9.37	-2.83	-14.04	859.73	F	-8.43	-18.41	861.71	F	-2.02	-13.33	909.77	F	
CC(C)CJOCCOCOC(C)(C)C	4	-734.60	-9.71	-3.10	-13.79	987.79	F	-9.66	-18.25	978.64	F	-2.17	-13.57	976.84	F	
CC(C)CJOCCOCOC(C)(C)C	4	-773.91	-9.87	-3.18	-13.37	1050.55	F	-10.43	-17.98	1031.02	F	-2.41	-13.28	1053.12	F	
CC(C)CJOCCOCOCOC(C)(C)C	5	-927.76	-9.42	-4.10	-13.34	1098.94	F	-12.63	-16.97	1201.93	F	-3.14	-12.79	1212.75	F	
CC(C)CJOCCOCOCOCOC(C)(C)C	4	-970.49	-9.24	-4.17	-12.92	1200.00	F	-12.63	-16.97	1201.93	F	-3.14	-12.79	1212.75	F	
CC(C)CJOCCOC(C)(C)C	3	-620.06	-9.63	-2.82	-13.92	865.11	F	-8.51	-18.49	876.71	F	-2.02	-13.46	923.95	F	
CC(C)CJOCCOCOCOC(C)(C)C	4	-813.22	-9.24	-3.68	-13.49	1064.41	F	-11.22	-17.76	1052.46	F	-2.47	-13.14	1056.92	F	
CC(C)CJOCCOCOCOC(C)(C)C	5	-927.76	-9.07	-4.06	-13.35	1091.35	F	-11.97	-17.37	1113.59	F	-2.84	-13.06	1145.17	F	
CC(C)CJOCCOCOCOCOC(C)(C)C	4	-813.22	-9.37	-3.62	-13.50	1028.88	F	-11.13	-17.76	1043.41	F	-2.63	-13.19	1098.51	F	
CC(C)CJOCCOCOCOCOC(C)(C)C	5	-967.07	-9.07	-4.25	-13.19	1139.91	F	-12.31	-17.76	1043.41	F	-2.95	-13.19	1182.13	F	
CC(C)CJOCCOCOC(C)(C)C	3	-659.37	-9.51	-3.10	-13.75	914.10	F	-9.37	-18.30	928.91	F	-2.23	-13.39	992.56	F	
CC(C)CJOCCOCOC(C)(C)C	5	-888.45	-9.77	-3.31	-13.60	1032.80	F	-11.01	-17.65	1054.62	F	-2.51	-13.23	1107.39	F	
CC(C)CJOCCOCOCOC(C)(C)C	4	-891.84	-8.97	-4.29	-13.12	1139.76	F	-12.31	-17.31	1116.51	F	-3.09	-12.94	1159.55	F	
CC(C)CJOCCOCOCOCOC(C)(C)C	2	-584.14	-9.21	-2.96	-13.82	911.35	F	-8.96	-18.27	906.28	F	-2.03	-13.23	930.86	F	
CC(C)CJOCCOCOCOC(C)(C)C	3	-777.32	-9.24	-3.71	-13.37	1059.61	F	-11.01	-17.67	1061.95	F	-2.60	-12.89	1073.13	F	
CC(C)CJOCCOCOCOC(C)(C)C	5	-888.46	-9.43	-3.64	-13.54	1080.58	F	-11.01	-17.65	1054.62	F	-2.51	-13.24	1087.72	F	
CC(C)CJOCCOCOCOCOC(C)(C)C	4	-931.16	-9.01	-4.41	-13.16	1164.15	F	-12.31	-17.76	1042.37	F	-3.15	-13.08	1140.26	F	
CC(C)CJOCCOCOCOCOC(C)(C)C	4	-852.52	-9.21	-4.24	-13.28	1082.37	F	-12.31	-17.76	1042.37	F	-3.15	-13.08	1140.26	F	
CC(C)CJOCCOCOC(C)(C)C	4	-773.91	-9.44	-3.44	-13.65	1006.00	F	-10.46	-17.96	1016.66	F	-2.49	-13.33	1013.83	F	
CC(C)CJOCCOCOCOC(C)(C)C	3	-698.67	-9.32	-3.67	-13.62	984.58	F	-10.49	-18.03	982.95	F	-2.64	-13.34	1020.39	F	
CC(C)CJOCCOCOCOCOC(C)(C)C	5	-1006.38	-9.12	-4.22	-12.81	1207.04	F	-12.94	-16.95	1167.17	F	-3.16	-12.81	1251.58	F	
CC(C)CJOCCOCOC(C)(C)C	2	-505.51	-9.64	-4.21	-13.49	827.68	F	-7.28	-18.72	799.70	F	-1.72	-13.52	872.45	F	
CC(C)CJOCCOCOCOCOC(C)(C)C	4	-970.48	-9.41	-4.24	-13.08	1195.80	F	-12.56	-17.08	1197.01	F	-3.12	-12.89	1286.97	F	
