

Supporting Information

Mechanistic Studies on N-Heterocyclic Carbene-Catalyzed Umpolung of β,γ -Unsaturated α -Diketones

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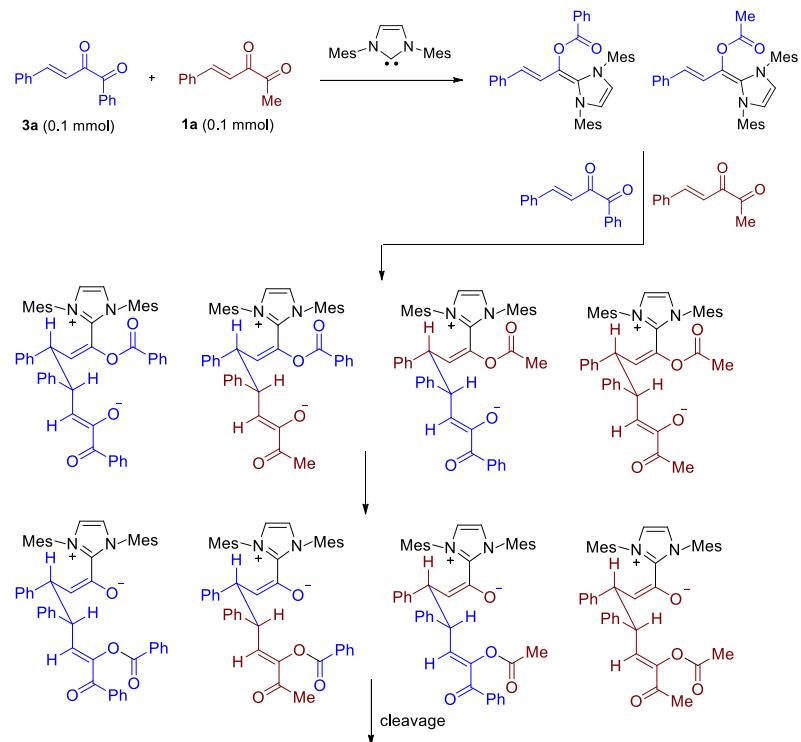
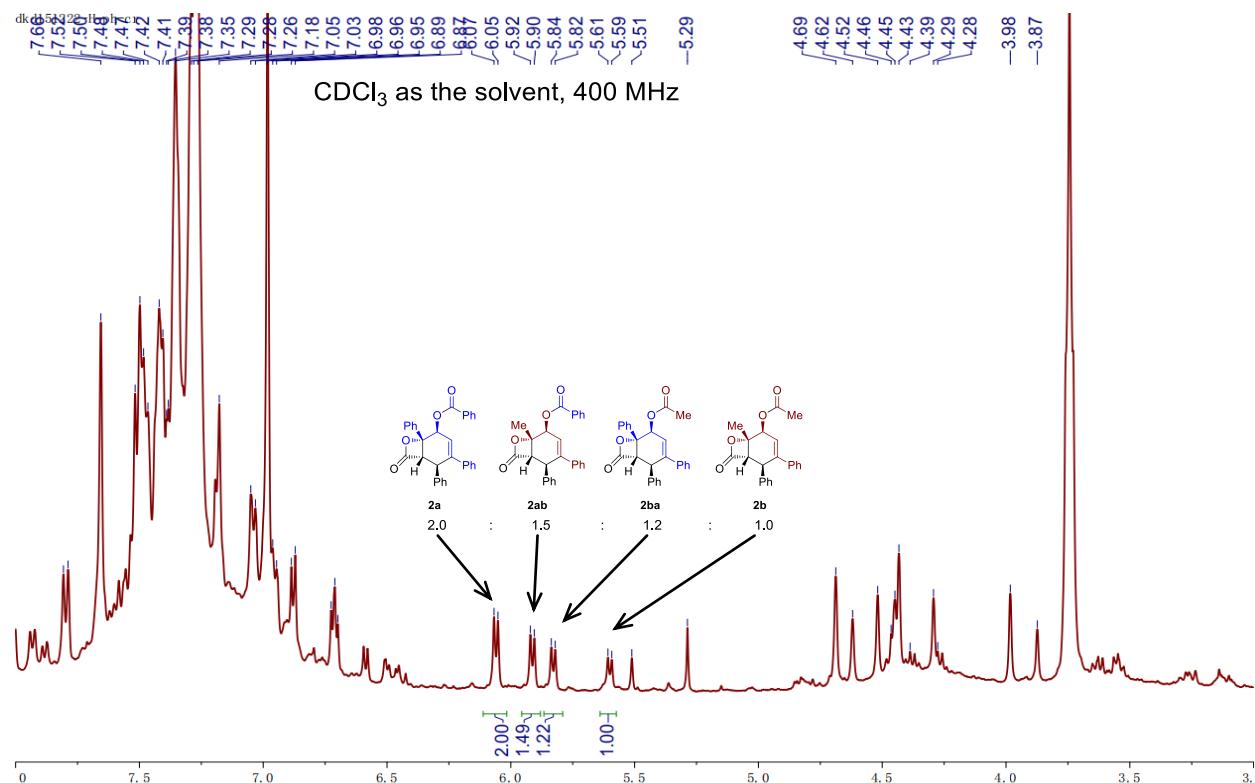
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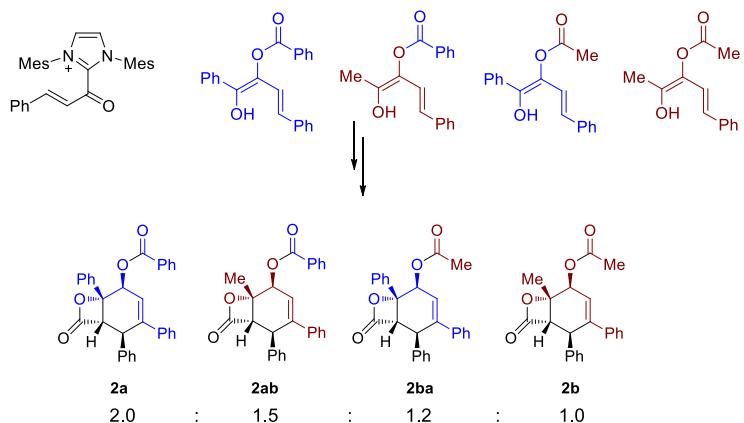
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I. Control experiments.

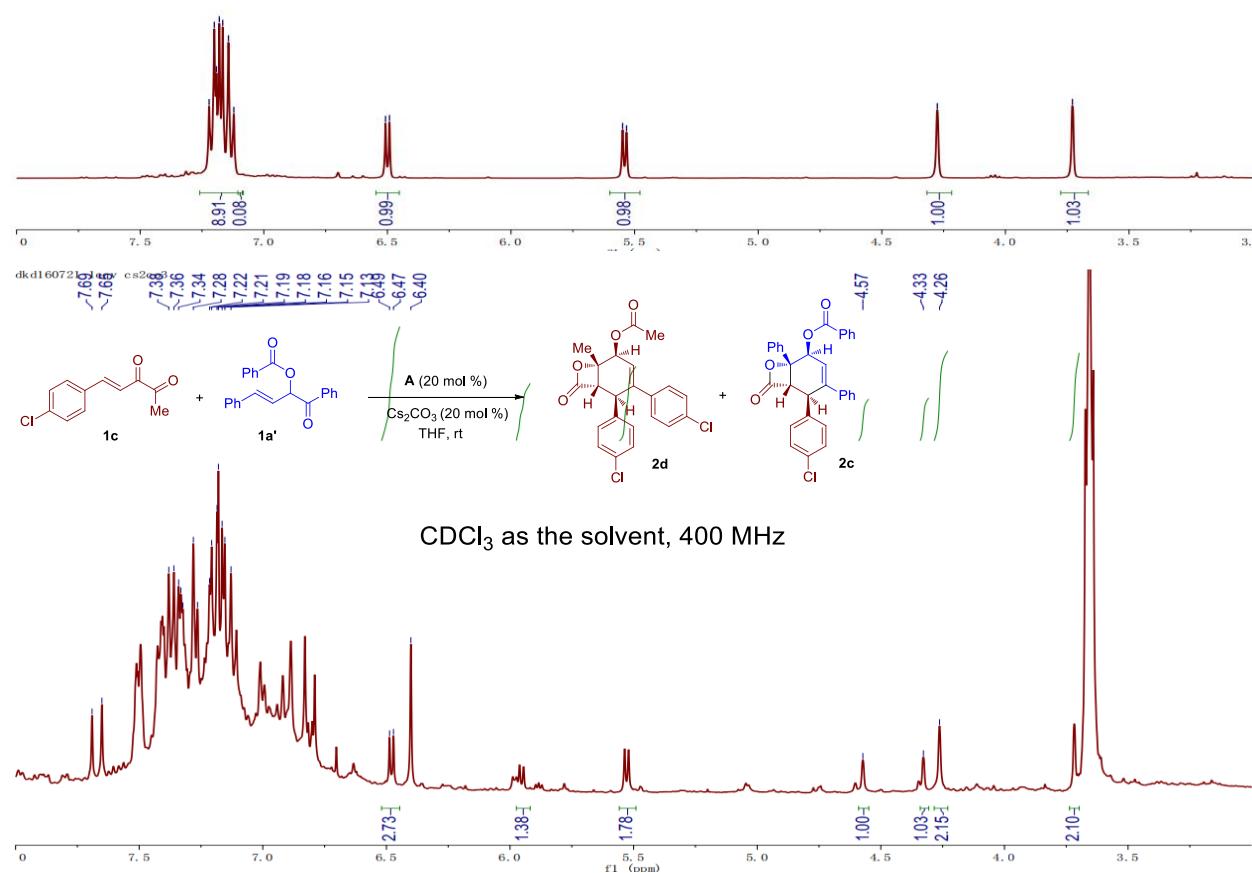
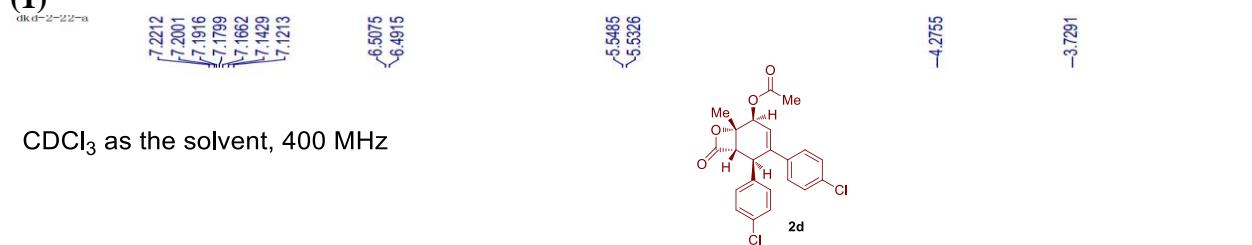
1. The ^1H NMR analysis and detailed description of eq 1 (Scheme 2):

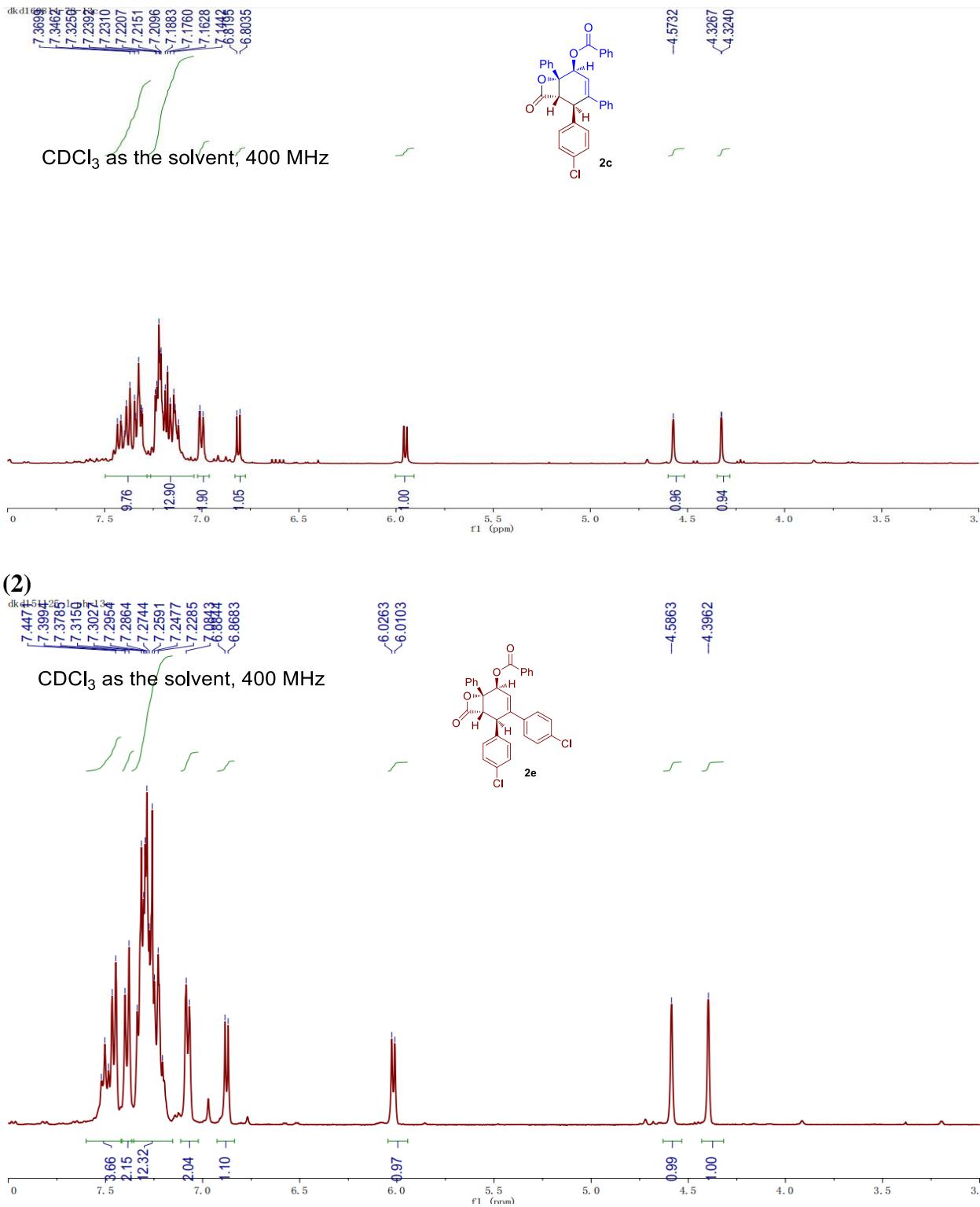


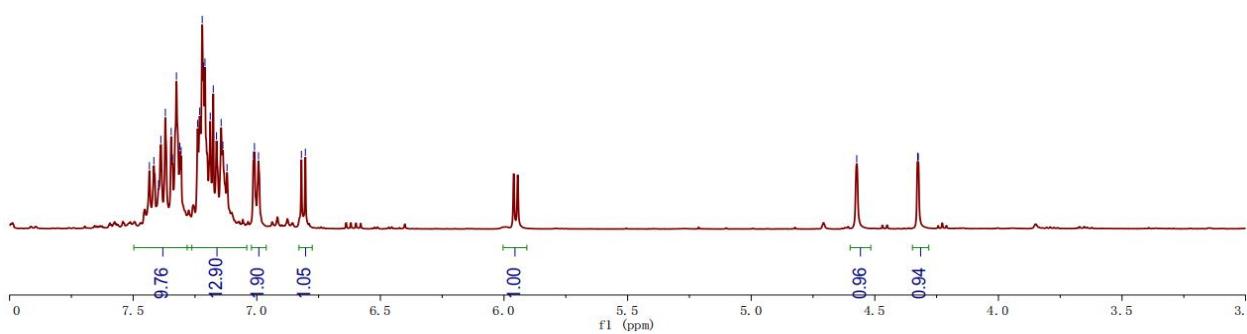
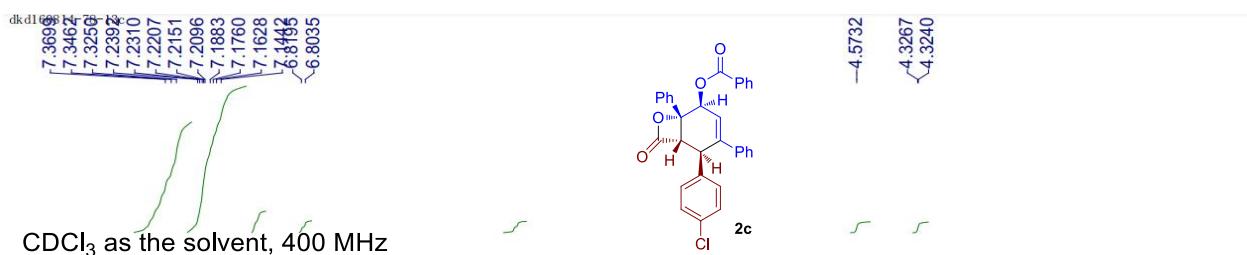
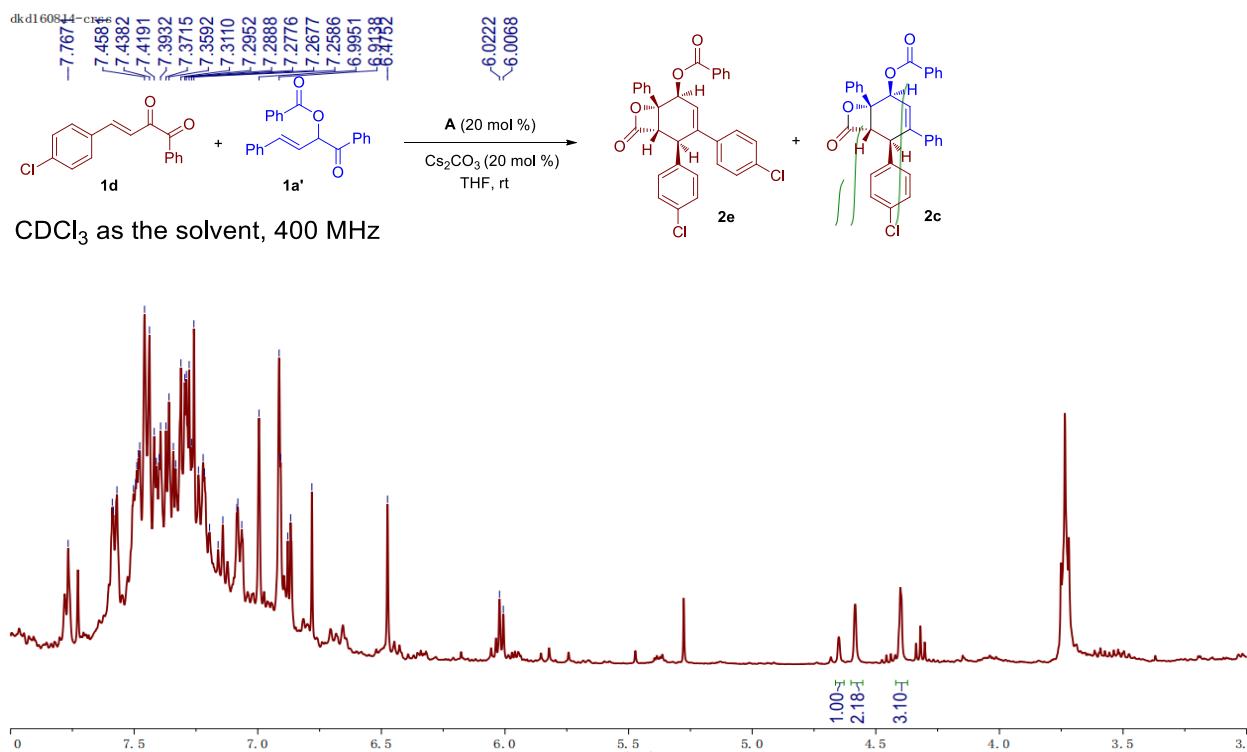


