

## Supporting Information

### **Computational insight into the cooperative role of noncovalent interactions in the aza-Henry reaction catalyzed by quinine-derivatives: mechanism and enantioselectivity**

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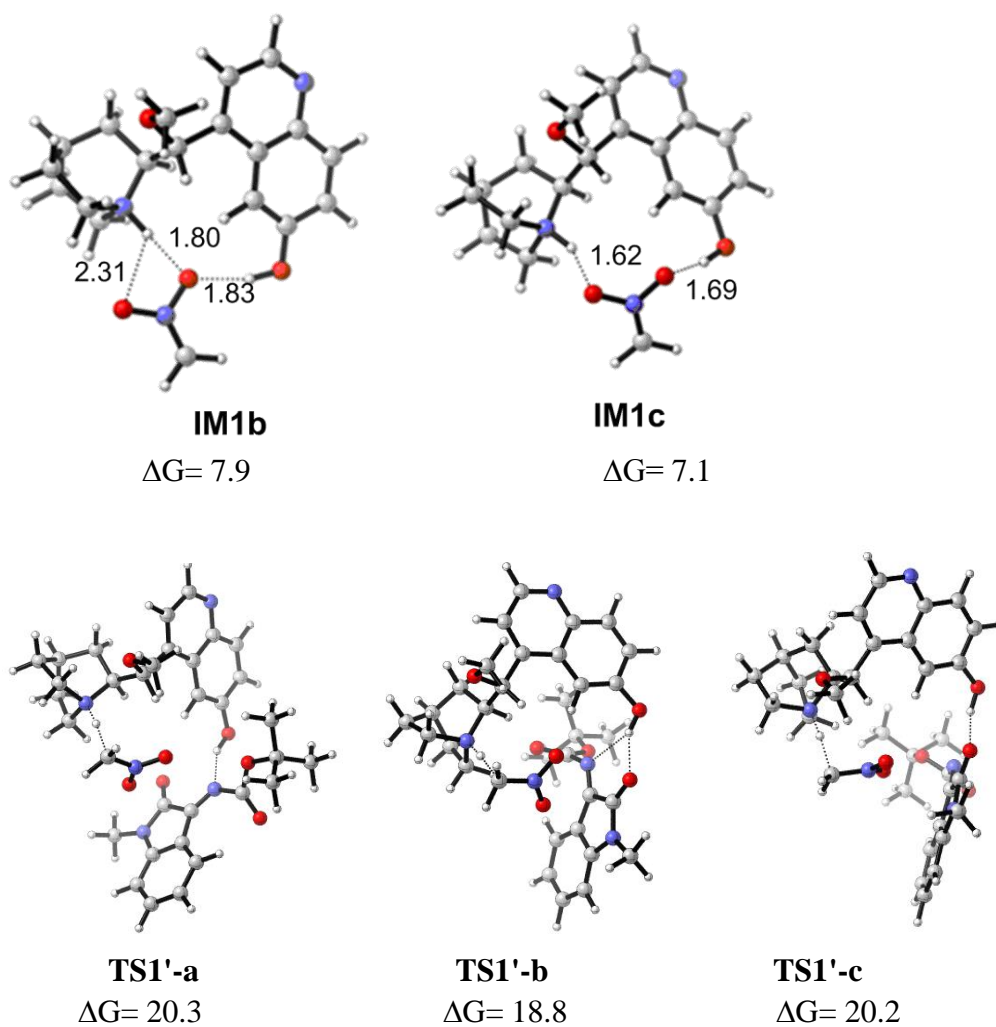
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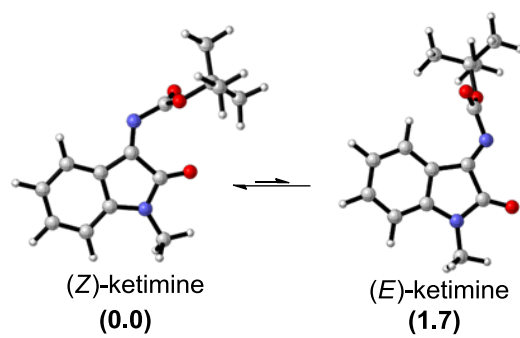
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### **Complete citing of reference 10.**

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, revision D.01, 2013.

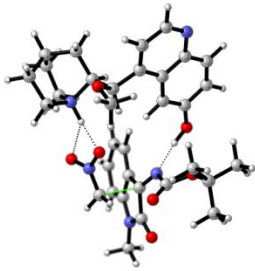
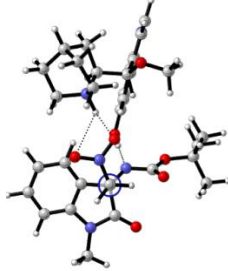
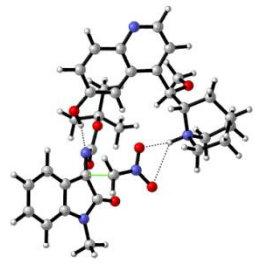
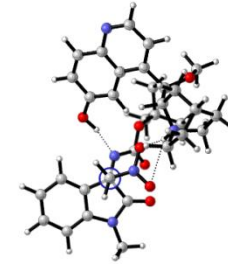
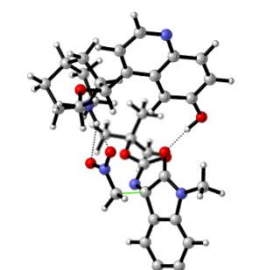

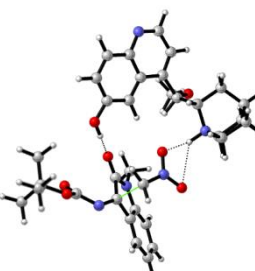



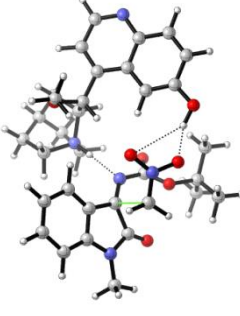
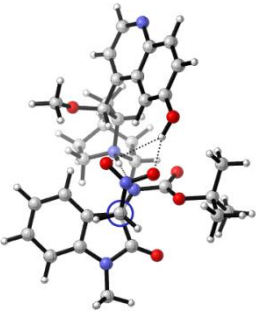
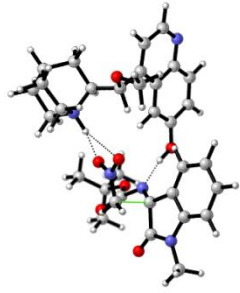
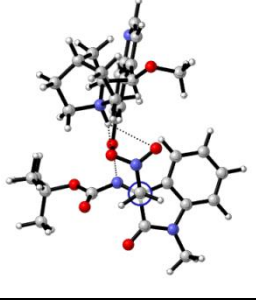
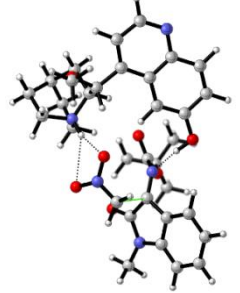
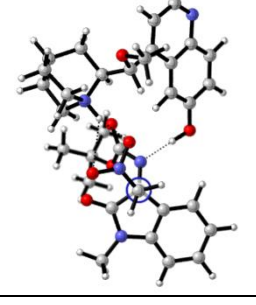
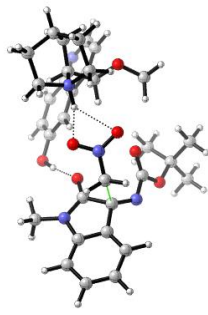
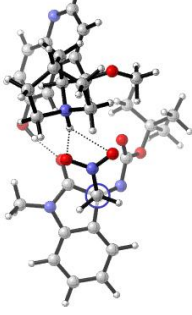
**Fig. S1.** The located less-stable conformations and the relative free energy for **IM1a** and **TS1'**.



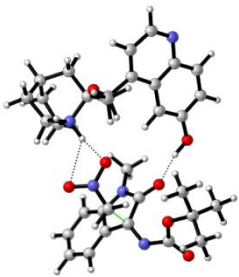
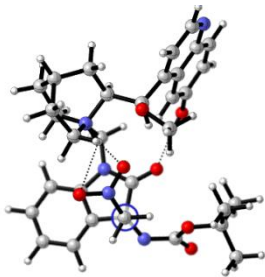
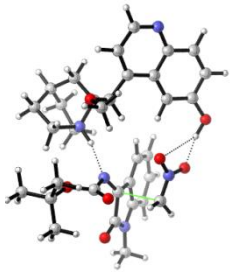
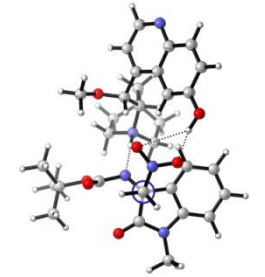
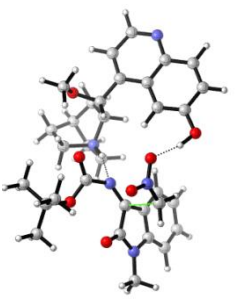
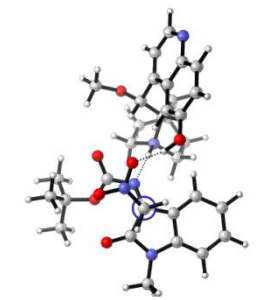
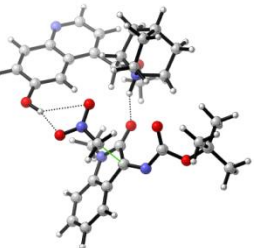
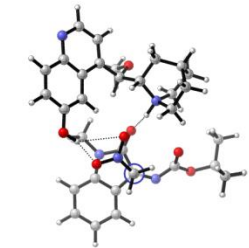
**Fig.S2** Two isomers of isatin-derived *N*-Boc ketimine (**1**) and the relative free energy with respect to the most stable *Z*-form.

**Table S1** The optimized structure of TS2s and their relative free energy with respect to the lowest-energy TS2 (**si-TS2a**) involving the Z-ketimine (Z-TS2s). See the main text for nomenclature of the transition states.

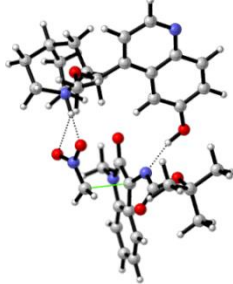
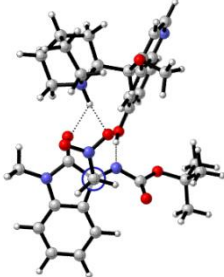
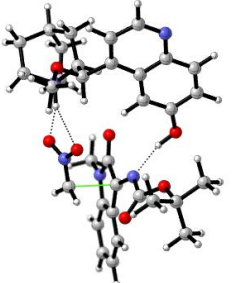
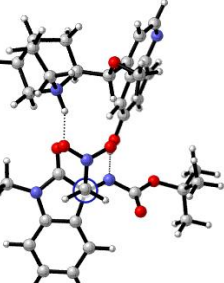
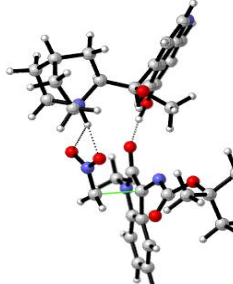
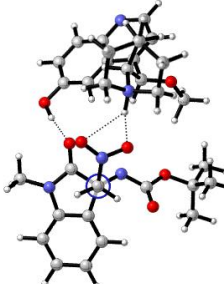
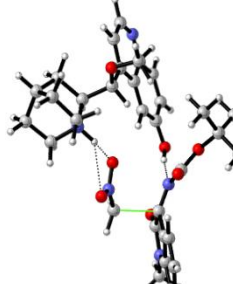
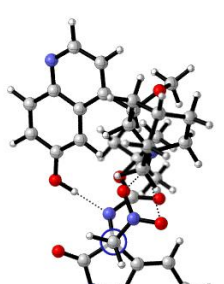
nomenclature	Normal	Newman	$\Delta\Delta G^\ddagger$	D(NCCN)
<b>a'-N-gau1-syn-R</b>			2.2	66.1
<b>a'-N-gau2-syn-R</b>			10.8	-61.6
<b>a'-N-anti-R</b>	the same with <b>a'-N-gau1-syn-R</b>			
<b>a'-O-gau1-syn-R</b>	failed to locate			
<b>a'-O-gau2-syn-R</b>			13.7	-53.8
<b>a'-O-snti-R</b>			15.9	-176.5

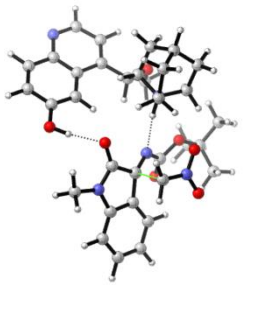
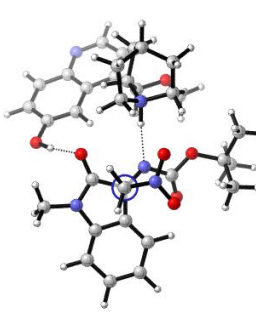
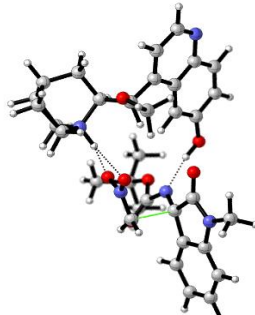
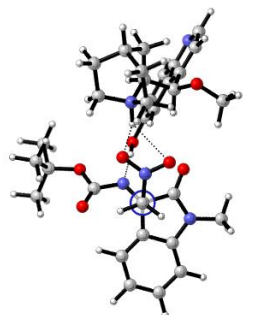
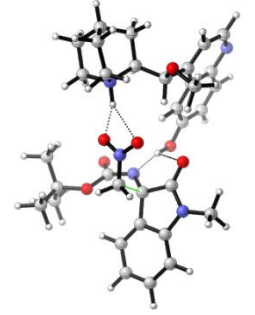
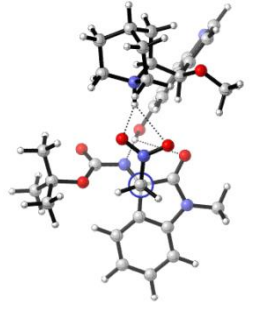
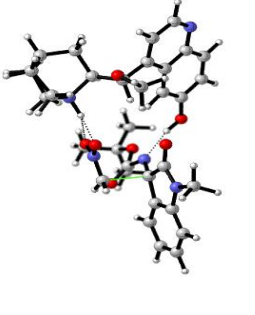
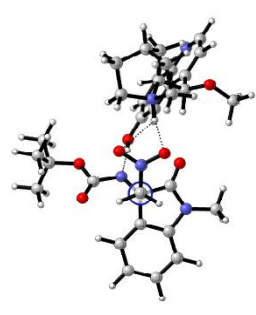
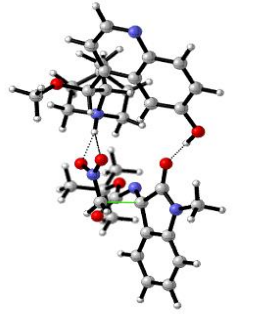
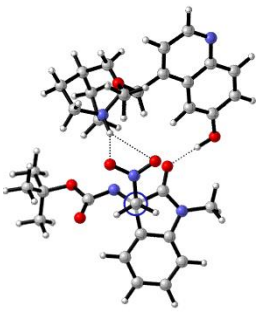
<b>b'-N-gau1-syn-R</b>			8.2	19.4
<b>b'-N-gau2-syn-R</b>	failed to locate			
<b>b'-N-snti-R</b>	failed to locate			
<b>b'-O-gau1-syn-R</b>	failed to locate			
<b>b'-O-gau2-syn-R</b>	failed to locate			
<b>b'-O-snti-R</b>	failed to locate			
<b>a'-N-gau1-syn-S</b>			5.0	-53.1
<b>a'-N-gau2-syn-S</b>			6.2	42.7
<b>a'-N-anti-S</b>	failed to locate			
<b>a'-O-gau1-syn-S</b>	failed to locate			
<b>a'-O-gau2-syn-S</b>			12.5	74.4

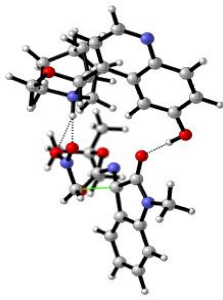
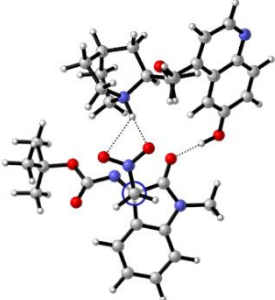
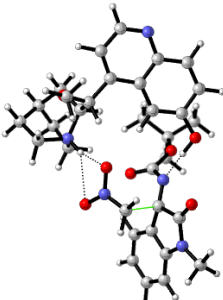

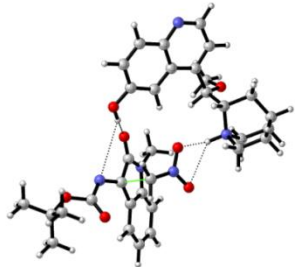
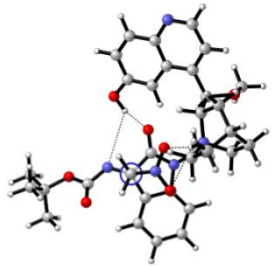
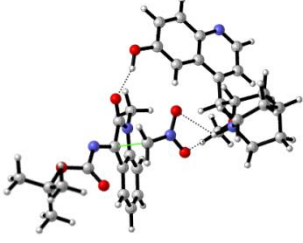
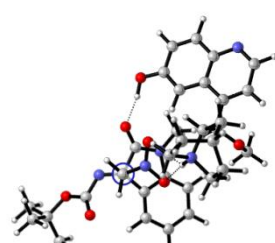


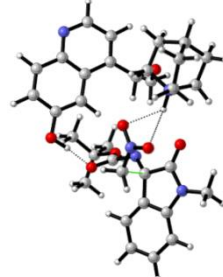
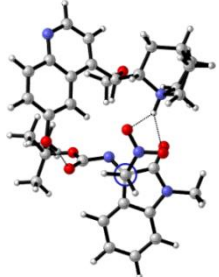
<b>a'-O-anti-S</b>			12.4	172.3
<b>b'-N-gau1-syn-S</b>			6.0	-66.7
<b>b'-N-gau2-syn-S</b>			16.2	20.7
<b>b'-N-anti-S</b>	failed to locate			
<b>b'-O-gau1-syn-S</b>	failed to locate			
<b>b'-O-gau2-syn-S</b>	the same with <b>b'-O-anti-S</b>			
<b>b'-O-anti-S</b>			4.9	148.7

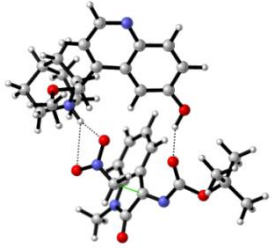
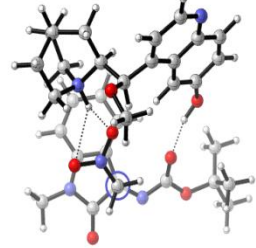
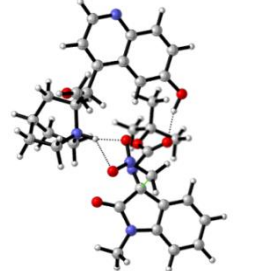
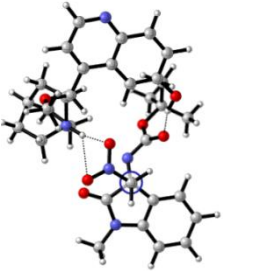
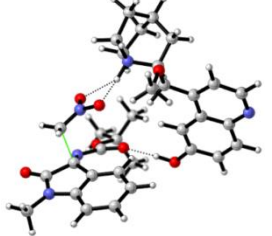

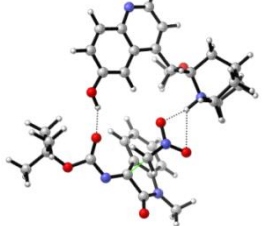
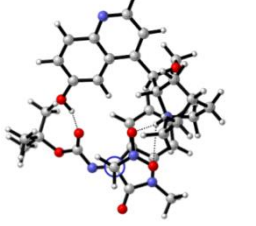
**Table S2.** The optimized structure and relative free energy of the C-C formation transition states (**TS2**) involved in the mode **a** for *E*-ketimine. See the main text for nomenclature of the transition states.

nomenclature	Normal View	Newman projection	$\Delta\Delta G^\ddagger$ (kcal/mol)	$D_{(NCCN)}$ (degree)
<b>a-N-gau1-syn-S</b> (si-TS2a)			<b>0.0</b>	<b>75.2</b>
<b>a-N-gau1-anti-S</b> (si-TS2c)			<b>1.0</b>	<b>58.5</b>
<b>a-O-gau1-syn-S</b>			<b>6.9</b>	<b>53.3</b>
<b>a-O-gau1-anti-S</b>	<i>the same with a-N-gau1-anti-S</i>			
<b>a-N-gau2-syn-S</b>			<b>8.5</b>	<b>-47.9</b>
<b>a-N-gau2-anti-S</b>	<i>the same with a-N-gau2-syn-S</i>			

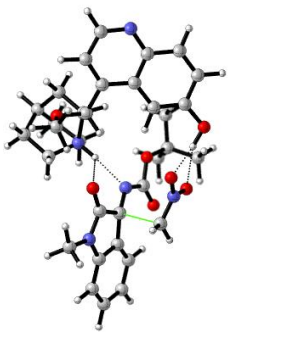
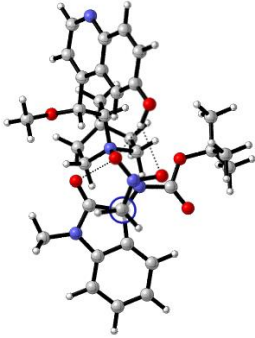
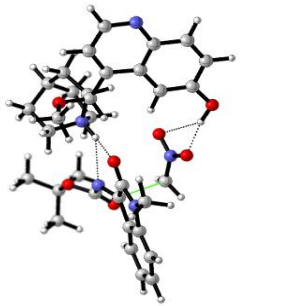
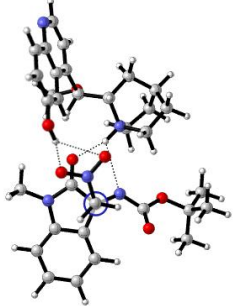
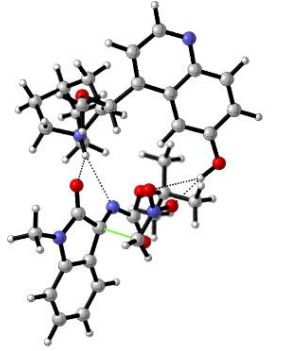
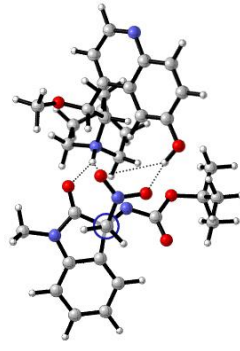
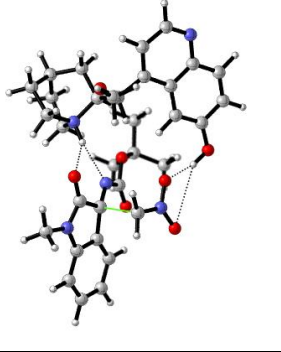
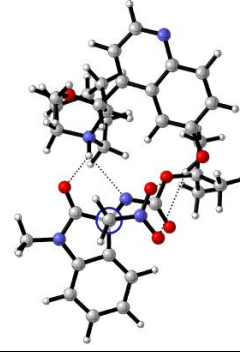
<b>a-O-gau2-syn-S</b> (a structure with only ketimine binding to catalyst)			<b>7.9</b>	<b>-36.4</b>
<b>a-O-gau2-anti-S</b>	<i>the same with a-O-gau1-syn-S</i>			
<b>a-N-anti-S</b>	<i>the same with a-N-gau1-anti-S</i>			
<b>a-O-anti-S</b>	<i>the same with a-N-gau1-anti-S</i>			
<b>a-N-gau1-syn-R</b>			<b>2.1</b>	<b>-49.2</b>
<b>a-N-gau1-syn-R-Boc-rotator</b>			<b>4.2</b>	<b>-45.4</b>
<b>a-N-gau1-anti-R</b>			<b>3.3</b>	<b>-45.3</b>
<b>a-O-gau1-syn-R</b>			<b>4.0</b>	<b>-49.7</b>

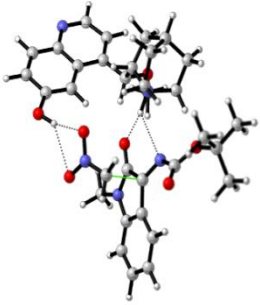
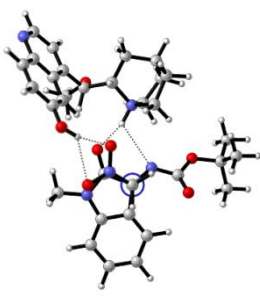
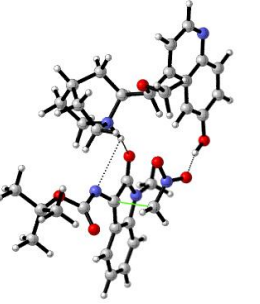
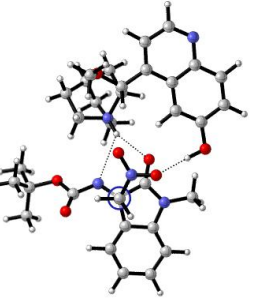
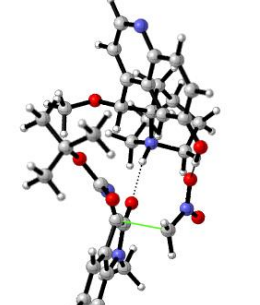
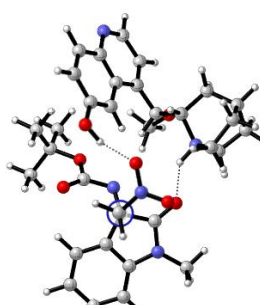
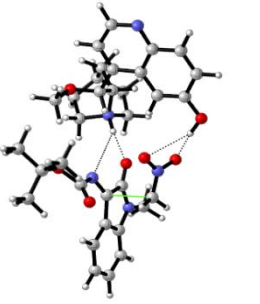
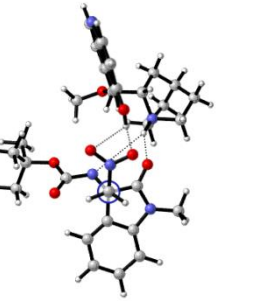
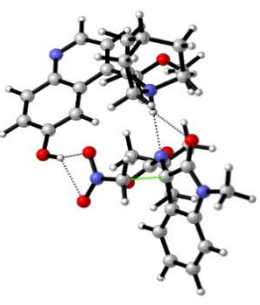
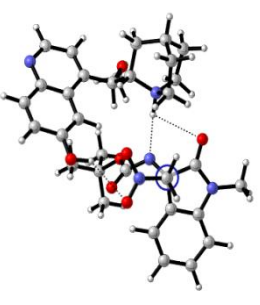
<b>a-O-gau1-anti-R</b>			<b>6.5</b>	<b>-35.2</b>
<b>a-N-gau2-syn-R</b>			<b>5.1</b>	<b>48.1</b>
<b>a-N-gau2-anti-R</b>	<i>the same with a-N-gau1-syn-R</i>			
<b>a-O-gau2-syn-R</b>	<i>the same with a-N-gau2-syn-R</i>			
<b>a-O-gau2-anti-R</b>	<i>the same with a-O-anti-R</i>			
<b>a-N-anti-R</b>	failed to locate			
<b>a-O-anti-R-1</b>			<b>10.6</b>	<b>-158.0</b>
<b>a-O-anti-R-2</b>			<b>11.2</b>	<b>-162.5</b>

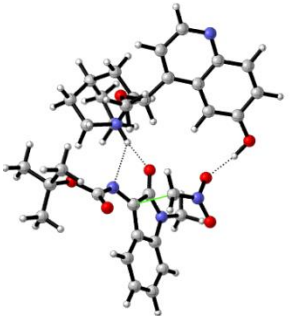
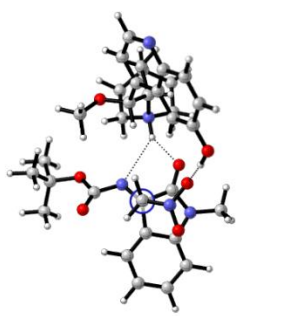
	<b>Normal</b>	<b>Newman project</b>	$\Delta\Delta G$	$D_{(NCCN)}$ (degree)
<b>TS2-a-Boc-O-gau1-R</b>			<b>4.6</b>	<b>-72.1</b>

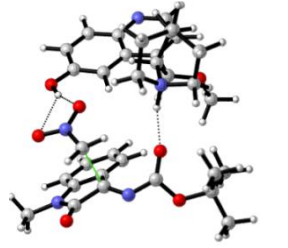
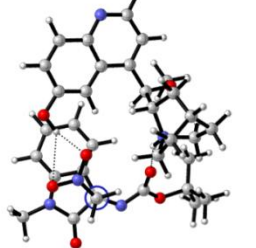
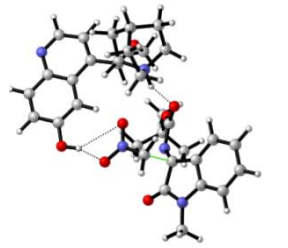
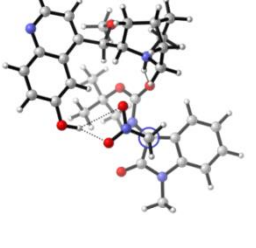
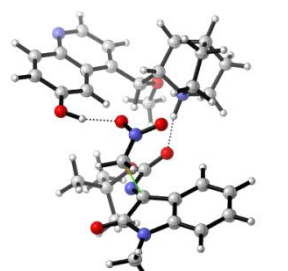
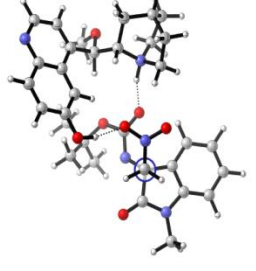
TS2-a-Boc-O-gau2-R	<i>the same with TS2-a-Boc-O-anti-R</i>			
TS2-a-Boc-O-anti-R			9.2	151.8
TS2-a-Boc-O-gau1-S			5.4	51.0
TS2-a-Boc-O-gau2-S			8.5	-54.7
TS2-a-Boc-O-anti-S			9.5	-152.9

**Table S3.** The optimized structure and relative free energy of transition states involved in the mode **b** for *E*-ketimine. See the main text for nomenclature of the transition states.