CO(C)CJOCCOC(C)(C)C	5	-738.00	-9.24	-3.66	-13.37	1031.27	F	-10.79	-17.79	1031.87	F	-2.58	-13.18	1074.48	F	
COCC(C)COC(C)C	4	-891.84	-8.96	-4.25	-13.19	1133.70	F	-11.72	-16.83	1126.33	F	-3.19	-13.02	1135.26	F	
COCC(C)COC(C)C	4	-891.85	-9.33	-2.12	-11.83	1133.52	F	-11.94	-14.44	1144.48	F	-2.82	-12.77	1195.85	F	
COCC(C)COC(C)C	3	-541.39	-9.01	-3.36	-14.04	795.39	F	-9.42	-18.49	793.11	F	-2.37	-13.63	841.65	F	
CC(C)CJOCCC(C)(C)C	4	-1009.79	-9.20	-1.90	-11.03	1348.22	F	-12.31	-17.84	953.49	F	-2.33	-13.43	906.94	F	
CCOCOCOCOCOC	2:3:2:1:2	4	-655.95	-9.60	-3.36	-13.94	851.11	F	-10.34	-18.39	868.95	F	-2.56	-13.35	949.96	F
CCOCOCOCOCOC	2:2:3:2	4	-695.25	-9.47	-3.74	-13.37	908.69	F	-11.00	-18.07	923.55	F	-2.70	-13.35	949.96	F
CCOCOCOCOCOC	2:2:3:1:2	4	-695.25	-9.37	-3.42	-13.30	923.70	F	-11.05	-18.05	931.33	F	-2.51	-13.27	944.54	F
CCOCOCOCOCOCOC	2:3:3:1:2	4	-734.58	-9.41	-3.69	-13.45	956.21	F	-11.32	-17.86	958.13	F	-2.67	-13.06	993.60	F
CCOCOCOCOCOCOC	2:3:1:2:2	4	-695.26	-9.35	-3.53	-13.41	900.21	F	-10.93	-18.09	902.61	F	-2.66	-13.19	950.91	F
CCOCOCOCOCOCOC	2:3:2:2:2	4	-734.56	-9.12	-4.07	-13.48	943.73	F	-11.81	-17.85	967.61	F	-3.03	-13.29	989.43	F
CCOCOCOCOCOCOC	2:3:3:2:2	4	-733.88	-9.03	-3.96	-13.28	1013.15	F	-12.17	-17.69	1005.37	F	-2.97	-13.00	1048.14	F
CCOCOCOCOCOCOC	2:3:1:3:2	4	-734.58	-9.39	-3.67	-13.40	940.60	F	-11.32	-17.84	953.49	F	-2.54	-13.24	981.94	F
CO(C)CJOCCOCOCOC	2:3:2:2:2	4	-773.89	-8.99	-4.13	-13.37	969.08	F	-12.01	-17.71	981.93	F	-2.85	-13.01	1046.85	F
CO(C)CJOCCOCOCOC	2:3:1:1:2	5	-707.49	-9.65	-3.61	-13.69	913.05	F	-11.05	-18.07	942.02	F	-2.49	-13.29	973.88	F
COOCOCOCOCOCOC	2:3:2:1:2:2	5	-809.80	-9.12	-3.59	-13.39	997.17	F	-11.75	-17.65	969.47	F	-3.03	-13.31	1006.84	F
COOCOCOCOCOCOC	2:3:1:3:1:2	5	-707.49	-9.69	-3.48	-13.74	943.80	F	-11.16	-18.03	944.14	F	-2.52	-13.19	1011.72	F
COOCOCOCOCOCOCOC	2:3:3:1:2:2	5	-809.80	-9.29	-3.88	-13.51	986.50	F	-11.86	-17.74	985.09	F	-2.86	-13.35	1020.18	F
COOCOCOCOCOCOCOC	2:3:1:2:2:2	5	-849.11	-9.17	-4.22	-13.14	1020.15	F	-12.34	-17.39	1016.29	F	-2.63	-13.20	1000.35	F
COOCOCOCOCOCOCOC	2:3:2:2:2:2	5	-888.43	-9.17	-3.97	-13.26	1024.88	F	-12.31	-17.43	1035.91	F	-2.99	-12.98	1072.36	F
COOCOCOCOCOCOCOC	2:3:2:1:2:2	5	-889.41	-9.51	-3.75	-13.54	974.96	F	-11.69	-17.74	1015.28	F	-2.47	-13.00	1061.09	F
CCOCOCOCOCOCOCOC	2:3:2:3:2:2	5	-888.42	-9.26	-4.36	-13.09	1044.47	F	-12.64	-17.21	1033.82	F	-3.09	-12.89	1115.15	F
COOCOCOCOCOCOCOC	2:2:1:3:1:2	5	-809.80	-9.34	-3.85	-13.35	1002.15	F	-12.29	-17.43	992.47	F	-2.73	-13.12	1026.94	F