2. ^1H NMR analysis of eq 3 (Scheme 2):

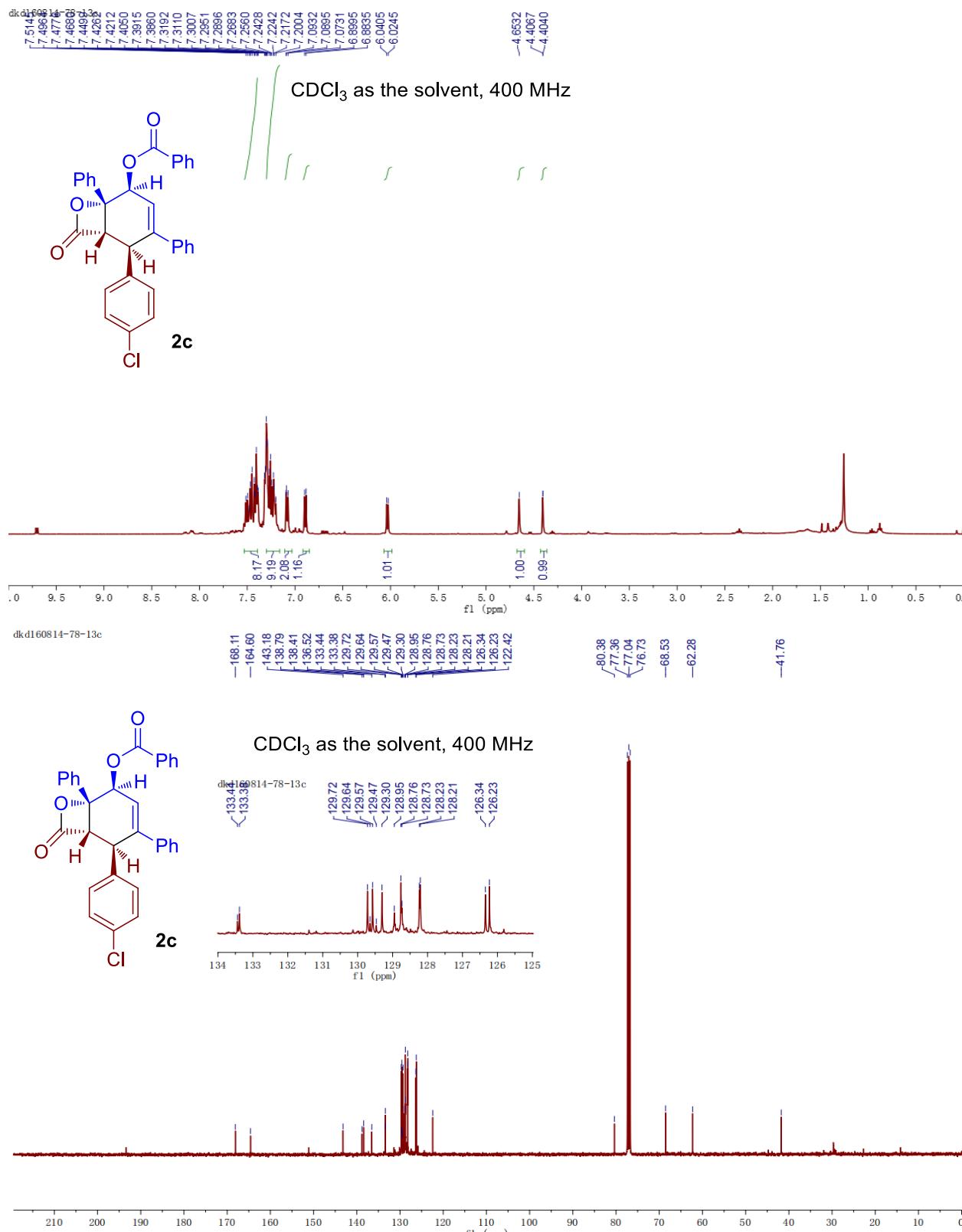
(1)







II. Characterization of 2c



III. Computational Details

All of the calculations were carried out at the DFT level of theory with the B3LYP hybrid functional.¹ To introduce the dispersion interaction, the functional was corrected with the empirical dispersion term (known as Grimme-D3),² as implemented in *Gaussian09* software package.³ The 6-311G(d,p) basis set⁴ was employed for the C, H, O, N, and Cl atoms. The transition states were located by means of the QST3 method⁵ and the Berny algorithm.⁶ All of the reactant, intermediate, transition state, and product structures were fully optimized without any symmetric restrictions. The solvent effect was introduced through IEF-PCM model⁷ with tetrahydrofuran (THF) as the solvent ($\epsilon = 7.4257$) for both optimization and single-point calculations.

Frequency calculations were made to ensure the structure obtained is a real minimum or a transition state. The transition states were identified with only one imaginary frequency (for TS2, there is another imaginary frequency at -5.11cm^{-1} , which is not easy to be eliminated and does not really affects the results). Intrinsic reaction coordinate (IRC) calculations⁸ were conducted to confirm that the transition state is connected to the correct reactant and product. All of the enthalpies and Gibbs energies shown in this article were calculated at 1 atm and 298.15K.

How to treat the entropy of solvated molecules has been raised as a question for a while.⁹ Unlike those in the gas phase, molecules in solution are closely surrounded by solvent molecules and therefore cannot freely have translational and rotational motions. Thereby, it is always a problem to calculate the exact contribution of translational and rotational motions to the entropy in solution. We have already noticed that, if the number of molecules changes during the reaction (like what can be seen from dissociation and addition reactions), the calculated entropy contribution to the Gibbs energy change is largely overestimated with the implicit solvation model. The overestimation even leads to the qualitatively incorrect conclusions, based on our test calculations of hydrogen bond energies. Many correction methods have been developed and employed in certain cases.¹⁰ In this article, we decided to use mainly the enthalpy to describe reaction pathways, with Gibbs energy shown in the parentheses as reference.¹¹

References

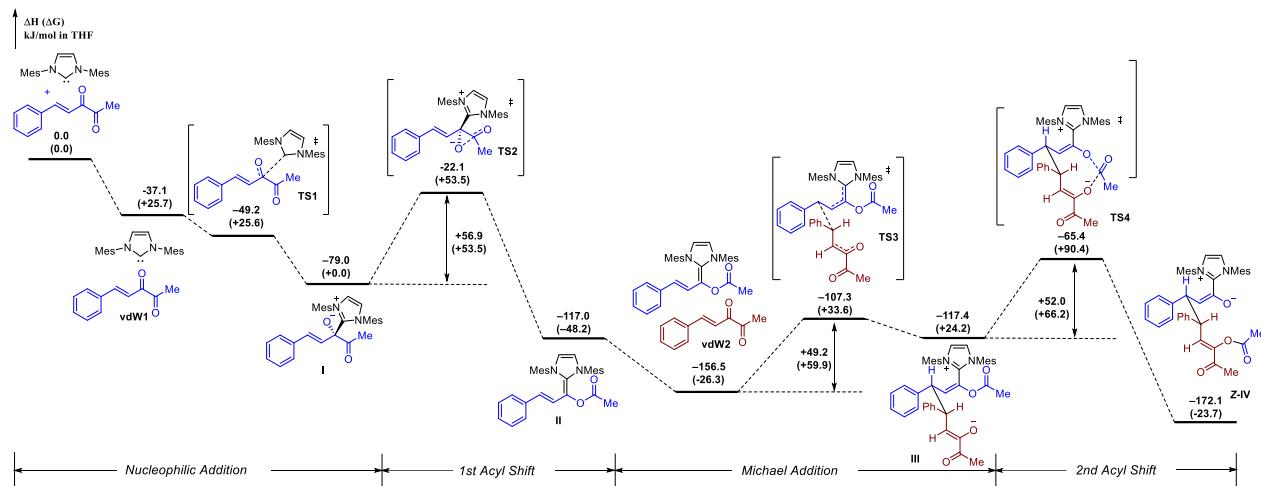
1. (a) Becke, A. D. Density-Functional Exchange-Energy Approximation with Correct Asymptotic Behavior. *Phys. Rev. A.* **1988**, 38, 3098. (b) Becke, A. D. A New Mixing of Hartree-Fock and Local Density-Functional Theories. *J. Chem. Phys.* **1993**, 98, 1372. (c) Lee, C.; Yang, W.; Parr, R. G. Development of the Colle-Salvetti Correlation-Energy Formula into a Functional of the Electron Density. *Phy. Rev. B.* **1988**, 37, 785.
2. Grimme, S.; Anthony, J.; Ehrlich, S.; Krieg, H. A Consistent and Accurate Ab Initio Parametrization of Density Functional Dispersion Correction (DFT-D) for the 94 Elements H-Pu. *J. Chem. Phys.* **2010**, 132, 154104.
3. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara,

- M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, M. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. *Gaussian 09, Revision D.01*; Gaussian, Inc.: Wallingford, CT, **2009**.
4. Krishnan, R.; Binkley, J. S.; Seeger, R.; Pople, J. A. Self-Consistent Molecular Orbital Methods. XX. A Basis Set for Correlated Wave Functions. *J. Chem. Phys.* **1980**, *72*, 650.
 5. (a) Peng, C.; Schlegel, H. B. Combining Synchronous Transit and Quasi-Newton Methods to Find Transition States. *Isr. J. Chem.* **1993**, *33*, 449. (b) Peng, C.; Ayala, P. Y.; Schlegel, H. B.; Frisch, M. J. Using Redundant Internal Coordinates to Optimize Equilibrium Geometries and Transition States. *J. Comput. Chem.* **1996**, *17*, 49.
 6. Schlegel, H. B. Optimization of Equilibrium Geometries and Transition Structures. *J. Comput. Chem.* **1982**, *3*, 214.
 7. (a) Mennucci, B.; Tomasi, J. Continuum Solvation Models: A New Approach to the Problem of Solute's Charge Distribution and Cavity Boundaries. *J. Chem. Phys.* **1997**, *106*, 5151. (b) Cossi, M.; Barone, V.; Mennucci, B.; Tomasi, J. Ab Initio Study of Ionic Solutions by a Polarizable Continuum Dielectric Model. *Chem. Phys. Lett.* **1998**, *286*, 253. (c) Cossi, M.; Scalmani, G.; Rega, N.; Barone, V. New Developments in the Polarizable Continuum Model for Quantum Mechanical and Classical Calculations on Molecules in Solution. *J. Chem. Phys.* **2002**, *117*, 43.
 8. Fukui, K. The Path of Chemical Reactions-the IRC Approach. *Acc. Chem. Res.* **1981**, *14*, 363.
 9. (a) Strajbl, M.; Sham, Y. Y.; Villa, J.; Chu, Z. . T.; Warshel, A. Calculations of Activation Entropies of Chemical Reactions in Solution. *J. Phys. Chem. B.* **2000**, *104*, 4578. (b) Mammen, M.; Shakhnovich, E. I.; Deutch, J. M.; Whitesides, G. M. Estimating the Entropic Cost of Self-Assembly of Multiparticle Hydrogen-Bonded Aggregates Based on the Cyanuric Acid Melamine Lattice. *J. Org. Chem.* **1998**, *63*, 3821. (c) Ribeiro, R. F.; Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Use of Solution-Phase Vibrational Frequencies in Continuum Models for the Free Energy of Solvation. *J. Phys. Chem. B* **2011**, *115*, 14556. (d) Su árez, E.; D áz, N.; Su árez, D. Entropy Calculations of Single Molecules by Combining the Rigid-Rotor and Harmonic-Oscillator Approximations with Conformational Entropy Estimations from Molecular Dynamics Simulations. *J. Chem. Theory Comput.* **2011**, *7*, 2638.
 10. (a) Sakaki, S.; Takayama, T.; Sumimoto, M.; Sugimoto, M. Theoretical Study of the Cp2Zr-Catalyzed Hydrosilylation of Ethylene. Reaction Mechanism Including New Sigma-Bond Activation. *J. Am. Chem. Soc.* **2004**, *126*, 3332. (b) Braga, A. A. C.; Ujaque, G.; Maseras, F. A DFT Study of the Full Catalytic Cycle of the Suzuki-Miyaura Cross-Coupling on a Model System. *Organometallics* **2006**, *25*, 3647. (c) Tanaka, R.; Yamashita, M.; Chung, L. W.; Morokuma, K.; Nozaki, K. Mechanistic Studies on the Reversible Hydrogenation of Carbon Dioxide Catalyzed by an Ir-PNP Complex. *Organometallics* **2011**, *30*, 6742. (d) Zhang, W.; Moore, J. S. Selective and Catalytic Arylation of N-Phenylpyrrolidine: (sp^3) C-H Bond Functionalization in the Absence of a Directing Group. *J. Am. Chem. Soc.* **2005**, *127*, 11863. (e) Ishikawa, A.; Nakao, Y.; Sato, H.; Sakaki, S. Oxygen Atom Transfer Reactions of Iridium and Osmium Complexes: Theoretical Study of Characteristic Features and Significantly

Large Differences Between These Two Complexes. *Inorg. Chem.* **2009**, *48*, 8154.

11. (a) Musaev, D. G.; Liebeskind, L. S. On the Mechanism of Palladium(0) Catalyzed, Copper(I) Carboxylate Mediated Thioorganic–Boronic Acid Desulfurative Coupling. A Noninnocent Role for the Carboxylate Ligand. *Organometallics* **2009**, *28*, 4639. (b) Jiang, J.; Ramozzi, R.; Moteki, S.; Usui, A.; Maruoka, K.; Morokuma, K. Mechanism of Metal-Free C–H Activation of Branched Aldehydes and Acylation of Alkenes Using Hypervalent Iodine Compound: A Theoretical Study. *J. Org. Chem.*, **2015**, *80*, 9264.

IV. Figures and Schemes



Scheme S1. Enthalpy profile from the start to the second acyl transfer (Gibbs free energy shown in parenthesis)

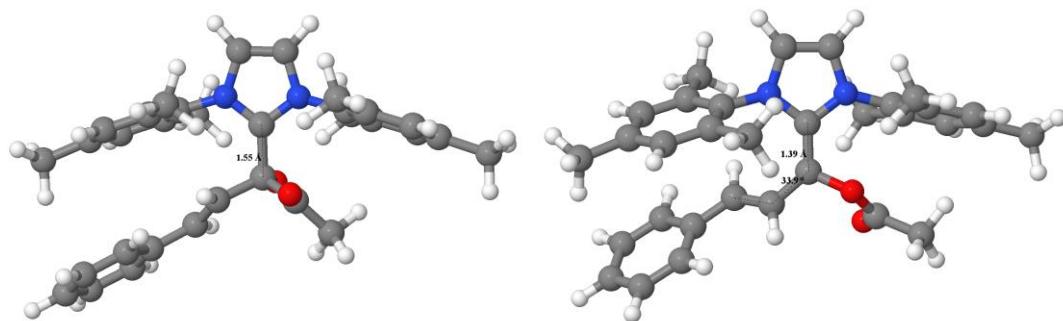
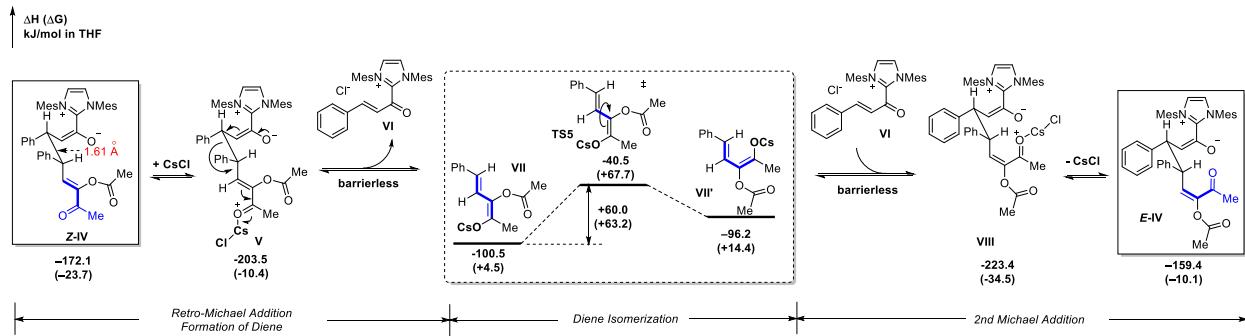


Figure S1. Optimized Structure of intermediates I and II



Scheme S2 Energy profile of the *cis-trans* isomerisation aided by Lewis acid.

Considering the CsCl in the system, we tried to use Cs^+ as Lewis acid to assist the formation of α,β -unsaturated acyl azolium intermediate. As shown in Scheme S2, **Z-IV** first complexes with CsCl to form **V**, and then undergoes barrierless C-C cleavage to form **VI** and **VII**. The free energy increase of the formation of azolium intermediate **VI** from **Z-IV** is 28.2 kJ/mol (6.7 kcal/mol), which is lower than the above case without assistance of Lewis/Brønsted acid(10.3 kcal/mol). The free energy barrier of the subsequent *cis-trans* isomerization of **VII** is 63.2 kJ/mol (15.1 kcal/mol, Scheme S4), which is also lower than the case without assistance of Lewis/Brønsted acid (19.7 kcal/mol, Scheme S4). Based on this, the interconversion between **Z-IV** and **E-IV** occurs with assistance of Lewis acid Cs^+ .

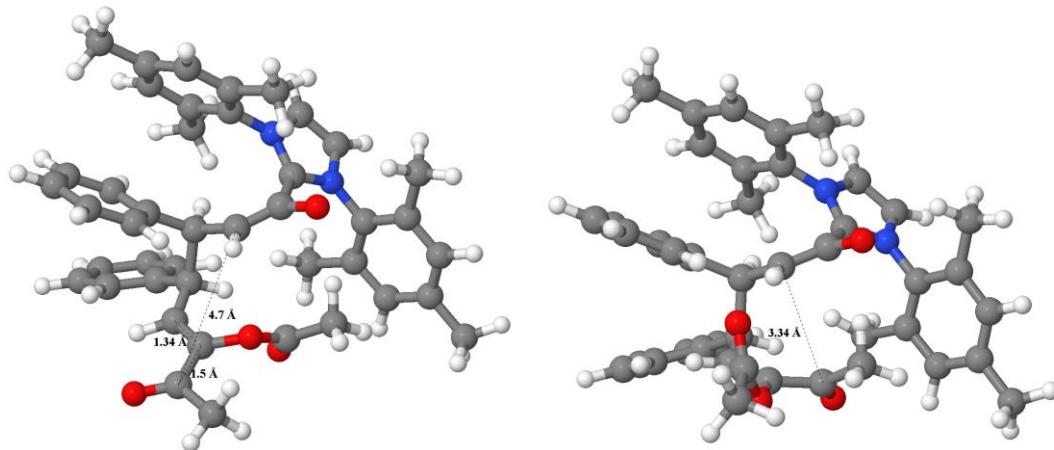
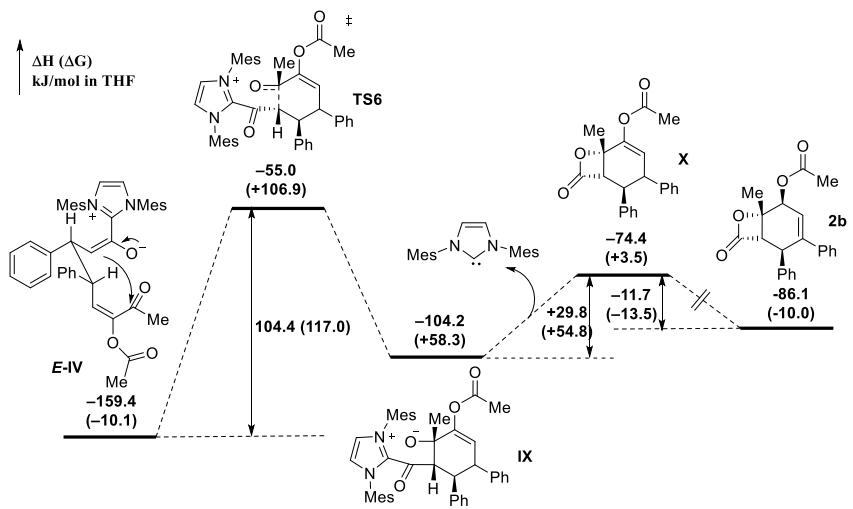


Figure S2. Optimized structure of Michael-type addition product **Z-IV** (with the C-C distance as 4.70 Å) and *cis-trans* isomerization product **E-IV** (with the new C-C distance as 3.34 Å to allow the following cyclization)



Scheme S3. Enthalpy (Gibbs free energy) profile from the aldol step to the final product.