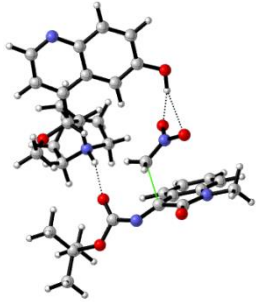
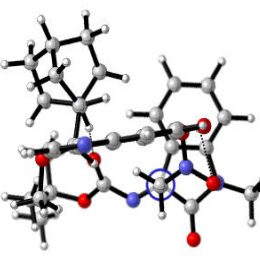
nomenclature	Normal View	Newman projection	$\Delta\Delta G^\ddagger$ (kcal/mol)	$D_{(NCCN)}$ (degree)
<b>b-N-gau1-syn-S</b>	<i>the same with b-O-anti-S</i>			
<b>b-N-gau1-anti-S</b>			<b>6.5</b>	<b>11.0</b>
<b>b-O-gau1-anti-S</b>			<b>0.3</b>	<b>82.2</b>
<b>b-O-gau1-syn-S</b>			<b>4.9</b>	<b>28.6</b>
<b>b-N-gau2-syn-S</b>			<b>6.8</b>	<b>-44.9</b>
<b>b-N-gau2-anti-S</b>	<i>the same with b-O-gau1-syn-S</i>			
<b>b-O-gau2-syn-S</b>	<i>the same with b-N-gau2-syn-S</i>			

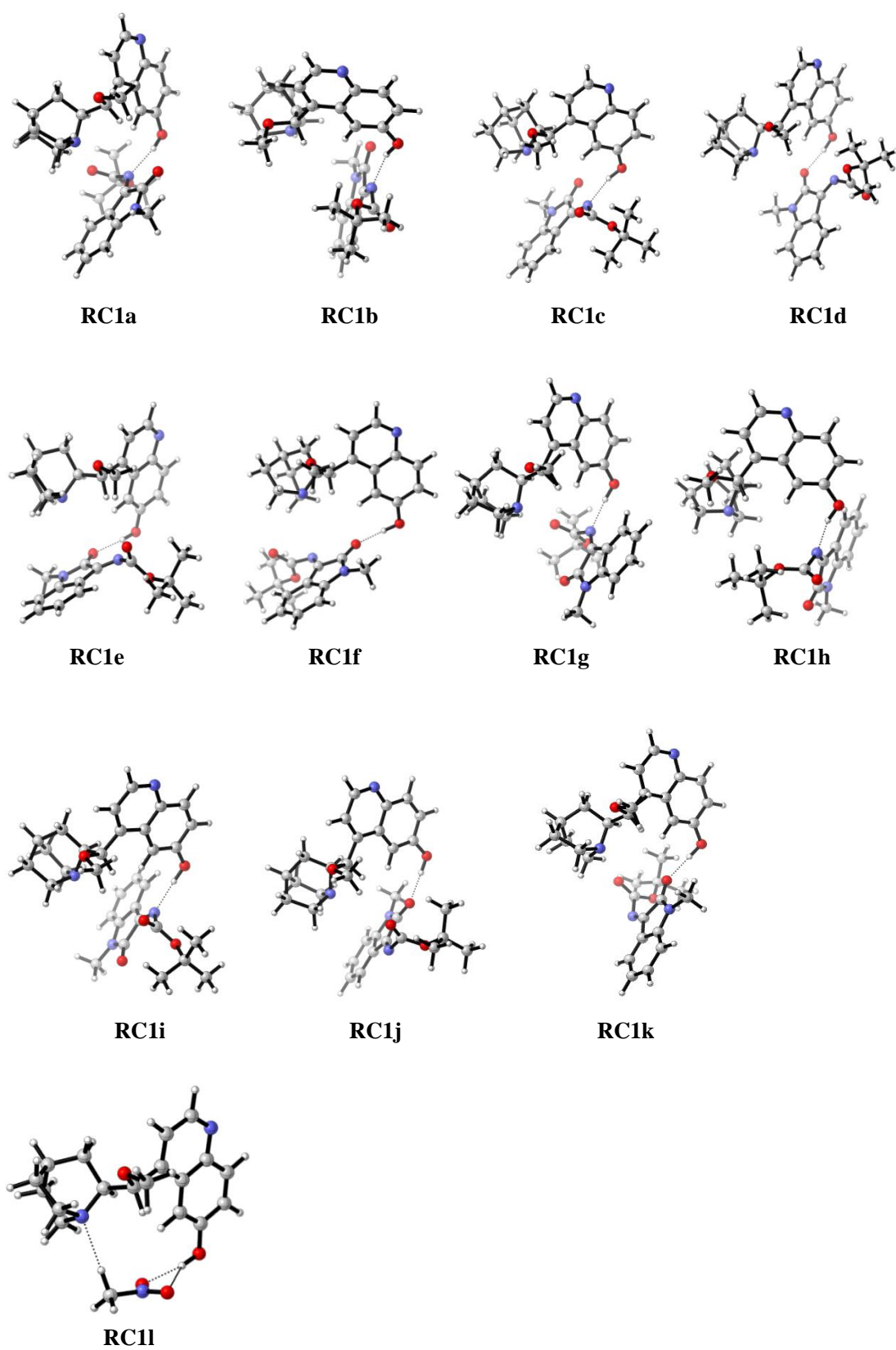
<b>b-O-gau2-anti-S</b>	<b>fail to located</b>			
<b>b-N-anti-S</b>	<i>the same with b-O-anti-S</i>			
<b>b-O-anti-S</b>			<b>2.8</b>	<b>108.0</b>
<b>b-N-gau1-syn-R</b>	<i>the same with b-O-anti-R</i>			
<b>b-N-gau1-anti-R (re-ts2b)</b>			<b>2.3</b>	<b>-82.8</b>
<b>b-O-gau1-syn-R</b>			<b>2.6</b>	<b>-65.5</b>
<b>b-O-gau1-anti-R</b>			<b>9.0</b>	<b>-43.9</b>
<b>b-N-gau2-syn-R</b>			<b>7.7</b>	<b>42.0</b>

<b>b-N-gau2-anti-R</b>	<i>the same with b-O-gau1-syn-R</i>			
<b>b-O-gau2-syn-R</b>	<i>the same with b-N-gau2-syn-R</i>			
<b>b-O-gau2-anti-R</b>	<i>the same with b-O-gau1-syn-R</i>			
<b>b-N-anti-R</b>	<i>the same with b-O-anti-R</i>			
<b>b-O- anti-R</b>			6.3	-148.9

	Normal	Newman project	$\Delta\Delta G$	D(N-C-C-N)
<b>TS2-b-Boc-O-gau1-R</b>	<i>the same with TS2-c-gau1-OS-R</i>			
<b>TS2-b-Boc-O-gau2-R</b>	<i>the same with TS2-a-N-gau2-syn-R</i>			
<b>TS2-b-Boc-O-anti-R</b>			16.9	154.3
<b>TS2-b-Boc-O-gau1-S</b>			7.8	20.4
<b>TS2-b-Boc-O-gau2-S</b>			6.3	-61.0



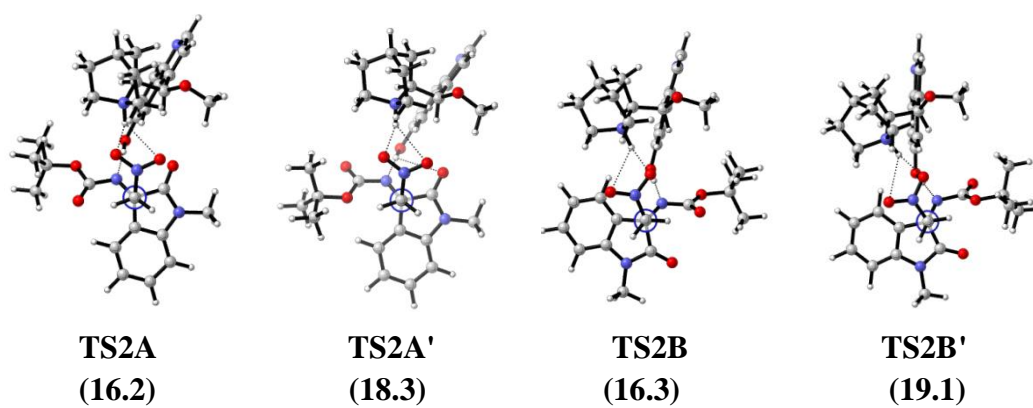
<b>TS2-b-Boc-O-anti-S</b>			13.1	-174.8
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**Fig.S3** The structure and relative energy of the possible complex of catalyst with substrates.

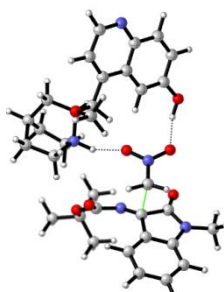
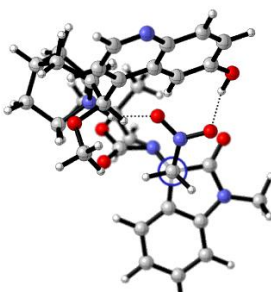
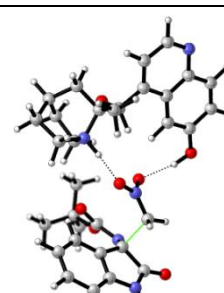
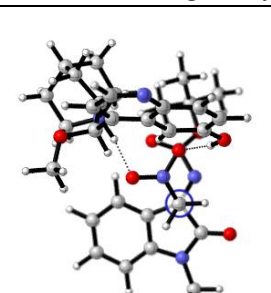
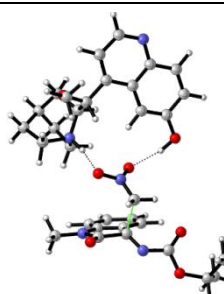
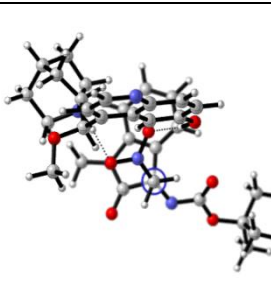
**Table S4** The relative energy, enthalpy and free energy (in kcal/mol) of the possible complex of catalyst with substrates.

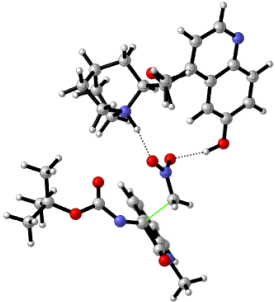
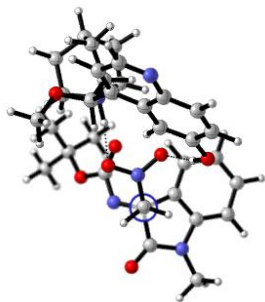
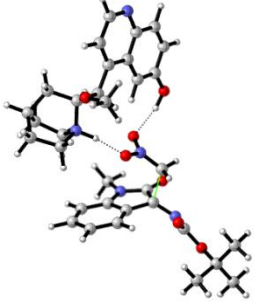
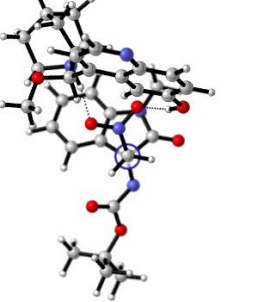
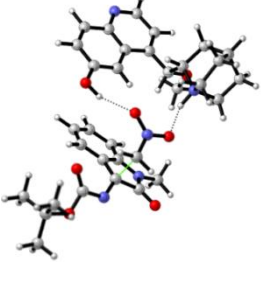
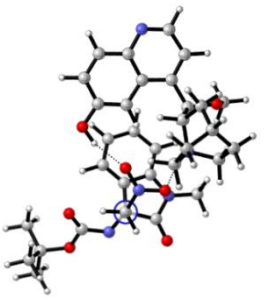
<b>RC1</b>		<b>Distance of the key HB</b>	<b>ΔE</b>	<b>ΔH</b>	<b>ΔG</b>
<b>RC1a</b>	cata- <i>E</i> -imine -N-com1	1.99	-11.6	-12.2	-0.1
<b>RC1b</b>	cata- <i>E</i> -imine -N-com2	1.99	-10.8	-11.4	0.6
<b>RC1c</b>	cata- <i>E</i> -imine -N-com2-Boc-rotator	2.07	-11.6	-12.2	-1.4
<b>RC1d</b>	cata- <i>E</i> -imine-O-com1	1.87	-11.8	-12.4	<b>-1.8</b>
<b>RC1e</b>	cata- <i>E</i> -imine-O-com1-Boc-rotator	1.86	-12.5	-13.1	-1.2
<b>RC1f</b>	cata- <i>E</i> -imine-O-com2	1.81	-9.5	-10.1	0.7
<b>RC1g</b>	cata- <i>Z</i> -imine -N-com1	1.91	-10.0	-10.6	<b>0.3</b>
<b>RC1h</b>	cata- <i>Z</i> -imine -N-com2	1.93	-10.0	-10.6	2.3
<b>RC1i</b>	cata- <i>Z</i> -imine -N-com2-Boc-rotator	1.92	-10.5	-11.1	1.2
<b>RC1j</b>	cata- <i>Z</i> -imine -O-com1	1.81	-11.1	-11.7	2.0
<b>RC1k</b>	cata- <i>Z</i> -imine -O-com2	1.81	-8.8	-9.4	2.5
<b>RC1l</b>	cata-CH <sub>3</sub> NO <sub>2</sub> -com1	1.93	-8.2	-8.8	3.3

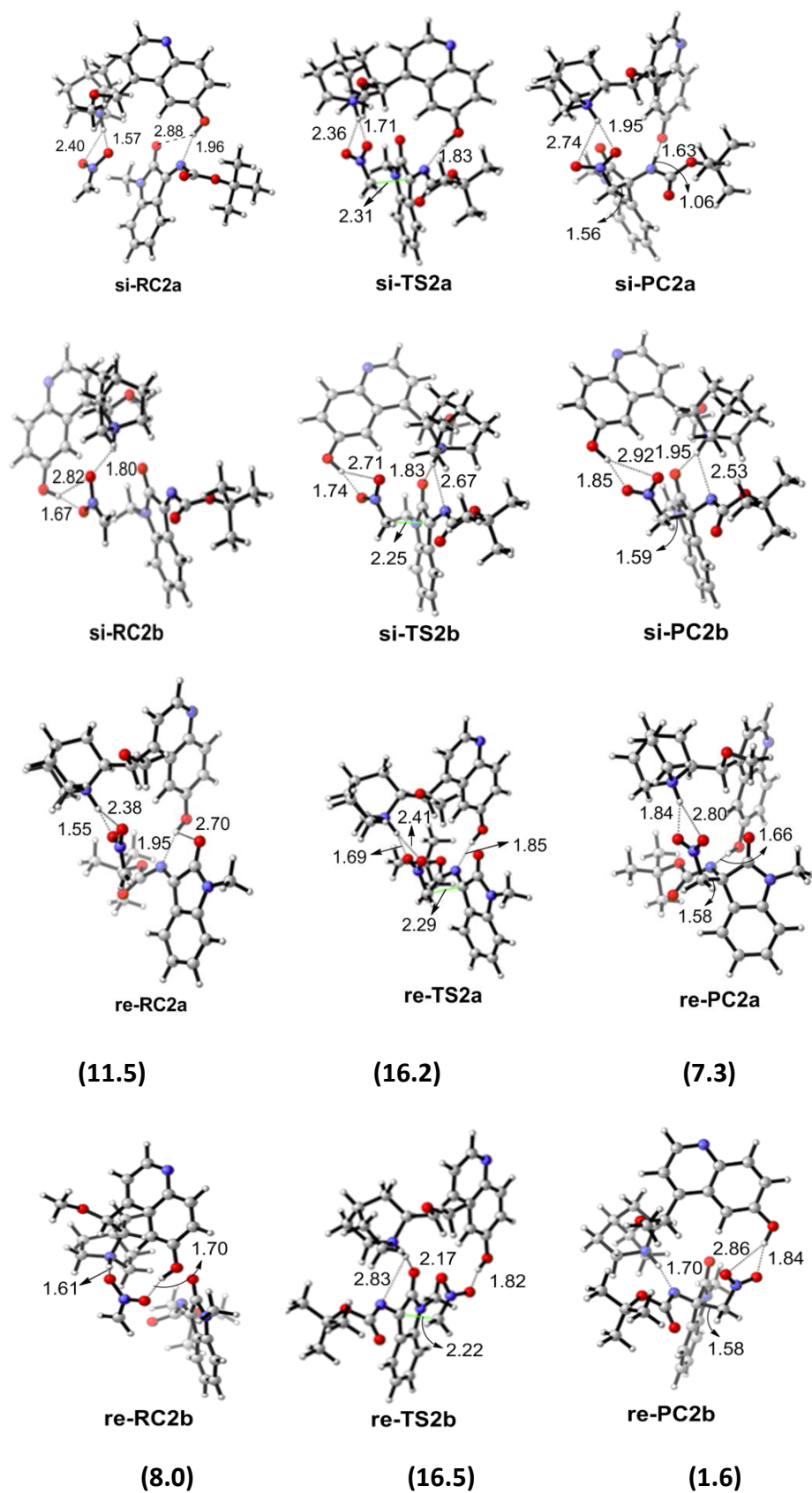


**Fig. S4** Comparison of two couples of transition states with different orient of Boc group. Values in parathesis are the relative Gibbs free energy (kcal/mol).

**Table S5** The optimized structure and relative free energy of transition states involved in the mode **c** for *E*-ketimine. See the main text for nomenclature of the transition states.

nomenclature	Normal View	Newman projection	$\Delta\Delta G^\ddagger$ (kcal/mol)	$D_{(NCCN)}$ (degree)
TS2-c-gau1-OS-R			10.0	-52.3
TS2-c-gau1-SS-R	<i>the same with TS2-b-O-gau1-syn-R</i>			
TS2-c-gau2-OS-R			14.0	59.3
TS2-c-gau2-SS-R	<i>the same with TS2-a-Boc-O-anti-R</i>			
TS2-c-anti-OS-R			13.7	175.8
TS2-c-anti-SS-R	<i>the same with TS2-a-O-anti-R</i>			
TS2-c-gau1-OS-S	<i>the same with TS2-b-N-gau1-syn-S</i>			
TS2-c-gau1-SS-S	<i>the same with TS2-b-N-gau1-anti-S</i>			

<b>TS2-c-gau2-OS-S</b>			13.0	-65.2
<b>TS2-c-gau2-SS-S</b>	<i>the same with TS2-a-N-gau2-syn-S</i>			
<b>TS2-c-anti-OS-S</b>			11.5	-173.7
<b>TS2-c-anti-SS-S</b>			12.6	-171.5

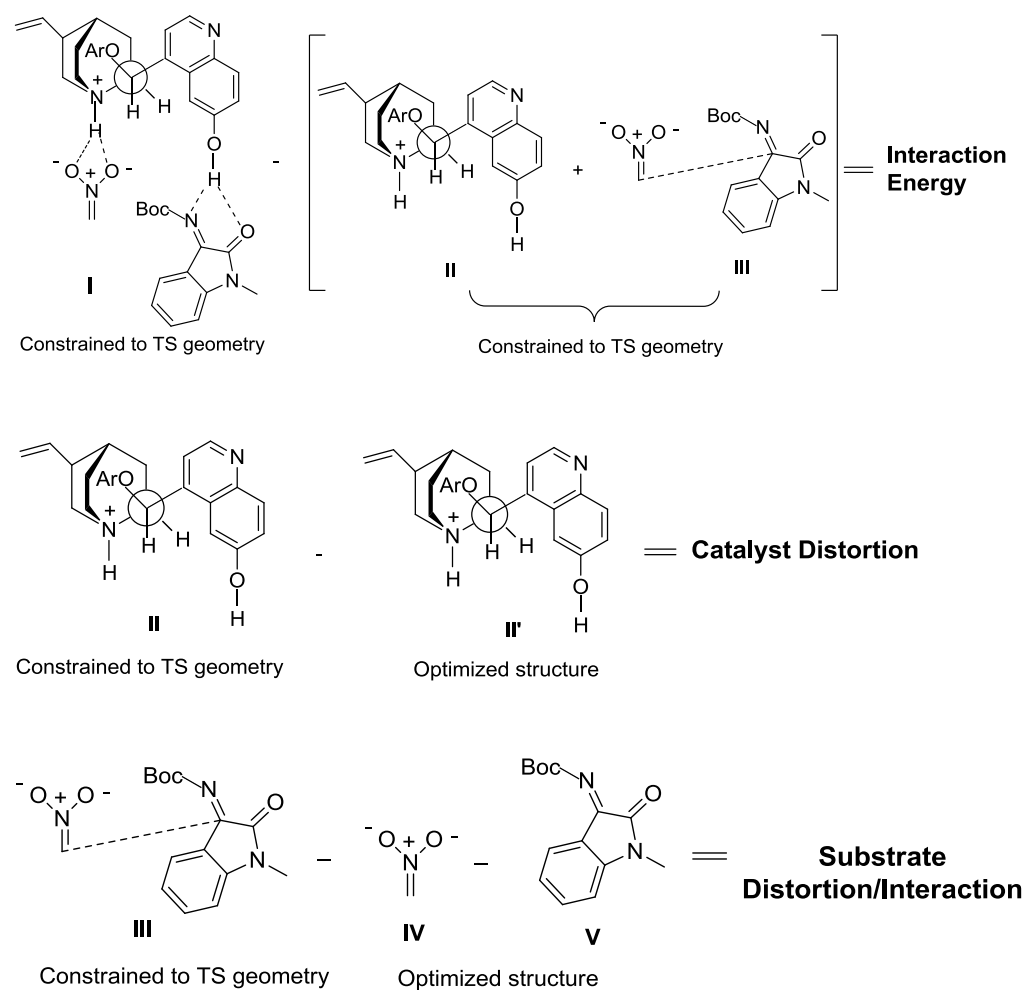


**Fig. S5** Optimized structure and relative free energy (in kcal/mol) of the stationary points for the C-C bond forming step leading to the *S*- and *R*-products in modes **a** and **b**. Bond distances are given in angstroms.

**Table S6.** NBO analysis of the lowest-energy transition states leading to the *S*-product for mode **a** and **b**.

Donor	Acceptor	$\Delta E_{\text{NBO}}$ (kcal/mol)	
		<i>si-TS2a</i>	<i>si-TS2b</i>
LP O1	BD*N-H1(O-H2)	36.21	0.35
LP O2	BD*N-H1(O-H2)	1.84	30.52
LP O3	BD*O-H2(N-H1)	0.11	22.07
LP N1	BD*O-H2(N-H1)	23.32	1.13

**Scheme S1.** Distortion/interaction analysis of the studied reaction.





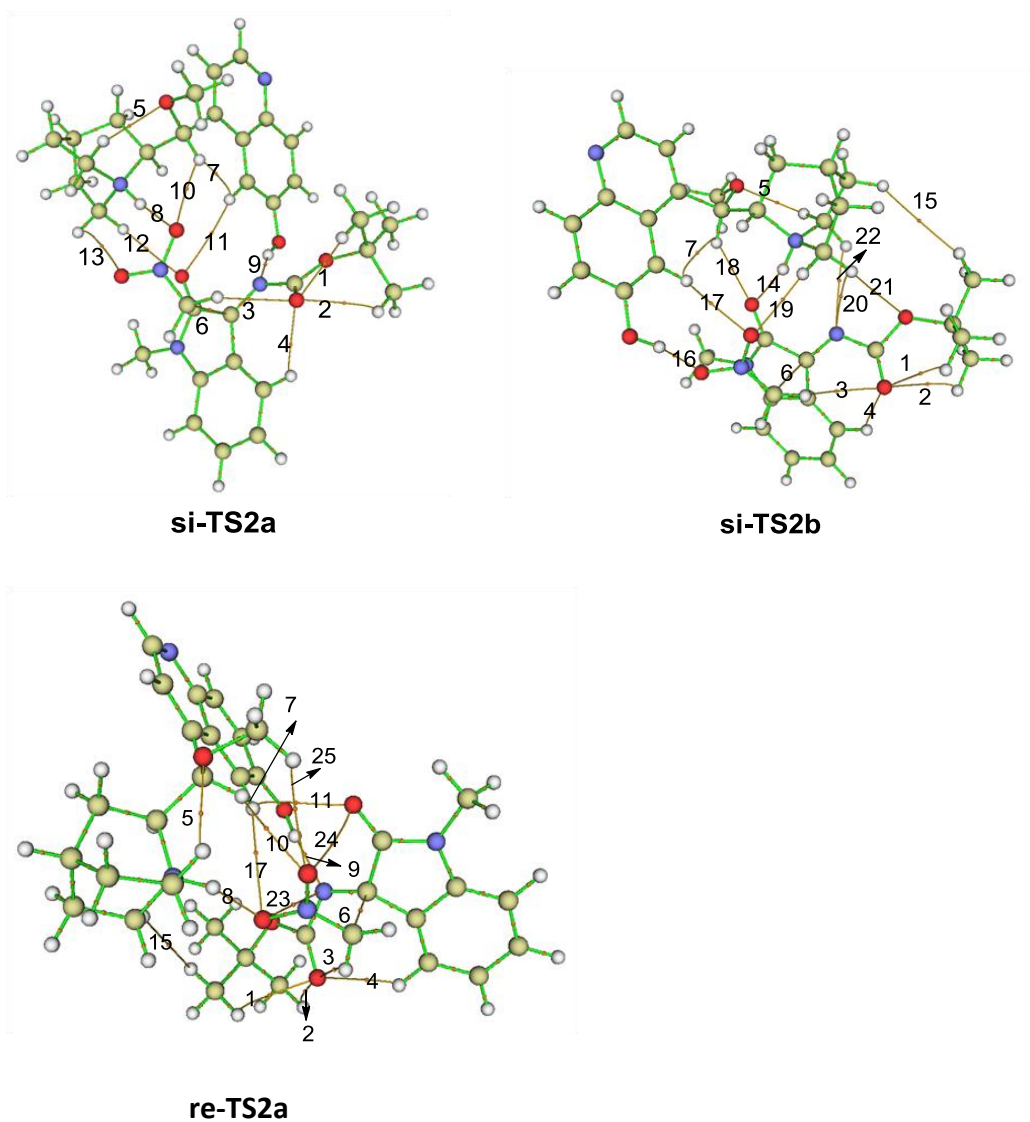
**Table S7** Distortion/interaction analysis of the five lowest energy transition states using the model catalyst at the SMD-D3-B3LYP-6311++G(d,p)// SMD-B3LYP-631G(d) level.

	<i>si-TS2a</i>	<i>si-TS2b</i>	<i>re-TS2a</i>	<i>si-TS2c</i>	<i>re-TS2b</i>	$\Delta\Delta E_1$	$\Delta\Delta E_2$	$\Delta\Delta E_3$	$\Delta\Delta E_4$
$\Delta E_{\text{int}}$	-71	-71.7	-69.2	-71.4	-70.3	0.7	1.8	0.4	1.2
$\Delta E_{\text{dist}}$	1.7	1.2	2.3	2.2	2.3	0.5	0.5	-0.5	0.0
$\Delta E_{\text{int/dist}}$	-5.3	-5.4	-5.4	-5.0	-4.7	0.1	-0.1	-0.3	-0.7
<b>total</b>	-74.5	-75.8	-72.3	-74.2	-72.7	1.3	2.2	-0.3	0.5

$\Delta\Delta E_1 = \Delta E(\text{si-TS2a}) - \Delta E(\text{si-TS2b})$ ;  $\Delta\Delta E_2 = \Delta E(\text{re-TS2a}) - \Delta E(\text{si-TS2a})$ ;  $\Delta\Delta E_3 = \Delta E(\text{si-TS2a}) - \Delta E(\text{si-TS2c})$ ;  $\Delta\Delta E_4 = \Delta E(\text{re-TS2a}) - \Delta E(\text{re-TS2b})$

**Table S8.** Comparison of the relative free energy of the lowest energy TSs leading to S-product in modes **a** and **b** at different level of theory.

method	$\Delta G^\ddagger$		$\Delta\Delta G^\ddagger$
	<b>si-TS2a</b>	<b>si-TS2b</b>	
SMD-D3-B3LYP-6311++G**//SMD-B3LYP-631G*	14.1	14.4	0.3
SMD-B3LYP-6311++G**//SMD-B3LYP-631G*	36.0	37.5	1.5



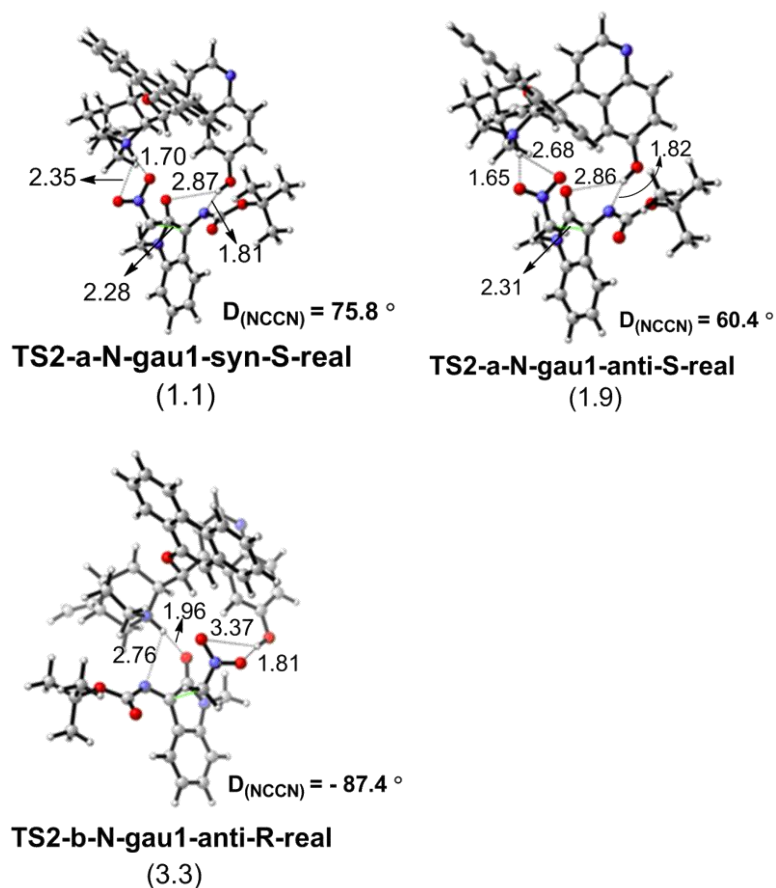
**Fig.S6** AIM plots depicting bond critical points (BCPs) along the bond paths in the transition states of **si-TS2a**, **si-TS2b** and **re-TS2a**.

**Table S9.** Summary of electron densities at the bond critical points (BCPs) along the bond paths, type and distance of interactions in **si-TS2a**, **si-TS2b** and **re-TS2a**.