COOCOCOCOCOCOCOC	2:3:1:3:1:2	5	-809.80	-9.48	-4.09	-13.04	1039.18	F	-13.04	-17.23	1061.19	F	-2.82	-12.92	1073.49	F
COOCOCOCOCOCOCOC	2:2:3:1:2:2	5	-849.11	-9.19	-4.31	-13.33	1009.85	F	-13.20	-17.14	1089.20	F	-3.39	-12.90	1125.67</td	

CCOCOCOCOCOCOCOCOCOCOC	2:1:3:2:1:2:2	6	-963.66	-9.36		-12.70	-17.21	1097.25	F	-2.94	-13.10	1142.27	F			
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:2:1:2	6	-1002.95	-9.05	-4.66	-12.99	1113.47	F	-13.45	-16.95	1119.05	F	-3.56	-12.87	1133.39	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:2:1:2	6	-1042.28	-9.25	-4.62	-13.01	1161.85	F	-13.43	-16.80	1137.51	F				
CCOCOCOCOCOCOCOCOCOCOC	2:2:1:3:1:2:2	6	-963.65	-9.28	-3.92	-13.08	1050.33	F	-12.78	-17.34	1078.25	F	-3.18	-12.98	1146.69	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:1:3:1:2:2	6	-1002.97	-9.26	-4.20	-12.96	1104.43	F	-12.96	-16.93	1115.73	F				
CCOCOCOCOCOCOCOCOCOCOC	2:1:2:3:1:2:2	6	-963.66	-9.39	-3.71	-13.05	1095.57	F	-12.69	-17.35	1062.94	F	-3.03	-13.03	1109.71	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:3:1:2:2	6	-1002.95	-9.02	-4.64	-12.84	1147.00	F	-13.42	-16.95	1121.51	F	-3.59	-12.85	1192.29	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:3:1:2:2	6	-1042.29	-9.21	-4.29	-12.76	1162.53	F	-13.44	-16.71	1130.67	F	-3.23	-12.75	1191.73	F
CCOCOCOCOCOCOCOCOCOCOC	2:1:3:3:1:2:2	6	-1002.97	-9.22	-4.12	-12.53	1162.88	F	-12.58	-16.54	1141.50	F	-3.13	-12.92	1168.87	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:3:1:2:2	6	-1042.28	-9.28	-4.23	-12.93	1159.58	F	-13.59	-16.80	1148.70	F				
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:3:1:2:2	6	-1081.60	-9.10	-4.38	-12.57	1232.97	F	-13.03	-15.11	1238.14	F	-3.33	-12.51	1219.88	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:1:1:3:1:2	6	-924.34	-9.61	-4.00	-13.24	1067.56	F	-12.46	-17.43	1039.19	F	-3.01	-13.25	1079.13	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:1:1:3:1:2	6	-963.66	-9.52	-4.04	-13.38	1074.96	F	-12.66	-17.23	1086.24	F	-2.97	-12.95	1141.26	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:2:1:3:1:2	6	-963.64	-9.21	-4.40	-12.91	1073.65	F	-12.77	-17.24	1075.61	F	-3.35	-13.05	1095.00	F
CCOCOCOCOCOCOCOCOCOCOC	2:1:3:1:3:1:2	6	-1002.97	-9.34	-3.84	-12.92	1137.21	F	-12.82	-16.95	1110.71	F	-3.25	-12.87	1147.26	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:1:3:1:2	6	-963.66	-9.69	-3.77	-13.04	1087.43	F								
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:1:3:1:2	6	-1002.97	-9.26	-4.02	-12.69	1145.17	F	-12.90	-16.97	1119.88	F				