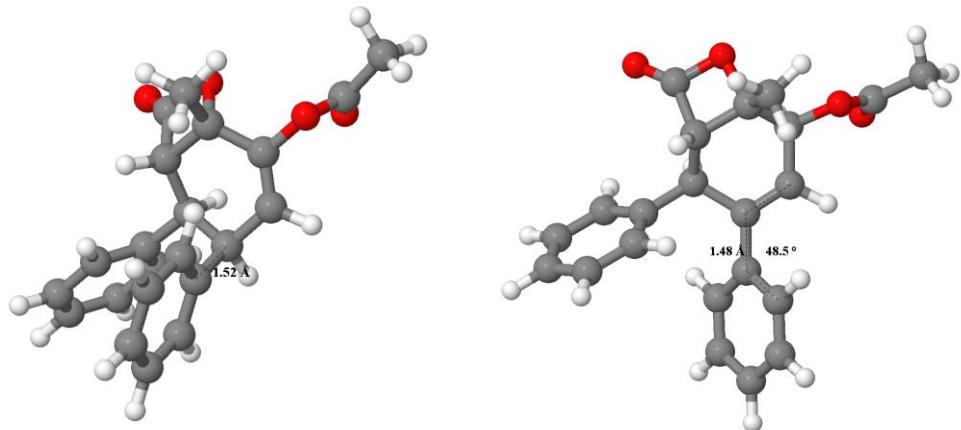


Figure S3 Optimized structures of products **X** and **2b**.

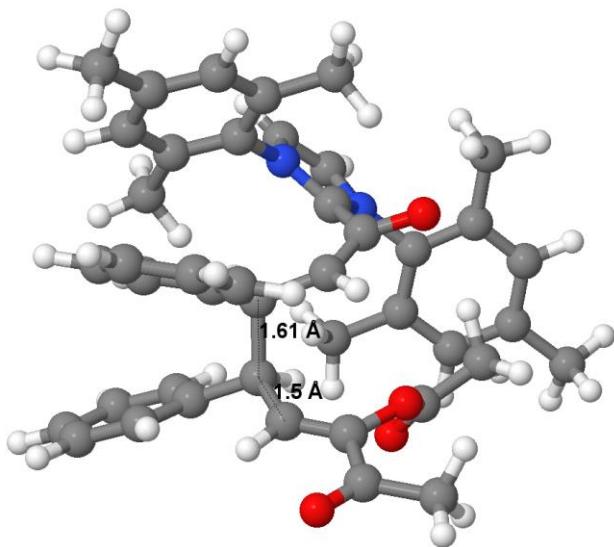


Figure S4. Optimized structure of intermediate **Z-IV**

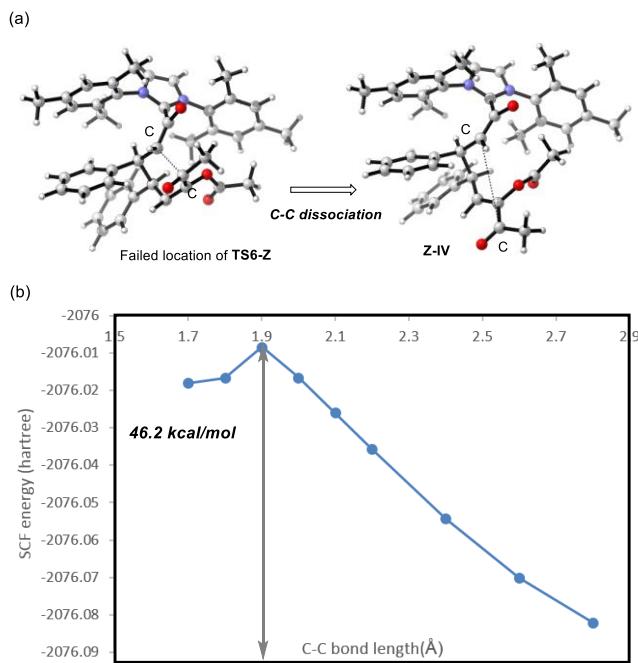
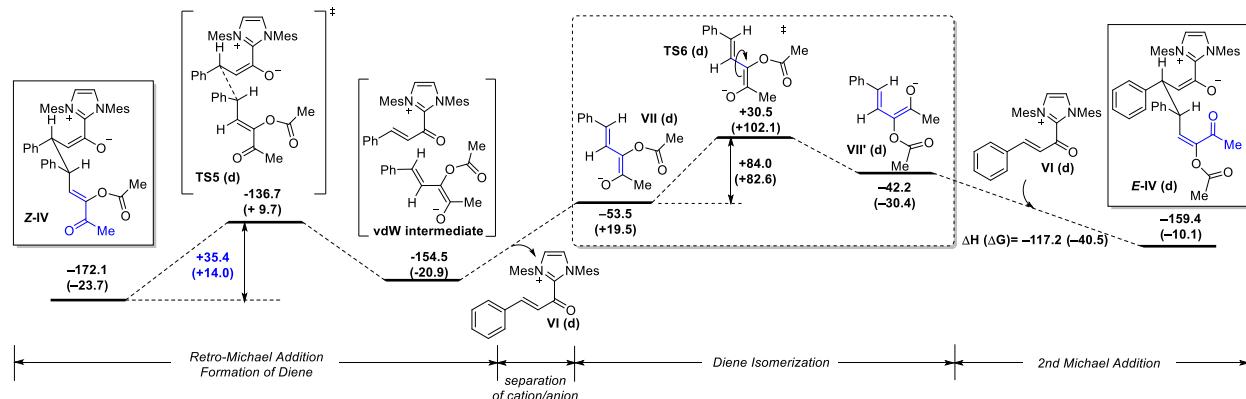


Figure S5 (a) The optimization of **TS6-Z**, (b) Energy scanning of stretching C-C bond

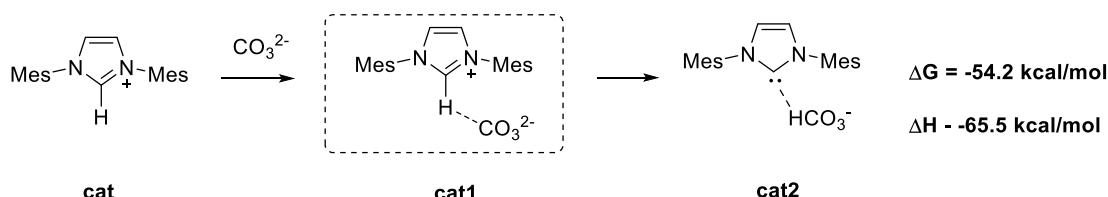
The energy demand with **Z-IV** for the intramolecular aldol-cyclization was investigated. As shown in Figure S5(a), during the optimization of the corresponding intramolecular aldol-cyclization transition state **TS6-Z**, the forming C-C bond gradually dissociates and the structure gradually turns back to **Z-IV**, indicating the high instability of **TS6-Z**. In order to estimate the

energy requirement, we scanned the process of gradual shortening of C-C bond and found that the highest energy point was reached at 1.9 Å (Figure S5(b)). The corresponding energy demand is 46.2 kcal/mol, which is higher than that for intramolecular aldol-cyclization with **E-IV**. Therefore, intramolecular aldol-cyclization with **Z-IV** is more favorable.



Scheme S4. Energy profile of the direct C-C cleavage pathway in which an enolate is involved

We investigated the formation of α,β -unsaturated acyl azonium intermediate, and **Z-IV** to **E-IV** conversion without any assistance of Lewis/Brønsted acid. As shown in Scheme S4, the free energy change of the formation of azonium intermediate **VI** is +43.2 kJ/mol (i.e. 10.3 kcal/mol).¹² It cannot happen spontaneously without the subsequent reactions. In this case, we wonder whether the cis-trans isomerization of the simultaneous formed enolate **VII(d)** can allow the following reaction. However, the free energy barrier of the isomerization **VII(d)→TS6(d)** is +82.6 kJ/mol (i.e. +19.7 kcal/mol). Therefore, for **Z-IV→TS6(d)**, the free energy requirement is as high as 30.0 kcal/mol.



Scheme S5. The reaction between cation **cat** and base CO_3^{2-}

The direct reaction mechanism from the catalyst cation to avoid the free carbene formation were investigated. As shown in Scheme S5, we tried to locate **cat1**, in which the hydrogen bond forms between the base CO_3^{2-} and the H of the cation. However, during optimization, H always

automatically transfers to CO_3^{2-} to deliver **cat2**. The process is extremely favourable with energy decrease of -54.2 (-65.5) kcal/mol. The strong base CO_3^{2-} used in the reaction system makes the formation of carbene inevitable.

References:

12. (a) Ruff, A.; Farkas, Ö. A DFT Study of Transition Structures and Reactivity in Solvolyses of tert-Butyl Chloride, Cumyl Chlorides, and Benzyl Chlorides. *J. Phys. Org. Chem.* **2008**, *21*, 53. (b) Martínez, A. G.; Vilar, E. T.; Barcina, J. O.; Cerero, S. M. Evidence for Different Types of Water Participation in the Solvolysis of 1-Adamantyl, tert-Butyl, and Methyl Chlorides from Density Functional Theory Computations. *J. Org. Chem.* **2005**, *70*, 10238. (c) da Silva, E. F.; Svendsen, H. F.; Merz, K. M. Explicitly Representing the Solvation Shell in Continuum Solvent Calculations. *J. Phys. Chem. A.* **2009**, *113*, 6404. (d) Thapa, B.; Schlegel, H. B. Density Functional Theory Calculation of $\text{p}K_{\text{a}}$'s of Thiols in Aqueous Solution Using Explicit Water Molecules and the Polarizable Continuum Model. *J. Phys. Chem. A.* **2016**, *120*, 5726. (e) Thapa, B.; Schlegel, H. B. Calculations of $\text{p}K_{\text{a}}$'s and Redox Potentials of Nucleobases with Explicit Waters and Polarizable Continuum Solvation. *J. Phys. Chem. A.* **2015**, *119*, 5134. (f) Baetzold, R. C. Silver-Water Clusters: A Theoretical Description of $\text{Ag}_n(\text{H}_2\text{O})_m$ for $n = 1-4$; $m = 1-4$. *J. Phys. Chem. C.* **2015**, *119*, 8299. (g) Gupta, M.; da Silva, E. F.; Svendsen, H. F. Explicit Solvation Shell Model and Continuum Solvation Models for Solvation Energy and $\text{p}K_{\text{a}}$ Determination of Amino Acids. *J. Chem. Theory Comput.* **2013**, *9*, 5021.

V. Enthalpy Corrections, Gibbs Free Energy Corrections, and Electronic Energies in Solvate of related compounds and Transition States

	Thermal Correction of Enthalpy (Hartree)	Thermal Correction of Gibbs Free Energies (Hartree)	Electronic Energy in solvent (Hartree)
NHC	0.419581	0.339136	-924.4519894
Substrate 1b	0.193172	0.139499	-575.7955537
vdW1	0.615329	0.505142	-1500.270059
I	0.615514	0.511504	-1500.28039
II	0.615785	0.507878	-1500.295117
vdW2	0.812065	0.673885	-2076.11544
III	0.813752	0.679822	-2076.095603
Z-IV	0.814176	0.682887	-2076.116867
V	0.820654	0.675992	-2556.380005
VII	0.246634	0.173995	-749.0667801
VII'	0.246461	0.175978	-749.0649718
VIII	0.8202	0.673979	-2556.389474
VI	0.569357	0.466519	-1807.266149
E-IV	0.814137	0.683159	-2076.111972
IX	0.815076	0.689132	-2076.091884
X	0.392214	0.314608	-1151.625388

2b	0.391917	0.313509	-1151.629442
TS1	0.614166	0.508562	-1500.267713
TS2	0.614479	0.509145	-1500.257677
TS3	0.811253	0.677109	-2076.089274
TS4	0.812162	0.683669	-2076.074195
TS5	0.245344	0.173944	-749.0426477
TS6	0.812725	0.686552	-2076.070786
CsCl	0.00426	-0.026131	-480.2464801
TS5(d)	0.811598	0.679547	-2076.100817
vdW intermediate	0.812981	0.676101	-2076.109009
VII(d)	0.243603	0.181815	-729.2152657
TS6(d)	0.242241	0.179878	-729.1818787
VII'(d)	0.24339	0.181435	-729.2107142
VI(d)	0.566747	0.468507	-1346.852613
	BSSE energy		
vdW1	0.005810008		
vdW2	0.006576217		
V	0.002468658		
VIII	0.004799638		

VI. Imaginary frequencies of Transition States

	Imaginary frequencies (cm ⁻¹)
TS1	-129.16
TS2	-204.13
TS3	-421.81
TS4	-300.66
TS5	-188.41
TS6	-240.40
TS5(d)	-230.21
TS6(d)	-217.44

VII. Full List of Coordinates for All Optimized Intermediates and TSs (including optimized geometries)

NHC

0 1

C 0.35567716 -0.77284757 -0.01011713
C 1.02911216 -0.77294157 2.19477287
C -0.32283284 -0.77292657 2.19320387
N -0.70705884 -0.77287757 0.85155587
H 1.73938516 -0.77298557 3.00395287
H -1.03499984 -0.77296057 3.00071787
N 1.41641816 -0.77288957 0.85399187
C 2.78742516 -0.77288257 0.42653487

C	3.43848216	0.45131843	0.23261787
C	3.43841816	-1.99707357	0.23236487
C	4.77674816	0.42763843	-0.16562913
C	4.77668916	-1.97337857	-0.16587713
C	5.46110516	-0.77286757	-0.37018813
H	5.29535016	1.36881643	-0.31971613
H	5.29523816	-2.91455557	-0.32015213
C	-2.07730784	-0.77285657	0.42165387
C	-2.72654784	0.45135043	0.22175287
C	-2.72664584	-1.99704557	0.22196787
C	-4.06242684	0.42767743	-0.18443913
C	-4.06252684	-1.97334257	-0.18422313
C	-4.74711284	-0.77282457	-0.38795613
H	-4.57778184	1.36880443	-0.34931713
H	-4.57795584	-2.91445757	-0.34893713
C	-1.99043184	1.75208043	0.42300687
H	-1.61874284	1.84338743	1.44767387
H	-1.11871084	1.80675743	-0.23447513
H	-2.63801984	2.60497443	0.21549987
C	-6.20155184	-0.77279457	-0.79338613
H	-6.85005384	-0.77258757	0.08944987
H	-6.45111884	0.11247043	-1.38259013
H	-6.45124384	-1.65822557	-1.38228113
C	-1.99062084	-3.29779757	0.42341487
H	-1.11882884	-3.35256857	-0.23396913

H	-1.61904684	-3.38905757	1.44812487
H	-2.63822584	-4.15067557	0.21589487
C	2.70397516	-3.29794157	0.43878687
H	2.33336916	-3.38655157	1.46409887
H	1.83169716	-3.35560257	-0.21767513
H	3.35223016	-4.15079657	0.23321387
C	2.70410016	1.75217643	0.43930987
H	1.83177116	1.80997643	-0.21707013
H	2.33358016	1.84063043	1.46466887
H	3.35236816	2.60504343	0.23383187
C	6.89779516	-0.77286057	-0.83474813
H	6.95057416	-0.77272257	-1.92881713
H	7.43132816	0.11251043	-0.48162713
H	7.43125616	-1.65836957	-0.48186013

Substrate 1b

0 1			
C	0.56087551	-0.77291381	0.00000000
C	1.74860051	0.22815019	0.00003500
C	3.12199551	-0.38291081	0.00002700
H	3.23989951	-1.02734981	0.87515700
H	3.23989251	-1.02735981	-0.87509300
H	3.87540651	0.40275819	0.00002600
C	-0.77844049	-0.18132981	-0.00000600
H	-0.83014149	0.89917719	-0.00004300

O	0.80449651	-1.97077581	-0.00008500
O	1.53985651	1.42230919	0.00008500
C	-1.87433249	-0.96782181	0.00002400
H	-1.70096949	-2.04213281	0.00005600
C	-3.26999949	-0.55110981	0.00001800
C	-4.26802249	-1.54221981	0.00006700
C	-3.66732149	0.80012719	-0.00003500
C	-5.61613049	-1.19965081	0.00006400
H	-3.97576249	-2.58671581	0.00010800
C	-5.01258249	1.14010619	-0.00003700
H	-2.92100849	1.58506919	-0.00007300
C	-5.99202549	0.14250819	0.00001200
H	-6.37135049	-1.97683881	0.00010300
H	-5.30369149	2.18406419	-0.00007800
H	-7.04150949	0.41336719	0.00001000

vdW1

0 1			
C	-0.27359781	-0.55403556	0.00000000
C	0.06990619	-2.05101256	1.71474700
C	-1.26167781	-2.01289856	1.48364700
N	-1.44597281	-1.09966656	0.44435200
H	0.65261219	-2.61614256	2.42206800
H	-2.07865781	-2.53821156	1.94807300
N	0.64663019	-1.16006856	0.80683400

C	2.05205919	-0.86391956	0.77659700
C	2.52691919	0.22876544	1.51415500
C	2.90384519	-1.67140856	0.01813300
C	3.89629319	0.49027844	1.48742800
C	4.27157219	-1.38433456	0.03615300
C	4.78602019	-0.31302656	0.76646400
H	4.27978919	1.34315244	2.03819700
H	4.94479619	-2.00512756	-0.54639600
C	-2.72791981	-0.69415256	-0.05738200
C	-3.49375581	0.20351144	0.69788700
C	-3.16502781	-1.18049656	-1.29588800
C	-4.72745081	0.60887344	0.18347900
C	-4.40191181	-0.74241056	-1.77322200
C	-5.19766981	0.14809744	-1.04806800
H	-5.32795781	1.31051544	0.75411000
H	-4.75080681	-1.10492956	-2.73515800
C	-2.98424581	0.74003344	2.01200700
H	-2.94782881	-0.04200456	2.77576400
H	-1.97008581	1.13117444	1.90215800
H	-3.62432681	1.54374044	2.37768000
C	-6.54548181	0.58099144	-1.57274100
H	-7.32352081	-0.13130856	-1.27761500
H	-6.83079981	1.55941844	-1.18001800
H	-6.54941781	0.63502044	-2.66380000
C	-2.31297781	-2.13639456	-2.09189600

H	-1.36753781	-1.66663556	-2.37402000
H	-2.05998381	-3.02197156	-1.50186200
H	-2.82907081	-2.45983556	-2.99691500
C	2.34837119	-2.79334356	-0.82006000
H	1.82653319	-3.53342356	-0.20680000
H	1.62111919	-2.40172456	-1.53613500
H	3.14127619	-3.30042456	-1.37133200
C	1.57740119	1.10355644	2.29114300
H	0.84240919	1.55862744	1.62367400
H	1.02007719	0.52309344	3.03212500
H	2.11450219	1.89947744	2.80880000
C	6.26468719	-0.01027456	0.78595100
H	6.81242419	-0.63927556	0.08187500
H	6.44967119	1.03565244	0.52646400
H	6.68346719	-0.17849856	1.78293900
C	3.13400919	1.61231144	-1.73481400
C	4.65462019	1.90535544	-1.64884100
C	5.53701219	1.02216644	-2.48665000
H	5.33601619	-0.02477356	-2.25458100
H	5.28981119	1.16068844	-3.54330200
H	6.58268019	1.26726544	-2.31003800
C	2.25303419	2.56531644	-1.06263100
H	2.73219919	3.39344344	-0.55739700
O	2.76919419	0.62710744	-2.36048200
O	5.07378319	2.80097544	-0.94515800