Bond path	Type of Interaction	Distance (Å)			$\rho_{bcp} * 10^{-2}$ (in a.u)		
		si-TS2a	si-TS2b	re-TS2a	si-TS2a	si-TS2b	re-TS2a
1	CH...O	2.45	2.42	2.42	1.2140	1.2968	1.2943
2	CH...O	2.44	2.42	2.44	1.2645	1.2873	1.2392
3	CH...O	2.39	2.61	2.49	1.1970	0.7799	0.9801
4	CH...O	2.34	2.29	2.25	1.3328	1.4759	1.6018
5	CH...O	2.3	2.31	2.32	1.5395	1.5221	1.5115
6	C-C formation	2.31	2.25	2.29	4.7027	5.3797	4.8962
7	CH...HC	2.11	2.13	2.06	1.0398	1.0211	1.1076
8	NH...O	1.71	-	1.69	4.8320	<i>No bcp</i>	5.1033
9	OH...N	1.83	-	1.85	3.9520	<i>No bcp</i>	3.7411
10	CH...O	2.47	-	2.61	0.8869	<i>No bcp</i>	0.7884
11	CH...O	2.99	-	2.64	0.3289	<i>No bcp</i>	0.7604
12	CH...O	2.46	-	-	0.8883	<i>No bcp</i>	<i>No bcp</i>
13	CH...O	2.58	-	-	0.9168	<i>No bcp</i>	<i>No bcp</i>
14	NH...O	-	1.83	-	<i>No bcp</i>	3.5228	<i>No bcp</i>
15	CH...HC	-	3.11	4.27	<i>No bcp</i>	0.1046	0.0608
16	OH...O	-	1.74	-	<i>No bcp</i>	4.2578	<i>No bcp</i>
17	CH...O	-	2.72	3.13	<i>No bcp</i>	0.6035	0.2346
18	CH...O	-	2.29	-	<i>No bcp</i>	1.301	<i>No bcp</i>
19	CH...O	-	2.34	-	<i>No bcp</i>	1.1581	<i>No bcp</i>
20	CH...N	-	2.67	-	<i>No bcp</i>	0.8222	<i>No bcp</i>
21	CH...O	-	2.6	-	<i>No bcp</i>	0.7325	<i>No bcp</i>
22	CH...N	-	2.79	-	<i>No bcp</i>	0.6734	<i>No bcp</i>
23	anion(O)... $\pi$	-	-	3.01	<i>No bcp</i>	<i>No bcp</i>	0.9533
24	anion(O)... $\pi$	-	-	3.14	<i>No bcp</i>	<i>No bcp</i>	0.6099
25	CH...O	-	-	2.81	<i>No bcp</i>	<i>No bcp</i>	0.4228

**Table S10.** Comparison of the relative free energy and their difference for the lowest energy stereocontrol TSs at different level of theory.

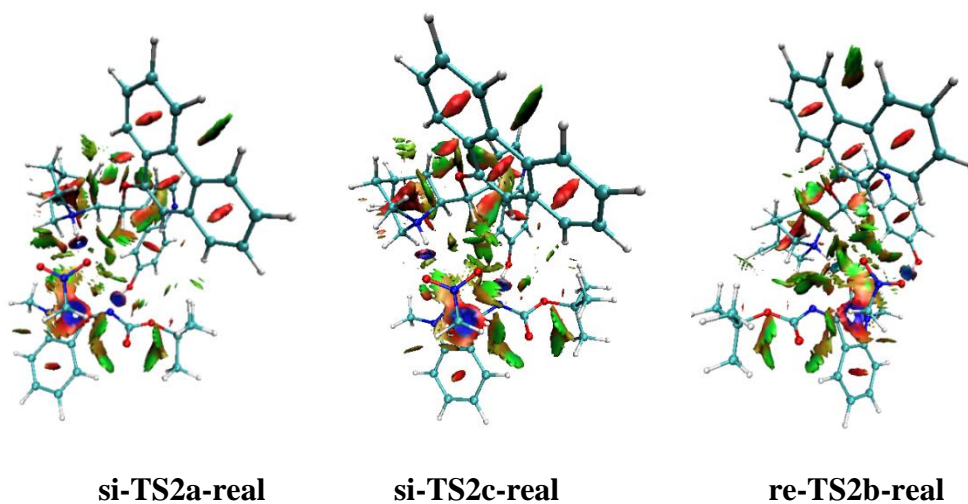
method	$\Delta G^\ddagger$		$\Delta\Delta G^\ddagger$	ee %
	<i>re</i> -TS2a	<i>si</i> -TS2a		
SMD-D3-B3LYP-6311++G**//SMD-B3LYP-631G*	16.2	14.1	2.1	94
SMD-M06-2X-6311++G**//SMD-M06-2X-631G*	20.2	18.0	2.2	95
SMD-D3-B3LYP-6311++G**//SMD-B3LYP-631+G**	17.0	14.4	2.6	97
SMD-M06-2X-6311++G**//SMD-B3LYP-631G*	21.4	19.9	1.5	85
SMD-wB97xd-6311++G**//SMD-B3LYP-631G*	21.7	19.8	1.9	92
SMD-B3LYP-6311++G**//SMD-B3LYP-631G*	37.4	36.0	1.4	83
SMD-D3-B3LYP-def2-TZVPP//SMD-B3LYP-631G*	19.3	17.2	2.1	94



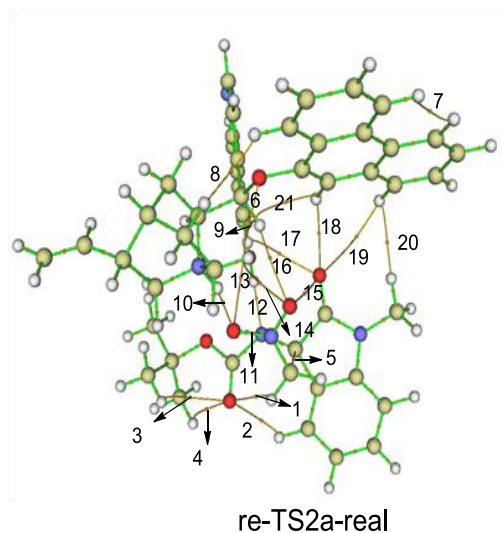
**Fig. S7** Optimized structure and relative free energy of the three less stable TS2s involving the real catalyst in modes **a** and **b**. Bond distances are given in angstroms.

**Table S11** Distortion/interaction analysis of *si-TS2b-real* and *re-TS2a-real* at the SMD-D3-B3LYP-6311++G(d,p)// SMD- B3LYP-631G(d) level.

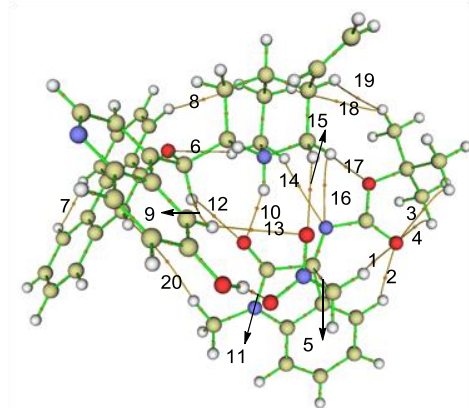
	<i>si-TS2b-real</i>	<i>re-TS2a-real</i>	$\Delta\Delta E(\text{si-re})$
$\Delta E_{\text{int}}$	-74.17	-71.3	-2.87
$\Delta E_{\text{dist}}$	1.37	2.66	-1.28
$\Delta E_{\text{int/dist}}$	-5.06	-5.38	0.32
<b>total</b>	<b>-77.87</b>	<b>-74.03</b>	<b>-3.84</b>



**Fig. S8.** NCI plots of the other three lowest-energy transition states involving the real catalyst. Strong and attractive interactions are blue, weak attractive interactions are green, and strong and repulsive interactions are red.

**Table S12.** AIM analysis for **re-TS2a-real**

Bond path	Type of Interaction	Distance (in Å)	$\rho_{\text{bcp}} * 10^{-2}$ (in a.u.)
1	CH...O	2.52	0.9297
2	CH...O	2.24	1.5863
3	CH...O	2.42	1.2930
4	CH...O	2.44	1.2418
5	C-C formation	2.28	4.9282
6	CH...O	2.44	1.1921
7	CH...HC	2.00	1.2392
8	CH...HC	2.35	0.4842
9	CH...HC	2.08	1.1237
10	NH...O	1.67	5.2458
11	anion (O)... $\pi$ (C=N)	3.00	0.9562
12	OH...N	1.83	3.8799
13	CH...O	3.08	0.2769
14	CH...O	2.77	0.6407
15	anion(O)... $\pi$ (C=O)	3.15	0.6209
16	CH...O	2.56	0.8354
17	CH...O	2.71	0.6769
18	CH...O	2.97	0.2748
19	CH...O	3.15	0.2422
20	CH...HC	2.48	0.3700
21	CH...HC	2.04	1.3726

**Table S13.** AIM analysis for **si-TS2b-real****si-TS2b-real**

Bond path	Type of Interaction	Distance (in Å)	$\rho_{\text{bcp}} * 10^{-2}$ (in a.u.)
1	CH...O	2.59	0.8078
2	CH...O	2.29	1.4207
3	CH...O	2.41	1.3067
4	CH...O	2.43	1.2652
5	C-C formation	2.27	4.9996
6	CH...O	2.39	1.2731
7	CH...HC( $\sigma \cdots \sigma$ )	2.00	1.2477
8	CH...HC( $\sigma \cdots \sigma$ )	2.56	0.3191
9	CH...HC( $\sigma \cdots \sigma$ )	2.12	1.1060
10	NH...O	1.81	3.5716
11	OH...O	1.73	4.1996
12	CH...O	2.30	1.2089
13	CH...O	2.72	0.6282
14	CH...N	2.76	0.7226
15	CH...O	2.39	1.0187
16	CH...N	2.63	0.8910
17	CH...O	2.58	0.7456
18	CH...HC( $\sigma \cdots \sigma$ )	3.21	0.0918
19	CH...HC( $\sigma \cdots \sigma$ )	3.18	0.0926
20	CH...HC( $\sigma \cdots \sigma$ )	3.27	0.1106

**Table S14.** Comparison of the relative free energy of the lowest energy TSs **si-TS2b-real** and **re-TS2a-real** at different level of theory.

method	$\Delta G^\ddagger$ (kcal/mol)		$\Delta\Delta G^\ddagger$ (kcal/mol)	ee (%)
	<b>si-TS2b-real</b>	<b>re-TS2a-real</b>		
SMD-D3-B3LYP-6311++G**// SMD-B3LYP-631G*	15.7	17.9	2.2	95
SMD-B3LYP-6311++G**// SMD-B3LYP-631G*	40.3	41.2	0.9	64
Exp.				90



**The optimized coordinates of all the stationary points in PES at the SMD-B3LYP-631G(d) level.**

**1. REACTANTS**

**2. STEP1 (protonation)**

**3. STEP2 (C-C bond formation) for model catalyst**

**3.1 MODE a**

**3.2 MODE b**

**3.3 MODE c**

**3.4 TS2s involving Z-ketimine**

**4. STEP3 (protonation of product) for model catalyst**

**5. Lowest-lying transition states for real catalyst**

**1. REACTANTS**

**Z-Ketimine**

C	4.04689000	-2.10683800	0.26267800
C	4.79376600	-0.93132700	0.39504800
C	4.19765300	0.33621000	0.31410100
C	2.82706200	0.38564600	0.09702700
C	2.06342300	-0.79222800	-0.03686600
C	2.66676300	-2.04272700	0.04323900
N	2.00140100	1.51996400	-0.02284300
C	0.68964200	1.15306100	-0.23558000
C	0.67806000	-0.38353700	-0.25558100
O	-0.26789900	1.89377100	-0.37653700
H	4.54111000	-3.07116400	0.33002000
H	5.86497700	-0.99583200	0.56552200
H	4.79062000	1.23885900	0.41806500
H	2.06923100	-2.94334800	-0.06444200
C	2.45078500	2.89582400	0.06701000
H	2.89504800	3.09575700	1.04840000
H	3.18906300	3.11377200	-0.71251300
H	1.58013500	3.53854900	-0.07206900
N	-0.33429600	-1.13593700	-0.42445300
C	-1.62785500	-0.64188100	-0.70326900
O	-2.03700400	-0.52299600	-1.83928400
O	-2.31113100	-0.51450800	0.43708900
C	-3.74309500	-0.12657500	0.44271400
C	-4.06172700	-0.07770500	1.93737800

H	-5.11126200	0.19673800	2.08759000
H	-3.88987400	-1.05251300	2.40633400
H	-3.43546500	0.66438900	2.44379500
C	-4.57004400	-1.20561100	-0.25947800
H	-4.33340200	-1.25883400	-1.32395400
H	-4.38674500	-2.18674500	0.19285600
H	-5.63663400	-0.97725600	-0.15197000
C	-3.91111600	1.25385000	-0.19567700
H	-4.94226400	1.59677700	-0.05249900
H	-3.23855400	1.97777700	0.27533700
H	-3.69869300	1.22778600	-1.26600200

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**E-Ketimine**

C	1.59767600	2.92163700	-0.12902400
C	2.96037100	2.75555300	0.13759500
C	3.53555300	1.48358300	0.26355900
C	2.70066300	0.38229900	0.12050800
C	1.31900100	0.53328900	-0.13984000
C	0.76657900	1.80639500	-0.27254300
N	3.04684400	-0.97458900	0.19402100
C	1.94054000	-1.77789900	-0.01420700
C	0.75864900	-0.81859500	-0.22683500
O	1.91700400	-2.99318000	-0.01933400
H	1.18324000	3.91983000	-0.22957900
H	3.59433400	3.63127900	0.24613200
H	4.59553000	1.36916000	0.46465300
H	-0.28657400	1.93365500	-0.49851600
C	4.38103300	-1.48730900	0.43328200
H	5.06963700	-1.16613800	-0.35637800
H	4.76122800	-1.14524500	1.40235300
H	4.31953200	-2.57679200	0.43501700
N	-0.40858500	-1.29720600	-0.40597200
C	-1.54387100	-0.51383900	-0.66852300
O	-1.78470900	-0.03759900	-1.76158200
O	-2.32531400	-0.50292700	0.41588600
C	-3.70029900	0.05740300	0.38672600
C	-4.17895800	-0.18458000	1.81836100
H	-5.20401100	0.18202100	1.93765100
H	-4.16414300	-1.25297700	2.05753400
H	-3.53966200	0.33877500	2.53734600
C	-4.54890300	-0.72668100	-0.61608400
H	-4.19670000	-0.57920400	-1.63909300
H	-4.52574500	-1.79732600	-0.38497200

H	-5.58964600	-0.38880200	-0.55596000
C	-3.65251900	1.55396900	0.07120100
H	-4.65360200	1.98328200	0.19237000
H	-2.97898600	2.07208300	0.76308000
H	-3.32116400	1.73727100	-0.95279900

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**nitromethane**

C	1.32572800	-0.00019700	-0.00224500
H	1.66797400	-0.90664000	-0.49859400
H	1.63199900	0.00145000	1.04696900
H	1.66814800	0.90469000	-0.50133800
N	-0.16865400	-0.00000100	-0.01200100
O	-0.73366700	1.09066500	0.00315100
O	-0.73407200	-1.09045300	0.00315300

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**nitronate**

C	-1.29332900	-0.00025600	-0.00089700
H	-1.80672200	0.95126000	0.00214700
H	-1.80637200	-0.95198100	0.00211900
N	0.04635800	-0.00013200	0.00000400
O	0.69082300	-1.11110800	0.00006900
O	0.69024800	1.11150600	0.00006600

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**QN-model**

C	0.49066600	-0.64068900	0.71728700
C	-0.83259300	-1.05207000	0.07759000
C	-1.94687600	-0.15308800	0.02510600
C	-0.98998700	-2.30653900	-0.47381200
C	-1.92263200	1.17019700	0.54424200
C	-3.15293500	-0.63337900	-0.58380300
C	-2.22236700	-2.67336500	-1.06208300
H	-0.17270800	-3.01920600	-0.44294700
C	-3.04410800	1.97413300	0.46874800
H	-1.01811500	1.56506800	0.99929700
C	-4.28639800	0.22394200	-0.63676900
H	-2.33403100	-3.66629300	-1.49656700
C	-4.24069900	1.49641400	-0.12540200
H	-5.18918300	-0.16426300	-1.09871000
H	-5.10224000	2.15587800	-0.16417800
C	1.33666900	0.24559700	-0.23507100
H	0.62138900	0.88892700	-0.75781700
C	2.16461400	-0.54863400	-1.29415600

C	2.71529300	2.19623700	-0.41729400
C	3.35065900	0.49210000	1.14114000
C	3.59737600	0.02488700	-1.31183000
H	2.20202400	-1.61345600	-1.04528500
H	1.70245700	-0.45784800	-2.28452100
C	3.53438200	1.54273600	-1.57443500
H	1.86268900	2.76361300	-0.80832500
H	3.33374100	2.89519700	0.15721700
C	4.23681600	-0.21351200	0.07007900
H	2.97316300	-0.22822200	1.86881000
H	3.92225000	1.24768600	1.69254200
H	4.18625500	-0.47100400	-2.09216400
H	4.54798900	1.96006800	-1.62068200
H	4.30200800	-1.28961300	0.27033000
H	5.26075900	0.18099500	0.08351600
O	-3.08008900	3.24943000	0.94821000
N	-3.27517500	-1.88223800	-1.12035900
N	2.19754500	1.18495300	0.52659600
H	-2.21415600	3.46994000	1.33213100
H	0.27947300	-0.03148000	1.60779500
O	1.25509100	-1.77522200	1.11445700
C	0.83083600	-2.35646300	2.33861900
H	-0.20381400	-2.72234300	2.28822600
H	1.49596500	-3.20280100	2.53249800
H	0.91095000	-1.64174100	3.17163700
H	3.06423100	1.73721300	-2.54673300

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**QN-real**

C	0.64662300	0.01422100	0.08855600
C	0.89936100	1.15543100	-0.88894300
C	1.64055200	2.31567700	-0.49056300
C	0.45179100	1.08887100	-2.19168000
C	2.15403300	2.52129800	0.81946300
C	1.86421500	3.32478300	-1.48497200
C	0.72928500	2.14472900	-3.09000000
H	-0.12221900	0.23440700	-2.53283000
C	2.85861000	3.67063600	1.12442100
H	2.00367300	1.77516400	1.59507600
C	2.59534800	4.49188400	-1.13019300
H	0.37057500	2.08159000	-4.11651100
C	3.08354100	4.66714800	0.13981600
H	2.75094500	5.24024600	-1.90119800
H	3.64212800	5.55592500	0.41670800
C	1.90447900	-0.87990000	0.24105000

H	2.73838700	-0.17254200	0.28884300
C	2.16482500	-1.86860800	-0.93387400
C	3.32381300	-2.03197400	1.77469300
C	1.05569900	-2.76783900	1.56304700
C	2.64152800	-3.20857600	-0.33249500
H	1.25223000	-2.04645800	-1.51162600
H	2.90655000	-1.45596900	-1.62566000
C	3.83900900	-2.99415700	0.63845400
H	3.96506800	-1.14570300	1.84778300
H	3.35870900	-2.53795200	2.74566100
C	1.47768400	-3.80801600	0.48145800
H	0.02748200	-2.43686000	1.41110900
H	1.11259200	-3.19869900	2.56879700
H	2.93951500	-3.89262900	-1.13481900
H	4.08206400	-3.97068800	1.07697100
H	0.63734000	-4.03883200	-0.18430400
H	1.78995500	-4.75292300	0.94335800
C	5.07861100	-2.47144000	-0.03533000
H	5.01001200	-1.47002500	-0.46466400
C	6.23716200	-3.12838800	-0.12859800
H	6.36612600	-4.12648500	0.28791000
H	7.10275500	-2.69509300	-0.62466200
O	3.37334300	3.92232400	2.36004800
N	1.40917500	3.22665200	-2.76700000
N	1.93878400	-1.58178000	1.54725700
H	3.15861400	3.18192400	2.95312800
H	0.42107500	0.41295900	1.08354000
O	-0.45848000	-0.79928900	-0.32715700
C	-5.12517800	2.78378100	1.41407000
C	-3.80897300	2.44559900	1.16398700
C	-3.46613600	1.16838600	0.65895100
C	-4.49652400	0.21861000	0.39909200
C	-5.83320500	0.59252800	0.67027100
C	-6.14515500	1.84604700	1.16771900
C	-2.09202700	0.83628600	0.41314400
C	-4.12358100	-1.08427800	-0.13946200
C	-2.74951600	-1.38411700	-0.37987400
C	-1.74180000	-0.38822300	-0.07638700
C	-2.38817300	-2.64392700	-0.91027700
H	-1.34089700	-2.85236900	-1.09461000
C	-3.34810000	-3.59685300	-1.19593200
C	-4.70400900	-3.31255800	-0.95882600
C	-5.07771300	-2.08407800	-0.44397200
H	-1.34773700	1.59642500	0.61906200

H	-5.37224100	3.76878600	1.80101400
H	-3.01233300	3.16128100	1.35299600
H	-6.64027600	-0.10907300	0.48880400
H	-7.18160100	2.10526900	1.36582300
H	-3.05433100	-4.56050800	-1.60301000
H	-5.46378100	-4.05682800	-1.18172900
H	-6.13147300	-1.89062500	-0.27677500

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## 2. STEP1 (protonation)

### RC1

C	0.46576800	-0.86248100	0.85648900
C	-0.83727200	-1.55485500	0.45377700
C	-1.95746400	-0.81386200	-0.04520500
C	-0.96642400	-2.92497400	0.55476700
C	-1.96157300	0.59556000	-0.20550500
C	-3.13690900	-1.55208300	-0.39226900
C	-2.17387300	-3.55437500	0.17312500
H	-0.14607100	-3.52157600	0.93909500
C	-3.08240000	1.25763600	-0.67649700
H	-1.07431000	1.16815700	0.03146700
C	-4.27101500	-0.84188700	-0.87537700
H	-2.26217900	-4.63734400	0.25488300
C	-4.25167900	0.52331100	-1.01436900
H	-5.15443800	-1.41996500	-1.12992100
H	-5.11667800	1.06741300	-1.38154400
C	1.33770900	-0.54207800	-0.38236300
H	0.64883600	-0.09811900	-1.10846200
C	2.01345200	-1.78471800	-1.03289300
C	2.77812100	1.05454100	-1.43592600
C	3.53879600	-0.00311000	0.58093000
C	3.41765100	-1.36836600	-1.51759200
H	2.10608100	-2.60100900	-0.30871900
H	1.40524100	-2.15344400	-1.86662500
C	3.30360800	-0.08348300	-2.36248500
H	1.93203700	1.58111000	-1.89109800
H	3.55991400	1.79864600	-1.24551800
C	4.28333100	-1.06860400	-0.27889700
H	3.20752700	-0.42742200	1.52881400
H	4.19020000	0.84982200	0.80367400
H	3.86496200	-2.17468600	-2.10963000
H	4.27910600	0.18122700	-2.78846100

H	4.44449700	-1.98591100	0.30017600
H	5.27135400	-0.70526100	-0.58926800
O	-3.13902700	2.60046600	-0.84193900
N	-3.22961400	-2.90851100	-0.28191700
N	2.34303500	0.52742000	-0.12049100
H	-2.28696100	3.00781000	-0.57847500
H	0.22643700	0.09708200	1.33714500
O	1.21567400	-1.65457400	1.77307500
C	0.74606400	-1.57977100	3.11214200
H	-0.28922200	-1.93371300	3.20906800
H	1.39648800	-2.22260500	3.71212600
H	0.80467700	-0.55163400	3.50013700
C	1.38674500	3.63232900	0.98065500
H	1.81619900	4.32889800	0.26174600
H	1.73875900	2.60706300	0.78314100
H	1.57093400	3.92656500	2.01225600
N	-0.08291700	3.59704400	0.76513700
O	-0.81637700	3.43166400	1.73045600
O	-0.48067500	3.67031000	-0.40721900
H	2.62050600	-0.24809100	-3.20512600

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**TS1**

C	0.39615000	-0.81639200	0.81974700
C	-0.91723200	-1.47578400	0.39269500
C	-2.00092700	-0.67883600	-0.09438100
C	-1.10148500	-2.83994800	0.46953500
C	-1.92898800	0.72500600	-0.21852000
C	-3.21570900	-1.34920000	-0.45150500
C	-2.33795800	-3.40427700	0.07021600
H	-0.31261500	-3.48198800	0.84792600
C	-3.01797000	1.47097300	-0.63515700
H	-1.02258200	1.24935500	0.03317300
C	-4.31379700	-0.56287500	-0.90087500
H	-2.47471600	-4.48360400	0.12873900
C	-4.22637900	0.80665500	-0.98812100
H	-5.22931800	-1.08341400	-1.16661600
H	-5.07029800	1.40440200	-1.31988400
C	1.25966400	-0.50322400	-0.42661300
H	0.58857100	-0.04848100	-1.15862000
C	1.96324200	-1.73883500	-1.05013700
C	2.77212900	1.08946700	-1.50798200
C	3.48078900	0.04731600	0.59134700
C	3.38106600	-1.33972200	-1.50299000
H	2.02640900	-2.54657700	-0.31566000

H	1.37324500	-2.10442200	-1.89619900
C	3.29083500	-0.07776000	-2.38160200
H	1.92939100	1.61895100	-1.95888400
H	3.55278300	1.82320700	-1.29181500
C	4.22388500	-1.01955400	-0.25232700
H	3.09421900	-0.36376200	1.52254100
H	4.10882500	0.91229400	0.82195700
H	3.83835400	-2.16045100	-2.06452500
H	4.27195700	0.17372500	-2.79841200
H	4.37317000	-1.92532100	0.34454100
H	5.21472300	-0.65684600	-0.54845300
O	-2.97975400	2.81529800	-0.71840200
N	-3.36465500	-2.70267300	-0.37096000
N	2.30333300	0.56669300	-0.17940700
H	-2.09452500	3.13638300	-0.40153600
H	0.16242500	0.13364300	1.32160200
O	1.14551600	-1.63275600	1.71156500
C	0.67599200	-1.58422500	3.05643900
H	-0.35544800	-1.94839600	3.14394000
H	1.33330100	-2.23322800	3.64125600
H	0.72661500	-0.56235500	3.45889200
C	1.55065800	2.95532400	0.99411400
H	2.07120700	3.64332700	0.33178700
H	1.87577400	1.52814500	0.38396800
H	1.89185900	2.93933700	2.02647600
N	0.16938900	3.13041800	0.92383900
O	-0.56029700	2.77298100	1.87263400
O	-0.33661400	3.55763800	-0.16302100
H	2.61560300	-0.25493700	-3.22600900

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**IM1**

C	0.39669900	-0.84078200	0.83908300
C	-0.92054300	-1.49051900	0.41065700
C	-1.99282600	-0.68159800	-0.08151400
C	-1.11479400	-2.85347000	0.48144600
C	-1.90633700	0.72138000	-0.19820300
C	-3.20798800	-1.34191300	-0.45696400
C	-2.35265400	-3.40604300	0.06971900
H	-0.33289600	-3.50339300	0.86108800
C	-2.98152300	1.47914400	-0.63274600
H	-1.00571400	1.24137700	0.08211100
C	-4.29234600	-0.54473600	-0.92033300
H	-2.49949300	-4.48423600	0.12433700
C	-4.19020200	0.82396600	-1.00522800



H	-5.20881300	-1.05613900	-1.20032000
H	-5.02351800	1.42942100	-1.34977900
C	1.24470400	-0.51862800	-0.41426100
H	0.57076200	-0.04604600	-1.13133000
C	1.94473900	-1.74014400	-1.06183500
C	2.74795300	1.10577800	-1.49203500
C	3.49601900	0.00864500	0.58179900
C	3.34908700	-1.32642800	-1.54371400
H	2.02916100	-2.55321100	-0.33542300
H	1.33714700	-2.10180600	-1.89655300
C	3.23362800	-0.04882300	-2.39749200
H	1.89761600	1.65303600	-1.90387200
H	3.53905100	1.82531800	-1.26977800
C	4.22364000	-1.02678200	-0.30944200
H	3.11656500	-0.43175500	1.50213200
H	4.11982000	0.87086400	0.82966200
H	3.79457700	-2.13454700	-2.13176700
H	4.20157100	0.20856000	-2.83983600
H	4.39860400	-1.94375000	0.26214000
H	5.20139700	-0.64514200	-0.62358000
O	-2.92777300	2.81990400	-0.71508400
N	-3.36810000	-2.69426700	-0.38158500
N	2.30294100	0.54622300	-0.16331800
H	-2.03269200	3.13281600	-0.39927500
H	0.16959200	0.10534400	1.35264700
O	1.15530800	-1.66761200	1.71196800
C	0.69908800	-1.63608500	3.06295500
H	-0.33204200	-1.99931600	3.15499300
H	1.36115800	-2.29425200	3.63169200
H	0.75620000	-0.61962900	3.47763000
C	1.52783200	3.05524400	1.06773800
H	2.07395200	3.69171300	0.37866100
H	1.90158000	1.40364200	0.38998500
H	1.85214400	3.02369700	2.10292300
N	0.16586500	3.15900900	0.93721200
O	-0.59890500	2.79706400	1.86610200
O	-0.32203600	3.54202000	-0.18671000
H	2.53150500	-0.20955200	-3.22262000

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**IM1a**

C	0.31288500	-1.08070600	0.82321300
C	-1.08906200	-1.54412000	0.43187100
C	-2.05286900	-0.58383100	-0.01145700

C	-1.46334200	-2.86936500	0.46960600
C	-1.77339300	0.79710800	-0.10400600
C	-3.34556600	-1.06525400	-0.39694600
C	-2.77539500	-3.23703900	0.07990100
H	-0.76348800	-3.63074600	0.79860900
C	-2.71330800	1.68974500	-0.59281000
H	-0.81030700	1.19572100	0.18159600
C	-4.30462000	-0.12242900	-0.86349200
H	-3.06761000	-4.28603400	0.11777700
C	-4.00282600	1.21546100	-0.96608400
H	-5.28350300	-0.49844400	-1.14694100
H	-4.73284400	1.92984800	-1.33554600
C	1.12636300	-0.70530400	-0.44533000
H	0.43619700	-0.21780900	-1.13475100
C	1.84289700	-1.87989100	-1.15492400
C	2.58897700	1.00880000	-1.44936400
C	3.36034800	-0.17830700	0.56434600
C	3.23433100	-1.40842300	-1.62384300
H	1.94914700	-2.72636300	-0.47142400
H	1.23698500	-2.21104000	-2.00389600
C	3.08415100	-0.09297800	-2.41414300
H	1.73220200	1.57318300	-1.81962300
H	3.37432500	1.72307000	-1.19042500
C	4.11030400	-1.14715800	-0.38122500
H	2.99232000	-0.67862400	1.45895400
H	3.96541000	0.67988800	0.86462300
H	3.69531000	-2.17626900	-2.25275100
H	4.04169700	0.20191100	-2.85589500
H	4.31696300	-2.08611600	0.14217500
H	5.07389800	-0.72179300	-0.68310100
O	-2.44806600	3.00370100	-0.73025200
N	-3.69028600	-2.38442400	-0.34111100
N	2.15834400	0.37356000	-0.15277200
H	-1.48016200	3.15838700	-0.52720700
H	0.21690600	-0.17316400	1.43677100
O	1.03408300	-2.05818100	1.56201500
C	0.68325600	-2.10950600	2.94197800
H	-0.36620100	-2.39452600	3.08877700
H	1.32521000	-2.86745200	3.39867300
H	0.85853400	-1.14269100	3.43538000
C	0.35842300	4.31334100	1.67819800
H	0.67645800	4.32498900	2.70988900
H	1.71652600	1.15223200	0.45524800
H	-0.15121600	5.13691100	1.20066000