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:3:1:3:2	6	-1042.30	-9.27	-3.72	-12.27	1212.79	F	-12.89	-16.72	1158.37	F	-3.03	-12.62	1187.57	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:2:3:1:2	6	-963.65	-9.37	-4.08	-12.95	1067.56	F	-12.75	-17.23	1079.93	F				
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:3:2:1:2	6	-1002.97	-9.39	-4.32	-13.10	1145.98	F	-13.08	-16.98	1128.97	F				
CCOCOCOCOCOCOCOCOCOCOC	2:2:2:3:3:1:2	6	-1002.96	-9.36	-4.22	-12.99	1127.63	F	-13.35	-16.95	1110.62	F				
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:3:2:1:2	6	-1042.28	-9.23	-4.50	-12.99	1149.66	F	-13.51	-16.84	1137.93	F				
CCOCOCOCOCOCOCOCOCOCOC	2:1:3:3:3:1:2	6	-1002.97	-9.36	-4.20	-13.02	1162.51	F	-13.06	-17.05	1127.94	F				
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:3:3:1:2	6	-1042.29	-9.35	-4.46	-12.89	1159.44	F	-13.36	-16.80	1174.48	F	-3.34	-12.74	1202.91	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:3:3:1:2	6	-1081.59	-9.15	-4.74	-12.74	1224.43	F	-14.00	-16.52	1180.81	F	-3.35	-12.57	1253.23	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:1:3:3:1:2	6	-1002.97	-9.39	-4.21	-12.82	1121.53	F	-12.97	-17.18	1100.38	F	-3.15	-12.89	1153.74	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:1:3:3:1:2	6	-1042.29	-9.39	-4.29	-12.98	1206.08	F	-13.17	-16.90	1171.29	F	-3.17	-12.65	1247.45	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:3:3:1:2	6	-1042.28	-9.06	-4.46	-12.86	1200.43	F	-13.52	-16.71	1140.21	F				
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:3:3:1:2	6	-1081.61	-8.90	-4.42	-12.57	1221.70	F	-13.30	-16.59	1193.28	F	-3.25	-12.82	1258.10	F
CCOCOCOCOCOCOCOCOCOCOC	2:1:3:3:3:2:2	6	-1042.30	-9.38	-4.11	-12.96	1147.80	F	-13.11	-16.93	1153.68	F	-3.06	-12.96	1182.56	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:3:3:2:2	6	-1081.60	-9.24	-4.40	-12.91	1204.05	F	-13.55	-16.72	1176.46	F	-3.24	-12.75	1291.73	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:3:3:2:2	6	-1120.91	-9.29	-4.65	-12.81	1262.56	F	-13.97	-16.58	1228.26	F	-3.70	-12.62	1265.70	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:1:1:1:3:2:2	6	-885.02	-9.46	-4.09	-13.57	968.72	F	-12.18	-17.73	981.25	F	-3.05	-13.19	1031.88	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:1:1:1:3:2:2	6	-924.34	-9.55	-4.22	-13.40	1015.31	F	-12.20	-17.28	1024.80	F	-3.13	-13.02	1052.87	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:2:1:1:3:2:2	6	-924.33	-9.21	-4.30	-13.36	1012.99	F	-12.69	-17.41	1030.10	F	-3.24	-13.07	1084.30	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:1:1:3:2:2	6	-963.65	-9.24	-4.22	-13.00	1096.36	F	-13.04	-17.18	1067.54	F	-3.21	-12.91	1098.86	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:1:1:3:2:2	6	-963.66	-8.99	-4.17	-13.01	1081.00	F	-12.74	-17.27	1099.69	F				