C	0.91639619	2.38457844	-1.07772100
H	0.54395219	1.48786444	-1.56139600
C	-0.09903481	3.23185144	-0.46365300
C	-1.44102881	2.81596744	-0.52544500
C	0.19853619	4.44228244	0.19079000
C	-2.45265881	3.58467944	0.04036000
H	-1.67592181	1.86776044	-0.99371700
C	-0.81244681	5.20627344	0.75822600
H	1.22385419	4.78680344	0.25226400
C	-2.14240881	4.78155244	0.68372300
H	-3.47834881	3.23946744	-0.01205000
H	-0.56837881	6.13645344	1.25863700
H	-2.92868981	5.38128344	1.12809700

TSI

0 1			
C	0.31463748	-0.07523940	0.00000000
C	-0.69104152	-0.70273740	-1.02227900
C	-1.73214752	-1.61011740	-0.42291700
H	-1.23309352	-2.52209240	-0.07760500
H	-2.18669052	-1.14815440	0.45156000
H	-2.48158452	-1.86023740	-1.17209000
C	1.70817548	-0.13305340	-0.55877500
H	1.80185648	0.05605760	-1.62038600
O	-0.56992752	-0.54479840	-2.22090300

C	2.74430748	-0.49402940	0.20519400
H	2.53561148	-0.66978640	1.25790900
C	4.13652048	-0.67759640	-0.21623600
C	5.09788248	-1.03003340	0.74472400
C	4.56302848	-0.52514540	-1.54739700
C	6.43118148	-1.23115140	0.39416200
H	4.79036848	-1.14696540	1.77875400
C	5.89163648	-0.72602240	-1.89906800
H	3.84988448	-0.24104440	-2.31123300
C	6.83417448	-1.08442040	-0.93152600
H	7.15344248	-1.50331040	1.15580400
H	6.19748848	-0.60175940	-2.93204500
H	7.87014348	-1.24095640	-1.20982500
C	-0.14865952	1.91855460	-0.47130500
C	-1.34075352	3.84519560	-0.31679500
C	-0.03163452	4.17959160	-0.30519200
N	0.68158448	2.98518660	-0.39671300
H	-2.23205652	4.44611960	-0.26728200
H	0.46199048	5.13368960	-0.24205800
N	-1.39256352	2.45554360	-0.41435400
C	-2.62772552	1.71573760	-0.41614500
C	-3.18793152	1.34773760	0.81334800
C	-3.23988452	1.42502460	-1.64074800
C	-4.39256152	0.64325960	0.78994300
C	-4.43982852	0.71207460	-1.61159700

C	-5.02644552	0.30975360	-0.40970000
H	-4.84094452	0.34160860	1.73110000
H	-4.92635052	0.46745660	-2.55026500
C	2.12033848	2.92909260	-0.37363500
C	2.76238648	2.80233960	0.86183200
C	2.81690248	2.99357060	-1.58282700
C	4.15565048	2.75854960	0.86334600
C	4.21125748	2.94281860	-1.53091600
C	4.89478148	2.82443460	-0.32004600
H	4.67605348	2.64524260	1.80895000
H	4.77298248	2.97901660	-2.45862600
C	1.96406948	2.63650460	2.12880900
H	1.24974548	3.45315960	2.26657300
H	1.38960248	1.70489660	2.08778200
H	2.61984748	2.60406360	2.99997500
C	6.39637348	2.69517860	-0.28994500
H	6.85682348	3.15066260	-1.16936300
H	6.82031048	3.16132460	0.60270800
H	6.67555948	1.63739160	-0.27825700
C	2.07857848	3.07760060	-2.89480600
H	1.41900048	2.21447060	-3.02507800
H	1.44614448	3.96874160	-2.94239600
H	2.77522648	3.10769360	-3.73332100
C	-2.61018052	1.85285860	-2.94021700
H	-2.43613552	2.93229660	-2.96115000

H	-1.64328652	1.36092160	-3.07067300
H	-3.24770052	1.59066660	-3.78536700
C	-2.48511352	1.66418760	2.10798400
H	-1.52490452	1.14109960	2.14006700
H	-2.28440752	2.73486260	2.20410800
H	-3.08643752	1.35036860	2.96230900
C	-6.30152052	-0.49746940	-0.40722700
H	-6.07622252	-1.56904840	-0.43248300
H	-6.89210652	-0.30845740	0.49186400
H	-6.91920952	-0.27195340	-1.27923000
O	0.09844248	-0.22336940	1.22418700

I

0 1			
C	-0.28727770	0.06155423	0.00080579
C	-1.14018070	0.98197223	0.96168779
C	-1.80790070	2.15683223	0.30707179
H	-1.14102870	2.60134823	-0.43269721
H	-2.68149170	1.79163223	-0.24114221
H	-2.11941270	2.87890923	1.06147879
C	1.12626930	0.34974623	0.54653579
H	1.28619730	0.16597923	1.60275479
O	-1.18365370	0.77099323	2.16028679
C	2.07070430	0.86778323	-0.24036021
H	1.79299930	1.01232423	-1.28146021

C	3.45162530	1.19488323	0.13192579
C	4.35167530	1.58855723	-0.87175021
C	3.93639930	1.10927423	1.44945279
C	5.68205830	1.88032223	-0.57808821
H	3.99925030	1.65748723	-1.89573821
C	5.26214530	1.40187923	1.74481579
H	3.27110530	0.80380623	2.24795279
C	6.14474830	1.78978623	0.73314879
H	6.35610030	2.17863323	-1.37359121
H	5.61260530	1.32627723	2.76844179
H	7.17895330	2.01583923	0.96675879
C	-0.68818670	-1.41357477	0.27529979
C	-1.93174970	-3.28610877	0.25129179
C	-0.63380070	-3.66120077	0.24188579
N	0.12388830	-2.49558677	0.26041379
H	-2.84074970	-3.86066477	0.24611879
H	-0.16887870	-4.63078277	0.22641879
N	-1.95559370	-1.89668377	0.27434079
C	-3.18602870	-1.13693477	0.27972679
C	-3.73586270	-0.73570277	-0.94477121
C	-3.82012470	-0.90407477	1.50752679
C	-4.92071470	0.00226023	-0.90362921
C	-5.00125270	-0.16180277	1.49185079
C	-5.55549670	0.31380123	0.30082779
H	-5.35818770	0.33658123	-1.83865521

H	-5.50004070	0.04622223	2.43263179
C	1.56821630	-2.49276477	0.26049879
C	2.23599930	-2.41704177	-0.96450721
C	2.23132830	-2.53452177	1.49039479
C	3.62810230	-2.35156777	-0.92914721
C	3.62446030	-2.46282477	1.47171179
C	4.33540530	-2.35271377	0.27517979
H	4.17120630	-2.26348977	-1.86437721
H	4.16269530	-2.46635277	2.41371679
C	1.46772230	-2.31683477	-2.25510421
H	0.79014230	-3.16638177	-2.38421721
H	0.85570230	-1.40714777	-2.24563021
H	2.14538930	-2.28689277	-3.10932621
C	5.83016830	-2.15987577	0.28482979
H	6.29019630	-2.62077277	1.16173279
H	6.29532430	-2.57749877	-0.61087721
H	6.05992230	-1.08966177	0.31274079
C	1.46254730	-2.60382377	2.78565279
H	0.76991430	-1.76216277	2.88066279
H	0.86218730	-3.51619877	2.84564579
H	2.13927930	-2.58561777	3.64029079
C	-3.25407170	-1.44328577	2.79479779
H	-3.23136070	-2.53720177	2.78608479
H	-2.23284370	-1.08914877	2.94365379
H	-3.85761570	-1.12350577	3.64485379

C	-3.06990470	-1.08420077	-2.24752521
H	-2.06251470	-0.65416977	-2.25259621
H	-2.97683870	-2.16910877	-2.36093721
H	-3.64445570	-0.70019677	-3.09163121
C	-6.80586770	1.15793323	0.31749179
H	-6.54951370	2.21800723	0.41740779
H	-7.37696670	1.04444323	-0.60639221
H	-7.45277070	0.89715423	1.15796779
O	-0.45353870	0.27137223	-1.30554221

TS2

0 1			
C	-0.27102200	-0.05204500	0.85616300
C	-0.55896400	-0.64643200	2.27088600
C	0.20639700	-0.03319200	3.42759000
H	0.60538000	0.95493400	3.20798900
H	-0.46934900	0.02973700	4.28409100
H	1.02918100	-0.70252500	3.69529100
C	0.87102600	0.83916900	0.53173600
H	1.76141000	0.35783500	0.15015000
O	-1.11974800	-1.76349200	2.41666700
C	0.83994300	2.16537800	0.72446400
H	-0.07732600	2.58854400	1.12463500
C	1.92611600	3.10975300	0.44218500
C	1.69840300	4.48411200	0.62640400

C	3.19582300	2.71090200	-0.01810700
C	2.69059000	5.42396500	0.35775600
H	0.72792300	4.81400000	0.98266900
C	4.18566800	3.64849800	-0.28577200
H	3.41429400	1.65917400	-0.16464800
C	3.94014700	5.01156200	-0.10077800
H	2.48721900	6.47847400	0.50812700
H	5.15617000	3.31664200	-0.63838600
H	4.71531600	5.73990600	-0.30974800
C	-0.63915300	-0.99447200	-0.23981500
C	-1.84107100	-2.17459100	-1.71318800
C	-0.58030300	-2.65972400	-1.73954000
N	0.15907600	-1.91915700	-0.82487300
H	-2.72216800	-2.44849900	-2.26511500
H	-0.12993100	-3.44999300	-2.31308200
N	-1.86528700	-1.14169200	-0.78218000
C	-3.03066500	-0.30253300	-0.59292500
C	-3.06571300	0.93590000	-1.23859900
C	-4.09622000	-0.79660200	0.16522900
C	-4.22344300	1.70329200	-1.09764700
C	-5.23050900	0.00837800	0.27390300
C	-5.31196500	1.25853800	-0.34511600
H	-4.27262000	2.67029600	-1.58767200
H	-6.06833500	-0.34856400	0.86433800
C	1.58143300	-2.08517200	-0.62907700

C	2.44688000	-1.38088100	-1.47926700
C	2.03685100	-2.95760500	0.36488800
C	3.81742200	-1.52259800	-1.26541600
C	3.42029900	-3.06154000	0.53684800
C	4.32093100	-2.34544100	-0.25302900
H	4.50607000	-0.97957100	-1.90418800
H	3.79933400	-3.72606200	1.30610300
C	1.91699900	-0.49100400	-2.57617300
H	1.29247000	-1.05235100	-3.27631400
H	1.29968300	0.31678300	-2.17307300
H	2.73627300	-0.04024800	-3.13624200
C	5.80708900	-2.44170000	-0.01223700
H	6.13920300	-1.63615400	0.65112400
H	6.07505200	-3.38865400	0.46041600
H	6.36843100	-2.34972700	-0.94470900
C	1.08036300	-3.77563500	1.19144700
H	0.34184500	-3.14921600	1.70062600
H	0.52361900	-4.47025500	0.55360300
H	1.62231400	-4.36254700	1.93419800
C	-3.99432100	-2.11929200	0.87680600
H	-3.87028700	-2.94759700	0.17218800
H	-3.11992000	-2.11617700	1.53561700
H	-4.89278600	-2.31064900	1.46535000
C	-1.88947600	1.44108900	-2.03521200
H	-1.05937300	1.70726500	-1.37411000

H	-1.51966700	0.68580900	-2.73441600
H	-2.16140200	2.32881600	-2.60726600
C	-6.53920700	2.12089900	-0.17575400
H	-7.44642900	1.51522300	-0.11500100
H	-6.47404700	2.70515800	0.74829100
H	-6.65062300	2.82511500	-1.00299200
O	-1.37844300	0.52413700	1.50328600

II

0 1

C	-0.28727770	1.04651161	0.00000000
C	-1.50550370	1.78371461	-0.00862500
H	-1.61177670	2.45155861	-0.86373800
C	-2.50049070	1.73286961	0.91426900
H	-2.31217170	1.19652161	1.83713500
C	-3.83665570	2.28788461	0.77772100
C	-4.68972970	2.32609061	1.90011800
C	-4.35977570	2.75691661	-0.44573300
C	-5.98651170	2.81911161	1.81168400
H	-4.32117570	1.95265461	2.85029100
C	-5.65326170	3.25899861	-0.53089600
H	-3.75665870	2.69624261	-1.34413000
C	-6.47988470	3.29365061	0.59472800
H	-6.61756170	2.83075361	2.69420700
H	-6.02811670	3.60893361	-1.48716600

H	-7.49267370	3.67320261	0.52159400
C	-0.03558170	-0.23745739	0.45800100
C	1.06291430	-2.14608639	1.05267600
C	-0.25115970	-2.41039339	1.11912300
N	-0.94660470	-1.25210439	0.74617100
H	1.92021730	-2.76051239	1.26325000
H	-0.77894170	-3.31289339	1.37038200
N	1.21534830	-0.81400439	0.64685000
C	2.48608530	-0.14894739	0.69011400
C	2.82523530	0.60818361	1.81792200
C	3.37028630	-0.32003739	-0.38287700
C	4.08888730	1.20389561	1.84912200
C	4.62822530	0.27741661	-0.29985600
C	5.00304630	1.04669861	0.80616200
H	4.36356130	1.80121861	2.71260500
H	5.32472730	0.15349461	-1.12319000
C	-2.34918670	-1.25478439	0.45668000
C	-3.25307470	-1.31101839	1.52826900
C	-2.78772670	-1.18441439	-0.87198200
C	-4.61601870	-1.24347839	1.24516900
C	-4.16224370	-1.10540439	-1.10379500
C	-5.08872470	-1.10956139	-0.06098300
H	-5.32363770	-1.25570039	2.06776300
H	-4.51490270	-1.02781739	-2.12764600
C	-2.76779070	-1.39634539	2.95396600

H	-2.39208470	-2.39646039	3.19133900
H	-1.94559570	-0.70007739	3.13731100
H	-3.57545270	-1.16905139	3.65103000
C	-6.55947970	-0.90939339	-0.32778800
H	-7.17640670	-1.46331739	0.38384400
H	-6.81316870	0.15173161	-0.22788100
H	-6.83207270	-1.22232939	-1.33809600
C	-1.81819770	-1.16230839	-2.02554800
H	-1.41815970	-0.15501339	-2.17347200
H	-0.96517570	-1.82092739	-1.84610800
H	-2.30953070	-1.47528739	-2.94833700
C	2.94148830	-1.08624239	-1.60724600
H	2.69033030	-2.12362339	-1.37008100
H	2.04494330	-0.62980339	-2.03646200
H	3.72750230	-1.08901939	-2.36357200
C	1.84154030	0.80126661	2.94236300
H	1.03536830	1.46510461	2.61786700
H	1.38908530	-0.14692439	3.24443000
H	2.32602830	1.24787461	3.81168000
C	6.34941530	1.72752661	0.84831600
H	6.30088230	2.70642861	0.35908200
H	6.68248230	1.89090061	1.87539900
H	7.11008430	1.14006961	0.32913700
O	0.79462230	1.62825961	-0.72603100
C	1.38300530	2.74812061	-0.22320800

C	2.48238130	3.21194161	-1.13872300
H	3.31244330	2.50515861	-1.06548100
H	2.14002930	3.22077861	-2.17432200
H	2.81751330	4.20178861	-0.83648300
O	1.06750530	3.27071961	0.81603600

vdW2

0 1

C	-1.02599179	-0.44459644	0.00000000
C	-2.08562979	0.37058056	-0.49067700
H	-1.78970779	0.89444856	-1.39660500
C	-3.34097779	0.61251456	-0.03391400
H	-3.70574579	0.10641656	0.84684300
C	-4.30477079	1.49911156	-0.67773000
C	-5.68282179	1.29998156	-0.44780500
C	-3.93453179	2.58823356	-1.49365500
C	-6.64168379	2.12815356	-1.02205900
H	-5.98925679	0.47574056	0.18672000
C	-4.89619779	3.41133656	-2.07005400
H	-2.88582379	2.82104356	-1.63374300
C	-6.25667879	3.18815356	-1.84454300
H	-7.69355079	1.94518056	-0.82783600
H	-4.58063079	4.24810156	-2.68457800
H	-7.00142779	3.83739656	-2.29074500
C	-0.94492379	-1.42826844	0.97884500

C	-0.04280179	-2.91701844	2.45249800
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N	-1.94179879	-2.21776244	1.53758600
H	0.74360921	-3.39735744	3.00720000
H	-1.97600879	-3.84851044	2.95180900
N	0.23791321	-1.87142544	1.56550300
C	1.46999521	-1.13445144	1.65920100
C	1.52142721	0.00353056	2.47477500
C	2.59032421	-1.60029644	0.96048700
C	2.73736421	0.68378356	2.56849700
C	3.78822121	-0.89923444	1.09938100
C	3.87848321	0.24840256	1.89259900
H	2.78672021	1.57914056	3.17947800
H	4.66494721	-1.24536344	0.56099800
C	-3.33523079	-2.26820244	1.21252700
C	-4.25405679	-1.86258344	2.19276800
C	-3.74714279	-2.71948644	-0.04810000
C	-5.61211079	-1.89868844	1.87489400
C	-5.11615879	-2.72691844	-0.32165700
C	-6.06112279	-2.31580444	0.62002200
H	-6.33061279	-1.56441044	2.61605900
H	-5.45103579	-3.06078444	-1.29866700
C	-3.78865079	-1.33211344	3.52501900
H	-3.35477479	-2.11863744	4.14868400
H	-3.01860679	-0.56845344	3.39155800

H	-4.61564179	-0.88186444	4.07101600
C	-7.52831179	-2.27944644	0.26901500
H	-8.15501579	-2.27853944	1.16306500
H	-7.76190479	-1.37446144	-0.30238300
H	-7.81156479	-3.13463444	-0.34927000
C	-2.75162679	-3.16728044	-1.08530600
H	-2.26248179	-2.30345044	-1.54428400
H	-1.96427679	-3.78178344	-0.64165200
H	-3.24252879	-3.74403644	-1.87039600
C	2.47646821	-2.79409744	0.04883900
H	2.18786121	-3.69583844	0.59607300
H	1.70363721	-2.61483044	-0.70377000
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C	0.29426221	0.49849056	3.19314200
H	-0.44454279	0.84964756	2.47049700
H	-0.16996479	-0.29592544	3.78505100
H	0.53661221	1.33443056	3.84875000
C	5.17000521	1.02519656	1.97849100
H	5.22609821	1.76928956	1.17637400
H	5.25121121	1.56099656	2.92662900
H	6.03808021	0.36981356	1.87770900
O	0.21327621	-0.26817844	-0.69832400
C	0.86554121	0.91273156	-0.57761400
C	2.10254821	0.95351556	-1.43240800
H	2.27997421	0.00712756	-1.93852400

H	1.99213221	1.75357656	-2.16786600
H	2.95085121	1.19560156	-0.79136900
O	0.49137021	1.81954956	0.12567500
C	-0.66592779	3.84857756	1.84097200
C	-0.39054479	4.41421656	0.42375400
C	1.00980921	4.89853756	0.17299000
H	1.26389721	5.68683756	0.88632000
H	1.70125421	4.07161156	0.33982400
H	1.09149021	5.26830656	-0.84807400
C	-2.01024779	3.30816156	2.07061900
H	-2.66279179	3.24456556	1.21070300
O	0.21675721	3.91173356	2.68384800
O	-1.28469579	4.47654156	-0.39298300
C	-2.38596979	2.92693256	3.30694300
H	-1.64471379	3.03177256	4.09623100
C	-3.67991679	2.39609756	3.71847200
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C	-5.09978679	1.55905756	5.50938000
H	-3.06322279	2.19037856	5.77290400
C	-5.96267279	1.70859056	3.25888700
H	-4.62627579	2.46386956	1.77540500
C	-6.14682579	1.38311856	4.60532000
H	-5.23476179	1.30574356	6.55455800
H	-6.76874279	1.56853756	2.54820100