N	0.59130600	3.23793400	0.97155000
O	0.23393000	3.14162500	-0.28026300
O	1.20101000	2.20961100	1.51267900
H	2.37469500	-0.22948600	-3.23761100

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**IM1b**

C	-0.14711900	-1.29097500	0.71919200
C	-1.62825200	-1.30113200	0.34636300
C	-2.27928500	-0.06032100	0.06426300
C	-2.36259700	-2.45982500	0.22710900
C	-1.61538700	1.18022100	0.14694700
C	-3.64638200	-0.09712600	-0.35552500
C	-3.72243100	-2.38409300	-0.16918000
H	-1.91096300	-3.42580100	0.42964500
C	-2.23455200	2.35579400	-0.23780500
H	-0.59792100	1.25307700	0.50192900
C	-4.28058300	1.13349400	-0.68839100
H	-4.30180800	-3.30256500	-0.25711800
C	-3.59746300	2.32824400	-0.64596500
H	-5.32130200	1.09711300	-0.99729700
H	-4.07988300	3.26055500	-0.92463200
C	0.72303300	-1.02547000	-0.54923100
H	0.12158400	-0.43510800	-1.24069100
C	1.26567500	-2.30062100	-1.25335000
C	2.63617700	0.21798100	-1.52246900
C	2.86590600	-0.75506300	0.73214800
C	2.80741200	-2.26766900	-1.27976800
H	0.92272300	-3.18982300	-0.72153100
H	0.87314600	-2.34970200	-2.27410200
C	3.27243900	-1.05851500	-2.11192000
H	1.89270900	0.66826300	-2.18299400
H	3.35421900	0.98922100	-1.24181400
C	3.33469400	-2.11345300	0.16091900
H	2.34548000	-0.85849000	1.68437100
H	3.66893000	-0.03069600	0.86325900
H	3.18640500	-3.19591800	-1.71866600
H	4.36520900	-0.98496600	-2.09210000
H	2.95759500	-2.93043600	0.78242200
H	4.42856200	-2.16290600	0.17132900
O	-1.56866500	3.52984400	-0.23976700
N	-4.35196900	-1.26097600	-0.45897700
N	1.90780900	-0.12239700	-0.24156900
H	-0.60625600	3.33259500	-0.07334600
H	0.01588900	-0.46375700	1.42486000

O	0.27881400	-2.49418700	1.33905600
C	-0.07729800	-2.58547500	2.71527900
H	-1.16417300	-2.55338300	2.86171400
H	0.30274200	-3.54596700	3.07280700
H	0.38317800	-1.77609400	3.30070200
C	2.03821400	4.38467800	0.98821600
H	2.92863800	4.82583900	1.41064700
H	1.58510000	0.81924700	0.11481400
H	1.12156000	4.93260100	0.83018200
N	2.08924100	3.11904500	0.64683200
O	1.02450800	2.52857000	0.10908600
O	3.13110200	2.39203100	0.80279700
H	2.97379800	-1.17670000	-3.15875500

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**IM1c**

C	0.28445900	-1.10605200	0.78335300
C	-1.09306600	-1.58072700	0.32326700
C	-2.10662800	-0.62495000	-0.00193800
C	-1.38364500	-2.91878700	0.16432900
C	-1.92510200	0.76831200	0.14035500
C	-3.35346800	-1.12491500	-0.50202700
C	-2.65655000	-3.30535100	-0.32242600
H	-0.64683200	-3.67627700	0.41117400
C	-2.92986700	1.66056200	-0.20333900
H	-1.01298300	1.18643700	0.54813300
C	-4.36541700	-0.18733500	-0.85117100
H	-2.88243100	-4.36421600	-0.44440100
C	-4.16453900	1.16561900	-0.71297600
H	-5.30566800	-0.57829500	-1.22917300
H	-4.94017800	1.87870100	-0.97707200
C	1.10834300	-0.66306500	-0.45456800
H	0.42527800	-0.12013000	-1.10994600
C	1.79901900	-1.82773000	-1.21813600
C	2.79877800	0.87652600	-1.38969800
C	3.24404700	-0.17619700	0.78970500
C	3.31701000	-1.57145000	-1.30194100
H	1.61338100	-2.77081900	-0.70025000
H	1.37409800	-1.91180500	-2.22337200
C	3.56556200	-0.26988800	-2.08553400
H	1.98301000	1.27162600	-1.99830300
H	3.43436500	1.71381100	-1.09924600
C	3.88375200	-1.41579200	0.12298800
H	2.78047200	-0.40865400	1.74685900
H	3.95429500	0.63998100	0.93914400

H	3.80324400	-2.41264100	-1.80570900
H	4.63740800	-0.04664200	-2.11722100
H	3.65939200	-2.30991900	0.71123400
H	4.97234600	-1.30245300	0.08750700
O	-2.78442700	2.99180200	-0.07185100
N	-3.61014400	-2.45611000	-0.65487400
N	2.17015100	0.36954700	-0.11218500
H	-1.88680900	3.18188800	0.33608900
H	0.15746100	-0.23627700	1.44353700
O	1.00720400	-2.11070800	1.48170600
C	0.60474900	-2.26728400	2.83925400
H	-0.44423600	-2.57802700	2.92283000
H	1.24242300	-3.04559400	3.26647300
H	0.74391300	-1.33605100	3.40739900
C	0.76312400	4.69651600	-0.07800300
H	-0.11974400	5.31653800	-0.12899000
H	1.75316200	1.25162600	0.33963800
H	1.70987300	4.97272100	-0.51750600
N	0.69485800	3.56758400	0.58557700
O	1.75975100	2.82092400	0.72891700
O	-0.40216500	3.16367200	1.15285900
H	3.22442400	-0.37625100	-3.12046900

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**TS1'**

C	-5.34648000	0.21931200	2.43294800
C	-5.42026700	-1.04320000	3.02901400
C	-4.73827200	-2.14454300	2.49569300
C	-3.98011500	-1.94056800	1.34993200
C	-3.89890500	-0.67068800	0.72643400
C	-4.58578300	0.41326600	1.27673700
N	-3.21180900	-2.88782800	0.66318900
C	-2.57814300	-2.30767400	-0.41389500
C	-3.00961100	-0.83189300	-0.42404300
O	-1.84315000	-2.86020100	-1.20957000
H	-5.88596700	1.05519700	2.86781600
H	-6.01968200	-1.17981400	3.92525800
H	-4.79759300	-3.11931800	2.96831900
H	-4.53409300	1.38501100	0.80493700
C	-3.04071400	-4.27276800	1.05039800
H	-4.00034600	-4.80168900	1.04390600
H	-2.37038000	-4.73659000	0.32497000
H	-2.59694800	-4.34480500	2.04994500
N	-2.54466800	-0.09346500	-1.36236400
C	-2.92571400	1.25242100	-1.54250800

O	-4.06026800	1.68230600	-1.43625800
O	-1.85547700	1.92736800	-1.96635300
C	-1.92822700	3.36327500	-2.31184000
C	-0.48019800	3.68100300	-2.68874700
H	-0.39377300	4.72699000	-3.00134500
H	0.18880800	3.51838000	-1.83682600
H	-0.14657500	3.04300100	-3.51365300
C	-2.36909800	4.17671800	-1.09222900
H	-3.41638100	3.99186400	-0.84595900
H	-1.75560700	3.92248200	-0.22137400
H	-2.24546800	5.24511500	-1.30294300
C	-2.85477800	3.55633800	-3.51537400
H	-2.81487500	4.60146900	-3.84317000
H	-2.53403900	2.92573700	-4.35196700
H	-3.88898400	3.31126100	-3.26621100
C	2.54969100	-0.75630700	1.00301800
C	3.15691600	-1.48829400	-0.19567700
C	2.50267900	-1.56766500	-1.46921400
C	4.41025600	-2.05552700	-0.06709500
C	1.18709700	-1.09498300	-1.73143000
C	3.25155600	-2.17587900	-2.53760300
C	5.03628000	-2.65801400	-1.17910700
H	4.91774100	-2.03379700	0.89124000
C	0.63806500	-1.20683400	-3.00290000
H	0.57846100	-0.68094800	-0.93293000
C	2.67076000	-2.23823700	-3.83344500
H	6.02508600	-3.10176400	-1.06641200
C	1.40751400	-1.76311000	-4.06442500
H	3.25954100	-2.68885900	-4.62690100
H	0.95043800	-1.82218500	-5.04772900
C	2.80112500	0.76533800	0.86506700
H	2.18192100	1.07827500	0.02008300
C	4.25800900	1.22530300	0.61653800
C	1.97718700	2.96009700	1.55146700
C	3.25737500	1.65073900	3.17855600
C	4.44115800	2.63703500	1.21665900
H	4.97041400	0.53248500	1.07740800
H	4.45494100	1.22424500	-0.45945600
C	3.23095500	3.51615500	0.83413400
H	1.09851700	2.89274100	0.90685700
H	1.70680100	3.54924400	2.43156200
C	4.47479600	2.50063900	2.75075100
H	3.52732900	0.62648800	3.42526000
H	2.71412800	2.08334900	4.02312900

H	5.36877600	3.08693900	0.85014100
H	3.39921200	4.55581000	1.13402000
H	5.39866600	2.00980400	3.07453700
H	4.44979200	3.49007700	3.22202700
O	-0.60386600	-0.81195400	-3.33398000
N	4.49775800	-2.70556500	-2.38164000
N	2.27417900	1.56880700	2.04090000
H	-1.16856700	-0.63279700	-2.54040300
H	1.46241100	-0.91096500	1.02899900
O	3.10223500	-1.20824500	2.23503200
C	2.51927900	-2.42538700	2.69503300
H	2.73712900	-3.26256500	2.01889100
H	2.95949100	-2.63499100	3.67365700
H	1.43044400	-2.32495900	2.79628700
C	-0.16411100	0.75469700	3.09657900
H	-0.53044300	1.67820900	3.53755800
H	1.29565400	1.14700500	2.47275700
H	-0.06237900	-0.10115300	3.75669500
N	-0.81827500	0.44409400	1.91440900
O	-0.80870800	-0.75512000	1.50239100
O	-1.31621600	1.36555200	1.21689000
H	3.08802100	3.51149000	-0.25221200

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**TS1'a**

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**TS1'b**

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**TS1'c**

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**TS1'd**

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**TS1'e**

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**TS1'f**

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### 3. STEP2 (C-C bond formation) for model catalyst

#### 3.1 MODE a

##### a-N-gau1-syn-S (si-TS2a)

C	-3.05524200	0.02132100	0.88140100
C	-3.54299800	1.21984800	0.07049600
C	-2.68470500	1.87085800	-0.87362400
C	-4.84105300	1.66921200	0.19817000
C	-1.32358300	1.52579400	-1.07814900
C	-3.26599700	2.92539300	-1.65697600
C	-5.29930200	2.73617900	-0.60800800
H	-5.51093700	1.20657800	0.91522500
C	-0.56099500	2.18785300	-2.03121000
H	-0.84810600	0.74071300	-0.49975000
C	-2.46191200	3.57066200	-2.63654300
H	-6.32486400	3.08816700	-0.50111300
C	-1.15176200	3.21227000	-2.82578000
H	-2.92140000	4.36012000	-3.22409800
H	-0.53166000	3.70691200	-3.56764600
C	-3.10891200	-1.24360400	-0.00407800
H	-2.60177800	-0.98401100	-0.93549100
C	-4.52085800	-1.80131700	-0.30093200
C	-1.95069200	-3.34150600	-0.56889500
C	-2.96189000	-3.13086900	1.66632000
C	-4.45160400	-3.34222000	-0.34175900
H	-5.22584100	-1.48246900	0.47276100
H	-4.87266300	-1.40111800	-1.25629000
C	-3.27455000	-3.76990700	-1.24202400
H	-1.25761800	-2.82867500	-1.23728100
H	-1.41681500	-4.17299500	-0.10942300
C	-4.19579100	-3.86031300	1.08814000
H	-3.23005200	-2.39059300	2.41802300
H	-2.21287700	-3.80844900	2.08083400
H	-5.39176500	-3.74853600	-0.72726600
H	-3.27857300	-4.85507500	-1.38899400
H	-5.06688700	-3.67036900	1.72337300
H	-4.03273500	-4.94357400	1.07185600



O	0.73272300	1.91269000	-2.26497700
N	-4.55623100	3.34241700	-1.51324200
N	-2.27053100	-2.38392900	0.55419700
H	1.11677800	1.36663500	-1.52326000
H	-2.01012900	0.18473600	1.17428400
O	-3.83523400	-0.19790400	2.05052700
C	-3.47264800	0.64789000	3.13923200
H	-3.60049300	1.70941100	2.89096400
H	-4.13815800	0.39347900	3.96838900
H	-2.43130000	0.47502100	3.44474600
C	2.17309100	-1.67556300	1.68511700
H	2.33372500	-0.76398800	2.24241400
H	-1.37022800	-1.99661200	0.94766500
H	2.89160700	-2.48231200	1.70866400
N	0.88130600	-2.08033300	1.55913900
O	-0.05932300	-1.22533200	1.73555000
O	0.60361300	-3.25944400	1.20432400
H	-3.37158700	-3.30860100	-2.23097500
C	6.48690900	-0.99654100	0.21375900
C	6.57081700	-2.16912800	-0.54113300
C	5.43326500	-2.73293100	-1.13455100
C	4.21811600	-2.08461800	-0.94849400
C	4.11287200	-0.90190700	-0.17930700
C	5.25552200	-0.35715800	0.40370600
N	2.96723000	-2.45038700	-1.46199000
C	2.00201800	-1.52660700	-1.11352300
C	2.68995300	-0.48719700	-0.23025000
O	0.83159600	-1.53972100	-1.46609600
H	7.38207300	-0.57897600	0.66534500
H	7.53225900	-2.65797300	-0.67383300
H	5.50438600	-3.64192600	-1.72325500
H	5.18224800	0.53733700	1.00974800
C	2.70723100	-3.61750300	-2.27865300
H	3.30229200	-3.59052100	-3.19870800
H	2.93816300	-4.53715400	-1.72944600
H	1.64748400	-3.60936800	-2.53760900
N	2.11240400	0.69566400	-0.14596000
C	2.56815000	1.64851400	0.74353700
O	3.16906000	1.43183800	1.79433800
O	2.17107700	2.86611800	0.32381300
C	2.39614800	4.08075400	1.12467000
C	1.79271400	5.17469200	0.24049600
H	1.88407600	6.14941100	0.73156600
H	2.30947200	5.22310900	-0.72389700

H	0.73196600	4.98040000	0.05062100
C	3.89596600	4.31853300	1.32704600
H	4.33622900	3.56160900	1.97852800
H	4.41808600	4.30224100	0.36361700
H	4.05379100	5.30420000	1.77989600
C	1.63805500	3.97920200	2.45176800
H	1.70843900	4.93209900	2.98884000
H	0.57793700	3.76916500	2.27092700
H	2.05012500	3.19145200	3.08540700

**a-N-gau1-anti-S(si-TS2c)**

C	-3.02570600	0.04189400	0.93899400
C	-3.44900400	1.32382400	0.22409000
C	-2.58684800	1.96088900	-0.72666500
C	-4.70071300	1.86324000	0.43894400
C	-1.26182100	1.53567800	-1.00531200
C	-3.12783600	3.08376600	-1.44087400
C	-5.11354400	3.00024600	-0.29260400
H	-5.37118600	1.41265100	1.16299300
C	-0.50306300	2.17527600	-1.97649000
H	-0.80957000	0.71496200	-0.45841300
C	-2.32998900	3.70515000	-2.44048000
H	-6.10143000	3.42425400	-0.11477700
C	-1.06066100	3.26139200	-2.71077900
H	-2.76028500	4.54612700	-2.97651900
H	-0.44498700	3.73678100	-3.46878000
C	-3.16317300	-1.14437600	-0.03943400
H	-2.59817700	-0.86907500	-0.93197500
C	-4.60834300	-1.53697100	-0.42616300
C	-2.18940700	-3.29572400	-0.73107100
C	-3.28117400	-3.16363300	1.47247200
C	-4.68483100	-3.06749600	-0.60311000
H	-5.30865800	-1.21787700	0.35192400
H	-4.88394100	-1.02182700	-1.35090100
C	-3.51349700	-3.53262900	-1.49289400
H	-1.41775200	-2.80238500	-1.32429600
H	-1.76942200	-4.21827200	-0.32413200
C	-4.54503200	-3.72671900	0.78301000
H	-3.51782700	-2.45795400	2.26581200
H	-2.62667200	-3.94258500	1.86885900
H	-5.63988100	-3.34465200	-1.05934500
H	-3.61412400	-4.59512600	-1.73763900
H	-5.42449500	-3.51241200	1.39873000

H	-4.47731500	-4.81545500	0.67879400
O	0.75624500	1.82196200	-2.28546900
N	-4.37442500	3.58776600	-1.21326100
N	-2.46497700	-2.40344400	0.45575900
H	1.15263000	1.25661300	-1.56569500
H	-1.97159200	0.11040500	1.23619700
O	-3.81747400	-0.21729900	2.09476300
C	-3.36419100	0.48184200	3.25281600
H	-3.41490500	1.56997000	3.11660000
H	-4.02859700	0.19486900	4.07239200
H	-2.33195000	0.20225600	3.50272000
C	2.04804100	-1.59415400	1.80425900
H	2.57197600	-0.77852800	2.28076900
H	-1.52177000	-2.19498300	0.89429000
H	2.42788300	-2.60582000	1.81245300
N	0.69793500	-1.48089300	1.76750300
O	-0.00408600	-2.52672400	1.50560800
O	0.14965400	-0.35565000	1.92022000
H	-3.51652200	-2.97922400	-2.43827200
C	6.40828000	-1.54867200	0.25434500
C	6.35099000	-2.78707100	-0.38954600
C	5.15102600	-3.26644900	-0.93103500
C	4.02071000	-2.46684700	-0.80968200
C	4.05561800	-1.21652700	-0.14811600
C	5.26036900	-0.75764600	0.38347100
N	2.73440300	-2.73152500	-1.29784700
C	1.88143600	-1.67861400	-1.03147200
C	2.68888800	-0.64795600	-0.24233700
O	0.71447900	-1.59047000	-1.38581400
H	7.34933800	-1.19666900	0.66672200
H	7.24900700	-3.39294000	-0.47562300
H	5.11195800	-4.22623000	-1.43612000
H	5.29479600	0.19078200	0.90391200
C	2.35480100	-3.91026700	-2.04794800
H	2.98432700	-4.02201500	-2.93807400
H	2.44236600	-4.81380500	-1.43373100
H	1.31662600	-3.78563300	-2.35900200
N	2.22248100	0.58207300	-0.23339200
C	2.79306200	1.55316400	0.57193200
O	3.46854000	1.35997900	1.57966300
O	2.42535900	2.76478400	0.11451200
C	2.80747100	4.00930900	0.80111300
C	2.16370400	5.08314500	-0.07929600
H	2.37878300	6.07869000	0.32364000

H	2.55304500	5.03137300	-1.10160400
H	1.07728700	4.95303500	-0.11979700
C	4.33144800	4.16346300	0.80832000
H	4.80715300	3.40494900	1.43268900
H	4.72878800	4.08378300	-0.21008600
H	4.59803200	5.15245900	1.19844900
C	2.20863600	4.03814900	2.21077600
H	2.37528000	5.02355600	2.66146300
H	1.12766000	3.86351000	2.16805900
H	2.66058200	3.27987900	2.85271000

**a-O-gaul-syn-S**

C	-2.59437500	0.68583600	-0.16337700
C	-3.35851300	-0.05975200	-1.25953800
C	-2.98374300	-1.37658400	-1.67820700
C	-4.46668500	0.51932100	-1.84402700
C	-1.84181300	-2.06380400	-1.19489400
C	-3.82546100	-2.01659900	-2.65080300
C	-5.21467000	-0.19748600	-2.80563000
H	-4.76541600	1.52540800	-1.56975200
C	-1.53801700	-3.33662900	-1.65318000
H	-1.16565300	-1.59540600	-0.48900700
C	-3.49765300	-3.33291800	-3.07738300
H	-6.08982900	0.26657100	-3.25924100
C	-2.38979200	-3.98083600	-2.59260800
H	-4.15091200	-3.80118500	-3.80768500
H	-2.12858900	-4.98135700	-2.92451500
C	-3.10550800	0.21380900	1.21626600
H	-2.98522800	-0.87215400	1.22511400
C	-4.56638100	0.59264400	1.56045800
C	-2.47430600	-0.21795900	3.55537200
C	-2.50345200	2.11723600	2.76935600
C	-4.67068800	0.89515200	3.06933700
H	-4.87467600	1.47172900	0.98651600
H	-5.22674700	-0.23303700	1.28055600
C	-3.98974300	-0.23865700	3.86120700
H	-2.06307800	-1.19441400	3.30045900
H	-1.88200100	0.19020700	4.37676400
C	-3.92791300	2.21369900	3.35878500
H	-2.38029900	2.71471200	1.86876100
H	-1.72333300	2.38574600	3.48436000
H	-5.72178600	0.98254100	3.36082700
H	-4.15108300	-0.10738100	4.93613400
H	-4.45659000	3.05839000	2.90556200

H	-3.88896900	2.39437400	4.43883000
O	-0.44731400	-4.02382200	-1.24978700
N	-4.92578800	-1.42377400	-3.19535200
N	-2.23007900	0.68537600	2.37022500
H	0.12940900	-3.43517700	-0.70730900
H	-1.52375800	0.44670700	-0.22941000
O	-2.75740300	2.09352700	-0.26140500
C	-1.93118500	2.68538300	-1.26562800
H	-2.21410600	2.34681900	-2.27060600
H	-2.08610100	3.76515900	-1.19711400
H	-0.87310400	2.44967200	-1.09456600
C	2.46187400	0.00221200	2.20592100
H	2.88939700	0.98994200	2.10378500
H	-1.20431200	0.63320200	2.11662600
H	2.96373900	-0.76184000	2.78484600
N	1.09756700	-0.01045500	2.33503900
O	0.49453700	-1.01176100	2.79792100
O	0.44693000	0.99576200	1.88623900
H	-4.42351600	-1.20541100	3.58328300
C	6.67823900	-0.27050700	0.38596700
C	6.87295500	-1.63919900	0.58117400
C	5.78608200	-2.52225500	0.61949600
C	4.51410400	-1.98769100	0.45350800
C	4.29411500	-0.60689500	0.26112500
C	5.38847600	0.25507400	0.23000100
N	3.29422200	-2.68513400	0.44102300
C	2.24862600	-1.83324500	0.19187900
C	2.81560100	-0.41605100	0.10316200
O	1.07226600	-2.16499900	0.05924900
H	7.53347200	0.39876700	0.36068400
H	7.87885100	-2.03106700	0.70555400
H	5.93714500	-3.58719400	0.76508000
H	5.23268500	1.31840000	0.10143900
C	3.15919500	-4.11653200	0.62610900
H	2.09613600	-4.35834100	0.65395000
H	3.63124200	-4.66463000	-0.19718100
H	3.62014200	-4.42352800	1.57099200
N	2.11670600	0.44448600	-0.62023000
C	2.51249600	1.75132000	-0.69995200
O	3.24507100	2.36512200	0.07967500
O	1.90447100	2.33595000	-1.76909400
C	2.18497700	3.72472400	-2.14825800
C	1.33502400	3.90403900	-3.41008400
H	1.45670000	4.91630000	-3.81099500

H	1.63351800	3.18799900	-4.18320200
H	0.27299500	3.74593000	-3.19130400
C	3.67141300	3.89732700	-2.48181900
H	4.29365300	3.78034000	-1.59291900
H	3.98309500	3.15913600	-3.22976000
H	3.84413400	4.89608500	-2.89935700
C	1.72723000	4.69235200	-1.05080100
H	1.83413800	5.72610100	-1.40066800
H	0.67151700	4.52576000	-0.80856200
H	2.31720900	4.56522700	-0.14191300

**a-N-gau2-syn-S**

C	3.09872700	0.39488900	0.52862400
C	3.66153000	-0.83989800	-0.17759300
C	2.83035900	-1.75222300	-0.90997200
C	5.01958800	-1.08632900	-0.12131900
C	1.41744200	-1.64485800	-1.02523100
C	3.50161500	-2.85249400	-1.55172400
C	5.56765000	-2.20022000	-0.79310100
H	5.66849600	-0.43417200	0.45344400
C	0.68495100	-2.59629200	-1.72883700
H	0.88088800	-0.81949800	-0.57354000
C	2.72666400	-3.79174700	-2.28641600
H	6.64064700	-2.38346200	-0.74738800
C	1.36543600	-3.67209000	-2.37372200
H	3.25461500	-4.61058100	-2.76633800
H	0.76792400	-4.39298200	-2.92388900
C	3.08140800	1.60414700	-0.43914800
H	2.69215200	1.23948900	-1.39175800
C	4.44222400	2.32652000	-0.63082500
C	1.91294600	3.67886900	-1.10915500
C	2.40159000	3.33825300	1.27914700
C	4.28557200	3.82914900	-0.31644300
H	5.19068600	1.89372400	0.03557800
H	4.79146600	2.18748200	-1.65855100
C	3.24553800	4.44487700	-1.27085900
H	1.62310400	3.13319800	-2.00891700
H	1.07723000	4.31612900	-0.81417500
C	3.79540500	3.99258800	1.13666600
H	2.37121200	2.59006700	2.06834600
H	1.60287500	4.06247500	1.45144300
H	5.25077900	4.32987900	-0.44141900
H	3.10365600	5.50627500	-1.04196300
H	4.50061300	3.51310500	1.82154000

H	3.74103500	5.05363100	1.40189800
O	-0.64628400	-2.58928300	-1.87155700
N	4.84724400	-3.05621900	-1.49132200
N	2.05764400	2.64964500	-0.01383300
H	-1.12088300	-1.91171600	-1.30883500
H	2.06532700	0.19235200	0.84290000
O	3.87117000	0.75990600	1.66705100
C	3.66665600	-0.07396900	2.80321200
H	3.93658600	-1.11721000	2.59762700
H	4.31744400	0.31211900	3.59236500
H	2.62365600	-0.03378600	3.14582000
C	-2.18762000	1.66967700	-1.47621900
H	-2.95311600	2.42871700	-1.57299000
H	1.12608200	2.15991100	0.04218900
H	-1.85890800	1.12227700	-2.34823400
N	-1.16471000	2.01308200	-0.63463100
O	-0.13468700	1.24873500	-0.63543600
O	-1.24143000	2.98335600	0.15704700
H	3.59281600	4.37859700	-2.30703500
C	-5.38350100	1.84729100	1.98346200
C	-6.52706300	1.83015300	1.18385700
C	-6.50726000	1.24125700	-0.08719300
C	-5.31580800	0.66938400	-0.51783200
C	-4.15299800	0.65169000	0.28697200
C	-4.18853600	1.26528300	1.53823400
N	-5.07380500	0.05781800	-1.75465500
C	-3.77313900	-0.39423800	-1.84305300
C	-3.08880000	-0.04082700	-0.50619500
O	-3.28340800	-0.97249500	-2.79709600
H	-5.41407900	2.31983000	2.96115400
H	-7.44752900	2.28219700	1.54407300
H	-7.39315700	1.23603000	-0.71431200
H	-3.29808300	1.28114900	2.15020300
C	-6.05276700	-0.10851100	-2.80933900
H	-6.90736300	-0.69714000	-2.45691100
H	-6.41282500	0.86352300	-3.16642900
H	-5.56596600	-0.63657400	-3.63084700
N	-2.14219200	-0.90488200	-0.14751200
C	-1.70952500	-1.03198200	1.15790700
O	-1.73308900	-0.20616700	2.06270900
O	-1.20703300	-2.28810000	1.29523900
C	-0.83987400	-2.84023100	2.60388000
C	-0.43878100	-4.27730300	2.25820800
H	-0.12437000	-4.81159100	3.16161500

H	-1.27967300	-4.81815500	1.81114100
H	0.39094900	-4.28599000	1.54371700
C	-2.05475900	-2.83341300	3.53840100
H	-2.35356500	-1.81601600	3.79785600
H	-2.90344800	-3.33911900	3.06376000
H	-1.81401900	-3.37262200	4.46179600
C	0.35060600	-2.08262300	3.19976400
H	0.67603000	-2.57395200	4.12436300
H	1.19184100	-2.09134800	2.49871700
H	0.08485500	-1.04862300	3.42704100

**a-O-gau2-syn-S**

C	2.46623500	-0.92277300	-0.53634600
C	3.69580300	-0.09187800	-0.90973800
C	3.67086800	1.33424700	-0.79759100
C	4.86430900	-0.68815200	-1.33231000
C	2.53877000	2.05878400	-0.35524500
C	4.87102800	2.04709800	-1.12056600
C	5.98823100	0.11357900	-1.64750900
H	4.92678200	-1.76707000	-1.42598400
C	2.59709900	3.42965600	-0.17746700
H	1.60721900	1.55636200	-0.12625700
C	4.88200100	3.46266600	-0.97547200
H	6.90549100	-0.36417700	-1.98982500
C	3.78206000	4.14124800	-0.50820000
H	5.79826300	3.98704900	-1.23018300
H	3.79734700	5.21896400	-0.37582900
C	2.28811700	-0.92821600	0.99829500
H	2.40967700	0.10344300	1.32838500
C	3.26198500	-1.83642600	1.78266900
C	0.66282500	-0.72581800	2.83276800
C	0.63659900	-2.77869900	1.45224100
C	2.53963300	-2.37928700	3.03335900
H	3.59720000	-2.66743500	1.15475400
H	4.14450600	-1.25208600	2.05985000
C	1.81167800	-1.21852700	3.74043200
H	0.62499900	0.35971400	2.72953200
H	-0.32133200	-1.07847600	3.14137400
C	1.48646000	-3.40678400	2.57771800
H	0.92355900	-3.13629300	0.46680200
H	-0.43578100	-2.91099600	1.58250800
H	3.26155000	-2.84542900	3.71070800
H	1.40104900	-1.55186600	4.69910600
H	1.97112900	-4.31477200	2.20404800