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:1:1:3:2:2	6	-1002.97	-9.07					-12.93	-17.00	1103.10	F	-3.23	-12.90	1141.53	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:1:2:1:3:2:2	6	-924.33	-9.44	-4.34	-13.30	1026.00	F	-12.57	-17.31	1032.80	F	-3.12	-13.11	1116.66	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:1:2:1:3:2:2	6	-963.65	-9.40	-4.18	-13.18	1105.27	F	-12.77	-17.09	1069.47	F	-3.22	-13.05	1123.36	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:2:2:1:3:2:2	6	-963.64	-9.25	-4.30	-13.21	1069.54	F	-12.89	-17.20	1082.62	F	-3.20	-12.97	1129.76	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:2:1:3:2:2	6	-1002.96	-9.08	-4.45	-13.07	1119.59	F	-13.23	-16.83	1127.84	F	-3.41	-12.92	1137.82	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:2:1:3:2:2	6	-1002.96	-9.20	-4.59	-12.92	1109.30	F	-13.27	-16.99	1113.24	F				
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:2:1:3:2:2	6	-1042.27	-9.41	-4.80	-12.91	1132.01	T	-13.65	-16.89	1147.63	F				
CCOCOCOCOCOCOCOCOCOCOC	2:2:1:3:2:3:2:2	6	-963.65	-9.38	-4.08	-13.03	1051.18	F	-12.58	-17.18	1001.86	F	-3.11	-12.91	1114.24	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:1:3:2:3:2:2	6	-1002.97	-9.36	-4.18	-12.95	1109.51	F	-12.82	-16.96	1117.89	F	-3.05	-12.95	1151.71	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:2:3:2:3:2:2	6	-1042.27	-9.02	-4.18	-12.87	1119.96	F	-13.19	-17.13	1116.75	F	-3.25	-12.78	1181.75	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:3:2:3:2:2	6	-1042.27	-9.11	-4.64	-12.87	1162.10	F	-13.71	-16.70	1144.42	F	-3.67	-12.87	1179.83	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:3:2:3:2:2	6	-1042.28	-9.28	-4.45	-12.98	1152.09	F	-13.39	-16.86	1156.52	F				
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:3:2:3:2:2	6	-1081.60	-9.40	-4.45	-12.75	1168.50	F	-13.46	-16.49	1188.85	F	-3.44	-12.60	1225.91	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:3:2:3:2:2	6	-1081.58	-8.73	-4.76	-12.62	1190.49	F	-13.86	-16.57	1183.66	F	-3.71	-12.53	1254.33	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:1:3:2:3:2:2	6	-1042.28	-9.19	-4.33	-12.77	1135.28	F	-13.18	-16.68	1133.04	F	-3.31	-12.86	1193.01	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:2:3:2:3:2:2	6	-1042.27	-8.85	-4.66	-12.85	1131.24	F	-13.80	-16.82	1140.93	F	-3.70	-12.73	1205.54	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:3:2:3:2:2	6	-1081.59	-9.14	-4.61	-12.36	1224.45	F	-13.70	-16.39	1169.50	F	-3.50	-12.58	1215.14	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:3:2:3:2:2	6	-1120.91	-8.99	-4.77	-12.76	1182.52	F	-14.05	-16.70	1175.69	F	-3.70	-12.74	1234.84	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:3:2:3:2:2	6	-1081.60	-9.23	-4.20	-12.57	1202.73	F	-13.98	-16.60	1209.71	F				