H -7.09918979 0.99218956 4.94494100

TS3

0 1

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C 0.32941133 -0.70271974 -0.07226900
H 0.38660033 -1.52744574 -0.77191500
C 1.45017733 -0.54744874 0.81161200
C 2.83140733 -0.57989674 0.28323500
C 3.86934433 -0.02258774 1.04545000
C 3.16925933 -1.21435374 -0.92290100
C 5.19255033 -0.08751974 0.62062700
H 3.63096633 0.46668026 1.98111600
C 4.49312233 -1.27792474 -1.35092900
H 2.39694233 -1.65667474 -1.53813400
C 5.51245333 -0.71539874 -0.58346500
H 5.97386833 0.35578126 1.22844200
H 4.72859233 -1.77138274 -2.28755900
H 6.54206633 -0.76425274 -0.91975500
C -1.34864767 1.08003126 0.58361500
C -2.65957867 2.73056526 1.37794100
C -1.41624767 3.23527526 1.23831700
N -0.60900267 2.22289226 0.73447400
H -3.57463467 3.17674726 1.72421500
H -1.02371467 4.21882426 1.42228500

N	-2.61900967	1.40385526	0.97143700
C	-3.79411467	0.56377726	1.01865000
C	-4.07446967	-0.12262674	2.20281400
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C	-5.23350267	-0.89853174	2.23897800
C	-5.76835867	-0.28325374	-0.02203200
C	-6.08468467	-0.99817774	1.13725500
H	-5.46489067	-1.44946674	3.14426800
H	-6.42544267	-0.34681974	-0.88317000
C	0.73645333	2.48579726	0.28433300
C	1.71128033	2.77362326	1.24950700
C	1.00388033	2.52172526	-1.09024100
C	2.99478133	3.07834626	0.80070900
C	2.31238633	2.80941026	-1.48208500
C	3.32010233	3.07964626	-0.55640700
H	3.76770033	3.28724626	1.53248600
H	2.54535233	2.82606626	-2.54166100
C	1.40438933	2.73443726	2.72713900
H	0.87650833	3.63606926	3.05260900
H	0.77494933	1.88115426	2.99083800
H	2.32535933	2.66248626	3.30651700
C	4.74077433	3.30748026	-1.00321400
H	5.26278133	4.00264326	-0.34180500
H	5.28667833	2.35830926	-0.98263900
H	4.78523133	3.69751226	-2.02212900

C	-0.06030767	2.26312526	-2.12640900
H	-0.20650067	1.18990926	-2.27542800
H	-1.02482667	2.68445926	-1.83362800
H	0.22557533	2.70081826	-3.08350300
C	-4.27994267	1.26243226	-1.36502400
H	-4.09465867	2.32150026	-1.16672400
H	-3.37089267	0.84884126	-1.80929600
H	-5.08544667	1.18806926	-2.09603300
C	-3.12556067	-0.07047774	3.36975300
H	-2.18690767	-0.55382974	3.08950500
H	-2.89980067	0.95658026	3.66859200
H	-3.53590067	-0.59722874	4.23137900
C	-7.30248667	-1.88778974	1.18146500
H	-7.68306267	-1.99406074	2.19933900
H	-8.10493467	-1.49794574	0.55142000
H	-7.05568467	-2.89039674	0.81637200
O	-1.92152867	-0.86449974	-0.69639500
C	-2.39841867	-2.00025074	-0.06426500
C	-3.08354367	-2.89996374	-1.04255200
H	-3.54385167	-2.33613274	-1.85281100
H	-2.30294167	-3.54930374	-1.44905700
H	-3.82117067	-3.50893974	-0.52320200
O	-2.25381967	-2.19921674	1.10938400
C	1.17101733	-3.97279474	0.09800400
C	1.95606233	-5.12660074	-0.54345600

C	1.26112633	-5.81738674	-1.69716600
H	0.29909233	-6.21543374	-1.36477400
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H	1.89351433	-6.61579074	-2.08478700
C	1.81235533	-3.31361074	1.14502500
H	2.82555433	-3.61723574	1.36613000
O	0.02947533	-3.71415174	-0.39532100
O	3.06380433	-5.47637074	-0.16968000
C	1.22143433	-2.19936774	1.83567000
C	1.75780233	-1.77265774	3.15896000
C	0.90472833	-1.12825174	4.06938500
C	3.10357933	-1.93251874	3.51938200
C	1.37363833	-0.65841974	5.29222300
H	-0.13990067	-0.99900174	3.80831400
C	3.57636533	-1.46259374	4.74310000
H	3.78907833	-2.41468474	2.83510700
C	2.71690633	-0.82162374	5.63454100
H	0.69203933	-0.16857074	5.97913300
H	4.62161133	-1.59693174	4.99957400
H	3.08729233	-0.45802174	6.58644900
H	0.13493133	-2.21471474	1.82099500
H	1.31695033	0.19599626	1.58768800

Intermediate III

0 1

C	-0.06839945	0.19835841	0.00000000
C	-1.18942945	0.92131841	-0.01185400
H	-1.21344645	1.76598441	-0.70554600
C	-2.35235645	0.89242841	0.92370900
C	-3.67747445	0.65624441	0.22085300
C	-4.70190645	-0.01837959	0.89023000
C	-3.93788245	1.15612941	-1.06156000
C	-5.94949945	-0.20465759	0.29878600
H	-4.52556945	-0.39409459	1.88930000
C	-5.17979345	0.95860141	-1.66140900
H	-3.18082245	1.73462741	-1.57694400
C	-6.19160545	0.27634541	-0.98602100
H	-6.72643645	-0.73397459	0.83953200
H	-5.36119045	1.35265041	-2.65557900
H	-7.15916045	0.12812841	-1.45294100
C	0.30012255	-0.94620859	0.82764700
C	1.53722355	-2.35736059	2.04764600
C	0.32727655	-2.93205459	1.85743900
N	-0.43150645	-2.05560659	1.09467600
H	2.41040255	-2.69368359	2.57756600
H	-0.06507245	-3.88189659	2.17208200
N	1.51402155	-1.13405959	1.40097500
C	2.64577655	-0.23250359	1.37694600
C	2.67826755	0.83441941	2.27683400
C	3.67062655	-0.48661859	0.45644900

C	3.79946455	1.66469441	2.24789000
C	4.76428555	0.37732441	0.46319500
C	4.84635355	1.45536941	1.35026100
H	3.84325455	2.50432141	2.93292400
H	5.56793555	0.20790241	-0.24550300
C	-1.73255545	-2.41887459	0.57760300
C	-2.76346645	-2.65293859	1.49656900
C	-1.88172645	-2.63086359	-0.80057600
C	-3.98253845	-3.10344459	0.99230800
C	-3.13418145	-3.04944759	-1.24911900
C	-4.19344545	-3.29018759	-0.37334000
H	-4.79917445	-3.27695859	1.68468100
H	-3.27858645	-3.20566459	-2.31282500
C	-2.59719045	-2.41720759	2.97904200
H	-2.13212745	-3.27561359	3.47299700
H	-1.97702945	-1.54440859	3.19342100
H	-3.56863845	-2.25709759	3.44793800
C	-5.54929045	-3.68817259	-0.89496200
H	-6.09892545	-4.28805459	-0.16657200
H	-6.14095545	-2.78987059	-1.09941800
H	-5.47173845	-4.25510859	-1.82501900
C	-0.75009145	-2.44477959	-1.78037300
H	-0.62258745	-1.39253159	-2.04560600
H	0.20184755	-2.79773059	-1.37530500
H	-0.95053445	-2.99830459	-2.69806000

C	3.56932255	-1.61807859	-0.53371800
H	3.51080555	-2.58985359	-0.03634700
H	2.66867055	-1.50912759	-1.14448300
H	4.43435655	-1.63067959	-1.19683500
C	1.51643855	1.12751741	3.18495700
H	0.73259455	1.62356141	2.60564400
H	1.09054655	0.22031441	3.61980200
H	1.80912055	1.79487441	3.99566500
C	6.02191955	2.39905741	1.30392400
H	5.82466155	3.21620441	0.60214600
H	6.21355455	2.84583741	2.28149800
H	6.92945355	1.89110541	0.97107100
O	0.94980555	0.48658341	-0.93341500
C	1.59321555	1.71065041	-0.85637400
C	2.51440755	1.86790441	-2.02970800
H	3.08880955	0.95584941	-2.19083300
H	1.91333855	2.05222341	-2.92389300
H	3.17759655	2.71188241	-1.85553500
O	1.40851055	2.49829341	0.02544900
C	-2.60272845	4.00125041	-0.16272700
C	-3.38775745	5.24776841	-0.58191700
C	-3.09713445	5.74453241	-1.98544800
H	-2.02044445	5.83287841	-2.13813500
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C	-2.96166045	3.47529841	1.05407000
H	-3.73550345	4.00707141	1.58987600
O	-1.73905045	3.57287941	-1.01826000
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C	-2.34597245	2.28761341	1.74517700
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H	-4.99538745	2.40149441	2.50064300
C	-4.10363145	1.31359541	5.59241700
H	-2.07907245	0.92085641	6.21470100
H	-5.98847945	1.80568941	4.67622600
H	-4.54037945	1.04995741	6.54925400
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H	-2.21300945	0.10826741	1.66839800

TS4

0 1			
C	-0.36932539	0.30779753	-0.00483473
C	-1.57504839	0.88883153	-0.19584073
H	-1.57429139	1.54850653	-1.04964073
C	-2.63186739	1.15833953	0.81121927

C	-4.03364839	1.32111553	0.26444327
C	-5.12290439	0.89779153	1.03317627
C	-4.29245239	1.92722153	-0.97054673
C	-6.43055039	1.05211553	0.58050927
H	-4.94248039	0.44673553	2.00097227
C	-5.59976739	2.08799753	-1.42704773
H	-3.47452939	2.28566453	-1.58204373
C	-6.67466439	1.64695553	-0.65635973
H	-7.25645339	0.70981153	1.19422327
H	-5.77731739	2.55925953	-2.38744473
H	-7.69080839	1.76847853	-1.01461273
C	-0.08762139	-0.81697547	0.87964227
C	1.01321761	-2.36183947	2.07784327
C	-0.25021839	-2.81076247	1.90646727
N	-0.92430539	-1.85991847	1.15695527
H	1.85737961	-2.78951347	2.58858227
H	-0.73246439	-3.71627347	2.22736927
N	1.10985661	-1.13674047	1.43757827
C	2.36081561	-0.40491147	1.43063027
C	2.64415461	0.43696753	2.50751627
C	3.27246761	-0.66237447	0.40239427
C	3.89655361	1.05229953	2.52777827
C	4.51088561	-0.02439647	0.46955027
C	4.83769361	0.83820953	1.51974627
H	4.13572561	1.72096653	3.34786727

H	5.23401361	-0.20200347	-0.31990673
C	-2.26679039	-2.07844747	0.66944727
C	-3.31683739	-2.08544347	1.59687927
C	-2.46151439	-2.33953047	-0.69365673
C	-4.60374839	-2.31432847	1.11178927
C	-3.77313639	-2.53818847	-1.12659673
C	-4.85548139	-2.51310347	-0.24571473
H	-5.43354839	-2.30436847	1.81014227
H	-3.94985739	-2.72130247	-2.18120973
C	-3.08901839	-1.84957547	3.07097427
H	-2.76477339	-2.76654647	3.57264727
H	-2.32308339	-1.09363947	3.25659427
H	-4.01034439	-1.51943347	3.55216127
C	-6.26987439	-2.64305147	-0.74900073
H	-6.90061939	-3.18081747	-0.03735773
H	-6.70383339	-1.64667147	-0.88572173
H	-6.31059239	-3.16072747	-1.70934573
C	-1.31494539	-2.40610847	-1.66984773
H	-1.00165139	-1.40364247	-1.97290473
H	-0.44265739	-2.90186147	-1.23682973
H	-1.60831039	-2.95442847	-2.56565273
C	2.91008061	-1.55640647	-0.75337673
H	2.54176161	-2.52920247	-0.41553473
H	2.11481261	-1.08636747	-1.33782373
H	3.77037461	-1.72441747	-1.40199973

C	1.62242261	0.70243153	3.58019227
H	0.79459561	1.27027253	3.15004427
H	1.22108161	-0.22283947	4.00270027
H	2.05401161	1.28860553	4.39207727
C	6.16673561	1.55242653	1.54035827
H	6.10295761	2.49334953	0.98343427
H	6.47472361	1.79502653	2.55956427
H	6.95133661	0.95020853	1.07673027
O	0.70495061	0.79959953	-0.67249773
C	1.06142761	2.26735353	-0.17829973
C	2.24351061	2.62625053	-1.04864273
H	3.08212761	1.99276253	-0.75412673
H	2.01840361	2.47428753	-2.10224673
H	2.50050561	3.67060653	-0.87201973
C	-1.05147239	3.94266153	-0.34817073
C	-1.13014539	5.34173953	-0.93896773
C	-0.09124639	5.67453853	-1.98921673
H	0.91318561	5.54439853	-1.57896373
H	-0.17028139	4.97786653	-2.82685673
H	-0.23507839	6.70029653	-2.32743273
C	-1.88583839	3.69416453	0.69618527
H	-2.49453739	4.55364753	0.94876227
O	-0.18763139	3.16325253	-1.00037173
O	-1.97110939	6.16271953	-0.60915973
C	-2.07830139	2.47805553	1.56899227

C	-2.94606939	2.73499953	2.78537627
C	-2.59434639	2.14407353	4.00506227
C	-4.13281039	3.47475153	2.72661727
C	-3.39706439	2.28851253	5.13491327
H	-1.67733139	1.56640953	4.06798327
C	-4.93773439	3.62522853	3.85416527
H	-4.44071739	3.92181653	1.78912327
C	-4.57460539	3.03219553	5.06271527
H	-3.10065139	1.82676353	6.07046027
H	-5.85377239	4.20162453	3.78583827
H	-5.20125239	3.15033853	5.93965727
H	-1.09539739	2.16335253	1.91779727
H	-2.64830039	0.39826353	1.58949927
O	1.00568861	2.44710653	1.02530527

Z-IV

0 1			
C	-0.19151847	0.33515731	0.00000000
C	-1.11993747	1.33345731	0.02034000
H	-1.06300647	1.98166931	-0.84552100
C	-2.12811247	1.69355631	1.06798000
C	-3.55488847	1.80221931	0.53846100
C	-4.63503147	1.46467131	1.36025400
C	-3.83562347	2.28073931	-0.74725500
C	-5.95008547	1.58769731	0.91806900

H	-4.44404847	1.10404531	2.36232700
C	-5.14904347	2.41082231	-1.19504200
H	-3.02498047	2.55151731	-1.41095300
C	-6.21403347	2.06254131	-0.36476500
H	-6.76605847	1.30842031	1.57565700
H	-5.33937747	2.78238731	-2.19603700
H	-7.23587147	2.15884431	-0.71467800
C	-0.08869847	-0.69923769	1.09749300
C	0.89111253	-2.15599769	2.49487400
C	-0.38797847	-2.55810369	2.32171900
N	-0.98673947	-1.64749769	1.45659600
H	1.69300853	-2.56434169	3.08379800
H	-0.92999647	-3.39851069	2.71564700
N	1.06689553	-1.01296069	1.72929800
C	2.32005053	-0.29296469	1.67061500
C	2.52262853	0.75661931	2.56981000
C	3.30709953	-0.72989069	0.78010600
C	3.76461753	1.39307031	2.55646500
C	4.53000253	-0.05907869	0.80201500
C	4.77649853	1.00149731	1.67873500
H	3.93569953	2.21877231	3.23853500
H	5.30920053	-0.37322169	0.11513900
C	-2.35722647	-1.76504769	1.01602900
C	-3.37342247	-1.59251369	1.96391400
C	-2.61791647	-2.10966169	-0.31747600

C	-4.69139347	-1.73416569	1.52993100
C	-3.95539947	-2.21093369	-0.70184900
C	-5.00282647	-2.01429969	0.20020500
H	-5.49395947	-1.58362069	2.24383300
H	-4.18225347	-2.45719169	-1.73381400
C	-3.08235047	-1.25519869	3.40684500
H	-2.80087447	-2.14640569	3.97583500
H	-2.26488647	-0.53821669	3.50708800
H	-3.96435447	-0.82621069	3.88383600
C	-6.43799047	-2.05014369	-0.25833600
H	-7.09627947	-2.45160969	0.51560900
H	-6.77727947	-1.03358069	-0.48454600
H	-6.55781247	-2.65149969	-1.16180500
C	-1.50943447	-2.39923669	-1.29772400
H	-0.94161847	-1.50276169	-1.55460900
H	-0.79478747	-3.11322069	-0.87697200
H	-1.91689947	-2.82731969	-2.21421700
C	3.04434053	-1.86707169	-0.16962500
H	2.83691653	-2.79715569	0.36878500
H	2.16874853	-1.62197369	-0.77548900
H	3.90242653	-2.03679169	-0.82113700
C	1.43381353	1.17940231	3.51812300
H	0.52227953	1.40765231	2.96591900
H	1.19470253	0.38477631	4.23185500
H	1.72107553	2.07116931	4.07358400

C	6.09381853	1.73647731	1.64472900
H	6.05654853	2.55469631	0.91726500
H	6.33317153	2.17298631	2.61665700
H	6.91246153	1.07560431	1.35152600
O	0.68549753	0.11115731	-0.91629300
C	1.27139353	3.66156231	0.41355300
C	2.27956653	2.87853631	-0.36380400
H	3.17694853	2.74413531	0.23318600
H	1.84775653	1.89817431	-0.60658600
H	2.50600953	3.38559131	-1.30333300
C	-0.89424847	4.69830031	0.04339100
C	-1.15938247	5.97296231	-0.70082600
C	-0.09861447	6.42312331	-1.67837300
H	0.86194053	6.53956231	-1.16878900
H	0.04770753	5.66467931	-2.45171000
H	-0.40265547	7.36701931	-2.12739500
C	-1.75634447	4.25583331	0.96622000
H	-2.60699347	4.91850831	1.07242900
O	0.24661853	4.04570331	-0.41439500
O	-2.18156647	6.61093131	-0.52045900
C	-1.70708347	3.03713531	1.83897700
C	-2.51361347	3.19952031	3.12015400
C	-2.04623747	2.59326731	4.29310300
C	-3.74732447	3.85903731	3.17086300
C	-2.78233447	2.63849331	5.47498300

H	-1.09303147	2.07853731	4.28364200
C	-4.48593347	3.91182731	4.35158000
H	-4.15778547	4.31719131	2.28003300
C	-4.00898647	3.30022131	5.50927900
H	-2.39452047	2.16201231	6.36866100
H	-5.44005047	4.42693931	4.36208600
H	-4.58405947	3.34133331	6.42742000
H	-0.66939847	2.87453631	2.12350400
H	-2.12479447	0.93341631	1.85183800
O	1.30469053	3.93410431	1.58626800

Intermediate V

0 1

C	-1.98985200	0.60210700	-1.22276400
C	-0.77748200	0.09638200	-0.85985700
H	-0.31798500	-0.52930900	-1.61595600
C	-0.05091300	0.21542700	0.44626500
C	1.35398800	0.82059800	0.31508300
C	2.15510600	1.05583500	1.44367000
C	1.85229600	1.22467400	-0.92889500
C	3.40280300	1.66727600	1.33087900
H	1.79867600	0.77810400	2.42558600
C	3.10113100	1.83537900	-1.04673100
H	1.23948200	1.09416600	-1.81091100
C	3.88588000	2.06075700	0.08246400