H	0.85448800	-3.69886300	3.42399500
O	1.55085100	4.13458900	0.31472100
N	6.00922400	1.42850100	-1.54806100
N	0.87090400	-1.28249900	1.43841600
H	0.86451000	3.49733600	0.62454900
H	1.57683200	-0.44727200	-0.97641200
O	2.55568000	-2.25936900	-1.00346500
C	2.19904800	-2.40308300	-2.37658300
H	2.85792900	-1.81967600	-3.03259100
H	2.30794900	-3.46344100	-2.61768100
H	1.16061200	-2.09204700	-2.54430300
C	-3.03738900	0.50866700	2.14086500
H	-3.94125700	1.10113100	2.15148300
H	0.15282100	-0.84678400	0.80904800
H	-2.23922000	0.72446400	2.83822200
N	-3.22990500	-0.83032500	1.88932400
O	-2.28021200	-1.63070300	2.12719200
O	-4.28332000	-1.21379400	1.32154200
H	2.51474000	-0.40542900	3.95376900
C	-5.60185200	1.74967200	-1.40524600
C	-5.57149300	3.11093500	-1.09620200
C	-4.45888400	3.67762800	-0.46118000
C	-3.39332700	2.83812100	-0.16451600
C	-3.38849200	1.46633400	-0.49341500
C	-4.51578700	0.91877900	-1.10525200
N	-2.20946800	3.17711100	0.51603700
C	-1.39210800	2.08972400	0.64403600
C	-2.10497600	0.90264400	0.01556100
O	-0.25194200	2.11803100	1.13284600
H	-6.47735900	1.32535500	-1.88816000
H	-6.41943900	3.74291200	-1.34589500
H	-4.43674100	4.73320800	-0.21010000
H	-4.55076000	-0.13182300	-1.35071600
C	-1.90437900	4.49869500	1.03195400
H	-1.65857700	5.19313400	0.22097200
H	-2.76224100	4.88734200	1.58926800
H	-1.05219600	4.41884800	1.70782900
N	-1.39014700	-0.16351700	-0.29883800
C	-1.84837400	-1.05455400	-1.26647800
O	-2.51003100	-0.77502400	-2.25487800
O	-1.35291100	-2.29607400	-1.02423200
C	-1.95051200	-3.46981300	-1.69823700
C	-1.27295200	-4.65376700	-1.00413900
H	-1.62394600	-5.59173000	-1.44768100

H	-0.18477900	-4.61017000	-1.12277700
H	-1.51014500	-4.67150400	0.06421600
C	-1.62253400	-3.47407700	-3.19461600
H	-2.04782700	-2.60250400	-3.69321500
H	-0.53916600	-3.48344100	-3.35808100
H	-2.03633900	-4.37927500	-3.65517700
C	-3.46108000	-3.49962300	-1.43360700
H	-3.85228700	-4.49859900	-1.65800200
H	-3.66697000	-3.26867100	-0.38298400
H	-3.99312900	-2.77757100	-2.05639000

**a-N-gau1-syn-R**

C	-2.97534000	-0.97730100	-0.35421100
C	-3.42877100	-1.03279300	1.10403500
C	-2.56948500	-0.60729200	2.16853900
C	-4.69644100	-1.47588100	1.42173700
C	-1.22906500	-0.18370400	1.98281000
C	-3.11509800	-0.64664200	3.49774000
C	-5.12976700	-1.46939400	2.76704900
H	-5.35955600	-1.83806000	0.64318800
C	-0.43617400	0.15318900	3.07066800
H	-0.77561900	-0.17530900	0.99924200
C	-2.28960400	-0.24987200	4.58535400
H	-6.13569500	-1.81097700	3.00934900
C	-0.98938900	0.13694300	4.38329300
H	-2.72113500	-0.27948400	5.58160200
H	-0.34877700	0.42146700	5.21303600
C	-3.25663800	0.43728300	-0.91486600
H	-2.88871300	1.14478400	-0.16824500
C	-4.73988200	0.72945900	-1.26155300
C	-2.44635300	2.23958600	-2.39457500
C	-2.89765400	0.02670000	-3.37930800
C	-4.81936400	1.46186700	-2.61576400
H	-5.29969100	-0.20719000	-1.32017100
H	-5.18685600	1.33655300	-0.46868400
C	-3.90959800	2.70420300	-2.57487800
H	-1.94851500	2.71030400	-1.54443200
H	-1.83450200	2.40966800	-3.28283400
C	-4.32447900	0.51291800	-3.72580300
H	-2.85787900	-1.03501700	-3.15058700
H	-2.16951400	0.24828700	-4.16232800
H	-5.85347300	1.76079700	-2.81350500
H	-4.00665200	3.28013900	-3.50090100
H	-4.99621000	-0.34697300	-3.81280000

H	-4.32924500	1.03046000	-4.69134000
O	0.85730700	0.50117300	2.97040400
N	-4.38315900	-1.06370500	3.77585000
N	-2.42175000	0.75173300	-2.14681200
H	1.18813000	0.44427500	2.03127500
H	-1.89621800	-1.16474800	-0.41481100
O	-3.64964600	-1.93226200	-1.16559700
C	-3.11782300	-3.25042900	-1.03892900
H	-3.23838500	-3.63923900	-0.01934300
H	-3.68363400	-3.88190900	-1.72929100
H	-2.05383000	-3.27356900	-1.30755800
C	2.05232200	-0.70531700	-2.23721400
H	2.36350300	-1.65807800	-2.64254100
H	-1.40693100	0.50718900	-1.97042800
H	2.61395100	0.20030700	-2.41192400
N	0.70799000	-0.53520400	-2.14008300
O	0.27143600	0.63361400	-1.83617400
O	-0.09634000	-1.49853500	-2.27253800
H	-4.20562600	3.36093300	-1.74999800
C	6.49954500	-0.88902100	-0.94816500
C	6.57880100	-2.28144500	-0.86736900
C	5.45397600	-3.05185000	-0.54724900
C	4.25618200	-2.38584500	-0.31097900
C	4.15319500	-0.97649900	-0.39866100
C	5.28640900	-0.22888900	-0.71814900
N	3.02669500	-2.95044400	0.04170700
C	2.07559100	-1.96767700	0.25472700
C	2.74947900	-0.62869400	-0.05451600
O	0.92966000	-2.15369500	0.62608500
H	7.38422000	-0.31026000	-1.19759100
H	7.52573800	-2.78093400	-1.05446100
H	5.51952100	-4.13307000	-0.47936200
H	5.21562400	0.84783100	-0.80156300
C	2.76994800	-4.36496900	0.21387600
H	3.40898800	-4.78617700	0.99863700
H	1.72406400	-4.47548100	0.50498400
H	2.94482100	-4.91136400	-0.72020100
N	2.19571400	0.44617300	0.47649600
C	2.63474600	1.70954200	0.13417400
O	3.29910400	2.02064400	-0.85145800
O	2.15275000	2.58998300	1.03855500
C	2.39612700	4.03366500	0.92624300
C	1.65800000	4.58911700	2.14705300
H	1.76917700	5.67783500	2.19404200

H	0.58995300	4.35130100	2.09716000
H	2.05906800	4.15880900	3.07062300
C	1.78104300	4.57634500	-0.36823200
H	2.29851600	4.18879200	-1.24741000
H	0.72289300	4.29737800	-0.43223400
H	1.84349700	5.67076500	-0.37617400
C	3.89638900	4.32924300	1.02521300
H	4.05768100	5.41288500	1.06243000
H	4.31167700	3.89367700	1.94116800
H	4.43806200	3.92689000	0.16711200

**a-N-gau1-syn-R-Boc-rotator**

C	-3.04266200	-0.24538500	-0.85296300
C	-3.64385800	-1.30500800	0.07085600
C	-2.88566200	-1.86736600	1.14771900
C	-4.94827300	-1.72209900	-0.09934300
C	-1.52562600	-1.56002000	1.39767000
C	-3.55879700	-2.81352800	1.99405400
C	-5.51153000	-2.65953900	0.79691600
H	-5.54161200	-1.33908600	-0.92304100
C	-0.83327900	-2.18906300	2.42195000
H	-0.97747500	-0.88742600	0.75077200
C	-2.83268500	-3.40688100	3.06313300
H	-6.54506200	-2.97717800	0.66176600
C	-1.51025500	-3.10827900	3.27391200
H	-3.35870400	-4.11453200	3.69738000
H	-0.94721600	-3.57286200	4.07819500
C	-3.18913000	1.14099400	-0.18417500
H	-2.83151500	1.02951500	0.84200300
C	-4.62266800	1.73182700	-0.20171700
C	-2.15885100	3.35503800	0.17476200
C	-2.69556900	2.67375500	-2.13299200
C	-4.55901600	3.23463200	-0.53853500
H	-5.22903000	1.21605300	-0.95070100
H	-5.09268900	1.57375000	0.77351600
C	-3.57325000	3.92788400	0.42077800
H	-1.68074300	2.98579900	1.08392700
H	-1.48481300	4.07406900	-0.29524500
C	-4.05298200	3.39952600	-1.98515700
H	-2.75281400	1.79819200	-2.77462500
H	-1.89966500	3.32793000	-2.49487200
H	-5.55447100	3.67828300	-0.43875700
H	-3.57099500	5.00976600	0.25331500
H	-4.77684100	2.97441900	-2.68762300

H	-3.94753400	4.46292000	-2.22661000
O	0.47220100	-1.98780600	2.66634700
N	-4.85792700	-3.18662500	1.81427100
N	-2.25269600	2.18617600	-0.77641700
H	0.87121800	-1.35043600	2.01244300
H	-1.97472000	-0.44852000	-1.00360100
O	-3.68514900	-0.21063200	-2.12175100
C	-3.23852500	-1.23848700	-3.00502300
H	-3.47555800	-2.23740900	-2.61667600
H	-3.76881100	-1.08936800	-3.94958900
H	-2.15676200	-1.16844000	-3.17721600
C	2.15109900	0.72966600	-1.83287900
H	2.42353100	0.26239900	-2.76987500
H	-1.27204200	1.80825000	-0.85911500
H	2.80305800	1.45150200	-1.36604300
N	0.81864300	1.01980000	-1.71871000
O	0.44719200	1.74360000	-0.73173300
O	-0.03297000	0.52476300	-2.50155600
H	-3.87671200	3.75890100	1.45927200
C	6.35398400	-0.90693500	-0.57786400
C	6.37129500	-1.95534000	-1.50089400
C	5.18151400	-2.53946500	-1.95207600
C	3.98242900	-2.04012000	-1.45311100
C	3.94321200	-0.96262900	-0.53765300
C	5.13980500	-0.40688700	-0.09112900
N	2.69189600	-2.49988000	-1.72865500
C	1.75214200	-1.81625700	-0.97508900
C	2.50946100	-0.73046000	-0.19933700
O	0.55642000	-2.05079500	-0.95030200
H	7.28848800	-0.47482300	-0.23180900
H	7.32038700	-2.33143700	-1.87345300
H	5.19706100	-3.36483400	-2.65679600
H	5.12702000	0.40772300	0.62101900
C	2.36521000	-3.60915100	-2.60045900
H	2.84113100	-4.53365900	-2.25310400
H	1.28146300	-3.73492200	-2.57970000
H	2.68646600	-3.40710800	-3.62861300
N	1.92432600	-0.28651100	0.90263700
C	2.36848500	0.74774600	1.69468400
O	2.00680900	0.87695100	2.85560400
O	3.17568000	1.64201600	1.04972700
C	3.53469700	2.93043800	1.66933900
C	4.33929800	3.62709300	0.56808800
H	4.69643800	4.60066700	0.92154000

H	5.21025300	3.02916900	0.27857300
H	3.72353600	3.79202100	-0.32288400
C	4.40597900	2.70331300	2.90897300
H	3.85124500	2.17966500	3.68886000
H	5.29565200	2.11503500	2.65524800
H	4.74455000	3.66836500	3.30414700
C	2.26674000	3.72938500	1.98884100
H	2.53799200	4.74891700	2.28691500
H	1.62708900	3.78663200	1.10135200
H	1.70168500	3.26624300	2.79945200

**a-N-gau1-anti-R**

C	3.06901900	-0.94992300	-0.28720400
C	3.50393800	-0.07277200	-1.46235900
C	2.60658700	0.85470700	-2.08369400
C	4.79647700	-0.15514900	-1.94051600
C	1.24413900	1.00468800	-1.72007700
C	3.13749400	1.64803100	-3.15914700
C	5.21336500	0.68211600	-2.99953700
H	5.49193500	-0.86968400	-1.51324200
C	0.41893400	1.87712200	-2.41557300
H	0.80208400	0.39526400	-0.94181100
C	2.27389000	2.56157200	-3.82364800
H	6.23802900	0.61756100	-3.36437400
C	0.95453200	2.67415100	-3.46822900
H	2.69419800	3.15568200	-4.62986300
H	0.28635400	3.35802100	-3.98364800
C	3.23847800	-0.16405400	1.03217000
H	2.70735400	0.78092900	0.89382800
C	4.69882400	0.09707500	1.47667800
C	2.31104500	0.21524300	3.28222300
C	3.25982100	-1.99800700	2.77329000
C	4.79478800	-0.02674800	3.01126700
H	5.37201200	-0.62630000	1.00775500
H	5.00318100	1.09460300	1.14664100
C	3.68255300	0.82222200	3.65698800
H	1.59901600	0.94324000	2.89559900
H	1.83815800	-0.30586300	4.11720300
C	4.58286500	-1.50314800	3.40039600
H	3.42091500	-2.69052900	1.95031300
H	2.58716200	-2.45816000	3.50013000
H	5.77740500	0.31447300	3.35144400
H	3.79454900	0.84027900	4.74594300
H	5.41470200	-2.11536400	3.03722200

H	4.55496800	-1.60464700	4.49093700
O	-0.89208000	2.02671800	-2.16600900
N	4.42719600	1.56006700	-3.59176200
N	2.51247500	-0.81773600	2.20118200
H	-1.21033700	1.44038300	-1.42508300
H	2.00766400	-1.21138300	-0.39447400
O	3.83482600	-2.14764100	-0.20559200
C	3.41315200	-3.15210300	-1.12516900
H	3.52735600	-2.82450400	-2.16641100
H	4.05261200	-4.02187300	-0.95263100
H	2.36452000	-3.43141200	-0.95290800
C	-2.07375900	-1.71928800	1.67939000
H	-2.20269000	-2.78533200	1.55376100
H	1.56418600	-1.17379500	1.88882000
H	-2.80274300	-1.11079700	2.19301700
N	-0.79057800	-1.29505400	1.80832900
O	-0.55466800	-0.09506700	2.11363100
O	0.17803600	-2.09754800	1.53827800
H	3.74993900	1.85814300	3.30723200
C	-6.42183400	-1.67847400	-0.03681800
C	-6.30805000	-2.87144600	-0.75452300
C	-5.07204700	-3.29569100	-1.25797400
C	-3.96326500	-2.49121700	-1.01885900
C	-4.05494400	-1.28628200	-0.28203900
C	-5.29661300	-0.88208200	0.20824300
N	-2.65297900	-2.70182500	-1.46065100
C	-1.83716200	-1.64312600	-1.10495300
C	-2.69518600	-0.68379400	-0.27642400
O	-0.66323100	-1.51637400	-1.41278100
H	-7.39029400	-1.36602200	0.34300200
H	-7.18960600	-3.48198200	-0.93121700
H	-4.98666000	-4.21736700	-1.82454900
H	-5.37794500	0.03162300	0.78215500
C	-2.20833200	-3.82567100	-2.25773500
H	-2.33856900	-4.76817900	-1.71363200
H	-2.76374300	-3.87981500	-3.20132900
H	-1.14906600	-3.67736300	-2.47343700
N	-2.26141000	0.55842100	-0.17067000
C	-2.88586700	1.44755500	0.68615700
O	-3.64802300	1.17312500	1.60923100
O	-2.47440700	2.69612900	0.38161900
C	-2.89749200	3.86815900	1.15879500
C	-2.16908200	5.01311800	0.44961800
H	-2.40384800	5.96850100	0.93133700

H	-1.08472200	4.86345100	0.48614500
H	-2.46888000	5.07026100	-0.60197600
C	-2.41819400	3.74094800	2.60862800
H	-2.92770900	2.92633400	3.12620400
H	-1.33905800	3.55192300	2.63648800
H	-2.61351300	4.67630400	3.14612900
C	-4.41551700	4.05277100	1.06112500
H	-4.70321600	4.99889300	1.53411800
H	-4.72943000	4.08951200	0.01169000
H	-4.94813600	3.24012900	1.55852600

**a-O-gau1-syn-R**

C	-3.05255600	-0.83402600	1.00431900
C	-4.27746700	-0.01539500	0.59642500
C	-4.13722400	1.20815000	-0.13525600
C	-5.54994800	-0.44814600	0.90436600
C	-2.88716900	1.75907500	-0.51852900
C	-5.34328000	1.89069000	-0.50765600
C	-6.67101800	0.31495100	0.50171000
H	-5.69345300	-1.36953200	1.45846500
C	-2.82996100	2.91156900	-1.28469400
H	-1.95483300	1.30753500	-0.19828900
C	-5.24390200	3.09299200	-1.26096400
H	-7.67277800	-0.03027000	0.75543600
C	-4.02488900	3.58850600	-1.65124600
H	-6.16808300	3.59759400	-1.52664000
H	-3.94530600	4.49782400	-2.23956400
C	-2.45839700	-1.54352700	-0.23042800
H	-2.34145700	-0.77843000	-0.99941300
C	-3.25979900	-2.73363500	-0.80258000
C	-0.34353000	-2.15181700	-1.32496900
C	-0.98694100	-3.35514800	0.73631800
C	-2.26760100	-3.77087000	-1.37223600
H	-3.87169300	-3.19324300	-0.02016200
H	-3.93540800	-2.36826000	-1.58157400
C	-1.21162300	-3.05016100	-2.23721100
H	-0.21017900	-1.13885600	-1.70701600
H	0.64881200	-2.56044000	-1.12988700
C	-1.54785800	-4.45290600	-0.19312000
H	-1.57872300	-3.23047800	1.64127900
H	0.05698300	-3.51613300	1.01153200
H	-2.80329200	-4.51422400	-1.97028800
H	-0.57365500	-3.77945900	-2.74689300
H	-2.24175400	-5.08839500	0.36659100



H	-0.74203100	-5.09575200	-0.56463400
O	-1.66538200	3.44473900	-1.72038800
N	-6.58887300	1.43986600	-0.18100400
N	-1.03432600	-2.02867100	0.01300900
H	-0.90697100	2.86420400	-1.46214900
H	-2.28436100	-0.15279800	1.39688900
O	-3.36012500	-1.81016400	1.99346900
C	-3.33527100	-1.29600300	3.32405800
H	-4.07561300	-0.49836200	3.46732600
H	-3.57893600	-2.13124600	3.98599800
H	-2.33981200	-0.90855400	3.57937100
C	1.85927400	1.13216800	2.00302600
H	1.81947000	2.16593200	2.32071700
H	-0.50068400	-1.34641000	0.61069200
H	2.64748800	0.47737600	2.34682500
N	0.63410100	0.52820200	1.89510300
O	0.61336100	-0.74173400	1.76377200
O	-0.42094300	1.20954000	1.82996500
H	-1.70244400	-2.45169200	-3.01256400
C	6.04435800	2.64362200	0.82935600
C	5.68203000	3.96772700	0.57407700
C	4.38617700	4.29002900	0.15137200
C	3.47960000	3.24801500	-0.00371900
C	3.82387500	1.90378000	0.25060800
C	5.11764700	1.60442200	0.67449800
N	2.14280900	3.34294500	-0.42926200
C	1.58121300	2.09652100	-0.54744800
C	2.61154000	1.07887100	-0.05011300
O	0.45957500	1.84375600	-0.98884800
H	7.05394700	2.41323800	1.15757700
H	6.41117800	4.76334000	0.70150500
H	4.10624600	5.31795900	-0.05517800
H	5.38942600	0.57998500	0.89265800
C	1.48181700	4.59704100	-0.74064000
H	1.87232700	5.02861500	-1.66972000
H	0.41242400	4.42186900	-0.85119000
H	1.63610000	5.30963800	0.07564200
N	2.47750500	-0.15614600	-0.50941200
C	3.31027200	-1.14861000	-0.06957200
O	4.00292800	-1.16124700	0.94876000
O	3.21834700	-2.21243200	-0.92065100
C	4.05565300	-3.40476600	-0.74893800
C	3.66824400	-4.26466100	-1.95597600
H	4.23277900	-5.20344100	-1.95018300

H	2.59984000	-4.50802200	-1.93608800
H	3.88216700	-3.73880600	-2.89264800
C	3.70935600	-4.12744300	0.55768500
H	3.94143100	-3.50629800	1.42398200
H	2.64361000	-4.38464700	0.58448500
H	4.28126800	-5.06023400	0.62822900
C	5.54128700	-3.03276100	-0.82370800
H	6.14875500	-3.94437400	-0.86014200
H	5.74376100	-2.45550800	-1.73320400
H	5.84938900	-2.44380200	0.04165900

**a-O-gau1-anti-R**

C	-3.37879700	-0.65242300	1.08251400
C	-4.51511500	0.12664100	0.42318100
C	-4.24313000	1.25957900	-0.40989500
C	-5.82705200	-0.26186500	0.59235600
C	-2.93956500	1.75991100	-0.66508900
C	-5.36889100	1.89820100	-1.02927400
C	-6.86204400	0.45385600	-0.05345600
H	-6.06711400	-1.11405300	1.21905700
C	-2.74975000	2.82325700	-1.53285700
H	-2.06724400	1.32450200	-0.18954000
C	-5.13810500	3.00781100	-1.88879100
H	-7.89696700	0.14437100	0.08781800
C	-3.86683800	3.45669500	-2.14346400
H	-6.00390100	3.47933400	-2.34410000
H	-3.68496100	4.29435100	-2.81010500
C	-2.64480400	-1.50447900	0.02438300
H	-2.43210600	-0.83978100	-0.81420000
C	-3.38709500	-2.76009000	-0.48326900
C	-0.41953400	-2.23704800	-0.72247400
C	-1.31390000	-3.16543200	1.38201000
C	-2.34252000	-3.85407900	-0.79655600
H	-4.09024700	-3.12071000	0.27384700
H	-3.96341500	-2.49792500	-1.37551900
C	-1.19012600	-3.23544800	-1.61681600
H	-0.21100800	-1.28172800	-1.20650500
H	0.52690600	-2.62903300	-0.35237600
C	-1.77116300	-4.37480400	0.53765900
H	-2.00821200	-2.93504300	2.18851200
H	-0.30944300	-3.27392900	1.79236200
H	-2.81023100	-4.67101600	-1.35426800
H	-0.50621200	-4.01512500	-1.96723500
H	-2.53142200	-4.93900400	1.08750000

H	-0.93260300	-5.05388100	0.34882900
O	-1.52728200	3.30730800	-1.84594700
N	-6.65697900	1.49172800	-0.84025300
N	-1.26636400	-1.94370300	0.49565800
H	-0.82023200	2.75080900	-1.43183200
H	-2.65667000	0.06549500	1.49647500
O	-3.83482900	-1.50240700	2.12559700
C	-3.99862400	-0.83625200	3.37550500
H	-4.72977100	-0.02012900	3.31118400
H	-4.36362200	-1.58509400	4.08323100
H	-3.04199700	-0.43358300	3.73663500
C	2.08900800	0.77780600	2.08431700
H	1.74814000	1.72740600	2.47791900
H	-0.81517400	-1.16650800	1.03960400
H	3.02555000	0.36234800	2.42903600
N	1.09767300	-0.17107300	1.97131300
O	1.42495100	-1.36137600	1.75424300
O	-0.12902100	0.18389700	1.94488900
H	-1.58825300	-2.73132000	-2.50433300
C	6.04128100	2.80403700	0.97810900
C	5.56991600	4.11435500	0.88320100
C	4.23416300	4.37268500	0.55073300
C	3.40418300	3.28214500	0.31902800
C	3.85718400	1.95076800	0.41127000
C	5.18856400	1.71531400	0.74999700
N	2.04467300	3.31876700	-0.04236300
C	1.56387900	2.05450800	-0.26271800
C	2.68356200	1.06128800	0.09216600
O	0.44330100	1.77309700	-0.68992400
H	7.08027300	2.62124000	1.23766000
H	6.24174200	4.94830000	1.06782500
H	3.86640700	5.39059000	0.47122700
H	5.54460800	0.69751800	0.83732700
C	1.29860600	4.54917900	-0.22898200
H	1.70877800	5.12866600	-1.06391800
H	0.25848700	4.30808600	-0.44315300
H	1.34111000	5.15667800	0.68126300
N	2.61027600	-0.10038700	-0.55663400
C	3.56066800	-1.06493900	-0.36002600
O	4.42655100	-1.12192900	0.51424800
O	3.38619900	-2.04237800	-1.29775800
C	4.27428300	-3.20330300	-1.36442300
C	3.72197700	-3.98058100	-2.56354100
H	4.30536000	-4.89315200	-2.72823700

H	2.67783500	-4.26620600	-2.39355500
H	3.76553100	-3.37385700	-3.47456600
C	4.16485400	-4.04622600	-0.08811800
H	4.54543900	-3.50157600	0.77709500
H	3.12025800	-4.31867000	0.10319200
H	4.73878500	-4.97331300	-0.20447300
C	5.71767700	-2.76420400	-1.63968300
H	6.34563900	-3.64462100	-1.82042000
H	5.76008000	-2.12966300	-2.53269000
H	6.12944600	-2.20897000	-0.79537400

**a-N-gau2-syn-R**

C	-3.04230400	0.68088100	-1.16714400
C	-3.69187800	-0.67301400	-0.87599600
C	-2.91886200	-1.86501900	-0.67530500
C	-5.06871900	-0.76213500	-0.81371200
C	-1.49808600	-1.92531500	-0.72409800
C	-3.66165600	-3.07391500	-0.43342500
C	-5.68843200	-2.00202700	-0.54757100
H	-5.67923100	0.11689800	-0.99124700
C	-0.83212100	-3.13630500	-0.55805500
H	-0.90843700	-1.03330600	-0.90914600
C	-2.94990500	-4.29434600	-0.27199800
H	-6.77496500	-2.06150500	-0.49268700
C	-1.58258300	-4.32947600	-0.33706100
H	-3.53130200	-5.19502900	-0.09791000
H	-1.03347200	-5.25868100	-0.21654400
C	-2.71547000	1.42083800	0.15378800
H	-2.21461500	0.69791000	0.80157000
C	-3.92705900	2.05906200	0.87828500
C	-1.08792900	2.89869500	1.29699900
C	-2.21246300	3.74037600	-0.72093200
C	-3.53244700	3.45491000	1.40286000
H	-4.76951500	2.15451800	0.18846500
H	-4.24186800	1.41040200	1.70090500
C	-2.23768200	3.33969500	2.23067000
H	-0.52151800	2.04023400	1.65996300
H	-0.37701300	3.70072500	1.09086200
C	-3.27805700	4.38423900	0.19840600
H	-2.62613500	3.42043600	-1.67495600
H	-1.35337600	4.38981500	-0.90214000
H	-4.34092200	3.85823700	2.02043900
H	-1.99244900	4.30058400	2.69500200

H	-4.20560700	4.53736700	-0.36239000
H	-2.93979600	5.36620700	0.54667000
O	0.49804700	-3.29021800	-0.60499500
N	-5.02157600	-3.12486000	-0.36414500
N	-1.66816200	2.51115200	-0.04171900
H	1.00194400	-2.42874500	-0.53124000
H	-2.10597100	0.51618600	-1.71330600
O	-3.88797300	1.52010700	-1.94937700
C	-3.92909900	1.16637700	-3.32837500
H	-4.32785600	0.15538800	-3.47960800
H	-4.59103200	1.88718100	-3.81552700
H	-2.93084300	1.22691700	-3.78540300
C	2.27806400	0.90908600	-2.14868600
H	1.91197100	0.14845500	-2.82480400
H	-0.88879600	2.09741000	-0.61935000
H	3.13923300	1.49968000	-2.43296800
N	1.26824900	1.64752700	-1.58044000
O	1.46422800	2.78526500	-1.10072300
O	0.12395600	1.08257000	-1.48563300
H	-2.37426900	2.61416100	3.04002700
C	5.29411900	2.15209800	1.19722100
C	6.44992600	1.80410200	0.49695600
C	6.42441700	0.80492100	-0.48531300
C	5.21269100	0.17022700	-0.73266000
C	4.03314900	0.50302800	-0.02874800
C	4.07624600	1.50933300	0.93354700
N	4.96048800	-0.84025600	-1.67012000
C	3.63903400	-1.23906200	-1.63347900
C	2.94161200	-0.36288100	-0.57469900
O	3.13916400	-2.11944000	-2.31156000
H	5.33288700	2.93438400	1.95005300
H	7.38617600	2.31358600	0.70932200
H	7.32312600	0.53690800	-1.03169700
H	3.17367100	1.78711800	1.46023800
C	5.94670600	-1.42121300	-2.55841100
H	6.75669000	-1.89041500	-1.98853400
H	5.44241100	-2.18062700	-3.15811500
H	6.37234200	-0.65873500	-3.22092600
N	1.93597100	-0.97373300	0.05417600
C	1.43386100	-0.53279300	1.25919800
O	1.30910400	0.62270700	1.65993900
O	1.03668200	-1.62074100	1.96485500
C	0.55726200	-1.53810000	3.35020000
C	0.34687000	-3.01064200	3.71455000

H	-0.00275200	-3.09868000	4.74886100
H	-0.39703300	-3.47192900	3.05687400
H	1.28360600	-3.56895400	3.61633400
C	-0.77038600	-0.77779900	3.42310600
H	-0.63252400	0.28160900	3.19959800
H	-1.49289000	-1.20397400	2.71856400
H	-1.19103100	-0.86621400	4.43176500
C	1.63071900	-0.91359200	4.24806000
H	1.31600500	-0.97598900	5.29625900
H	2.57680700	-1.45699800	4.14584200
H	1.80069300	0.13526200	3.99748700