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:3:3:2:3:2:2	6	-1081.60	-9.16	-4.82	-12.30	1223.92	F	-14.36	-16.65	1209.30	F	-3.83	-12.50	1254.10	F
CCOCOCOCOCOCOCOCOCOCOC	2:2:3:3:3:2:3:2:2	6	-1120.90	-8.99	-4.81	-12.70	1235.33	F	-14.19	-16.52	1206.11	F	-3.79	-12.55	1277.49	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:3:3:2:3:2:2	6	-1160.22	-9.26	-4.97	-12.37	1310.39	F	-14.61	-16.44	1243.60	T				
CCOCOCOCOCOCOCOCOCOCOC	2:3:1:1:3:2:3:2:2	6	-963.65	-9.27	-4.22	-13.27	1078.12	F	-12.78	-17.33	1051.16	F	-3.14	-13.07	1100.68	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:1:3:2:3:2:2	6	-1002.96	-9.41	-4.77	-12.98	1088.21	T	-13.45	-17.17	1094.18	F	-3.59	-12.73	1165.67	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:3:1:3:2:3:2:2	6	-1042.29	-9.40	-4.50	-13.02	1136.35	F	-13.31	-16.92	1143.30	F	-3.43	-12.78	1188.95	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:1:3:2:3:2:2	6	-1002.97	-9.52	-4.24	-13.19	1099.92	F	-12.89	-17.07	1107.27	F	-3.26	-12.86	1125.84	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:2:1:3:2:3:2:2	6	-1042.28	-9.11	-4.49	-12.87	1129.29	F	-13.20	-16.80	1127.75	F	-3.43	-12.65	1203.82	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:2:2:2:1:3:2:3:2:2	6	-1081.60	-9.07	-4.41	-12.63	1166.85	F	-12.61	-15.16	1233.13	F	-3.62	-12.59	1224.48	F
CCOCOCOCOCOCOCOCOCOCOC	2:3:1:3:1:3:2:3:2:2	6	-1042.28	-9.												

CCOCOCOCOCOCOCOCOCOC	2:2:3:4:1:2	S	-927.75	-9.05	-4.15	-13.14	1114.37	F	-12.73	-17.10	1101.94	F	-2.87	-12.71	1122.49	F
CCOCOCOCOCOCOCOCOCOC	2:3:3:4:1:2	S	-967.07	-9.37	-4.14	-13.02	1126.22	F	-12.88	-16.96	1129.88	F	-3.03	-12.77	1224.98	F
CCOCOCOCOCOCOCOCOCOC	2:4:3:4:1:2	S	-1006.39	-9.07	-4.06	-12.81	1172.08	F	-12.86	-16.83	1183.84	F	-2.87	-12.97	1183.93	F
CCOCOCOCOCOCOCOCOCOC	2:1:4:4:1:2	S	-927.75	-9.43				F				F				
CCOCOCOCOCOCOCOCOCOC	2:2:4:4:1:2	S	-967.06	-9.33	-4.14	-13.06	1141.03	F	-12.97	-17.05	1168.72	F	-3.13	-12.93	1180.21	F
CCOCOCOCOCOCOCOCOCOC	2:3:4:4:1:2	S	-1006.38	-9.32	-3.94	-12.74	1175.54	F	-12.96	-16.80	1189.79	F				F
CCOCOCOCOCOCOCOCOCOC	2:4:4:4:1:2	S	-1045.69	-9.15	-4.20	-12.13	1279.20	F	-13.06	-16.71	1217.95	F	-3.27	-12.71	1284.14	F