H	3.99443900	1.84440200	2.22258400
H	3.45644300	2.14526600	-2.02331400
H	4.85638300	2.53399300	-0.00951600
C	-2.75085000	1.52338200	-0.29777100
C	-4.50017700	2.45835500	0.74624900
C	-3.48896600	3.35770300	0.76144700
N	-2.40886500	2.76561400	0.11457200
H	-5.49980800	2.50351200	1.14051200
H	-3.42559900	4.35350600	1.16192400
N	-4.03417400	1.33205300	0.08293300
C	-4.83221000	0.14718400	-0.14360900
C	-4.77243400	-0.88600600	0.79549900
C	-5.67441000	0.11038600	-1.25987900
C	-5.58318000	-2.00163200	0.58412600
C	-6.46552400	-1.02682200	-1.42711600
C	-6.43102800	-2.09047800	-0.52150100
H	-5.54076500	-2.82042500	1.29431800
H	-7.12146000	-1.08340000	-2.28970400
C	-1.14641600	3.43314200	-0.11684400
C	-0.29000400	3.66229100	0.96274600
C	-0.85298500	3.87144000	-1.41985500
C	0.91844000	4.31758200	0.70333300
C	0.36381100	4.51517100	-1.62045500
C	1.26688900	4.73947000	-0.57433600
H	1.60619800	4.47882600	1.52603300

H	0.61418000	4.85801000	-2.61927600
C	-0.60222000	3.24458700	2.37910500
H	-0.74218500	4.12520200	3.01268500
H	-1.50207100	2.63710200	2.45957400
H	0.22948500	2.67180800	2.79465800
C	2.58805000	5.41335100	-0.84395100
H	3.10437500	5.66925800	0.08271500
H	3.24312900	4.75070900	-1.41662900
H	2.45269600	6.32760000	-1.42828200
C	-1.82666700	3.68100800	-2.55573500
H	-1.94700300	2.62699100	-2.81701700
H	-2.81938300	4.05543900	-2.28701300
H	-1.48909000	4.22231300	-3.44018700
C	-5.69660800	1.24252700	-2.25069000
H	-5.97340000	2.18775500	-1.77411600
H	-4.69455900	1.35653300	-2.67171800
H	-6.40813300	1.04515500	-3.05335500
C	-3.86099300	-0.79494400	1.98935200
H	-2.83269500	-0.63101000	1.66920700
H	-4.13610700	0.04005200	2.64093500
H	-3.88486300	-1.71316200	2.57478600
C	-7.25968900	-3.32941100	-0.75582100
H	-6.68245800	-4.07565000	-1.31268200
H	-7.56496100	-3.78973500	0.18638000
H	-8.15617200	-3.10688300	-1.33823900

O	-2.62470900	0.40888600	-2.32377300
C	-1.96121900	-3.09045700	-0.79921000
C	-3.00078400	-2.80968000	-1.83516700
H	-3.98076800	-3.07587400	-1.44913100
H	-2.97504100	-1.73816500	-2.07611000
H	-2.77769800	-3.36142100	-2.75019000
C	0.46881100	-2.96173400	-0.61866900
C	1.49804300	-3.87778000	-1.20660100
C	1.03525000	-4.83020500	-2.27879000
H	0.19264300	-5.42743000	-1.91993500
H	0.67231400	-4.26740300	-3.14299500
H	1.86144400	-5.47628500	-2.56972600
C	0.76597300	-2.19636200	0.43893200
H	1.78898600	-2.32900200	0.76507400
O	-0.70857200	-2.95778200	-1.35445800
O	2.65927600	-3.84585500	-0.82816200
C	-0.06919300	-1.20344300	1.18257200
C	0.24693200	-1.13796400	2.67844700
C	-0.54426800	-0.31383100	3.49285400
C	1.27042200	-1.86448300	3.29569700
C	-0.30435900	-0.19157400	4.85711700
H	-1.35507600	0.25373100	3.05504000
C	1.51595200	-1.74655300	4.66505100
H	1.89401400	-2.53763200	2.72241600
C	0.73668000	-0.90456600	5.45217300

H	-0.93110000	0.46038500	5.45533700
H	2.31998500	-2.31974300	5.11315700
H	0.92971200	-0.81079300	6.51458600
H	-1.10687000	-1.52081000	1.11167200
H	-0.61667700	0.87503100	1.10682400
O	-2.13718000	-3.38363500	0.35433600
Cl	7.66026700	0.74649800	-1.41728800
Cs	4.97144400	-1.61193200	-0.60736500

VI

0 1

C	0.76607387	-0.04787962	0.00000000
C	-0.46162313	-0.78538762	0.21663000
H	-0.83813213	-0.73185662	1.23222600
C	-1.10517713	-1.44610662	-0.76867900
C	-2.40493913	-2.09138062	-0.68329200
C	-2.82912013	-2.90919962	-1.74557500
C	-3.28190113	-1.85996162	0.39358500
C	-4.08895013	-3.49577362	-1.73002800
H	-2.16424613	-3.07819262	-2.58612300
C	-4.54286613	-2.44185762	0.39904600
H	-2.99266513	-1.19597962	1.20165900
C	-4.94930813	-3.26214962	-0.65675600
H	-4.40336413	-4.12685962	-2.55305300
H	-5.21650713	-2.24829062	1.22563000

H	-5.93604813	-3.71088362	-0.64547000
C	1.08175487	0.48351638	-1.38932000
C	2.30452887	1.29485138	-3.06266800
C	1.01773487	1.68267138	-3.26477500
N	0.26611687	1.16529338	-2.22644000
H	3.19631387	1.46142738	-3.64047700
H	0.56985587	2.27843738	-4.03965600
N	2.32864987	0.56341838	-1.89244100
C	3.50889587	-0.08643562	-1.35827000
C	3.70939787	-1.43630862	-1.65708900
C	4.39316587	0.67084438	-0.58300900
C	4.86487487	-2.03605162	-1.15125300
C	5.53088687	0.02415138	-0.10469500
C	5.78446887	-1.32367762	-0.37979500
H	5.04488887	-3.08431362	-1.36406400
H	6.23015687	0.58282338	0.50829900
C	-1.16885013	1.33292238	-2.09478600
C	-1.98853713	0.66408738	-3.01822400
C	-1.67756913	2.08883938	-1.03471400
C	-3.36505113	0.74509838	-2.82688000
C	-3.06682213	2.13046038	-0.89106700
C	-3.92167013	1.45520538	-1.75965200
H	-4.01786013	0.21374338	-3.51086700
H	-3.48029713	2.68646138	-0.05712400
C	-1.42809713	-0.14152662	-4.16539800

H	-1.13248213	0.50318838	-4.99855000
H	-0.54383213	-0.71644662	-3.87940700
H	-2.17721613	-0.84018462	-4.53832400
C	-5.40987113	1.43830338	-1.52218000
H	-5.96490613	1.36889838	-2.46024700
H	-5.67714713	0.56808838	-0.91341800
H	-5.74076213	2.32965538	-0.98609800
C	-0.80951013	2.79500738	-0.02559000
H	-0.79358713	2.22534938	0.91000100
H	0.21433487	2.94209438	-0.37099900
H	-1.23050813	3.77500038	0.20671300
C	4.09478587	2.10738138	-0.24468000
H	3.99718387	2.72427838	-1.14231600
H	3.15193787	2.16783538	0.30533000
H	4.88474687	2.53307038	0.37389100
C	2.70743087	-2.22611062	-2.46263000
H	1.82575287	-2.46684262	-1.85997900
H	2.36319987	-1.67353162	-3.34057200
H	3.14028787	-3.16727862	-2.80153600
C	7.03994687	-1.98353662	0.13385100
H	6.94135887	-3.07032562	0.15370200
H	7.89264587	-1.73806862	-0.50782800
H	7.28180087	-1.64074362	1.14242100
O	1.55054887	0.26704738	0.87949400
H	-0.62959113	-1.50585762	-1.74376000

Cl -2.27266913 0.81048938 2.90853400

VII

0 1

C -2.53564200 2.98190100 -0.04547200
C -2.97870600 4.00953000 -1.05674400
H -3.38029900 4.88138400 -0.54470300
H -2.12964400 4.30142500 -1.67900700
H -3.73570200 3.57860200 -1.71535900
C -1.55064000 0.80621500 0.11092000
C -2.42884700 -0.17583300 0.60752700
C -3.92502300 0.03778500 0.40208800
H -4.15929200 0.30647800 -0.63153400
H -4.45314500 -0.87652800 0.67371500
H -4.28020700 0.85615800 1.03684500
C -0.15647600 0.79209200 0.28941900
H 0.16630400 -0.02084400 0.93410100
O -2.08981600 1.86914200 -0.67648400
O -2.03268600 -1.21640300 1.20703300
C 0.77969300 1.64384100 -0.22922300
C 2.21226700 1.56421400 -0.01281400
C 3.07673500 2.44428500 -0.70481800
C 2.82756600 0.63547100 0.86209600
C 4.45726500 2.39388400 -0.54581000
H 2.64380400 3.17601300 -1.38045800

C	4.20728900	0.58599600	1.01652100
H	2.21219900	-0.04587200	1.43910400
C	5.04087500	1.46169500	0.31430800
H	5.08344700	3.08838900	-1.09693300
H	4.63979500	-0.13798900	1.70021700
H	6.11659400	1.42259500	0.44162800
H	0.43947900	2.44069100	-0.88541300
O	-2.58167000	3.11905500	1.15246600
Cs	0.00567100	-3.05875100	-0.32371500

TS5

0 1

C	3.92951900	1.24523100	-0.49996900
C	5.16956500	2.00875200	-0.09756800
H	5.71270000	2.32017800	-0.98807300
H	4.87439200	2.89557000	0.47015300
H	5.80649600	1.40032600	0.54619600
C	2.18037400	-0.14027000	0.36210900
C	2.16982700	-1.50899100	0.46722600
C	3.45931800	-2.25243300	0.80562000
H	4.30758600	-1.59832600	1.01285300
H	3.27871700	-2.89168900	1.67624500
H	3.71845300	-2.91455200	-0.02807400
C	1.00111200	0.65186300	-0.03575300
H	0.81856400	0.77615200	-1.10601600

O	3.41012500	0.59272200	0.55166700
O	1.11385900	-2.22382400	0.29823700
C	0.12522800	1.18372800	0.83016100
C	-1.13504000	1.86909600	0.49368500
C	-2.12745400	1.99377400	1.48122000
C	-1.42253400	2.36418100	-0.79200900
C	-3.36493400	2.56673000	1.19518000
H	-1.92346400	1.62761000	2.48243800
C	-2.65755800	2.93614800	-1.07791900
H	-0.66911000	2.30958600	-1.56879300
C	-3.63831100	3.03705900	-0.08817500
H	-4.11368700	2.64824200	1.97541900
H	-2.85476800	3.31387500	-2.07524900
H	-4.59848700	3.48664500	-0.31401300
H	0.30508000	1.03154300	1.89269900
O	3.45139200	1.25325600	-1.61424000
Cs	-1.82909400	-1.94748400	-0.29316300

VII'

O 1			
C	-3.93586700	1.56268700	-0.16817000
C	-5.00275200	1.92971400	-1.16973600
H	-5.64240700	2.70745200	-0.75736900
H	-4.55199300	2.26075600	-2.10637000
H	-5.60517400	1.04339800	-1.38688500

C	-1.89664900	0.31573600	0.05265600
C	-2.09846700	-0.86826500	0.78563700
C	-3.49001300	-1.49616200	0.76319900
H	-3.90126500	-1.54949900	-0.24840800
H	-3.42860000	-2.49776100	1.18994300
H	-4.18386000	-0.89868000	1.36368000
C	-0.71299600	1.07424500	-0.07983000
H	-0.78734800	1.85916300	-0.83184800
O	-2.99349300	0.78610600	-0.75007900
O	-1.18290100	-1.43868400	1.44425700
C	0.47315700	0.93697400	0.59645200
C	1.69633700	1.67543200	0.34386700
C	2.80394500	1.49286100	1.20629400
C	1.88241100	2.56597000	-0.74116400
C	4.00838900	2.15860400	1.00692700
H	2.69872400	0.81898300	2.05169900
C	3.08517100	3.23442300	-0.93354400
H	1.07484500	2.72967000	-1.44603600
C	4.16348600	3.03999000	-0.06498300
H	4.83108100	1.99227700	1.69524400
H	3.18716000	3.91217700	-1.77537800
H	5.10059000	3.56159700	-0.22204400
H	0.50140000	0.22329700	1.41123900
O	-3.93574600	1.88849400	0.99418700
Cs	1.26812900	-2.39606200	-0.40054600

VIII

0 1

C	-0.19536800	-1.29540600	-0.76220500
C	-0.69204900	-0.02664200	-0.77499000
H	-0.25449800	0.61403100	-1.53562400
C	-1.67736900	0.61817300	0.15611300
C	-2.93563800	1.15489700	-0.53094100
C	-4.08899400	1.42294900	0.21907000
C	-2.98455500	1.39348500	-1.90836700
C	-5.24426000	1.91534600	-0.38032300
H	-4.08778600	1.23339000	1.28446500
C	-4.13921400	1.88870800	-2.51485600
H	-2.12184200	1.16792900	-2.52170700
C	-5.27476100	2.15435100	-1.75347100
H	-6.12388400	2.10397400	0.22547100
H	-4.15089900	2.05775400	-3.58615500
H	-6.17451200	2.53453600	-2.22430500
C	-0.68804600	-2.31300100	0.24136600
C	-0.59596800	-3.98557000	1.73038400
C	-1.85892100	-3.94028700	1.24640500
N	-1.90456200	-2.89776800	0.32627100
H	-0.13558000	-4.62791200	2.45975600
H	-2.72454900	-4.54198600	1.45699800

N	0.11906000	-2.97942600	1.09708600
C	1.52149900	-2.71535900	1.33114600
C	1.88914400	-1.73689700	2.25862500
C	2.46323300	-3.49474800	0.64000400
C	3.25698000	-1.53046100	2.47462200
C	3.81195000	-3.26304900	0.90579100
C	4.23012700	-2.28045300	1.81452000
H	3.56051800	-0.76148100	3.17712600
H	4.55728000	-3.85203800	0.38123000
C	-3.08379000	-2.53886200	-0.42834400
C	-4.16683300	-1.97295400	0.25403600
C	-3.11581900	-2.81217900	-1.80321800
C	-5.28956100	-1.62190100	-0.49591000
C	-4.25840500	-2.42872000	-2.50520300
C	-5.34499700	-1.81780800	-1.87462300
H	-6.12813000	-1.15645800	0.00938600
H	-4.30079700	-2.61745100	-3.57281600
C	-4.15728900	-1.75432900	1.74730100
H	-4.42254600	-2.67297500	2.27975300
H	-3.17942700	-1.44232500	2.11750900
H	-4.88316200	-0.99016000	2.02519300
C	-6.53672500	-1.34658800	-2.66829900
H	-7.46285200	-1.44821300	-2.09780300
H	-6.41891500	-0.28703700	-2.91714900
H	-6.64282100	-1.90143700	-3.60277700

C	-1.98304400	-3.52350400	-2.50007200
H	-1.08256000	-2.90762000	-2.55577800
H	-1.70778600	-4.43595800	-1.96209700
H	-2.27725400	-3.80346300	-3.51224200
C	2.02339400	-4.51500400	-0.37628700
H	1.40381800	-5.29467700	0.07660000
H	1.42905900	-4.01273700	-1.14374600
H	2.88446600	-4.99481900	-0.84279300
C	0.88323100	-0.93902500	3.04737200
H	-0.11586500	-0.99904300	2.61952200
H	0.82652200	-1.30911500	4.07577900
H	1.18034700	0.10950900	3.08137200
C	5.69696200	-2.00989700	2.03443000
H	6.06540400	-1.27550700	1.30875700
H	5.88056700	-1.60837700	3.03333800
H	6.29020200	-2.91905700	1.91251300
O	0.70250400	-1.80168600	-1.53386400
C	1.81501800	3.94832600	-2.04866000
C	2.00468300	5.13602500	-2.94236500
H	2.43863400	4.81782800	-3.88725600
H	1.05201500	5.64168800	-3.10547100
H	2.67630000	5.84405800	-2.44973200
C	0.85655700	3.24953900	-0.00512600
C	2.03136100	2.88118300	0.84382800
C	3.19871700	3.83982000	0.85729100

H	3.77159500	3.73021600	-0.06868900
H	2.86441500	4.87728400	0.91568300
H	3.84639200	3.59271100	1.69640900
C	-0.39525200	2.79340800	0.07966000
H	-1.10309000	3.23534700	-0.61730200
O	1.09695700	4.28258300	-0.93991000
O	2.04867400	1.84876700	1.49346000
C	-0.93337900	1.74571800	1.00533400
C	-1.80223400	2.32629800	2.11299500
C	-2.03234100	1.54995100	3.25625100
C	-2.42155700	3.57677800	2.02839500
C	-2.87239300	1.99580900	4.27248000
H	-1.55392900	0.58193100	3.34861100
C	-3.26056500	4.02987800	3.04619500
H	-2.26335700	4.20582100	1.16117700
C	-3.49519100	3.24010400	4.16920300
H	-3.03658700	1.37518800	5.14643900
H	-3.73391900	5.00132500	2.95677200
H	-4.14933000	3.59158900	4.95894300
H	-0.09770000	1.23517600	1.47254900
H	-2.00491900	-0.11025500	0.90109600
O	2.24283800	2.83489500	-2.23537300
Cl	6.93918700	0.53977000	-0.70776500
Cs	3.39028100	-0.08949100	-1.40149700

E-IV

0 1

C	1.14911081	1.58002734	0.00000000
C	0.21268181	2.56664434	0.09245600
H	0.26624981	3.27771634	-0.72253000
C	-0.78186719	2.86405234	1.16918600
C	-2.20659319	3.06011334	0.66196100
C	-3.29019319	2.71149434	1.47592900
C	-2.48089619	3.62989634	-0.58745400
C	-4.60401119	2.90428234	1.05757000
H	-3.10131219	2.28765934	2.45436700
C	-3.79524019	3.82907434	-1.00989000
H	-1.66773319	3.92696234	-1.23593600
C	-4.86385919	3.46398434	-0.19217300
H	-5.42297419	2.61454334	1.70702200
H	-3.98240219	4.26996634	-1.98327900
H	-5.88532419	3.61429934	-0.52417200
C	1.22764481	0.44560634	0.99603200
C	2.16830581	-1.14861566	2.26212700
C	0.88909381	-1.52038366	2.02514300
N	0.31427081	-0.52322866	1.24332700
H	2.95431881	-1.62017766	2.82464500
H	0.33256981	-2.38981166	2.32496300
N	2.36632081	0.06208834	1.61688800
C	3.60454281	0.80668734	1.65496100

C	3.75811181	1.78477434	2.63920900
C	4.60726981	0.49254034	0.72961900
C	4.96358681	2.48850334	2.66644800
C	5.79325581	1.22097634	0.80133800
C	5.98502681	2.22643034	1.75483300
H	5.09297981	3.27090834	3.40521100
H	6.58310281	1.00442034	0.08926600
C	-1.05392119	-0.56236966	0.78247300
C	-2.07546519	-0.44537466	1.73314900
C	-1.30955519	-0.75942966	-0.58112300
C	-3.39185619	-0.49029666	1.27476500
C	-2.64470419	-0.77223666	-0.98625500
C	-3.69579319	-0.62475466	-0.07927500
H	-4.19780619	-0.37891766	1.99195500
H	-2.86664519	-0.90371666	-2.04006700
C	-1.79065519	-0.26566466	3.20524000
H	-1.56685719	-1.22201566	3.68761300
H	-0.93635119	0.39052834	3.38341800
H	-2.65592419	0.16360934	3.71161100
C	-5.12542319	-0.55839566	-0.55178300
H	-5.80549719	-1.03006066	0.16155300
H	-5.43022619	0.48851134	-0.65429400
H	-5.25209919	-1.04124966	-1.52287100
C	-0.19853319	-0.97844966	-1.57669100
H	0.38208881	-0.06968166	-1.74876100