**a-O-anti-R-1**

C	-3.73711300	-0.04671000	0.49327900
C	-4.12523700	1.43306500	0.48712000
C	-3.14625800	2.47675000	0.39488400
C	-5.45932800	1.78690600	0.53282900
C	-1.74249800	2.26571200	0.41753400
C	-3.64578800	3.82196100	0.29087100
C	-5.83438000	3.14590200	0.44285500
H	-6.22474200	1.02594500	0.64368800
C	-0.86275100	3.33664400	0.34798700
H	-1.32421600	1.26992100	0.49353100
C	-2.71498100	4.89071900	0.17315300
H	-6.88945000	3.41577900	0.47335900
C	-1.36363200	4.66078300	0.19880500
H	-3.11500000	5.89616100	0.08187600
H	-0.64923200	5.47574300	0.12977500
C	-3.75557700	-0.59733500	-0.95653900
H	-3.27466600	0.15735700	-1.58234000
C	-5.15574200	-0.96974000	-1.51337100
C	-2.65620600	-2.10228500	-2.58557700
C	-3.38923900	-3.04247600	-0.42755600
C	-5.10811600	-2.37670000	-2.14366100
H	-5.89213800	-0.96167700	-0.70685300
H	-5.46417300	-0.22666700	-2.25476500
C	-4.02294400	-2.41421800	-3.23563300
H	-2.17264000	-1.22037000	-3.00977000
H	-1.94931100	-2.93250000	-2.63778200
C	-4.75900200	-3.40548500	-1.04941700
H	-3.46502300	-2.80818100	0.63250300
H	-2.63610300	-3.82072400	-0.56739400
H	-6.08379400	-2.61475600	-2.57810900

H	-3.99736000	-3.39942700	-3.71242700
H	-5.53068800	-3.40226500	-0.27359500
H	-4.72543200	-4.41285800	-1.47700900
O	0.47806900	3.20783500	0.40392100
N	-4.97225500	4.13469700	0.30841800
N	-2.85460500	-1.81638800	-1.11613600
H	0.73992100	2.31672700	0.74394200
H	-2.71777200	-0.15293800	0.88658600
O	-4.61977200	-0.83745100	1.28150400
C	-4.44393200	-0.66844400	2.68465400
H	-4.65554000	0.35993800	3.00263500
H	-5.15084200	-1.34542900	3.17108600
H	-3.42173500	-0.93190300	2.99371500
C	1.69078300	-0.53540700	-1.14331200
H	2.43632600	-1.01636900	-1.76118100
H	-1.89892700	-1.55394700	-0.74883200
H	1.50621600	0.52212700	-1.27440600
N	0.53088700	-1.26178000	-0.98234600
O	-0.52031200	-0.62992500	-0.59281600
O	0.50380200	-2.50507300	-1.12602900
H	-4.24630800	-1.68051500	-4.01703000
C	4.38024400	-3.91441000	0.72670600
C	3.47764500	-4.44004500	1.65416500
C	2.43510600	-3.65882600	2.16904500
C	2.33428400	-2.34674800	1.72258100
C	3.23080900	-1.80029500	0.78438200
C	4.26057600	-2.59096800	0.28216400
N	1.39551300	-1.37601000	2.12181200
C	1.64252200	-0.17203600	1.51576300
C	2.83153600	-0.37200300	0.56801000
O	0.99910500	0.85569200	1.71774900
H	5.18146600	-4.53804500	0.34037700
H	3.58068700	-5.47008600	1.98493000
H	1.73686500	-4.06572100	2.89368600
H	4.94624800	-2.18226900	-0.45014400
C	0.32049200	-1.59950200	3.06587200
H	0.71685700	-1.92546500	4.03386700
H	-0.20963100	-0.65483400	3.19446500
H	-0.37288300	-2.36060800	2.68992500
N	3.59901800	0.70184200	0.39315400
C	4.65103500	0.66583700	-0.47321200
O	4.79682500	-0.09016500	-1.44095900
O	5.51526700	1.66769500	-0.16642400
C	6.68835900	1.95856300	-0.99397200

C	7.32589800	3.14413600	-0.26275400
H	8.23419100	3.46786000	-0.78273400
H	6.63222800	3.99055500	-0.21723300
H	7.59430600	2.86800300	0.76280500
C	6.25517000	2.37267300	-2.40526500
H	5.80950000	1.53427400	-2.94353000
H	5.52225300	3.18615700	-2.35433900
H	7.12262300	2.73313400	-2.97070500
C	7.64903900	0.76365400	-1.01037500
H	8.58010100	1.04169300	-1.51829600
H	7.90021600	0.46225200	0.01325200
H	7.20904000	-0.08949900	-1.52950200

**a-O-anti-R-2**

C	-3.22679300	-0.42376800	0.65119300
C	-4.14098800	0.73919400	0.25687400
C	-3.69454300	1.83531500	-0.55187900
C	-5.45478000	0.73418700	0.68399500
C	-2.36006900	2.00217800	-1.01368700
C	-4.67491600	2.83460300	-0.88187100
C	-6.33060500	1.77232800	0.29877600
H	-5.81590000	-0.06154600	1.32637300
C	-2.00440700	3.12259500	-1.75081600
H	-1.60104600	1.25648800	-0.80007300
C	-4.28273400	3.94440200	-1.68008700
H	-7.36671600	1.75502100	0.63484100
C	-2.98784200	4.08937000	-2.10320400
H	-5.04349700	4.67890100	-1.92677400
H	-2.67722300	4.94396800	-2.69672900
C	-3.24879600	-1.50762700	-0.44775700
H	-2.93817000	-1.00790400	-1.36725700
C	-4.59150500	-2.24282500	-0.66182300
C	-1.89730900	-3.23422600	-1.56374900
C	-2.58378700	-3.63118200	0.76748000
C	-4.30667300	-3.70930800	-1.05159200
H	-5.19122900	-2.21817400	0.25306900
H	-5.15990100	-1.73130500	-1.44345400
C	-3.23062900	-3.74552300	-2.15529300
H	-1.40216100	-2.48774800	-2.18561700
H	-1.19047900	-4.04132600	-1.35868500
C	-3.76516600	-4.44394700	0.19012500
H	-2.84445100	-3.10407000	1.68231100
H	-1.69358100	-4.23871600	0.94358800



H	-5.22572600	-4.18728600	-1.40331800
H	-3.09982000	-4.76498900	-2.53186400
H	-4.54865500	-4.54056900	0.94842800
H	-3.44417800	-5.45609200	-0.07931100
O	-0.75030500	3.38525600	-2.17452800
N	-5.97073300	2.78624800	-0.46329300
N	-2.17988500	-2.57323100	-0.23418700
H	-0.07250100	2.80944000	-1.74812600
H	-2.19086900	-0.07114100	0.74153100
O	-3.62673800	-1.01547300	1.88214300
C	-3.21730800	-0.27799900	3.03049700
H	-3.63329600	0.73751300	3.03225500
H	-3.59539200	-0.81914500	3.90158500
H	-2.12119600	-0.21865600	3.09163800
C	2.03276700	-0.85344700	-0.75199800
H	2.69809100	-1.61237600	-0.36458300
H	-1.28422500	-2.12858200	0.09414900
H	2.19839000	-0.45175700	-1.74202600
N	0.70473400	-1.05682500	-0.48115600
O	-0.18493500	-0.50017200	-1.19126800
O	0.36178200	-1.76031700	0.53117400
H	-3.53733300	-3.12297400	-3.00268500
C	3.14920300	-0.64203300	3.87728900
C	2.09333100	0.11288900	4.39198300
C	1.36487400	0.98754900	3.57453100
C	1.73126000	1.07344400	2.23644200
C	2.79350000	0.32074300	1.69936300
C	3.50657900	-0.54305500	2.52570300
N	1.15646000	1.89103000	1.24466300
C	1.79517600	1.72696000	0.03934600
C	2.93250300	0.71807500	0.26179700
O	1.50099700	2.28268500	-1.01385300
H	3.69920600	-1.31571800	4.52819700
H	1.82798400	0.02585200	5.44230300
H	0.54951100	1.57965400	3.97800100
H	4.31947200	-1.13128200	2.11745600
C	0.12802600	2.88210600	1.49732600
H	0.45261800	3.56511900	2.29044700
H	-0.02840500	3.45092500	0.58100000
H	-0.81434700	2.41246500	1.79657800
N	4.04525100	0.96326800	-0.42382800
C	5.11414600	0.11934600	-0.33876300
O	5.09279900	-1.08532400	-0.06078600
O	6.23861800	0.78858200	-0.69772300

C	7.53960700	0.12292300	-0.80504400
C	8.46445700	1.27157000	-1.21945300
H	9.49011000	0.90880500	-1.34800000
H	8.13226200	1.71331000	-2.16496400
H	8.46876800	2.05888000	-0.45786700
C	7.49865600	-0.95209900	-1.89683200
H	6.82699200	-1.76772900	-1.62288500
H	7.15904700	-0.51994200	-2.84518300
H	8.50331200	-1.36294500	-2.05230600
C	7.97102200	-0.44630600	0.55163200
H	9.00400400	-0.80884400	0.48999000
H	7.93197900	0.33272700	1.32183100
H	7.32878100	-1.27395300	0.85756800

**a-Boc-O-gau1-R**

C	2.35237600	0.53529000	0.78948600
C	3.36012600	-0.48997700	0.25873900
C	3.01672900	-1.46980200	-0.72918500
C	4.65343200	-0.48565000	0.74471600
C	1.70728100	-1.66052700	-1.24242700
C	4.07224300	-2.33549400	-1.18337100
C	5.61055900	-1.38714700	0.22867200
H	4.94122100	0.20117500	1.53299900
C	1.44402500	-2.68302600	-2.13841100
H	0.89741200	-0.99651300	-0.96466000
C	3.77643800	-3.32496400	-2.16087000
H	6.63071300	-1.36393800	0.61051500
C	2.49769400	-3.50322200	-2.62456400
H	4.59332500	-3.95365600	-2.50243300
H	2.25906600	-4.27937300	-3.34565800
C	2.50924100	1.87380900	0.02988700
H	2.46858900	1.63139300	-1.03316400
C	3.78281000	2.68844900	0.36946400
C	1.31646400	3.85307100	-0.86513200
C	1.31726300	3.48847900	1.57318800
C	3.43962700	4.19032500	0.42205300
H	4.18193600	2.37686100	1.33808500
H	4.54849100	2.49053700	-0.38613700
C	2.67927300	4.57760000	-0.85914800
H	1.07655200	3.33381300	-1.79058200
H	0.48278600	4.51811400	-0.63455100
C	2.53055400	4.44370400	1.64118200
H	1.36202800	2.70244800	2.32328700
H	0.35847000	4.00100900	1.64931200

H	4.35932800	4.77666400	0.51148400
H	2.52220100	5.66051100	-0.90213400
H	3.08392400	4.26863300	2.56961300
H	2.19794700	5.48758500	1.65167500
O	0.19680000	-2.96674600	-2.58816000
N	5.34976500	-2.27339000	-0.71206000
N	1.31396000	2.80255000	0.22744900
H	-0.47334400	-2.59100000	-1.97375300
H	1.33140500	0.17211600	0.62231300
O	2.53365800	0.77659000	2.18192900
C	2.03166200	-0.27249900	3.00697000
H	2.59108500	-1.20589600	2.86045200
H	2.15515500	0.05815300	4.04162000
H	0.96728800	-0.45963300	2.80823200
C	-2.15390900	0.64217900	-2.07035800
H	-3.06141200	1.03903300	-2.50479100
H	0.42880000	2.27209800	0.13178100
H	-1.90803800	-0.40442300	-2.17158000
N	-1.08816400	1.50266100	-2.10437000
O	0.06425000	1.06054300	-1.79331200
O	-1.27062000	2.72489500	-2.34534400
H	3.26596900	4.29922200	-1.74175700
C	-6.09241300	-1.07584400	-0.43186000
C	-6.73892700	0.16104600	-0.36417800
C	-6.02244100	1.34349100	-0.13297800
C	-4.64575400	1.24223200	0.02712500
C	-3.97603500	0.00102300	-0.04598600
C	-4.70294200	-1.16334500	-0.27620500
N	-3.72767800	2.27349600	0.27324200
C	-2.45057200	1.77400600	0.40173600
C	-2.53488100	0.27459300	0.18350200
O	-1.45341900	2.43982300	0.67378000
H	-6.66921700	-1.97780600	-0.61467200
H	-7.81682200	0.21308800	-0.49171200
H	-6.52994600	2.30151600	-0.07906300
H	-4.19904500	-2.11990300	-0.35460400
C	-4.05158100	3.68400000	0.33339800
H	-4.74450000	3.89086100	1.15668400
H	-3.12204400	4.23018200	0.49880300
H	-4.50263100	4.01782600	-0.60756000
N	-1.59010300	-0.47941100	0.69344900
C	-1.54783000	-1.83024200	0.48760300
O	-1.68391100	-2.40075700	-0.60481200
O	-1.24195600	-2.46528700	1.63326800

C	-1.12273700	-3.93517000	1.73062900
C	-0.84125200	-4.13700900	3.22176000
H	-0.72796100	-5.20363200	3.44268000
H	0.08127100	-3.62481900	3.51576200
H	-1.66170200	-3.74288400	3.83094900
C	0.05167100	-4.43623500	0.88756100
H	-0.14284300	-4.32628100	-0.18004100
H	0.96738300	-3.89107200	1.13932000
H	0.22309600	-5.49820700	1.09867500
C	-2.44447900	-4.60107000	1.33687800
H	-2.39948100	-5.67003200	1.57484000
H	-3.27820700	-4.16522300	1.89903500
H	-2.64342100	-4.49484200	0.26872900

**a-Boc-O-gau2-R**

C	3.22292000	0.21532400	-0.96488700
C	3.64669200	1.62386400	-0.54914500
C	2.72675000	2.55904700	0.02968100
C	4.96692700	2.00199900	-0.69286300
C	1.32935200	2.32934100	0.18668600
C	3.28140200	3.81015500	0.47234500
C	5.39465500	3.26927300	-0.24122100
H	5.67837900	1.32665200	-1.15564300
C	0.52189100	3.29865300	0.76263200
H	0.87196700	1.40382100	-0.15134800
C	2.42455400	4.76362700	1.08692500
H	6.43884100	3.55820200	-0.35538900
C	1.08577300	4.51725300	1.23426100
H	2.86887000	5.69551400	1.42329300
H	0.42136400	5.24439900	1.69111700
C	3.33312300	-0.73348700	0.25459600
H	2.85253600	-0.21851100	1.08983500
C	4.76680500	-1.17434500	0.64145300
C	2.27059400	-2.62321000	1.43385600
C	3.13314900	-3.00025700	-0.84355600
C	4.74790900	-2.66138200	1.05266100
H	5.44531200	-1.03770400	-0.20483200
H	5.12926200	-0.55012200	1.46333000
C	3.64031600	-2.88382200	2.10097600
H	1.63596000	-1.94050500	2.00202500
H	1.70431700	-3.53913600	1.25229100
C	4.43600200	-3.51847900	-0.19085600
H	3.31695400	-2.48394100	-1.78387600

H	2.38661800	-3.77925200	-1.00641600
H	5.72072100	-2.94203500	1.46720600
H	3.67586400	-3.90773700	2.48652000
H	5.25806700	-3.45726600	-0.91104400
H	4.33092500	-4.57059600	0.09572300
O	-0.81332900	3.18392400	0.93453600
N	4.59560900	4.14478600	0.33539700
N	2.49587200	-1.99540100	0.08187400
H	-1.23213600	2.43983100	0.44619200
H	2.17601000	0.22704400	-1.29241400
O	4.03099000	-0.30389200	-2.01515400
C	3.70478600	0.22163000	-3.29915300
H	3.84992500	1.30841500	-3.34366400
H	4.37966700	-0.25710400	-4.01327900
H	2.66592100	-0.01172800	-3.57234500
C	-1.74888600	-1.06782700	-1.88014500
H	-1.73972400	0.01208200	-1.87363300
H	1.55017000	-1.70618300	-0.29520700
H	-2.18200500	-1.60556100	-2.71270200
N	-0.58022900	-1.61336500	-1.41222800
O	-0.29768800	-2.82335400	-1.57980600
O	0.18227800	-0.86621200	-0.69739800
H	3.78662200	-2.21007100	2.95202800
C	-1.43867300	-1.44802600	2.90362800
C	-1.47643100	-2.84035000	3.01213100
C	-2.06360500	-3.62829300	2.01294700
C	-2.61515900	-2.97688300	0.91415000
C	-2.58618600	-1.57016500	0.78712400
C	-1.98771100	-0.80561600	1.78420100
N	-3.29073800	-3.55468800	-0.16679100
C	-3.78056900	-2.58757600	-1.02570200
C	-3.30715200	-1.22732800	-0.47480900
O	-4.44263100	-2.79640100	-2.02630400
H	-0.98439700	-0.85468100	3.69240100
H	-1.05050100	-3.32571900	3.88672900
H	-2.10102300	-4.70923000	2.10430400
H	-1.94725600	0.27207500	1.69162200
C	-3.47401000	-4.97521800	-0.37549200
H	-4.01764000	-5.42909900	0.46114700
H	-4.05612400	-5.09921300	-1.29014800
H	-2.50714400	-5.47860900	-0.49073300
N	-4.11051700	-0.19538700	-0.72994000
C	-3.75838100	1.06799600	-0.39810200
O	-2.60146100	1.49590500	-0.22481300

O	-4.85644800	1.85678700	-0.37551600
C	-4.80975600	3.29774900	-0.10382900
C	-6.27836500	3.70459300	-0.26405000
H	-6.39874600	4.77592600	-0.07012800
H	-6.63093400	3.49457500	-1.27953800
H	-6.91173400	3.15237700	0.43847900
C	-3.94223200	4.02599400	-1.13678300
H	-2.88274800	3.80379700	-1.00389400
H	-4.23899900	3.74161300	-2.15288400
H	-4.08442700	5.10826900	-1.03460300
C	-4.34267900	3.54995900	1.33341200
H	-4.46759400	4.61061300	1.58141500
H	-4.94645000	2.96520200	2.03678200
H	-3.29119000	3.29274900	1.47031600

**a-Boc-O-anti-R**

C	3.22267000	0.21464600	-0.96481700
C	3.64688700	1.62310500	-0.54925700
C	2.72726000	2.55866100	0.02946900
C	4.96724800	2.00078400	-0.69302500
C	1.32977100	2.32947500	0.18645000
C	3.28235500	3.80960100	0.47206100
C	5.39541700	3.26794200	-0.24148200
H	5.67846600	1.32516100	-1.15575900
C	0.52265200	3.29912100	0.76231600
H	0.87205900	1.40411100	-0.15157100
C	2.42584800	4.76340600	1.08660300
H	6.43970000	3.55650700	-0.35567800
C	1.08698000	4.51752100	1.23393500
H	2.87050100	5.69514000	1.42295000
H	0.42283200	5.24492400	1.69076200
C	3.33277000	-0.73409600	0.25473000
H	2.85239200	-0.21896100	1.08999200
C	4.76637800	-1.17527300	0.64148300
C	2.26984900	-2.62347700	1.43420600
C	3.13222600	-3.00094800	-0.84318200
C	4.74714900	-2.66224100	1.05291300
H	5.44480300	-1.03895300	-0.20492200
H	5.12911800	-0.55100400	1.46320100
C	3.63954900	-2.88425800	2.10131100
H	1.63533400	-1.94062400	2.00232800
H	1.70343300	-3.53933600	1.25273500
C	4.43496900	-3.51942700	-0.19047600
H	3.31613500	-2.48478000	-1.78356200

H	2.38550100	-3.77977800	-1.00594200
H	5.71991200	-2.94307200	1.46745200
H	3.67489200	-3.90811400	2.48703500
H	5.25701900	-3.45850100	-0.91070600
H	4.32963600	-4.57148100	0.09623800
O	-0.81262200	3.18496400	0.93412000
N	4.59667700	4.14376400	0.33509400
N	2.49520900	-1.99584400	0.08215400
H	-1.23166600	2.44075500	0.44614100
H	2.17572500	0.22659700	-1.29221500
O	4.03047200	-0.30487200	-2.01514800
C	3.70418900	0.22058400	-3.29915300
H	3.84931100	1.30736900	-3.34372300
H	4.37903900	-0.25817300	-4.01329400
H	2.66531300	-0.01280400	-3.57227600
C	-1.74933000	-1.06780900	-1.88036500
H	-1.73990800	0.01209600	-1.87407400
H	1.54956900	-1.70644800	-0.29495300
H	-2.18261200	-1.60559000	-2.71280800
N	-0.58075200	-1.61352200	-1.41243600
O	-0.29849200	-2.82359300	-1.57981600
O	0.18194800	-0.86638900	-0.69779400
H	3.78603100	-2.21039900	2.95224600
C	-1.43875600	-1.44856600	2.90340800
C	-1.47697200	-2.84089500	3.01170500
C	-2.06452900	-3.62848700	2.01247100
C	-2.61599200	-2.97672200	0.91383800
C	-2.58656300	-1.56999300	0.78702400
C	-1.98771900	-0.80579700	1.78414900
N	-3.29189500	-3.55412700	-0.16711100
C	-3.78167300	-2.58670100	-1.02570600
C	-3.30758400	-1.22671800	-0.47475700
O	-4.44413100	-2.79513900	-2.02612500
H	-0.98420300	-0.85549600	3.69222900
H	-1.05110800	-3.32653900	3.88618200
H	-2.10232000	-4.70942500	2.10367600
H	-1.94694600	0.27189600	1.69173900
C	-3.47587700	-4.97455200	-0.37589100
H	-4.01995000	-5.42818400	0.46059900
H	-4.05783600	-5.09821200	-1.29069100
H	-2.50924500	-5.47843500	-0.49091100
N	-4.11050000	-0.19436900	-0.72966900
C	-3.75769000	1.06880400	-0.39772400
O	-2.60049100	1.49606800	-0.22460300

O	-4.85538900	1.85808400	-0.37480300
C	-4.80810300	3.29907200	-0.10337400
C	-6.27657600	3.70645400	-0.26347500
H	-6.39660500	4.77776500	-0.06920600
H	-6.62922600	3.49688100	-1.27902600
H	-6.91011500	3.15422200	0.43888700
C	-3.94045700	4.02680500	-1.13658100
H	-2.88104700	3.80410700	-1.00395400
H	-4.23762600	3.74251700	-2.15259000
H	-4.08207300	5.10915700	-1.03442300
C	-4.34076300	3.55132800	1.33377300
H	-4.46499800	4.61211300	1.58155400
H	-4.94483200	2.96709000	2.03731800
H	-3.28942400	3.29351100	1.47066800

**a-Boc-O-gau1-S**

C	3.01550800	-1.32941900	-0.62328000
C	4.04977600	-0.20979700	-0.74549500
C	3.66186800	1.15250300	-0.97074100
C	5.39581500	-0.49986900	-0.66183200
C	2.31443600	1.59353400	-1.07871400
C	4.71969300	2.11322300	-1.11506900
C	6.35202900	0.53216100	-0.79736800
H	5.72413400	-1.52326700	-0.51497700
C	2.02469800	2.92325600	-1.33661300
H	1.48942300	0.89579600	-0.99849500
C	4.38348800	3.46788800	-1.38690600
H	7.41269600	0.29370600	-0.72486500
C	3.07592300	3.86689700	-1.49890800
H	5.20020900	4.17461000	-1.49993900
H	2.81546500	4.90078800	-1.70481300
C	2.45374100	-1.41051800	0.81906600
H	2.30291100	-0.38366000	1.16066200
C	3.31512000	-2.20174100	1.83536100
C	0.38962200	-1.69280100	2.15993600
C	1.03456800	-3.49364400	0.60414400
C	2.39924300	-3.10886500	2.68307800
H	4.04959800	-2.81378500	1.30586100
H	3.86089300	-1.49996000	2.47347500
C	1.27000300	-2.25906700	3.29832200
H	0.26032100	-0.61110100	2.20841900
H	-0.60449500	-2.13803100	2.10728600
C	1.77375600	-4.18477500	1.77225900
H	1.51449900	-3.66981400	-0.35614000
H	-0.01760800	-3.77021500	0.52628500



H	2.98542700	-3.58592000	3.47473900
H	0.65881600	-2.86733900	3.97306900
H	2.55212700	-4.84666000	1.37906700
H	1.07886900	-4.80442800	2.34953000
O	0.76506000	3.40812400	-1.45750700
N	6.04249500	1.79401900	-1.01989400
N	1.04971800	-2.00336700	0.83739000
H	0.08739600	2.78661200	-1.10396600
H	2.17713800	-1.10842700	-1.29463800
O	3.55605900	-2.59975300	-0.96973300
C	3.61185300	-2.82896900	-2.37504900
H	4.26772400	-2.10840700	-2.88061900
H	4.01728100	-3.83509300	-2.51135100
H	2.61086500	-2.77811700	-2.82633500
C	-2.13466200	-0.50160500	-2.08036700
H	-1.96223700	0.55929100	-2.19317700
H	0.50405300	-1.54084900	0.06825600
H	-2.84751400	-1.00922500	-2.71818400
N	-0.99748400	-1.22436700	-1.82331800
O	-0.92960100	-2.45594400	-2.02302800
O	-0.04371500	-0.59793500	-1.23820100
H	1.69630400	-1.44361800	3.89297900
C	-5.90159400	1.92789800	-1.30550800
C	-6.82244200	0.88998100	-1.46863800
C	-6.47087200	-0.44060400	-1.20424600
C	-5.17382700	-0.69296300	-0.76951300
C	-4.23179400	0.34477200	-0.60265500
C	-4.59558900	1.65971400	-0.87363500
N	-4.60408600	-1.92948300	-0.43419200
C	-3.30865400	-1.77148300	0.02511200
C	-2.96602400	-0.28501200	-0.12157000
O	-2.60004000	-2.65876700	0.47697500
H	-6.19662900	2.95112400	-1.51954700
H	-7.83084200	1.11263500	-1.80716900
H	-7.19113200	-1.24282900	-1.33056800
H	-3.87171200	2.45936600	-0.76403200
C	-5.29419800	-3.20233600	-0.46750700
H	-6.15505500	-3.20065700	0.21155000
H	-5.64048300	-3.43028100	-1.48183200
H	-4.58659600	-3.96898300	-0.14771900
N	-2.06519500	0.17698400	0.73174500
C	-1.62775900	1.46112000	0.75354700
O	-1.45345100	2.22128800	-0.21222900
O	-1.30958600	1.78987100	2.03328300

C	-1.00758400	3.15936300	2.47547900
C	-0.97519200	3.00528800	3.99934600
H	-0.75585100	3.96824000	4.47282600
H	-1.93962800	2.64683000	4.37436700
H	-0.20231500	2.28951500	4.30053800
C	-2.12665900	4.11973600	2.06083500
H	-2.15514100	4.25686600	0.97829800
H	-3.10040300	3.74438100	2.39630000
H	-1.96179400	5.09689000	2.52893900
C	0.35886500	3.61199700	1.95688100
H	0.65746800	4.53501200	2.46778900
H	1.12058100	2.85245300	2.16605800
H	0.34008700	3.80978900	0.88496900

**a-Boc-O-gau2-S**

C	-2.71462700	-0.75098300	-1.05544400
C	-3.45737400	-1.40971400	0.10623200
C	-2.91494500	-1.41558700	1.43154300
C	-4.67970500	-2.01397200	-0.10437700
C	-1.66400900	-0.84180700	1.78300500
C	-3.69856600	-2.05386800	2.45113800
C	-5.36557800	-2.61387300	0.97619600
H	-5.10912100	-2.04115700	-1.10015100
C	-1.20013200	-0.89992700	3.08921600
H	-1.04284400	-0.35542900	1.03860400
C	-3.19608900	-2.08661100	3.78161900
H	-6.32989300	-3.08999800	0.80250200
C	-1.98421100	-1.52843800	4.09677700
H	-3.80639300	-2.57262000	4.53696600
H	-1.59413300	-1.55498400	5.10973700
C	-2.89186200	0.78132700	-1.00195700
H	-2.60188000	1.08943000	0.00510800
C	-4.30212000	1.32145400	-1.33154200
C	-1.74993300	2.92281800	-1.40943600
C	-2.32688100	1.52510800	-3.35320300
C	-4.15931000	2.66425000	-2.07895000
H	-4.84866400	0.60677100	-1.95466600
H	-4.86414200	1.44860900	-0.40171900
C	-3.15543700	3.56327700	-1.32738500
H	-1.23853300	2.87559800	-0.44721800
H	-1.08855200	3.42696300	-2.11510200
C	-3.60721000	2.37988500	-3.48925200
H	-2.48315400	0.48783100	-3.64114500
H	-1.48151600	1.92920100	-3.91367200

H	-5.13239500	3.15962800	-2.14699100
H	-3.12999200	4.56365500	-1.77133900
H	-4.34768600	1.83972000	-4.08777400
H	-3.39141000	3.32089500	-4.00708400
O	-0.01728700	-0.38684600	3.48299000
N	-4.90676900	-2.63836500	2.21220600
N	-1.89897600	1.50598700	-1.90380300
H	0.48148800	0.00945100	2.72519200
H	-1.64197600	-0.96614400	-0.95850500
O	-3.16863700	-1.22043000	-2.31758600
C	-2.55597100	-2.44339300	-2.72421800
H	-2.77022900	-3.25947400	-2.02234800
H	-2.97877200	-2.69403300	-3.70050800
H	-1.46800300	-2.32534000	-2.81830200
C	2.63536300	0.27858100	-2.42445500
H	2.63543000	-0.66470500	-2.95479600
H	-0.96552600	1.01499500	-1.86800700
H	3.33722300	1.05268400	-2.70178000
N	1.38676700	0.75884600	-2.12929200
O	1.25721300	1.94323700	-1.73515200
O	0.37725400	-0.03336400	-2.16635700
H	-3.46338500	3.67980800	-0.28268700
C	1.65307300	-3.41040100	0.35216500
C	2.65084700	-4.26030900	-0.12619100
C	3.82755600	-3.74365300	-0.68401200
C	3.96760800	-2.36137100	-0.74141600
C	2.97448900	-1.48053800	-0.25293500
C	1.80963000	-2.01913600	0.28746100
N	5.05051300	-1.64747600	-1.26658100
C	4.85326800	-0.28445200	-1.15384500
C	3.46515600	-0.08371700	-0.49555800
O	5.63889600	0.57442800	-1.51154500
H	0.74618900	-3.82569000	0.78258800
H	2.52052200	-5.33777800	-0.06736600
H	4.60413100	-4.40384800	-1.05721600
H	1.04575400	-1.35780700	0.66480700
C	6.24777300	-2.23794800	-1.82796700
H	6.75824600	-2.86355300	-1.08667800
H	6.01005800	-2.84979100	-2.70612200
H	6.90752100	-1.42116700	-2.12531400
N	3.36509800	1.05801900	0.17802000
C	2.40845300	1.34382000	1.09764900
O	1.41958500	0.67243300	1.44516100
O	2.70510100	2.54861600	1.64269000

C	1.95996700	3.16893000	2.73794900
C	2.63919000	4.53850200	2.85350300
H	2.19172400	5.11801000	3.66829900
H	3.70905000	4.42310500	3.05643700
H	2.52739100	5.10415400	1.92231600
C	2.16178700	2.37071600	4.03057000
H	1.67219500	1.39614600	3.99581700
H	3.23033000	2.21976000	4.21954600
H	1.74241500	2.92523100	4.87819100
C	0.47885900	3.35042900	2.38564300
H	0.00341100	3.99882600	3.13087200
H	0.38181300	3.83343100	1.40644400
H	-0.05447600	2.39953700	2.36645300