CCOCOCOCOCOCOCOCOCOC	2:4:1:1:2:2	S	-849.12	-9.41	-3.83	-13.36	1010.07	F	-11.64	-17.44	1031.19	F	-2.85	-13.15	1049.31	F
CCOCOCOCOCOCOCOCOCOC	2:4:2:1:2:2	S	-888.42	-9.18	-4.22	-13.03	1048.91	F	-12.46	-17.24	1061.36	F	-1.13	-10.84	1332.47	F
CCOCOCOCOCOCOCOCOCOC	2:4:3:1:2:2	S	-927.74	-9.31	-4.26	-13.03	1088.62	F	-12.66	-17.22	1100.66	F	-3.14	-12.94	1134.42	F
CCOCOCOCOCOCOCOCOCOC	2:4:2:1:2:2	S	-888.42	-9.26	-4.10	-13.13	1091.58	F	-12.62	-17.40	1053.32	F	-3.13	-13.16	1106.12	F
CCOCOCOCOCOCOCOCOCOC	2:4:4:1:2:2	S	-927.74	-9.00	-4.17	-13.09	1064.32	F	-12.84	-17.28	1099.97	F				F
CCOCOCOCOCOCOCOCOCOC	2:4:4:1:2:2	S	967.06	9.12	-4.41	-13.10	1130.03	F	-12.82	-17.06	1132.21	F	-3.11	-12.81	1179.71	F
CCOCOCOCOCOCOCOCOCOC	2:4:1:2:2:2	S	-888.42	-9.37	-4.07	-13.17	1051.53	F	-12.26	-17.19	1073.66	F	-3.03	-12.84	1104.71	F
CCOCOCOCOCOCOCOCOCOC	2:4:1:3:2:2	S	-927.74	-9.22	-4.21	-13.01	1104.83	F	-12.53	-16.91	1119.61	F	-3.33	-12.93	1132.02	F
CCOCOCOCOCOCOCOCOCOC	2:3:1:4:2:2	S	-927.74	-9.15				F	-12.69	-17.12	1107.50	F	-3.16	-13.06	1141.76	F
CCOCOCOCOCOCOCOCOCOC	2:4:1:4:2:2	S	-967.06	-9.44	-4.03	-12.70	1135.83	F	-12.68	-17.02	1136.33	F	-3.07	-12.95	1161.03	F
CCOCOCOCOCOCOCOCOCOC	2:4:1:1:3:2	S	-888.43	-9.40	-4.05	-13.29	1045.63	F	-12.25	-17.44	1044.36	F	-1.38	-10.97	1311.35	F
CCOCOCOCOCOCOCOCOCOC	2:4:2:1:3:2	S	-927.73	-9.37	-3.76	-12.58	1089.83	F	-12.95	-17.19	1093.88	F	-3.45	-12.95	1134.99	F
CCOCOCOCOCOCOCOCOCOC	2:4:3:1:3:2	S	-967.06	-9.36	-4.50	-13.05	1139.00	F	-13.01	-16.95	1135.55	F	-3.38	-12.92	1170.69	F
CCOCOCOCOCOCOCOCOCOC	2:3:4:1:3:2	S	-967.06	-9.27	-4.15	-12.94	1140.30	F	-12.85	-17.01	1145.05	F	-3.05	-12.99	1165.65	F
CCOCOCOCOCOCOCOCOCOC	2:4:4:1:3:2	S	-1006.38	-9.42	-4.41	-13.01	1171.47	F	-13.02	-16.85	1186.07	F	-3.26	-12.83	1214.80	F
CCOCOCOCOCOCOCOCOCOC	2:4:1:2:3:2	S	-927.75	-9.21	-4.03	-13.09	1109.52	F	-12.53	-17.22	1100.66	F	-2.51	-11.83	1247.04	F
CCOCOCOCOCOCOCOCOCOC	2:4:1:3:3:2	S	-967.07	-9.30	-3.94	-12.98	1137.10	F	-12.79	-16.96	1123.93	F	-2.97	-12.96	1155.48	F
CCOCOCOCOCOCOCOCOCOC	2:4:1:4:3:2	S	-1006.38	-9.24	-4.15	-12.73	1189.69	F	-12.89	-16.87	1193.41	F				F
CCOCOCOCOCOCOCOCOCOC	2:4:1:1:4:2	S	-927.75	-9.42	-4.04	-13.19	1065.86	F	-12.39	-17.37	1079.74	F	-2.98	-13.07	1127.33	F
CCOCOCOCOCOCOCOCOCOC	2:4:2:1:4:2	S	-967.07	-8.90	-3.84	-13.02	1136.56	F	-12.59	-17.20	1120.63	F	-3.00	-12.79	1170.59	F
CCOCOCOCOCOCOCOCOCOC	2:4:3:1:4:2	S	-1006.38	-9.26	-3.88	-13.11	1164.67	F	-11.77	-14.72	1262.05	F	-3.03	-12.85	1215.18	F
CCOCOCOCOCOCOCOCOCOC	2:4:4:1:4:2	S	-1045.70	-9.15	-4.18	-12.89	1201.32	F	-12.94	-16.71	1211.49	F	-3.12	-12.69	1279.76	F