H	0.50397381	-1.73652066	-1.21764200
H	-0.60563419	-1.31644566	-2.53030900
C	4.39228781	-0.57239966	-0.31184600
H	4.20616481	-1.54898866	0.14576100
H	3.51865881	-0.30391066	-0.91057800
H	5.26356881	-0.66287266	-0.96185200
C	2.67363281	2.05821634	3.64839100
H	1.69675281	2.12815234	3.16890500
H	2.61586481	1.25377234	4.38916300
H	2.85768681	2.99801034	4.16572700
C	7.25653981	3.03939234	1.76778000
H	7.16660581	3.90081834	1.09705000
H	7.47553981	3.42351634	2.76633900
H	8.11172381	2.44986734	1.42949400
O	2.03594681	1.44508434	-0.92109100
C	0.70256681	6.39957334	-1.64969000
C	0.99242381	7.59129134	-2.51717200
H	0.49415981	7.47400434	-3.47659300
H	0.65513681	8.50262934	-2.02015800
H	2.07147881	7.67633534	-2.66523800
C	1.12487381	5.58466334	0.57328200
C	2.43437181	4.92623134	0.91588400
C	3.31150081	4.48906634	-0.22607700
H	2.88380781	3.57188634	-0.65788700
H	3.36147881	5.24455734	-1.01190300

H	4.30754481	4.26053734	0.15196700
C	-0.06122019	5.29881234	1.11134300
H	-0.92138719	5.83196634	0.72153800
O	1.25513581	6.58291034	-0.40916500
O	2.73875481	4.74390934	2.08220800
C	-0.30098219	4.14213734	2.03052600
C	-1.23345819	4.41715134	3.19332100
C	-1.06861019	3.66961434	4.36684800
C	-2.29644719	5.32426134	3.13475400
C	-1.93978519	3.81313434	5.44369800
H	-0.24786119	2.96286834	4.43519000
C	-3.16739319	5.47719634	4.21240200
H	-2.46519519	5.90886334	2.23916300
C	-2.99662519	4.72049834	5.37002800
H	-1.79052019	3.22205534	6.34067900
H	-3.98567319	6.18540734	4.14260000
H	-3.67606719	4.83863934	6.20659400
H	0.65352281	3.84051334	2.45090100
H	-0.80115419	2.05198234	1.89920100
O	0.09321581	5.41551234	-1.97397800

TS6

0 1			
C	-2.02462381	-0.03419973	0.00000000
C	-1.09261481	1.23238927	-0.05851600

C	0.17681319	0.97066627	-0.81607200
C	0.32691519	0.06600027	-1.77293600
C	-0.60959581	-1.00289073	-2.33980800
C	-2.21527281	-0.66715173	-1.36976800
H	1.02456919	1.60320827	-0.57241500
H	-0.81510681	1.43612527	0.98086500
H	-1.49272681	-0.73901273	0.64049500
H	-2.67112981	0.03099627	-2.06610600
C	-1.79677581	2.49205927	-0.56154800
C	-2.34395381	3.40043427	0.35198400
C	-1.94122281	2.75972427	-1.92617100
C	-3.03590181	4.52849027	-0.08171400
H	-2.24428681	3.20871327	1.41457100
C	-2.63896881	3.88333527	-2.36683100
H	-1.49029181	2.09220127	-2.64856500
C	-3.19268981	4.77125627	-1.44596900
H	-3.45514981	5.21535927	0.64532600
H	-2.74296881	4.06762527	-3.43056000
H	-3.73318781	5.64707727	-1.78727400
C	-3.32498581	0.37506027	0.69026800
C	-3.35611481	0.52137627	2.08263100
C	-4.45814381	0.76393927	-0.03447800
C	-4.47155681	1.05012527	2.72990700
H	-2.48537281	0.24796827	2.66670100
C	-5.56939781	1.30631927	0.60570000

H	-4.47092981	0.66501027	-1.11166600
C	-5.58070581	1.45706427	1.99053700
H	-4.46857881	1.15357127	3.80947900
H	-6.42889681	1.60955427	0.01836600
H	-6.44665381	1.87769027	2.48912500
O	1.56351219	-0.02887873	-2.44811600
C	2.58211019	-0.71811373	-1.86419400
C	3.54948719	-1.19436773	-2.91223400
H	3.70780019	-0.42815873	-3.67204000
H	4.49254619	-1.48251773	-2.45182100
H	3.09983419	-2.06282173	-3.40178400
O	2.68216419	-0.90775173	-0.67940800
C	-2.94986981	-1.91181273	-1.49789100
O	-3.48239581	-2.26296973	-2.54762800
C	-4.25930381	-4.41791973	0.89332900
C	-2.96789881	-4.43558173	1.29120900
H	-5.11820181	-4.96896073	1.23225900
H	-2.45594181	-5.02744273	2.02850300
N	-2.28151581	-3.51548273	0.51322700
N	-4.35474281	-3.49805373	-0.13241900
C	-3.13854781	-2.93087673	-0.35896000
C	-5.62245481	-3.22002773	-0.77916000
C	-6.53037781	-2.39393773	-0.10959500
C	-5.93664081	-3.88881973	-1.96954700
C	-7.74881081	-2.13434573	-0.74170500

C	-7.17038381	-3.60226873	-2.55262700
C	-8.07501381	-2.70871773	-1.97095000
H	-8.46090881	-1.47941273	-0.25079800
H	-7.43376881	-4.09564873	-3.48236700
C	-0.82890581	-3.49426473	0.57156800
C	-0.20094981	-2.86779073	1.65067900
C	-0.13422281	-4.27345373	-0.36243600
C	1.18982519	-2.96022673	1.72542600
C	1.24806219	-4.35532073	-0.22332200
C	1.92941919	-3.69002373	0.79683000
H	1.70143919	-2.45441873	2.53777000
H	1.80852919	-4.93836273	-0.94611000
C	-5.00451181	-4.90560873	-2.57379300
H	-4.08791981	-4.42312473	-2.91356400
H	-4.72630681	-5.66705373	-1.83893200
H	-5.47660381	-5.40732473	-3.41909100
C	-6.25369381	-1.87826973	1.27860300
H	-6.37424681	-2.68450773	2.00984100
H	-5.24249981	-1.48650073	1.38347900
H	-6.94746781	-1.08229173	1.54092700
C	-9.37513181	-2.37644273	-2.66021400
H	-9.22749681	-1.56787873	-3.38391300
H	-9.76702881	-3.23645873	-3.20805600
H	-10.13349481	-2.04619073	-1.94742700
C	-0.84551481	-4.98184273	-1.48331200

H	-0.18681981	-5.71297673	-1.95394700
H	-1.74309681	-5.50435773	-1.14015200
H	-1.12706681	-4.23857273	-2.23203400
C	-0.95642781	-2.16436873	2.75196400
H	-0.50553481	-1.19235373	2.96487400
H	-2.00714781	-2.00936273	2.51363600
H	-0.91130481	-2.75189973	3.67410800
C	3.43378419	-3.72361873	0.86991200
H	3.83169419	-2.84717873	0.35048900
H	3.78699819	-3.69157573	1.90357400
H	3.83996019	-4.61825273	0.39257400
C	-1.05855181	-0.64611973	-3.77712400
H	-1.81422281	-1.36446273	-4.09725000
H	-1.45923381	0.36543127	-3.88710300
H	-0.17938981	-0.74773673	-4.41873000
O	-0.14076881	-2.18951273	-2.21290900

IX

0 1

C	-0.45143639	0.95075238	0.00000000
C	0.82497261	1.86609838	0.02758100
C	2.01106161	1.10445538	-0.51364000
C	1.86497361	0.14395338	-1.42581800
C	0.56073061	-0.19653462	-2.09342400
C	-0.69311839	0.34562138	-1.37843900

H	2.98670861	1.34989738	-0.12529800
H	1.02806161	2.05772738	1.08687600
H	-0.18776839	0.13054738	0.66630300
H	-1.28437439	0.99664738	-2.01804000
C	0.61969161	3.23336638	-0.61836300
C	0.07804961	4.28234838	0.13690600
C	0.92760161	3.47804038	-1.95913600
C	-0.16963839	5.52704538	-0.43539900
H	-0.16466039	4.11566738	1.18033900
C	0.67968161	4.72244738	-2.53847300
H	1.38175961	2.69551738	-2.55124400
C	0.12566161	5.75140238	-1.78016400
H	-0.59365239	6.32155638	0.16877700
H	0.92617561	4.88695338	-3.58174200
H	-0.06668039	6.71970738	-2.22849800
C	-1.64012039	1.66472038	0.61927000
C	-1.70669239	1.77109338	2.01556000
C	-2.62814539	2.30478938	-0.13414800
C	-2.72163239	2.49090938	2.63980000
H	-0.94620439	1.29187938	2.62186600
C	-3.64741139	3.02623138	0.48515700
H	-2.60693639	2.25421838	-1.21450500
C	-3.69872839	3.12527138	1.87329200
H	-2.75032939	2.55548238	3.72193100
H	-4.40225539	3.51287538	-0.12234900

H	-4.49266839	3.68599138	2.35351600
O	2.87558861	-0.64461362	-1.97938500
C	4.14916961	-0.75298062	-1.52694000
C	4.88060561	-1.77575762	-2.35407700
H	4.80994561	-1.51907462	-3.41262400
H	5.92233961	-1.82142362	-2.04539900
H	4.40578661	-2.74943462	-2.21755000
O	4.61727561	-0.13320962	-0.60423700
C	-1.27817439	-1.13219362	-1.51181600
O	-2.16853839	-1.32237062	-2.39647800
C	-2.77003839	-3.11116562	1.30628400
C	-1.46676539	-3.26027162	1.62485200
H	-3.66380939	-3.49872362	1.76147200
H	-0.98247239	-3.80934162	2.41244400
N	-0.73128839	-2.55240462	0.68235100
N	-2.82510539	-2.32022762	0.16975900
C	-1.57192739	-1.96347462	-0.21115800
C	-4.10058539	-2.08856362	-0.48700500
C	-4.95993139	-1.12667162	0.04443000
C	-4.48389739	-2.95573462	-1.52040500
C	-6.21420039	-0.97498562	-0.55747400
C	-5.74693239	-2.77203362	-2.07646500
C	-6.61883239	-1.77540862	-1.62327000
H	-6.88837939	-0.21806362	-0.16979400
H	-6.05895339	-3.42241762	-2.88748700

C	0.71720961	-2.67150162	0.68180100
C	1.46636361	-1.95797262	1.62139400
C	1.29385861	-3.63839862	-0.15617800
C	2.84845061	-2.16392062	1.64044500
C	2.67416861	-3.81366262	-0.08678800
C	3.47147161	-3.07560562	0.79305900
H	3.44722261	-1.59664262	2.34573200
H	3.13771561	-4.55209962	-0.73275600
C	-3.55689439	-4.02887862	-2.02248600
H	-2.70171539	-3.54730862	-2.50154200
H	-3.18137039	-4.65088362	-1.20410100
H	-4.06162639	-4.67765762	-2.73956900
C	-4.59401539	-0.32028162	1.26217900
H	-4.75073839	-0.90845162	2.17310700
H	-3.55205439	-0.00861462	1.24937600
H	-5.20763139	0.57659838	1.33477800
C	-7.96009839	-1.57390062	-2.28510800
H	-7.84867939	-1.00963062	-3.21701700
H	-8.42563239	-2.52972462	-2.53874300
H	-8.64524039	-1.01814062	-1.64167700
C	0.45888861	-4.46155362	-1.10106500
H	1.03991661	-5.29079362	-1.50681600
H	-0.42273739	-4.87555662	-0.60387400
H	0.11562261	-3.83400862	-1.92496400
C	0.86494261	-1.01695162	2.63768500

H	1.26056961	-0.00659562	2.50520300
H	-0.22131239	-0.96960262	2.58576900
H	1.13399161	-1.33839062	3.64733400
C	4.96823961	-3.25910862	0.84325400
H	5.47245561	-2.31483462	0.62155100
H	5.29102561	-3.57817862	1.83849200
H	5.30629961	-4.00569862	0.12251900
C	0.60667461	0.09591238	-3.59789300
H	-0.35149439	-0.20168762	-4.02441500
H	0.78236161	1.15314838	-3.80834800
H	1.39978161	-0.49499162	-4.05987000
O	0.17981861	-1.57178162	-1.89840000

X

0 1			
C	-0.43771899	-0.08891929	0.00573006
C	-0.60018299	1.29147971	-0.71942194
C	-2.06399899	1.65516971	-0.75425894
C	-2.93169599	1.25585471	0.16880606
C	-2.54320599	0.54817771	1.42366206
C	-1.13677799	-0.09400329	1.38168706
H	-2.42131599	2.25473071	-1.58422894
H	-0.29355299	1.11093771	-1.75425994
H	-0.99522899	-0.77943729	-0.63347294
H	-0.48310499	0.20914171	2.19672906

C	0.29515901	2.40129071	-0.18499094
C	1.57052101	2.57850971	-0.73454394
C	-0.09231699	3.22546371	0.87504306
C	2.44165001	3.53817271	-0.22655794
H	1.88780001	1.94633771	-1.55655394
C	0.77813701	4.18512371	1.39040306
H	-1.08662399	3.13274671	1.29100606
C	2.05019501	4.34218671	0.84370306
H	3.42644301	3.65608571	-0.66432394
H	0.45788101	4.81365171	2.21381106
H	2.72728701	5.08934871	1.24172806
C	0.99056701	-0.59264529	0.06177606
C	1.42090201	-1.53353529	-0.87946194
C	1.91564001	-0.11703529	0.99875706
C	2.73811801	-1.98893329	-0.88891594
H	0.71539901	-1.91632129	-1.60970894
C	3.23197301	-0.57114429	0.99456706
H	1.61776401	0.62786071	1.72686106
C	3.64883301	-1.50843829	0.05012206
H	3.04941701	-2.72158929	-1.62496594
H	3.93349101	-0.18804429	1.72701106
H	4.67335301	-1.86284629	0.04838606
O	-4.28741999	1.59091371	0.09920506
C	-5.10680899	0.80236071	-0.67831994
C	-6.53282699	1.24554071	-0.52414094

H	-6.60998699	2.32253671	-0.68168094
H	-7.15978999	0.70997971	-1.23320694
H	-6.86454199	1.03515871	0.49547106
O	-4.70224899	-0.09698129	-1.36127694
C	-1.89758599	-1.39459529	1.61208206
C	-2.91605699	1.30551871	2.68657806
H	-2.62420499	0.72780771	3.56552506
H	-2.41490899	2.27376271	2.72154206
H	-3.99394199	1.46981571	2.71196906
O	-3.13949999	-0.83047729	1.52008806
O	-1.63995399	-2.54832029	1.77349506

Product 2b

0 1			
C	-0.12311902	0.26675786	0.00000000
C	-0.48420702	1.73645486	0.27133900
C	-1.78462602	2.04178686	0.37544200
C	-2.84293202	0.97978186	0.24413800
C	-2.47923802	-0.21533114	1.12193000
C	-1.00726402	-0.62756514	0.90914400
H	-2.12085302	3.06492886	0.49132700
H	-0.40002802	0.06272286	-1.04107200
H	-0.49198902	-0.83605014	1.84629200
C	0.55278598	2.79520686	0.32982000
C	1.56463598	2.87334786	-0.63839200

C	0.52456598	3.75786986	1.34817500
C	2.51246898	3.89079186	-0.59357300
H	1.60748598	2.13703186	-1.43127800
C	1.47643998	4.77399886	1.39515300
H	-0.23892202	3.69483086	2.11519000
C	2.47410598	4.84395086	0.42445100
H	3.28361998	3.93856986	-1.35405600
H	1.44272298	5.50534286	2.19485800
H	3.21831098	5.63120086	0.46250000
C	1.33465098	-0.11962014	0.16812400
C	2.00527698	-0.79603614	-0.85178300
C	2.02110398	0.16310186	1.35468500
C	3.33954198	-1.17375114	-0.69859600
H	1.48146598	-1.02980114	-1.77249000
C	3.35196898	-0.21000514	1.51066800
H	1.51568598	0.69500386	2.15362900
C	4.01713898	-0.87900314	0.48179300
H	3.84613398	-1.69715414	-1.50153400
H	3.87261498	0.02462586	2.43218300
H	5.05492898	-1.16818814	0.60200000
O	-4.13980402	1.47531086	0.63174200
C	-4.86785602	2.11404586	-0.31915500
C	-6.19908802	2.53988186	0.23479000
H	-6.75829202	1.65931986	0.55835800
H	-6.04836302	3.17498686	1.11003300

H	-6.75730302	3.07720986	-0.52836300
O	-4.47391402	2.29769886	-1.44436100
C	-1.60718802	-1.87805114	0.27901500
C	-2.97020602	-0.13384214	2.54858300
H	-2.61645802	-0.99680814	3.11504600
H	-2.58993902	0.77702186	3.01670000
H	-4.05918602	-0.10889714	2.57395900
O	-2.90632402	-1.50292614	0.48918700
O	-1.21912402	-2.86976214	-0.25918300
H	-2.90466002	0.63871686	-0.79423500

HCl

0 1			
Cl	-1.05468747	0.41015624	0.00000000
H	-1.05468747	0.41015624	-1.28926100

Z-IV (d)

0 1			
C	0.62208400	0.56760298	-0.00743033
C	-0.30633500	1.56590298	0.01290967
H	-0.24940400	2.21411498	-0.85295133
C	-1.31451000	1.92600198	1.06054967
C	-2.74128600	2.03466498	0.53103067
C	-3.82142900	1.69711698	1.35282367

C	-3.02202100	2.51318498	-0.75468533
C	-5.13648300	1.82014298	0.91063867
H	-3.63044600	1.33649098	2.35489667
C	-4.33544100	2.64326798	-1.20247233
H	-2.21137800	2.78396298	-1.41838333
C	-5.40043100	2.29498698	-0.37219533
H	-5.95245600	1.54086598	1.56822667
H	-4.52577500	3.01483298	-2.20346733
H	-6.42226900	2.39128998	-0.72210833
C	0.72490400	-0.46679202	1.09006267
C	1.70471500	-1.92355202	2.48744367
C	0.42562400	-2.32565802	2.31428867
N	-0.17313700	-1.41505202	1.44916567
H	2.50661100	-2.33189602	3.07636767
H	-0.11639400	-3.16606502	2.70821667
N	1.88049800	-0.78051502	1.72186767
C	3.13365300	-0.06051902	1.66318467
C	3.33623100	0.98906498	2.56237967
C	4.12070200	-0.49744502	0.77267567
C	4.57822000	1.62551598	2.54903467
C	5.34360500	0.17336698	0.79458467
C	5.59010100	1.23394298	1.67130467
H	4.74930200	2.45121798	3.23110467
H	6.12280300	-0.14077602	0.10770867
C	-1.54362400	-1.53260202	1.00859867

C	-2.55982000	-1.36006802	1.95648367
C	-1.80431400	-1.87721602	-0.32490633
C	-3.87779100	-1.50172002	1.52250067
C	-3.14179700	-1.97848802	-0.70927933
C	-4.18922400	-1.78185402	0.19277467
H	-4.68035700	-1.35117502	2.23640267
H	-3.36865100	-2.22474602	-1.74124433
C	-2.26874800	-1.02275302	3.39941467
H	-1.98727200	-1.91396002	3.96840467
H	-1.45128400	-0.30577102	3.49965767
H	-3.15075200	-0.59376502	3.87640567
C	-5.62438800	-1.81769802	-0.26576633
H	-6.28267700	-2.21916402	0.50817867
H	-5.96367700	-0.80113502	-0.49197633
H	-5.74421000	-2.41905402	-1.16923533
C	-0.69583200	-2.16679102	-1.30515433
H	-0.12801600	-1.27031602	-1.56203933
H	0.01881500	-2.88077502	-0.88440233
H	-1.10329700	-2.59487402	-2.22164733
C	3.85794300	-1.63462602	-0.17705533
H	3.65051900	-2.56471002	0.36135467
H	2.98235100	-1.38952802	-0.78291933
H	4.71602900	-1.80434602	-0.82856733
C	2.24741600	1.41184798	3.51069267
H	1.33588200	1.64009798	2.95848867