**a-Boc-O-anti-S**

C	-3.00512500	0.22307200	0.68267900
C	-3.30996600	1.72199700	0.67982500
C	-2.37683300	2.69986700	0.20038500
C	-4.54312100	2.15383000	1.12814200
C	-1.05131000	2.41328900	-0.23621400
C	-2.83587700	4.06366500	0.18015700
C	-4.87930100	3.52330300	1.07364300
H	-5.25555300	1.44217800	1.53103700
C	-0.21741100	3.43651700	-0.66301800
H	-0.66847200	1.39707300	-0.24300500
C	-1.96221700	5.07748300	-0.29981900
H	-5.85676400	3.85316200	1.42365300
C	-0.69186800	4.77742300	-0.71238600
H	-2.33583000	6.09684900	-0.31328800
H	-0.01289700	5.54779000	-1.06522300
C	-3.46634300	-0.40315000	-0.65768300
H	-3.09969900	0.25469100	-1.44912500
C	-4.99235800	-0.63655400	-0.80196900
C	-2.93765900	-2.07595900	-2.39760900
C	-3.27526000	-2.85960500	-0.08761700
C	-5.24471700	-2.02847400	-1.41635900
H	-5.47611200	-0.58131900	0.17632100
H	-5.42297900	0.14752000	-1.43169000
C	-4.44553600	-2.16229000	-2.72692000
H	-2.41851900	-1.30307600	-2.96794500
H	-2.40777900	-3.01841700	-2.54465300
C	-4.76516200	-3.10760900	-0.42411500
H	-3.12693500	-2.56744800	0.94997800

H	-2.63403100	-3.71370200	-0.31309600
H	-6.31350500	-2.15332300	-1.61476600
H	-4.66737200	-3.11689600	-3.21482900
H	-5.36218800	-3.06950700	0.49228800
H	-4.89662200	-4.10356800	-0.86038500
O	1.06013600	3.26603000	-1.06723400
N	-4.07027500	4.45315400	0.60640800
N	-2.76844100	-1.72620000	-0.93903600
H	1.45297000	2.39902400	-0.82084100
H	-1.92296800	0.06841800	0.78163500
O	-3.67051400	-0.45647600	1.74127300
C	-3.07400100	-0.25433100	3.01978500
H	-3.09314800	0.80192100	3.31651600
H	-3.66371900	-0.83571200	3.73337900
H	-2.03493700	-0.61138800	3.03306400
C	1.82169700	-1.41813800	-1.74038400
H	2.28962800	-2.09367300	-2.44372300
H	-1.73363700	-1.57903500	-0.78417000
H	1.92637800	-0.34997500	-1.85938500
N	0.55189700	-1.79061800	-1.37741300
O	-0.21257300	-0.89889000	-0.86055900
O	0.16086200	-2.98109800	-1.46348800
H	-4.72952700	-1.36716700	-3.42441600
C	1.00990200	-1.04586200	3.00017300
C	0.84623300	-2.40336900	3.28783700
C	1.41117200	-3.39041800	2.46913500
C	2.14540500	-2.97316200	1.36372200
C	2.31150200	-1.60576000	1.05220500
C	1.73810200	-0.63982800	1.87231500
N	2.84691100	-3.77186200	0.45277800
C	3.54871300	-2.99846500	-0.45472700
C	3.19097700	-1.53027400	-0.15069100
O	4.28630900	-3.42105900	-1.32692300
H	0.57635300	-0.29673600	3.65672800
H	0.27959400	-2.70496400	4.16510900
H	1.29513300	-4.44365100	2.70456000
H	1.85586000	0.41054200	1.63591700
C	2.88175600	-5.21876100	0.46325000
H	3.28836800	-5.59506800	1.40921200
H	1.87775600	-5.63251600	0.31460000
H	3.52816200	-5.53680500	-0.35644200
N	4.13032300	-0.63027800	-0.43850600
C	3.88678300	0.69612500	-0.33429300
O	2.77495300	1.25485000	-0.40139000

O	5.05208100	1.37167200	-0.22300300
C	5.13515200	2.83698100	-0.22113600
C	6.63478900	3.07600800	-0.01763500
H	6.85040600	4.14999100	-0.01318600
H	6.97011700	2.65230500	0.93521900
H	7.21409500	2.60929000	-0.82140900
C	4.33939400	3.43298900	0.94553100
H	3.26409900	3.33473200	0.79129300
H	4.61040700	2.93694300	1.88470500
H	4.57893400	4.49812200	1.04611100
C	4.68622700	3.39192300	-1.57706900
H	4.90045600	4.46601900	-1.62637800
H	5.23326500	2.90038400	-2.38952600
H	3.61585800	3.25260000	-1.73769000

### 3.2 MODE b

#### **b-N-gau1-anti-S**

C	2.23729000	-1.63426800	-0.28932300
C	3.58202000	-0.97942700	-0.60722000
C	3.66551700	0.37831800	-1.05489600
C	4.75761100	-1.67873900	-0.42021100
C	2.53851000	1.18139800	-1.36120400
C	4.98285800	0.93004800	-1.21794300
C	6.00115300	-1.04029500	-0.62890900
H	4.73302700	-2.72068700	-0.11942400
C	2.69877900	2.48014500	-1.82609900
H	1.53008700	0.79197300	-1.28068200
C	5.10916800	2.28170000	-1.64196800
H	6.92387700	-1.59840500	-0.47302500
C	4.00418700	3.03876600	-1.93650900
H	6.11250500	2.68493100	-1.74295800
H	4.09683500	4.06419400	-2.28217300
C	1.86354100	-1.31482400	1.17954400
H	2.02338700	-0.24356000	1.31679300
C	2.64298300	-2.13756200	2.24261300
C	0.07152800	-0.98283800	2.85655800
C	-0.09073300	-2.92041800	1.34839100
C	1.65932900	-2.89663900	3.15443600
H	3.30214900	-2.85164400	1.74608200
H	3.27100700	-1.46818000	2.83898300
C	0.77563600	-1.88000600	3.89720400
H	0.39973300	0.05458000	2.88440200
H	-1.01595200	-0.99183400	2.95088700

C	0.76322700	-3.80051100	2.28731400
H	-0.00792900	-3.20413700	0.30405700
H	-1.14692900	-2.91041400	1.62768100
H	2.22030700	-3.50372600	3.87175200
H	0.03548800	-2.40058200	4.51430200
H	1.38319000	-4.47810100	1.69367100
H	0.11192100	-4.41072500	2.92191600
O	1.66782400	3.26090900	-2.19120400
N	6.12549800	0.22018900	-0.99662500
N	0.37270300	-1.48732100	1.46114000
H	0.84495300	2.70703400	-2.27557400
H	1.45577000	-1.22516500	-0.93986500
O	2.27878800	-3.04768200	-0.44994200
C	2.17159200	-3.46692900	-1.80903600
H	3.00721900	-3.09534500	-2.41615900
H	2.19779900	-4.56015200	-1.80004400
H	1.22593600	-3.12791500	-2.25143100
C	-2.57257600	1.14138500	-2.43156500
H	-3.47412800	1.67134800	-2.16522200
H	-0.18268000	-0.88187500	0.80800900
H	-2.55170500	0.48177200	-3.28856500
N	-1.42104600	1.84101500	-2.21065400
O	-0.34828900	1.50065800	-2.80989900
O	-1.40990500	2.75107600	-1.34604700
H	1.38323000	-1.26397300	4.56806300
C	-6.39768200	0.11902000	0.03146800
C	-6.70460300	-0.99212800	-0.75615400
C	-5.69070200	-1.73992500	-1.36853500
C	-4.37605100	-1.34031000	-1.16321300
C	-4.04072700	-0.21111200	-0.37516100
C	-5.06912100	0.51749900	0.22519400
N	-3.22153100	-1.95684000	-1.66391000
C	-2.09370300	-1.31083600	-1.21261300
C	-2.55630500	-0.10797800	-0.39300400
O	-0.93758800	-1.68256000	-1.39206900
H	-7.19684000	0.68705600	0.49908100
H	-7.74094000	-1.28597200	-0.89971300
H	-5.92713700	-2.60597700	-1.97846800
H	-4.82479700	1.38307600	0.82485000
C	-3.19921700	-3.13037700	-2.51260500
H	-3.67128900	-3.98433000	-2.01302400
H	-3.72116200	-2.93836400	-3.45684100
H	-2.15526700	-3.36892100	-2.72153700
N	-1.62380800	0.43163800	0.36881100

C	-1.85913900	1.55017400	1.16261400
O	-2.91893800	2.11913600	1.37928800
O	-0.67849300	1.91254300	1.72745700
C	-0.53661200	3.17826900	2.46768000
C	0.95607200	3.19826000	2.81011200
H	1.21047500	4.12597500	3.33369700
H	1.22481500	2.35849000	3.46201300
H	1.56197200	3.13895000	1.89984000
C	-1.38266200	3.15465700	3.74487400
H	-2.44869600	3.14007200	3.51330900
H	-1.14294000	2.27420800	4.35319000
H	-1.16569800	4.04569900	4.34553200
C	-0.88442900	4.36151100	1.55901400
H	-0.64097600	5.29804900	2.07431200
H	-0.30578000	4.31351900	0.63169900
H	-1.94516700	4.36948900	1.30351100

**b-O-gau1-anti-S**

C	-2.65777800	0.78994800	-1.19039400
C	-4.09857200	0.50476300	-0.77024200
C	-4.39317800	-0.46392300	0.24280500
C	-5.14744800	1.18874900	-1.34900000
C	-3.40903900	-1.24208400	0.90441600
C	-5.77484200	-0.63523600	0.59564000
C	-6.47296800	0.93272800	-0.92893800
H	-4.95844700	1.91760000	-2.13000200
C	-3.76886700	-2.15382000	1.88720300
H	-2.35653200	-1.14084500	0.66594400
C	-6.10878600	-1.57910500	1.60585700
H	-7.29680900	1.47641800	-1.39021000
C	-5.13966400	-2.31572200	2.23779400
H	-7.15879100	-1.69419500	1.85848600
H	-5.39119500	-3.03702800	3.00978900
C	-1.99424000	1.72958700	-0.15691500
H	-2.20152300	1.30576800	0.82751400
C	-2.45944700	3.20516100	-0.22151900
C	0.09215600	2.28437000	1.05234300
C	0.06873700	2.51751900	-1.39730100
C	-1.25033800	4.13204200	0.01277100
H	-2.90278700	3.41688800	-1.19852100
H	-3.22962800	3.37197800	0.53732200
C	-0.51844900	3.68325200	1.29130000
H	-0.12966500	1.56464500	1.83985700
H	1.17171700	2.31594300	0.90974800



C	-0.29116600	4.00642400	-1.18762100
H	-0.38411300	2.10423500	-2.29586800
H	1.14320000	2.32850800	-1.40935200
H	-1.59045400	5.16742200	0.11372900
H	0.27603400	4.39143300	1.54944100
H	-0.76542700	4.40178400	-2.09180800
H	0.61379700	4.59718100	-1.00873800
O	-2.88023300	-2.91575600	2.54822300
N	-6.78970700	0.06151700	0.00917100
N	-0.46987000	1.71785200	-0.23376500
H	-1.95889700	-2.75912000	2.20597800
H	-2.09854800	-0.15224000	-1.20688100
O	-2.58043400	1.39635800	-2.47667500
C	-2.68288000	0.46689900	-3.55137400
H	-3.64721300	-0.05732700	-3.54883900
H	-2.59569500	1.04546300	-4.47499900
H	-1.87368100	-0.27558100	-3.51222700
C	1.74451200	-1.95099400	1.71191200
H	2.31923200	-1.20371500	2.24111300
H	-0.13452400	0.73523200	-0.34306800
H	2.09491400	-2.97276800	1.67747600
N	0.38115100	-1.84256800	1.85992000
O	-0.34272300	-2.85064800	1.56792000
O	-0.13906800	-0.75241500	2.20352700
H	-1.21796300	3.65873100	2.13402300
C	5.39217200	-3.45517900	-0.68792900
C	4.69635000	-4.46478100	-1.35639600
C	3.32785100	-4.33923300	-1.63272200
C	2.69246700	-3.17533200	-1.22113900
C	3.37668100	-2.14638400	-0.53502500
C	4.73586900	-2.29136400	-0.26629800
N	1.34256700	-2.82739700	-1.40528400
C	1.09768000	-1.57854800	-0.90830800
C	2.37659700	-1.07594000	-0.26392000
O	0.02952700	-0.96605700	-0.99636000
H	6.45173000	-3.57509100	-0.48137500
H	5.21835200	-5.36514100	-1.66859500
H	2.78972600	-5.12400700	-2.15454800
H	5.26443100	-1.51996100	0.27915500
C	0.33218200	-3.68337600	-1.99640500
H	0.58568700	-3.92337400	-3.03470100
H	0.23634000	-4.61134700	-1.42311600
H	-0.61695900	-3.14747400	-1.96989500
N	2.48244300	0.23674000	-0.14218500

C	3.55580900	0.79232400	0.50368800
O	4.28505000	0.25570200	1.33716800
O	3.65318300	2.10332000	0.14702700
C	4.72944600	2.96443100	0.66169100
C	4.46831200	4.29046500	-0.05731900
H	5.21886000	5.03301800	0.23378600
H	4.51484300	4.15996100	-1.14384900
H	3.47924200	4.68475200	0.20076100
C	6.09789400	2.40301300	0.26052900
H	6.31035300	1.46395800	0.77410500
H	6.13821900	2.23000000	-0.82100600
H	6.88144300	3.12504800	0.51711000
C	4.59617700	3.14071900	2.17783500
H	5.33839300	3.86570300	2.53178400
H	3.60236000	3.52581300	2.43474200
H	4.75210800	2.19644600	2.70197700

**b-O-gau1-syn-S**

C	2.45361600	-1.60855300	-0.25025000
C	3.74576500	-0.88996200	-0.64352600
C	3.72980200	0.45791300	-1.12416300
C	4.96624500	-1.51666800	-0.49571800
C	2.54278700	1.18947300	-1.36890100
C	5.00081700	1.07785000	-1.37666500
C	6.15852300	-0.81477800	-0.78853100
H	5.01518900	-2.54583600	-0.15643000
C	2.59833600	2.48694900	-1.85510500
H	1.56844000	0.73427200	-1.24365000
C	5.02249000	2.42121200	-1.84235800
H	7.11864200	-1.31515600	-0.66588700
C	3.85867300	3.11110000	-2.07437600
H	5.99251600	2.87637800	-2.01979100
H	3.87119000	4.13218500	-2.44434700
C	2.05313300	-1.16742700	1.17524400
H	2.00457000	-0.07647200	1.15593400
C	2.99348000	-1.64603500	2.30761800
C	0.16394200	-0.72150600	2.70165400
C	0.53890700	-3.03965100	1.95245800
C	2.15723800	-1.98636500	3.55699800
H	3.55340400	-2.52929000	1.98604100
H	3.71817900	-0.85724900	2.52786500
C	1.19299700	-0.82077700	3.84993100
H	0.02673300	0.28700100	2.31398600

H	-0.81865700	-1.10617900	2.98306000
C	1.32968300	-3.25256900	3.26316600
H	0.93947800	-3.61555000	1.12181500
H	-0.52577600	-3.25530000	2.05690900
H	2.81753100	-2.15756900	4.41249700
H	0.67124300	-0.98166800	4.79897600
H	1.98725500	-4.12145000	3.15717500
H	0.64818100	-3.45859900	4.09595500
O	1.49604600	3.20507300	-2.14244500
N	6.19187700	0.43782400	-1.20051700
N	0.63416300	-1.58420400	1.55177500
H	0.68469600	2.63147100	-2.05598800
H	1.64625700	-1.32232000	-0.93808900
O	2.60286500	-3.02320700	-0.27108400
C	2.45071100	-3.58491200	-1.57298300
H	3.18509200	-3.17825800	-2.28008100
H	2.61424500	-4.66100600	-1.47062800
H	1.43959900	-3.40555100	-1.96316500
C	-2.40327600	0.40165900	-2.49990900
H	-3.09906300	1.22132700	-2.40716100
H	-0.01029400	-1.44288200	0.74150600
H	-2.61056200	-0.43955600	-3.14753300
N	-1.08852000	0.75418400	-2.41259600
O	-0.17975500	-0.01551600	-2.81212700
O	-0.82114600	1.85268400	-1.81420900
H	1.75304300	0.11630400	3.94228800
C	-6.57763900	0.18034100	-0.47407300
C	-6.85491000	-1.10427100	-0.94558600
C	-5.82346500	-2.02540700	-1.16986300
C	-4.52274100	-1.61538100	-0.90674200
C	-4.21666600	-0.31587800	-0.43796900
C	-5.26057100	0.58437100	-0.22166800
N	-3.35175900	-2.37951500	-1.04116100
C	-2.25890100	-1.65901200	-0.63638000
C	-2.73662400	-0.25994100	-0.26775300
O	-1.11247400	-2.10568800	-0.54417000
H	-7.39061400	0.88109700	-0.30653600
H	-7.88193600	-1.39977400	-1.14260100
H	-6.03768400	-3.02560400	-1.53301400
H	-5.03826600	1.58448600	0.12452800
C	-3.30022500	-3.75803300	-1.48461900
H	-3.89219500	-4.40165300	-0.82377700
H	-3.68170700	-3.85130600	-2.50744800
H	-2.25750600	-4.07719100	-1.45924200

N	-1.89272600	0.44619000	0.45210800
C	-2.16254600	1.75915700	0.79319400
O	-3.09160800	2.46473000	0.41978500
O	-1.18538400	2.18628000	1.63639400
C	-1.10083000	3.59015000	2.06446000
C	0.16102700	3.60199300	2.93212200
H	0.34636600	4.61127100	3.31491100
H	0.05210400	2.92688700	3.78863300
H	1.03577600	3.29021400	2.35107800
C	-2.32652100	3.96780900	2.90308300
H	-3.23634900	3.96205100	2.30093600
H	-2.45194400	3.26595700	3.73618000
H	-2.19121200	4.97071100	3.32446500
C	-0.92001900	4.50422900	0.84760700
H	-0.71398200	5.52680200	1.18530300
H	-0.07566700	4.17089400	0.23449100
H	-1.81533300	4.51743700	0.22403400

**b-N-gau2-syn-S**

C	2.35667600	-1.45709300	-0.82671100
C	3.60153100	-0.58243000	-1.01388800
C	3.52666400	0.84488500	-1.11126100
C	4.84791400	-1.17420000	-1.07624900
C	2.31129400	1.57431200	-1.11820400
C	4.77049600	1.55700000	-1.22186700
C	6.00710200	-0.37467100	-1.19357500
H	4.94396000	-2.25397500	-1.04118900
C	2.31380900	2.95612500	-1.25851100
H	1.35849600	1.06545100	-1.04504500
C	4.73840400	2.97545300	-1.31984000
H	6.98580800	-0.85171600	-1.23338700
C	3.54936000	3.65876300	-1.33662700
H	5.68857200	3.49584500	-1.39492800
H	3.51999800	4.74040800	-1.42887100
C	2.00661100	-1.54897300	0.67685300
H	1.86791800	-0.52180400	1.02091000
C	3.05471000	-2.28280800	1.55100600
C	0.21192900	-1.84432700	2.34983300
C	0.67675300	-3.70920200	0.80796500
C	2.34032100	-3.14838800	2.60651400
H	3.68771800	-2.91980200	0.92702900
H	3.70291600	-1.54324500	2.02985100
C	1.30278100	-2.28818300	3.34938300
H	0.02238800	-0.77188800	2.35529100

H	-0.73646600	-2.36270200	2.50589900
C	1.61269900	-4.29984500	1.88688000
H	1.01309600	-3.92343200	-0.20270100
H	-0.35924300	-4.03235300	0.91304700
H	3.07390900	-3.55074900	3.31193300
H	0.84832800	-2.85700200	4.16726800
H	2.33978400	-4.96994900	1.41686100
H	1.04013500	-4.89260500	2.60850700
O	1.19214900	3.70325000	-1.32116000
N	5.98644400	0.94246500	-1.25353500
N	0.65183900	-2.20220200	0.94573200
H	0.39155900	3.11821200	-1.40234700
H	1.50346500	-1.00090200	-1.34740700
O	2.56035900	-2.77160700	-1.33011600
C	2.43815600	-2.86604600	-2.74684500
H	3.16568600	-2.22681100	-3.26252000
H	2.63202700	-3.90960300	-3.00809600
H	1.42528800	-2.59342900	-3.07594100
C	-2.26722900	0.41034100	-2.36439100
H	-3.20099600	0.37144000	-2.90941000
H	-0.07761100	-1.84113200	0.29299400
H	-1.47652400	-0.29056900	-2.59109200
N	-1.82143100	1.68166300	-2.09130900
O	-0.63807300	1.76941400	-1.61910600
O	-2.56571500	2.67560600	-2.20012500
H	1.78990400	-1.41336300	3.79385500
C	-6.29216600	1.16268800	-0.16831500
C	-6.90353000	0.01198500	-0.66676400
C	-6.14397800	-1.12214400	-0.98466700
C	-4.77303100	-1.05786000	-0.77748700
C	-4.13140300	0.09210900	-0.26117200
C	-4.90604700	1.21446000	0.03263100
N	-3.83281900	-2.06946100	-1.04563800
C	-2.57231800	-1.65745100	-0.71468100
C	-2.66985100	-0.22239800	-0.20911600
O	-1.55529100	-2.35416300	-0.78920000
H	-6.89455000	2.03612000	0.06486600
H	-7.97977900	-0.01089100	-0.81556800
H	-6.61422200	-2.01693400	-1.38022900
H	-4.43071700	2.10527600	0.41546400
C	-4.14824200	-3.37970600	-1.57870500
H	-4.82926900	-3.91651600	-0.90883600
H	-4.61447300	-3.29454500	-2.56657200
H	-3.21472700	-3.93719900	-1.66720200

N	-1.63815200	0.15734900	0.52648500
C	-1.64771200	1.31948600	1.27180900
O	-2.54979300	2.13260300	1.42440000
O	-0.44383600	1.42669500	1.90917100
C	-0.16322500	2.55202900	2.81691300
C	1.29152800	2.30330500	3.22558800
H	1.62460600	3.07981600	3.92248800
H	1.39997300	1.33281500	3.72374100
H	1.95164100	2.32285500	2.35199400
C	-1.08266300	2.47728900	4.04077400
H	-2.12673900	2.62436300	3.75861500
H	-0.98439900	1.50556600	4.53984000
H	-0.80351300	3.25528600	4.76093500
C	-0.28200300	3.89354800	2.08512600
H	0.11763000	4.69058500	2.72325200
H	0.29629700	3.88073800	1.15539700
H	-1.31948800	4.12697200	1.84385100

**b-O-anti-S**

C	-2.68726300	-0.21103500	1.54034400
C	-4.08441900	0.20176400	1.08087500
C	-4.26768300	0.92681700	-0.14061500
C	-5.20039800	-0.13250800	1.81865000
C	-3.20319500	1.32241500	-0.99070800
C	-5.61626800	1.24654700	-0.51284200
C	-6.48436600	0.24692000	1.36282000
H	-5.09506400	-0.68153000	2.74830600
C	-3.45614800	1.97790400	-2.18722600
H	-2.17051300	1.12444700	-0.72780600
C	-5.83843500	1.95048300	-1.72901500
H	-7.36201400	-0.01432500	1.95314800
C	-4.79502700	2.30298500	-2.54743000
H	-6.86471100	2.19090200	-1.99068100
H	-4.96290400	2.82932600	-3.48236800
C	-2.18338900	-1.39130600	0.67953400
H	-2.38533700	-1.12759900	-0.35962700
C	-2.80369700	-2.76952200	1.00332900
C	-0.22936300	-2.32511200	-0.49929500
C	-0.18665100	-2.25341400	1.96518400
C	-1.73030200	-3.85851900	0.80091400
H	-3.16524800	-2.79047000	2.03562900
H	-3.66251200	-2.93652300	0.34633900
C	-1.04132200	-3.63815400	-0.56156200
H	-0.37727200	-1.67287200	-1.36231900

H	0.83934100	-2.49660900	-0.37354900
C	-0.67694300	-3.71874300	1.91883900
H	-0.60003400	-1.70422900	2.80970600
H	0.89999400	-2.15990300	1.96228800
H	-2.19082000	-4.85039000	0.83713300
H	-0.37019000	-4.47148800	-0.79361900
H	-1.10867500	-3.99272600	2.88690100
H	0.16220400	-4.39819900	1.73189800
O	-2.48763700	2.33534500	-3.04959300
N	-6.70047100	0.90764800	0.24195100
N	-0.66582900	-1.54493800	0.71980100
H	-1.61613700	1.95989600	-2.76136200
H	-2.00514300	0.63406100	1.38931300
O	-2.65362900	-0.59141000	2.91154600
C	-2.54943100	0.51241100	3.80638700
H	-3.40512100	1.19414900	3.71875000
H	-2.52902300	0.09585000	4.81689500
H	-1.62411000	1.07925600	3.63174300
C	2.04360800	1.07770700	-2.01414000
H	2.11319100	0.02358400	-2.24119500
H	-0.21674300	-0.60056400	0.67884600
H	2.85703300	1.72877800	-2.29993300
N	0.80013400	1.62706400	-2.27022900
O	0.66233400	2.86940700	-2.34177700
O	-0.21009300	0.85451900	-2.36517200
H	-1.79080800	-3.59264500	-1.35929600
C	5.73754900	2.88943700	0.17050700
C	5.13307800	4.11669900	0.45104200
C	3.74657300	4.21475200	0.63084100
C	3.00031500	3.04944200	0.52192400
C	3.59001700	1.80170700	0.22249800
C	4.96979400	1.72376500	0.04689700
N	1.61130000	2.90566200	0.69326300
C	1.24417200	1.60074200	0.55063000
C	2.48123300	0.80520500	0.17452700
O	0.10390300	1.15451800	0.72347600
H	6.81394700	2.83665300	0.03470900
H	5.74163000	5.01321600	0.53240700
H	3.27749400	5.16794300	0.85188700
H	5.43133800	0.77659100	-0.20181000
C	0.68449000	3.99582300	0.93192000
H	0.92617800	4.50974900	1.86854800
H	0.71850900	4.71045300	0.10399400
H	-0.31880000	3.57437700	0.99975000

N	2.43424400	-0.49079400	0.44595000
C	3.45988900	-1.31833400	0.07609100
O	4.30644900	-1.12056500	-0.79449700
O	3.35517100	-2.48468900	0.77623400
C	4.33257100	-3.57104800	0.61481800
C	3.84570100	-4.61227700	1.62653300
H	4.49791300	-5.49199400	1.60975100
H	3.84896900	-4.20067200	2.64164000
H	2.82636700	-4.93825100	1.39068400
C	5.73722600	-3.08421600	0.98794000
H	6.10568800	-2.34692400	0.27280100
H	5.73287400	-2.63499200	1.98776700
H	6.43093300	-3.93279300	1.00141100
C	4.27561000	-4.13671400	-0.80813100
H	4.92541200	-5.01656000	-0.88268800
H	3.25531900	-4.45176000	-1.05695300
H	4.60285400	-3.39720200	-1.54072700

**b-N-gau1-anti-R (re-ts2b)**

C	-2.87017500	-1.37369900	0.58565800
C	-4.23651000	-0.73089500	0.35289200
C	-4.34820600	0.68699500	0.19936800
C	-5.38143900	-1.49055300	0.24269900
C	-3.25203300	1.57080500	0.33592000
C	-5.64477700	1.21930400	-0.10320400
C	-6.61692000	-0.85922900	-0.04036400
H	-5.34271000	-2.56686500	0.37467000
C	-3.41967800	2.93472400	0.17381100
H	-2.26690600	1.20618900	0.59997200
C	-5.77736800	2.62392700	-0.28296900
H	-7.51837900	-1.46485200	-0.12830100
C	-4.69738500	3.46411500	-0.15395500
H	-6.76490000	3.01029400	-0.51759600
H	-4.79963900	4.53791600	-0.28028800
C	-2.15932300	-1.55204400	-0.78286000
H	-2.37598300	-0.66090600	-1.37361300
C	-2.55842700	-2.84090000	-1.55289300
C	-0.02980500	-1.58655900	-2.05396000
C	-0.10072200	-2.68196500	0.15501600
C	-1.31409000	-3.72095800	-1.78816100
H	-3.29804300	-3.39806000	-0.97483700
H	-3.01733800	-2.57270600	-2.51002600
C	-0.32559500	-2.96108900	-2.68978900
H	-0.46795000	-0.75612300	-2.60743000



H	1.03111900	-1.38224100	-1.90936100
C	-0.63298100	-4.00677900	-0.43508300
H	-0.40994200	-2.52003400	1.18607800
H	0.98493800	-2.59662100	0.09680600
H	-1.61485000	-4.66074200	-2.26167900
H	0.60020600	-3.53583400	-2.80292200
H	-1.35032800	-4.46050100	0.25345700
H	0.19593200	-4.70936900	-0.57062100
O	-2.39378700	3.80465100	0.32027000
N	-6.75860000	0.43955400	-0.22146700
N	-0.63821300	-1.53496700	-0.66545000
H	-1.62328300	3.31410300	0.69151300
H	-2.26182800	-0.70740500	1.20892000
O	-2.96700700	-2.64023200	1.22521700
C	-3.18633200	-2.55363800	2.63018600
H	-4.13849400	-2.06133200	2.86619400
H	-3.21422200	-3.58026000	3.00468800
H	-2.37284000	-2.00871200	3.12972300
C	1.68338500	1.54027300	1.88602700
H	2.05911400	2.52329700	2.13366900
H	-0.33101700	-0.63957600	-0.24205900
H	2.17114500	0.66065800	2.28179100
N	0.31591600	1.47603800	1.80732600
O	-0.25070500	0.34634500	1.72394500
O	-0.34451300	2.55618800	1.74371700
H	-0.74737600	-2.82352100	-3.69089700
C	5.64037700	3.21566600	0.14173500
C	5.09010600	4.37917100	-0.40117200
C	3.75316500	4.42049700	-0.81874100
C	2.99654500	3.26393400	-0.67640000
C	3.53294200	2.07997800	-0.12129500
C	4.86348500	2.05942100	0.29095900
N	1.65628800	3.07091800	-1.04388000
C	1.26817800	1.77443300	-0.80725700
C	2.44370000	1.06335100	-0.14381900
O	0.17057300	1.29498900	-1.08069500
H	6.67858600	3.20717600	0.46084600
H	5.70353700	5.27035200	-0.50330100
H	3.32830500	5.32403900	-1.24405400
H	5.27861400	1.16487200	0.73809500
C	0.77942100	4.09739100	-1.57334100
H	1.13456400	4.45010900	-2.54829300
H	-0.21541600	3.66520900	-1.68561100
H	0.72415900	4.94543500	-0.88271600