H	2.00830500	0.61722198	4.22442467
H	2.53467800	2.30361498	4.06615367
C	6.90742100	1.96892298	1.63729867
H	6.87015100	2.78714198	0.90983467
H	7.14677400	2.40543198	2.60922667
H	7.72606400	1.30804998	1.34409567
O	1.49910000	0.34360298	-0.92372333
C	2.08499600	3.89400798	0.40612267
C	3.09316900	3.11098198	-0.37123433
H	3.99055100	2.97658098	0.22575567
H	2.66135900	2.13061998	-0.61401633
H	3.31961200	3.61803698	-1.31076333
C	-0.08064600	4.93074598	0.03596067
C	-0.34578000	6.20540798	-0.70825633
C	0.71498800	6.65556898	-1.68580333
H	1.67554300	6.77200798	-1.17621933
H	0.86131000	5.89712498	-2.45914033
H	0.41094700	7.59946498	-2.13482533
C	-0.94274200	4.48827898	0.95878967
H	-1.79339100	5.15095398	1.06499867
O	1.06022100	4.27814898	-0.42182533
O	-1.36796400	6.84337698	-0.52788933
C	-0.89348100	3.26958098	1.83154667
C	-1.70001100	3.43196598	3.11272367
C	-1.23263500	2.82571298	4.28567267

C	-2.93372200	4.09148298	3.16343267
C	-1.96873200	2.87093898	5.46755267
H	-0.27942900	2.31098298	4.27621167
C	-3.67233100	4.14427298	4.34414967
H	-3.34418300	4.54963698	2.27260267
C	-3.19538400	3.53266698	5.50184867
H	-1.58091800	2.39445798	6.36123067
H	-4.62644800	4.65938498	4.35465567
H	-3.77045700	3.57377898	6.41998967
H	0.14420400	3.10698198	2.11607367
H	-1.31119200	1.16586198	1.84440767
O	2.11829300	4.16654998	1.57883767

TS5 (d)

0 1			
C	0.71539660	0.58320372	0.00000000
C	-0.40066640	1.41071472	-0.09315500
H	-0.40840340	2.00618272	-0.99775200
C	-1.40407940	1.62580172	0.87533000
C	-2.75399840	2.08107172	0.50564900
C	-3.83605240	1.79354472	1.35266500
C	-3.00849640	2.81669772	-0.66569800
C	-5.12666840	2.21103472	1.03925000
H	-3.65987740	1.23788172	2.26385200
C	-4.29461540	3.24488472	-0.97179400

H	-2.19489740	3.06772072	-1.33345000
C	-5.36263240	2.94066272	-0.12402500
H	-5.94518040	1.97143872	1.70894800
H	-4.46660440	3.81862572	-1.87565400
H	-6.36560340	3.27127372	-0.36933600
C	0.83833960	-0.44738228	1.10276300
C	1.82116260	-1.84907828	2.54653500
C	0.55641760	-2.28885128	2.35038400
N	-0.04513840	-1.41506628	1.45478100
H	2.61880160	-2.22525928	3.16196900
H	0.03073860	-3.13936528	2.74500000
N	1.98772660	-0.71799928	1.76384700
C	3.24653660	-0.00313328	1.68576700
C	3.50369760	1.03214672	2.58538400
C	4.19946260	-0.45612228	0.75914400
C	4.75797360	1.64944472	2.51903500
C	5.42762660	0.19736172	0.73022900
C	5.72334060	1.25590072	1.59760500
H	4.96962160	2.46389672	3.20398000
H	6.17566660	-0.12849128	0.01491800
C	-1.38342940	-1.60900828	0.93988300
C	-2.46346640	-1.47190028	1.82296600
C	-1.54881640	-1.95895528	-0.40612300
C	-3.74601140	-1.63923028	1.30284600
C	-2.85578840	-2.10567428	-0.87412800

C	-3.96386540	-1.93243128	-0.04388500
H	-4.59644140	-1.51449028	1.96452800
H	-3.00760440	-2.36373528	-1.91686000
C	-2.27607740	-1.15545428	3.28680700
H	-2.02875640	-2.05627128	3.85693800
H	-1.47713040	-0.43330528	3.45984100
H	-3.19155140	-0.74116228	3.71002400
C	-5.36663440	-2.02286828	-0.58891200
H	-5.75309640	-1.01967328	-0.79755200
H	-5.40067240	-2.59242828	-1.51955400
H	-6.04424240	-2.49111028	0.12885600
C	-0.37932340	-2.18377228	-1.33174400
H	0.01084760	-1.24059528	-1.72034200
H	0.44739760	-2.68631728	-0.82380600
H	-0.68225640	-2.79951428	-2.17937100
C	3.89726160	-1.59988928	-0.17184000
H	3.65007960	-2.51140028	0.38079800
H	3.03963560	-1.33912128	-0.79533800
H	4.75297660	-1.81474728	-0.81264000
C	2.50099360	1.50825972	3.60302200
H	1.63850260	0.84767072	3.67446900
H	2.96077760	1.57014072	4.59214000
H	2.15210260	2.51022772	3.34172200
C	7.04678460	1.97337772	1.50539600
H	7.01517860	2.72977872	0.71365200

H	7.29204260	2.48334072	2.43889800
H	7.85856560	1.28337772	1.26378800
O	1.66576560	0.53450772	-0.82824500
C	2.20264960	4.06640272	0.61687500
C	3.30339860	3.38717672	-0.14542800
H	4.22278860	3.42057472	0.43166900
H	3.01788160	2.34961972	-0.33618200
H	3.43567860	3.87603772	-1.11272000
C	-0.06709940	4.82690272	0.26873000
C	-0.40024140	5.99370772	-0.55399400
C	0.58765160	6.37104372	-1.64277000
H	1.56943060	6.58911972	-1.21201700
H	0.72726360	5.54147872	-2.34069300
H	0.21487660	7.24709572	-2.17166400
C	-0.86362740	4.41556672	1.29075900
H	-1.74266640	5.04254072	1.39257700
O	1.08676860	4.14257972	-0.15766400
O	-1.42964740	6.64408472	-0.38175000
C	-0.73553640	3.28497872	2.14073200
C	-1.55336040	3.14337072	3.34790000
C	-1.14698540	2.25209672	4.36154100
C	-2.79330340	3.79075272	3.52278100
C	-1.92966240	2.01879272	5.48624200
H	-0.19811840	1.74049472	4.26010000
C	-3.57376040	3.56145672	4.65136400

H	-3.16351040	4.46773672	2.76377000
C	-3.15326840	2.67258172	5.64102900
H	-1.58339640	1.32570272	6.24559500
H	-4.52360140	4.07538972	4.75295400
H	-3.76573640	2.49472072	6.51753000
H	0.24683960	2.83856372	2.20153900
H	-1.38502540	0.98744972	1.74871700
O	2.26037360	4.47693672	1.75009700

vdW intermediate (d)

0 1

C	2.08398141	-0.53654743	0.00000000
C	2.38742441	-1.88583043	0.39098000
H	2.55451241	-2.03988743	1.44957700
C	2.50747341	-2.89061443	-0.51094200
C	2.84866841	-4.27237943	-0.23796400
C	2.92342141	-5.17310543	-1.31724200
C	3.13719641	-4.74156243	1.06080400
C	3.26943541	-6.50330343	-1.11246900
H	2.71970241	-4.81787243	-2.32160600
C	3.48278041	-6.07131343	1.25683000
H	3.14177441	-4.05411143	1.89978900
C	3.54971441	-6.95623143	0.17606500
H	3.33161641	-7.18220743	-1.95465200
H	3.71688741	-6.42043943	2.25579100

H	3.82890641	-7.99082643	0.33895900
C	1.71146141	-0.27250443	-1.45859000
C	1.72396141	0.49666957	-3.54505900
C	0.47304841	0.04372557	-3.28200000
N	0.48239241	-0.43544443	-1.97969800
H	2.15446441	0.93480957	-4.42785100
H	-0.41738259	0.01335157	-3.88425900
N	2.48130741	0.29639257	-2.39837900
C	3.87905641	0.66302957	-2.27439300
C	4.85539341	-0.23946643	-2.70891900
C	4.17915041	1.94460657	-1.79460200
C	6.18317841	0.18330257	-2.64782400
C	5.52391241	2.31097057	-1.74984200
C	6.53684841	1.44414357	-2.16893300
H	6.95600741	-0.50098643	-2.97749800
H	5.78203541	3.29865157	-1.38334700
C	-0.66650759	-0.95603243	-1.26604800
C	-1.04140859	-2.28977743	-1.44787100
C	-1.36951659	-0.07040943	-0.43236100
C	-2.14303259	-2.74784443	-0.71830400
C	-2.45739659	-0.58163643	0.26952100
C	-2.85136859	-1.91912743	0.14920600
H	-2.44861859	-3.78201643	-0.83819500
H	-3.01548859	0.08075357	0.92250900
C	-0.32711659	-3.23961743	-2.37794700

H	-1.04819359	-3.73480743	-3.03223000
H	0.41109741	-2.74740743	-3.01044100
H	0.18304441	-4.01953043	-1.80724200
C	-4.01015859	-2.44769243	0.95663300
H	-4.40927459	-3.36936543	0.52963500
H	-3.69138359	-2.66576543	1.98105900
H	-4.81848559	-1.71515343	1.01632700
C	-0.97216559	1.37931957	-0.31034700
H	-0.00439459	1.48240657	0.18616400
H	-0.88786459	1.85207257	-1.29297000
H	-1.71265059	1.93117257	0.26843500
C	3.09223941	2.88646257	-1.34424800
H	2.35503741	3.05472757	-2.13481100
H	2.56231441	2.47276957	-0.48286700
H	3.51162841	3.85186957	-1.06126800
C	4.53603541	-1.63321043	-3.18394200
H	4.67659441	-2.33896543	-2.36044500
H	3.51505541	-1.73016243	-3.55593400
H	5.21832341	-1.93189143	-3.98089500
C	7.98943941	1.83885157	-2.07774000
H	8.46880641	1.33290957	-1.23316300
H	8.53484341	1.54951957	-2.97922400
H	8.10744741	2.91407657	-1.93269500
O	2.05792941	0.43740357	0.74123900
C	6.84257341	0.62235357	2.13065200

C	7.12751341	2.03541957	1.68799700
H	8.15867041	2.29469357	1.92075800
H	6.92414541	2.15428757	0.62529600
H	6.45943041	2.70968957	2.23183600
C	5.28006941	-1.16507343	1.81943200
C	4.39158741	-1.29029143	2.90584200
C	4.06109641	-0.02866443	3.69479900
H	4.95774641	0.42135657	4.13071700
H	3.59576941	0.71283757	3.03889300
H	3.36725641	-0.29201543	4.49316900
C	5.71126041	-2.21240743	0.98941200
H	5.28120441	-3.17097443	1.25657800
O	5.74521541	0.14679957	1.50147400
O	3.82346541	-2.37273043	3.22299800
C	6.57706941	-2.12739043	-0.06692100
C	6.98392541	-3.20898243	-0.94089000
C	7.98010441	-2.97806943	-1.91936000
C	6.42346741	-4.50875043	-0.90533100
C	8.38123041	-3.96902743	-2.80843000
H	8.44793641	-1.99960943	-1.96565900
C	6.82761941	-5.49615943	-1.79450500
H	5.65254541	-4.74287243	-0.18277500
C	7.80725841	-5.24105643	-2.75900200
H	9.14993941	-3.74887243	-3.54261900
H	6.36463441	-6.47595643	-1.73708700

H	8.11681141	-6.01552543	-3.45156100
H	6.99999741	-1.15421743	-0.29589100
H	2.35132441	-2.66278043	-1.56011400
O	7.47786741	0.01609657	2.95947900

VI (d)

1 1			
C	-0.46656300	0.28771384	0.00000000
C	-1.56617000	1.21751784	-0.14211700
H	-1.77224500	1.49511384	-1.16869100
C	-2.24778200	1.74246584	0.90010000
C	-3.36600600	2.66744184	0.84852900
C	-3.86014100	3.19286484	2.05691900
C	-3.98986500	3.04227584	-0.35716700
C	-4.93836300	4.06981984	2.06276500
H	-3.39034600	2.91120384	2.99263900
C	-5.06777700	3.91486884	-0.34752400
H	-3.63866700	2.64167884	-1.29996400
C	-5.54459100	4.43208284	0.86071000
H	-5.30664500	4.46825884	3.00045300
H	-5.54299300	4.19348784	-1.28043800
H	-6.38786800	5.11268084	0.86199600
C	-0.22456300	-0.40261216	1.33089700
C	0.87627800	-1.30756416	3.03663800
C	-0.39855500	-1.77580916	3.07324600

N	-1.07390400	-1.19999616	2.01064500
H	1.71905200	-1.48660216	3.68050500
H	-0.88477500	-2.46378316	3.74136000
N	0.97095700	-0.46749516	1.94255800
C	2.16797000	0.25133184	1.55189500
C	2.33969600	1.55753484	2.01845000
C	3.10201400	-0.40896816	0.74607900
C	3.50993800	2.21913384	1.64185100
C	4.25341100	0.29731484	0.40178600
C	4.47262600	1.60843784	0.83556100
H	3.67173600	3.23331484	1.99069000
H	4.99563200	-0.18741416	-0.22332600
C	-2.45107300	-1.46912416	1.65048000
C	-3.46883500	-0.94358316	2.45789400
C	-2.70385300	-2.23524416	0.50552400
C	-4.78356400	-1.15491416	2.04458900
C	-4.03956000	-2.41835116	0.14360600
C	-5.08841700	-1.87346916	0.88609400
H	-5.58925300	-0.74381116	2.64325000
H	-4.26174500	-3.00736816	-0.73953600
C	-3.19349500	-0.20644816	3.74584700
H	-3.16717500	-0.90588316	4.58712300
H	-2.23812600	0.32019684	3.74200300
H	-3.98177800	0.51976584	3.94623300
C	-6.51998500	-2.03979416	0.44345300

H	-7.18806400	-2.16645316	1.29809500
H	-6.85298400	-1.15147616	-0.10326400
H	-6.63712400	-2.89946816	-0.21851100
C	-1.59942100	-2.85951416	-0.31332200
H	-1.20401200	-2.16298116	-1.05700800
H	-0.76228700	-3.18309016	0.30878600
H	-1.97738900	-3.73072116	-0.84884800
C	2.85642200	-1.81121816	0.25377800
H	2.70462500	-2.50945716	1.08160100
H	1.95938800	-1.83555616	-0.37005300
H	3.69940400	-2.16723716	-0.33810600
C	1.30317400	2.23241284	2.88178300
H	0.41259100	2.48857084	2.29985600
H	0.98392200	1.59205884	3.70803900
H	1.69656300	3.15701284	3.30373400
C	5.71378600	2.35507184	0.41532800
H	5.57400700	2.79894884	-0.57582300
H	5.94830600	3.16387584	1.10974300
H	6.57692300	1.68863284	0.35569700
O	0.29073300	-0.01700116	-0.90831200
H	-1.93685900	1.46564384	1.90204900

VII (d)

-1 1

C	-0.32659410	-0.14774494	0.00000000
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C	-0.73762910	1.18800806	-0.57149600
H	-1.09534610	1.83633206	0.22584400
H	0.10774590	1.65122206	-1.08419000
H	-1.52845310	1.03991506	-1.31081600
C	0.69315790	-2.22532494	-0.63066100
C	-0.21653610	-3.29936594	-0.49189800
C	-1.70528410	-2.99127594	-0.65503500
H	-1.90205110	-2.33068494	-1.50355100
H	-2.24237110	-3.93132394	-0.78581900
H	-2.08115210	-2.48976194	0.24285300
C	2.08374190	-2.33215594	-0.49917500
H	2.39888190	-3.35146694	-0.29248700
O	0.18160790	-0.93221694	-0.97343800
O	0.13417390	-4.47559294	-0.23004800
C	3.02015090	-1.33459594	-0.60337300
C	4.45257490	-1.48374294	-0.46077000
C	5.29562890	-0.35504894	-0.61186300
C	5.09884990	-2.71238894	-0.17116800
C	6.67713090	-0.44451494	-0.48554900
H	4.84189790	0.60672506	-0.83366100
C	6.47923690	-2.79721094	-0.04582300
H	4.50552790	-3.61053194	-0.04140600
C	7.28920190	-1.66732694	-0.20107000
H	7.28278990	0.44807806	-0.61040700
H	6.93262690	-3.75836994	0.17735400

H	8.36635090	-1.73969094	-0.10174200
H	2.66897590	-0.32891294	-0.82055400
O	-0.45754710	-0.47493894	1.15574800

TS6 (d)

-1 1

C	0.51321930	0.42768273	0.00000000
C	1.19364530	1.53199573	0.77885500
H	1.60124830	2.26899573	0.08856100
H	0.45482530	2.02028873	1.42105000
H	1.97946630	1.13150273	1.42068100
C	-0.36902870	-1.79725427	0.21778600
C	0.29270130	-2.98955927	0.02204100
C	1.77656830	-3.08364227	0.39796400
H	2.18166830	-2.18702027	0.87030600
H	1.91176630	-3.93614527	1.07224800
H	2.35625230	-3.29988527	-0.50680700
C	-1.76990170	-1.52900327	-0.15967100
H	-1.95965570	-1.17432527	-1.17525000
O	0.35156430	-0.65979127	0.76199400
O	-0.24712670	-4.04277127	-0.45697900
C	-2.80896670	-1.66504027	0.67769800
C	-4.23046170	-1.41354827	0.38870100
C	-5.15910570	-1.46052227	1.44247400
C	-4.72017370	-1.12908827	-0.89983900

C	-6.51488470	-1.22350327	1.22728800
H	-4.80682270	-1.68511327	2.44430900
C	-6.07274370	-0.89179827	-1.11597400
H	-4.03674970	-1.10303427	-1.74005000
C	-6.97986670	-0.93556727	-0.05438400
H	-7.20760370	-1.26571727	2.06093200
H	-6.42445870	-0.67666127	-2.11934000
H	-8.03446070	-0.75274627	-0.22754800
H	-2.59653170	-1.99156927	1.69410200
O	0.13237930	0.54207073	-1.14685600

VII' (d)

-1 1

C	1.36846753	-2.32503885	0.01791422
C	2.30839153	-3.35857185	-0.55552578
H	2.69788853	-3.98590485	0.24413122
H	1.80405253	-3.96461185	-1.30913278
H	3.14018153	-2.84423885	-1.04520378
C	-0.28070447	-0.69911285	-0.62996778
C	0.24465653	0.59690815	-0.44927878
C	1.76034953	0.77743115	-0.56628478
H	2.17593453	0.24863215	-1.42838878
H	1.97421353	1.84347115	-0.65102278
H	2.25825353	0.38737015	0.32768822
C	-1.62576647	-1.11662185	-0.58197078

H	-1.74405647	-2.18443185	-0.76264878
O	0.64989753	-1.74855985	-0.96638478
O	-0.46430747	1.60192915	-0.19190078
C	-2.75752547	-0.37275085	-0.35581478
C	-4.11322447	-0.88317385	-0.32825578
C	-5.18778147	0.01229515	-0.10092478
C	-4.46516647	-2.24446885	-0.51321578
C	-6.50983447	-0.41530885	-0.06307078
H	-4.96247447	1.06435415	0.04687922
C	-5.78733047	-2.66799285	-0.47502778
H	-3.68826547	-2.98083385	-0.68672978
C	-6.82906747	-1.76228485	-0.25004978
H	-7.29937147	0.30884915	0.11403522
H	-6.01112947	-3.72059685	-0.62122178
H	-7.85932847	-2.09863185	-0.22052478
H	-2.63026747	0.68869415	-0.18094278
O	1.29927953	-2.03432685	1.18904122