N	2.47520700	-0.25597900	-0.26804300
C	3.42582100	-0.99197800	0.38566300
O	4.04363000	-0.67633900	1.40359700
O	3.53459400	-2.21103600	-0.21338100
C	4.49633900	-3.21804100	0.25928300
C	4.31778800	-4.35368000	-0.75248000
H	4.98785000	-5.18533400	-0.50944900
H	3.28875900	-4.72930400	-0.74179900
H	4.54814100	-4.01101700	-1.76708900
C	4.12636200	-3.68985700	1.66939300
H	4.21160500	-2.87699900	2.39252600
H	3.09981900	-4.07412700	1.69083300
H	4.79504600	-4.50306700	1.97487900
C	5.92617400	-2.67018300	0.18994500
H	6.63809100	-3.47850400	0.39251100
H	6.13708000	-2.27704200	-0.81122500
H	6.08624700	-1.87569000	0.92033900

**b-O-gau1-syn-R**

C	-2.11380200	0.69749900	-1.09969500
C	-3.22649800	-0.26451000	-0.68038600
C	-3.12841200	-1.00071300	0.54323200
C	-4.36618700	-0.41714000	-1.44096100
C	-2.00318600	-0.93921700	1.39871500
C	-4.24431100	-1.82161800	0.91325800
C	-5.39879200	-1.27659600	-0.99395800
H	-4.47681400	0.12104300	-2.37625600
C	-1.98511400	-1.62365700	2.60288400
H	-1.12901100	-0.35858500	1.13309500
C	-4.18377600	-2.53418300	2.14343900
H	-6.29490800	-1.39613400	-1.60207600
C	-3.09234000	-2.43651200	2.97293000
H	-5.03591200	-3.15328300	2.40820800
H	-3.05228800	-2.97135300	3.91723900
C	-2.17878100	1.96349500	-0.21768700
H	-2.21282600	1.61997800	0.81670500
C	-3.36040100	2.92156800	-0.49196000
C	-0.82004900	3.64918500	0.96695000
C	-0.83822100	3.67495200	-1.50296500
C	-2.89384100	4.37299500	-0.25037200
H	-3.71043500	2.80819400	-1.52268300
H	-4.19036700	2.66162200	0.17128200
C	-2.13906500	4.44323900	1.09404500
H	-0.61129800	2.97870000	1.80195400

H	0.05060900	4.29268700	0.83162400
C	-1.92366200	4.76652600	-1.38229300
H	-0.99469300	3.02361300	-2.36080700
H	0.17595900	4.07440000	-1.53523700
H	-3.75505400	5.04747000	-0.23857500
H	-1.91641100	5.48223400	1.35745800
H	-2.45893300	4.85620600	-2.33313400
H	-1.47105400	5.74130200	-1.16932400
O	-0.94274600	-1.55222600	3.45780200
N	-5.36044400	-1.95073400	0.13914500
N	-0.90051300	2.79037000	-0.27856500
H	-0.31020100	-0.86785100	3.12784600
H	-1.14030300	0.21417800	-0.93061100
O	-2.20947700	1.07899600	-2.46619700
C	-1.62087600	0.13733400	-3.36336300
H	-2.14618700	-0.82572400	-3.34443400
H	-1.70509300	0.56864800	-4.36449200
H	-0.56284200	-0.03164900	-3.12359300
C	2.57012900	0.20435200	2.10588400
H	3.56326500	0.56351000	2.33917700
H	-0.04927300	2.19145500	-0.28917400
H	2.31863600	-0.83472300	2.27044500
N	1.57660200	1.10295700	2.41911400
O	0.36402600	0.69803200	2.48139600
O	1.84013800	2.32016700	2.54909300
H	-2.76047800	4.03141400	1.89680900
C	5.97124900	-1.90859200	-0.15872000
C	6.75829800	-0.77206000	-0.35448500
C	6.17702400	0.49963200	-0.44437300
C	4.79459300	0.58483300	-0.33792000
C	3.97997300	-0.55078700	-0.13736000
C	4.57839200	-1.80564700	-0.04289700
N	4.00467100	1.74351400	-0.41659700
C	2.67296100	1.43163900	-0.33139800
C	2.56360200	-0.06911800	-0.09757400
O	1.75576100	2.24342200	-0.45787900
H	6.44156000	-2.88507500	-0.08685000
H	7.83756000	-0.86841700	-0.43657600
H	6.78748500	1.38366700	-0.59838100
H	3.97036300	-2.68315200	0.13540700
C	4.51386300	3.09020800	-0.58321400
H	5.05894800	3.18663300	-1.52896100
H	3.66169500	3.77073600	-0.58704700
H	5.18215200	3.35424000	0.24362300

N	1.43935900	-0.64365700	-0.49355100
C	1.26162900	-1.99402500	-0.30764700
O	1.75589500	-2.68575800	0.58266500
O	0.38393600	-2.46228500	-1.23013800
C	0.06001200	-3.89472000	-1.32702400
C	-0.90761000	-3.93875800	-2.51292400
H	-1.21885900	-4.97076200	-2.70782300
H	-1.80357600	-3.34412600	-2.30565100
H	-0.43199300	-3.54594800	-3.41837300
C	-0.63308500	-4.38917100	-0.05369400
H	0.03188000	-4.32958400	0.80890200
H	-1.52942500	-3.79586900	0.15253900
H	-0.94263300	-5.43240700	-0.18812800
C	1.32627200	-4.69766600	-1.64391200
H	1.05830100	-5.73777100	-1.86242500
H	1.83088800	-4.28602600	-2.52574600
H	2.02364700	-4.69002500	-0.80404300

**b-O-gau1-anti-R**

C	-2.39719100	-0.02058700	-1.01775300
C	-3.59215100	-0.66521000	-0.31546100
C	-3.66160100	-0.72908400	1.11317000
C	-4.65273500	-1.15699500	-1.04758200
C	-2.62896400	-0.28268400	1.97318500
C	-4.86040000	-1.27987800	1.68178900
C	-5.77978700	-1.69150500	-0.38134000
H	-4.62517700	-1.13723200	-2.13200900
C	-2.76222200	-0.37609100	3.35232000
H	-1.68937700	0.08823300	1.58308600
C	-4.97320900	-1.34596200	3.09802100
H	-6.61463200	-2.07800300	-0.96519200
C	-3.96047900	-0.90540400	3.91222100
H	-5.88706900	-1.76319600	3.51090500
H	-4.04015900	-0.96254500	4.99388400
C	-2.55433800	1.51434500	-0.95834100
H	-2.79229100	1.76632200	0.07699900
C	-3.61399200	2.10671400	-1.92086500
C	-1.37156300	3.66799100	-0.71351400
C	-0.84447400	2.26026000	-2.67054000
C	-3.07533600	3.41261800	-2.53733100
H	-3.83971600	1.38976400	-2.71453800
H	-4.53870100	2.29260200	-1.36710700
C	-2.57965700	4.33572100	-1.40748800
H	-1.47078700	3.61434000	0.37181600

H	-0.42427300	4.15634100	-0.94514000
C	-1.89196200	3.07289400	-3.46530300
H	-0.79204200	1.22101900	-2.98755500
H	0.15506500	2.69765600	-2.70662100
H	-3.86653200	3.90819600	-3.10771000
H	-2.28278300	5.31039000	-1.80795500
H	-2.23932200	2.48586900	-4.32097800
H	-1.44531200	3.99267800	-3.85820200
O	-1.80754100	0.01654300	4.20952300
N	-5.89789400	-1.74822600	0.93118900
N	-1.24163300	2.24618700	-1.21263300
H	-0.98523400	0.29934900	3.71147700
H	-1.47114700	-0.29530800	-0.49112500
O	-2.29165600	-0.41034700	-2.37926700
C	-1.64403300	-1.67124700	-2.55865300
H	-2.19957600	-2.48059500	-2.06777500
H	-1.62230200	-1.85613300	-3.63589900
H	-0.61928000	-1.64648400	-2.16893500
C	2.47484300	-0.00164600	2.46422500
H	2.91651000	0.83532400	2.98692600
H	-0.46168400	1.81739100	-0.67202200
H	2.99337400	-0.94018200	2.34105000
N	1.12175800	-0.10695800	2.55808400
O	0.54483000	-1.14000900	2.13799400
O	0.44577100	0.89043600	3.01083900
H	-3.38471900	4.51216200	-0.68630900
C	6.60560300	-0.03803800	0.25377400
C	6.85989500	1.31124900	0.50979200
C	5.81033100	2.23124000	0.62846100
C	4.51382100	1.75389100	0.48016700
C	4.23203300	0.39056800	0.23732000
C	5.29305800	-0.50761000	0.12050000
N	3.32451400	2.49596200	0.52906500
C	2.24002800	1.69275000	0.27348900
C	2.75379000	0.27191900	0.10711200
O	1.08245300	2.10335100	0.16787700
H	7.43277900	-0.73660400	0.16615800
H	7.88393400	1.65793500	0.61927000
H	6.00747000	3.28094300	0.82184800
H	5.09743800	-1.55796300	-0.04938400
C	3.24144600	3.91584500	0.80224700
H	3.75560300	4.49504500	0.02633000
H	2.18657400	4.19192500	0.81945200
H	3.68900800	4.14732200	1.77498700

N	1.95913700	-0.60428600	-0.45625000
C	2.32803100	-1.93679400	-0.48546300
O	3.08152300	-2.50655400	0.29736400
O	1.67547300	-2.56406900	-1.49522300
C	1.84297000	-4.01030900	-1.72421900
C	0.97018800	-4.26666600	-2.95599800
H	1.04762500	-5.31704900	-3.25701500
H	-0.08249200	-4.05275700	-2.74404000
H	1.28983900	-3.64306300	-3.79806800
C	1.31629100	-4.79862600	-0.52084300
H	1.92690100	-4.62427700	0.36631500
H	0.28343800	-4.50942300	-0.29645800
H	1.32647000	-5.87084600	-0.74922700
C	3.30663400	-4.33758400	-2.04171700
H	3.38624500	-5.38215100	-2.36391100
H	3.67242500	-3.70401300	-2.85823100
H	3.94670500	-4.19306200	-1.17042700

**b-N-gau2-syn-R**

C	2.47603200	0.83290400	0.93693500
C	3.67012400	0.01197000	0.44732500
C	3.52977700	-0.93588900	-0.61839000
C	4.91487800	0.17432600	1.01864400
C	2.31295900	-1.18424100	-1.30250500
C	4.70803900	-1.65841100	-1.00696800
C	6.00720300	-0.59780000	0.55973000
H	5.05694000	0.88651700	1.82415900
C	2.25956200	-2.07623400	-2.36556400
H	1.39607400	-0.68248900	-1.01971500
C	4.61122700	-2.59711600	-2.07184100
H	6.98565200	-0.46934300	1.02142100
C	3.42903800	-2.79957400	-2.73769600
H	5.51161300	-3.13925700	-2.34573500
H	3.35754100	-3.50371700	-3.56138200
C	2.09038200	1.89530800	-0.11500600
H	2.09111500	1.40407500	-1.08804300
C	3.00752200	3.14199900	-0.14953000
C	0.22609400	3.04549200	-1.24910400
C	0.48319000	3.34180000	1.19581400
C	2.14715600	4.40085500	-0.36795900
H	3.56029900	3.22919600	0.78955400
H	3.73695900	3.02511200	-0.95679300
C	1.22743600	4.17405200	-1.58225500
H	0.18483900	2.25693500	-2.00272200

H	-0.78407900	3.40960600	-1.06945100
C	1.27890200	4.62965500	0.88455400
H	0.85419700	2.83257900	2.08263800
H	-0.58911000	3.50477300	1.29009100
H	2.79329600	5.26722000	-0.53943900
H	0.67887500	5.09018900	-1.82433700
H	1.91177000	4.88598300	1.74045700
H	0.59578500	5.47005500	0.71916100
O	1.14695400	-2.30409300	-3.08183900
N	5.92294300	-1.48407400	-0.41321200
N	0.64885100	2.37452100	0.04397500
H	0.43663900	-1.65541800	-2.83104900
H	1.61824500	0.15887300	1.07574900
O	2.74767000	1.49909500	2.16444100
C	2.52058100	0.70376100	3.32402000
H	3.15874200	-0.18904000	3.33928800
H	2.76998800	1.33085000	4.18441400
H	1.46920100	0.39747200	3.39075900
C	-2.60336000	0.60321900	-2.21695100
H	-2.19238200	1.60239600	-2.24149300
H	0.00877100	1.56453700	0.20705800
H	-3.61264100	0.44132900	-2.57149200
N	-1.71748800	-0.37187800	-2.61896700
O	-2.12136400	-1.47099100	-3.04408800
O	-0.46867500	-0.13901700	-2.46393400
H	1.82490100	3.91017400	-2.46169400
C	-5.43833300	-2.42540500	-0.13516000
C	-6.50489700	-1.54110200	0.02953600
C	-6.28215300	-0.16397200	0.16334000
C	-4.96708600	0.28160600	0.14001000
C	-3.87114800	-0.59711600	-0.00649100
C	-4.11600900	-1.96054600	-0.16391000
N	-4.52006100	1.60946100	0.23142000
C	-3.14986100	1.67605600	0.17152100
C	-2.63486900	0.24592200	0.00798400
O	-2.49060800	2.70694300	0.27389600
H	-5.63092400	-3.48764100	-0.25504200
H	-7.52407100	-1.91767500	0.04640600
H	-7.11113800	0.52700400	0.27923700
H	-3.29373900	-2.64216100	-0.33051700
C	-5.37763800	2.76613500	0.39268600
H	-5.95355000	2.69471500	1.32226200
H	-4.73939300	3.65007900	0.43172400
H	-6.07138300	2.85581300	-0.45075200

N	-1.42736800	0.00921800	0.50456000
C	-1.03154100	-1.31175400	0.69666300
O	-1.15205800	-2.23862100	-0.08806500
O	-0.43540300	-1.42758600	1.91511500
C	-0.15302900	-2.76433300	2.48635900
C	0.33124100	-2.43693700	3.90082400
H	0.52025900	-3.36342300	4.45371600
H	1.26173200	-1.86205300	3.87731200
H	-0.42153300	-1.85816200	4.44705500
C	0.94203800	-3.48112100	1.69307800
H	0.61749600	-3.69641000	0.67436100
H	1.85494900	-2.87771000	1.65384800
H	1.18891000	-4.42725800	2.18926000
C	-1.44280000	-3.59059600	2.55784700
H	-1.26104200	-4.49301000	3.15230000
H	-2.24057000	-3.01925200	3.04605500
H	-1.78342300	-3.89551900	1.56748600

**b-O- anti-R**

C	-2.28374800	0.99575400	-0.25154300
C	-3.65618000	0.45385200	-0.66568400
C	-3.93301000	-0.94875600	-0.77225600
C	-4.67289200	1.34441800	-0.95238700
C	-2.97174500	-1.97454600	-0.57209700
C	-5.27480700	-1.31493300	-1.14176500
C	-5.95596500	0.86996700	-1.30163300
H	-4.48701700	2.41261400	-0.92728800
C	-3.31224300	-3.30937400	-0.75225600
H	-1.94951400	-1.74552000	-0.29245200
C	-5.59680300	-2.69341800	-1.27865400
H	-6.75291800	1.58121000	-1.51556100
C	-4.64824000	-3.66449700	-1.09333500
H	-6.61756100	-2.94484700	-1.55091800
H	-4.88418100	-4.71764200	-1.21340800
C	-2.23762300	1.19518900	1.28225800
H	-2.58532700	0.25904400	1.72563100
C	-3.06725500	2.39429600	1.81275900
C	-0.84143800	1.12395700	3.32237500
C	-0.21132300	2.69850100	1.53000800
C	-2.27452900	3.13462000	2.90687600
H	-3.28737600	3.08617200	0.99644300
H	-4.02021800	2.02843200	2.20586400
C	-1.82264700	2.12178100	3.97397000
H	-1.11315700	0.08022900	3.48000700



H	0.18778600	1.26060000	3.65833100
C	-1.03013900	3.78217100	2.26876600
H	-0.22484600	2.81883300	0.45083700
H	0.82784700	2.63929900	1.85252400
H	-2.90600600	3.90385700	3.36183200
H	-1.33166300	2.63445700	4.80749500
H	-1.33270600	4.56147100	1.56176700
H	-0.41963700	4.26176400	3.04163300
O	-2.44328900	-4.32998400	-0.62492000
N	-6.26263300	-0.40960200	-1.38758200
N	-0.81863200	1.34689300	1.82506900
H	-1.52188800	-3.99194200	-0.48042600
H	-1.50611800	0.27093900	-0.52718700
O	-2.00189200	2.24110500	-0.87741600
C	-1.62938000	2.11828400	-2.24773800
H	-2.40855400	1.61987000	-2.83821700
H	-1.49431300	3.13420100	-2.62697500
H	-0.68792800	1.56159500	-2.35457800
C	1.27010900	-1.76534100	-1.30448400
H	2.00951000	-1.71755100	-2.09050700
H	-0.19724900	0.59569200	1.44843100
H	0.41660500	-1.10318500	-1.32757200
N	0.98777100	-3.03538400	-0.85472900
O	-0.05768300	-3.20416700	-0.13147800
O	1.79308600	-3.97100500	-1.05017300
H	-2.69022300	1.59274700	4.38249200
C	5.92245300	-1.93765000	-0.57683500
C	5.85698000	-3.03196500	0.29088500
C	4.71699800	-3.27267100	1.06636700
C	3.65676300	-2.38254500	0.94605500
C	3.69910700	-1.27797700	0.06756700
C	4.84283300	-1.05581400	-0.69833000
N	2.44420800	-2.39413400	1.65917800
C	1.67865600	-1.31330200	1.32163000
C	2.40833900	-0.55912800	0.22174200
O	0.59984600	-1.01067400	1.83503300
H	6.81732100	-1.77239100	-1.17006000
H	6.70061400	-3.71288100	0.36510300
H	4.66696800	-4.12330800	1.73810300
H	4.88012500	-0.22438000	-1.39092500
C	2.00241900	-3.46172500	2.53681300
H	2.72263000	-3.61823000	3.34666000
H	1.04088200	-3.16865800	2.95885200
H	1.87888800	-4.38851300	1.96829500

N	2.05846600	0.70476600	0.05316800
C	2.59870200	1.45044100	-0.96390800
O	3.02114800	1.03748000	-2.04265800
O	2.52370000	2.76912200	-0.63453300
C	3.03403900	3.81634300	-1.52979800
C	2.78367100	5.09562300	-0.72584800
H	3.12905700	5.97006800	-1.28774300
H	1.71561200	5.22329900	-0.51715400
H	3.32000100	5.06627000	0.22895000
C	2.23446900	3.83868500	-2.83634500
H	2.39437900	2.92551400	-3.41191600
H	1.16341000	3.94015700	-2.62592800
H	2.54064600	4.69731900	-3.44528700
C	4.53538600	3.62769000	-1.77382000
H	4.93436200	4.49586800	-2.31101900
H	5.07005300	3.54436000	-0.82061900
H	4.73237700	2.73277600	-2.36618700

**b-Boc-O-anti-R**

C	-2.32384300	0.93429700	-0.60701900
C	-3.46243300	-0.03198600	-0.92652700
C	-3.32343300	-1.42878300	-0.63132100
C	-4.66008000	0.41913300	-1.45354000
C	-2.15969900	-1.99591000	-0.05591600
C	-4.45311300	-2.27656200	-0.89962000
C	-5.70820700	-0.49966800	-1.70886500
H	-4.79989600	1.47249100	-1.66548900
C	-2.12692300	-3.33724300	0.30329000
H	-1.27126300	-1.40730600	0.12335400
C	-4.36664800	-3.65963100	-0.57385700
H	-6.64426200	-0.15162700	-2.13485900
C	-3.24034100	-4.17984800	0.02135000
H	-5.23029300	-4.27574000	-0.79590900
H	-3.17034300	-5.22520900	0.29789500
C	-2.21141000	1.12532700	0.91682500
H	-2.06610800	0.12890400	1.33869500
C	-3.42006000	1.80712800	1.59990000
C	-0.64329400	1.49004600	2.78584900
C	-1.13389300	3.40577200	1.25935800
C	-2.91347400	2.59751700	2.83269200
H	-3.92115500	2.48286600	0.89926200
H	-4.14234100	1.03956700	1.89297900
C	-1.91879300	1.72227200	3.63741200
H	-0.33087300	0.44326200	2.75684400

H	0.19830800	2.10814100	3.10756900
C	-2.16362700	3.85100700	2.32466000
H	-1.46932300	3.60802600	0.24391400
H	-0.14672200	3.84383800	1.40858600
H	-3.75587900	2.88951900	3.46701400
H	-1.65196900	2.21806200	4.57672300
H	-2.86741700	4.56213600	1.87947000
H	-1.67071500	4.36089500	3.16077600
O	-1.05613800	-3.90192400	0.93526100
N	-5.62134800	-1.80113100	-1.44370300
N	-0.94770500	1.89215800	1.34331100
H	-0.39995800	-3.21386100	1.24354900
H	-1.37422300	0.51416400	-0.97291200
O	-2.51074300	2.24293300	-1.21723700
C	-2.19436000	2.29293200	-2.64438100
H	-2.84684200	1.62693400	-3.21743400
H	-2.36084600	3.32646400	-2.94851200
H	-1.14616100	2.02110900	-2.81559700
C	2.40016000	-0.61993500	1.89724100
H	1.87597500	0.31796800	1.80841300
H	-0.11269900	1.65472100	0.75123900
H	3.31083800	-0.67561400	2.47579100
N	1.58458600	-1.72516600	1.99892900
O	2.06007400	-2.87915800	2.28770400
O	0.30797900	-1.59555900	1.67152000
H	-2.38399900	0.76555300	3.89928200
C	0.72937900	-2.35370400	-2.27525300
C	1.30506600	-3.62521900	-2.14748500
C	2.46392500	-3.82957400	-1.38222700
C	3.01942200	-2.72590400	-0.74142900
C	2.43019900	-1.44360800	-0.83441200
C	1.29079800	-1.25240900	-1.61020000
N	4.20511200	-2.65288400	0.01446900
C	4.46406000	-1.35036100	0.42571500
C	3.26435000	-0.50735000	-0.04123000
O	5.45080700	-0.98070900	1.07893300
H	-0.16289000	-2.22554100	-2.87770100
H	0.84916600	-4.47146800	-2.65056500
H	2.90608900	-4.81507800	-1.29741800
H	0.85083500	-0.26493100	-1.69466900
C	5.01741400	-3.79023700	0.41595100
H	5.37587200	-4.34331400	-0.45897900
H	5.87337100	-3.40002800	0.96903000
H	4.44083800	-4.45949900	1.06322300

N	3.45979500	0.79113900	-0.28252200
C	2.57700200	1.76187200	-0.49122500
O	1.38495000	1.86613800	-0.00694100
O	3.12094100	2.76186400	-1.27372700
C	2.54319100	4.13251700	-1.42990800
C	3.57736200	4.80651800	-2.34040400
H	3.28834000	5.84507200	-2.53778700
H	4.56282700	4.79561100	-1.86679500
H	3.64940100	4.27275600	-3.29249500
C	2.49189100	4.81579700	-0.05683600
H	1.83662500	4.26820800	0.62336500
H	3.49425700	4.85316000	0.38096900
H	2.12032500	5.84192400	-0.15993200
C	1.17354800	4.06072100	-2.11921600
H	0.81423300	5.07334000	-2.33816600
H	1.26353600	3.51816700	-3.06657600
H	0.44450300	3.54933100	-1.48985400

**b-Boc-O-gau1-S**

C	2.68030400	0.82304200	0.70444000
C	3.89368100	-0.05004400	0.36475400
C	3.78406800	-1.22407300	-0.45019800
C	5.14235800	0.29824200	0.83872800
C	2.56425500	-1.69779700	-0.99578000
C	4.99665200	-1.94410400	-0.72426100
C	6.26923300	-0.49058800	0.51240600
H	5.26199400	1.17326000	1.46817200
C	2.53669000	-2.82280700	-1.80712400
H	1.62975400	-1.18340000	-0.81084100
C	4.93016400	-3.10571700	-1.54275000
H	7.25004800	-0.20688500	0.89272200
C	3.74014600	-3.53586100	-2.07262700
H	5.85708400	-3.63776900	-1.73565100
H	3.68791000	-4.41793900	-2.70400900
C	2.31048200	1.71735400	-0.50009200
H	2.17109200	1.05174200	-1.35331400
C	3.33544700	2.82598700	-0.83929200
C	0.46239500	2.82325000	-1.70423600
C	0.98410600	3.59321700	0.57559900
C	2.58597900	4.09548400	-1.29150600
H	3.94975500	3.05234900	0.03704800
H	4.00280400	2.46557600	-1.62755800
C	1.54339900	3.71216900	-2.36014700
H	0.24899300	1.91122500	-2.26024800

H	-0.47509000	3.35803300	-1.53527900
C	1.85183600	4.69316400	-0.07555400
H	1.38715200	3.24715100	1.52373800
H	-0.05469800	3.89484700	0.71822100
H	3.29476300	4.82292500	-1.69857900
H	1.07704400	4.60819400	-2.78239100
H	2.57337800	5.07198100	0.65539000
H	1.23049200	5.53913100	-0.38982300
O	1.41624700	-3.30326100	-2.38015400
N	6.21600200	-1.57099000	-0.24162300
N	0.94683500	2.38980800	-0.33964300
H	0.63311900	-2.71318300	-2.23753100
H	1.81973300	0.17631800	0.92719000
O	2.93863600	1.66258700	1.82234900
C	2.73168000	1.02526300	3.08286900
H	3.36550900	0.13625600	3.19442400
H	3.00815600	1.75541100	3.84830700
H	1.67897100	0.74485500	3.20697400
C	-2.34505700	-0.13288700	-2.03057000
H	-2.27330000	0.93757700	-1.91481700
H	0.24705400	1.72416300	0.05945600
H	-3.04158300	-0.55309700	-2.74364000
N	-1.14009300	-0.78239200	-1.96325400
O	-1.01630200	-1.94978400	-2.42788900
O	-0.18974800	-0.22628900	-1.34007300
H	2.02805300	3.17887900	-3.18518300
C	-5.16170400	2.77045700	0.32635300
C	-6.33847300	2.28203900	-0.24798500
C	-6.43363000	0.95659600	-0.69083800
C	-5.31735200	0.13959500	-0.54033700
C	-4.11487000	0.62053600	0.02937300
C	-4.04102800	1.94169300	0.46608100
N	-5.19677400	-1.20969200	-0.88328500
C	-3.95254100	-1.70610200	-0.51507700
C	-3.15560000	-0.51563800	0.03778100
O	-3.60098100	-2.86799300	-0.59228900
H	-5.11357300	3.80118200	0.66599600
H	-7.19920300	2.93716300	-0.35355500
H	-7.35221000	0.57938100	-1.12903500
H	-3.12114500	2.31171800	0.90314900
C	-6.24604900	-2.02612100	-1.45668100
H	-7.12938500	-2.04345700	-0.80755500
H	-6.53851900	-1.65316400	-2.44519400
H	-5.85448000	-3.04003400	-1.55571000

N	-2.16027400	-0.82790900	0.84653900
C	-1.34302900	0.05858900	1.45816000
O	-1.09534700	1.23384500	1.13027000
O	-0.65363100	-0.40823800	2.52909500
C	-0.84847600	-1.72958000	3.17043600
C	-0.45007000	-2.86627200	2.22465600
H	-0.45143200	-3.81292800	2.77810000
H	-1.13823500	-2.94870700	1.38286100
H	0.56286400	-2.70665300	1.83777400
C	-2.28648500	-1.86677400	3.67930900
H	-2.55588700	-1.01054000	4.30863100
H	-2.99810400	-1.93774400	2.85504100
H	-2.37325400	-2.77434600	4.28765900
C	0.11961600	-1.66273500	4.35585900
H	0.04732900	-2.58065000	4.94885700
H	1.15416900	-1.56156200	4.01190000
H	-0.11675300	-0.81341600	5.00619000

**b-Boc-O-gau2-S**

C	2.98673600	0.68153800	0.80525900
C	3.99909700	-0.26133400	0.15110500
C	3.58080300	-1.28888700	-0.75427100
C	5.34588800	-0.14208900	0.42387700
C	2.23365700	-1.50033100	-1.13789200
C	4.60240200	-2.13469900	-1.30312200
C	6.26867800	-1.03024700	-0.17666800
H	5.69923900	0.62268900	1.10693100
C	1.89839500	-2.48900400	-2.05254400
H	1.43823800	-0.88189300	-0.74210100
C	4.22116600	-3.16602100	-2.20598600
H	7.33027300	-0.93149600	0.04744400
C	2.91104300	-3.34161300	-2.57538400
H	5.00745300	-3.80134100	-2.60291700
H	2.62058200	-4.11827300	-3.27663200
C	2.48652400	1.73304500	-0.21011600
H	2.18761400	1.19148000	-1.10878600
C	3.49375800	2.84940700	-0.57116600
C	0.50702400	3.01255500	-0.95914500
C	1.43958000	3.48719100	1.27378300
C	2.72416300	4.17144700	-0.77242400
H	4.23370200	2.96572100	0.22644200
H	4.02878600	2.56694600	-1.48272800
C	1.51898900	3.91402700	-1.69953100
H	0.10627000	2.19333700	-1.55870500

H	-0.33915500	3.57863200	-0.56406100
C	2.20318100	4.64921000	0.59834200
H	2.00802900	3.02997700	2.08122300
H	0.45718100	3.78298000	1.64752300
H	3.38590400	4.92630100	-1.20759700
H	1.03609500	4.85660900	-1.97665700
H	3.03522300	4.96025400	1.23805000
H	1.54841000	5.51800200	0.46932300
O	0.63750300	-2.69092100	-2.48103900
N	5.92612300	-1.99614100	-1.00657100
N	1.19632500	2.40732900	0.24699300
H	0.06829600	-1.92640200	-2.19581700
H	2.11886000	0.09161000	1.13601500
O	3.54030900	1.36028300	1.92690200
C	3.52359500	0.59560500	3.12996900
H	4.08473500	-0.34161500	3.02694500
H	3.99978100	1.21155700	3.89742700
H	2.49472000	0.36626500	3.43794100
C	-2.77242800	-0.75124400	-2.12529200
H	-3.66426800	-0.38192000	-2.61160700
H	0.53435900	1.70184600	0.64961600
H	-2.53924800	-1.80583500	-2.10868300
N	-1.70784100	0.09378100	-2.15772600
O	-0.54700800	-0.35043400	-1.82662700
O	-1.86211900	1.31024500	-2.43189400
H	1.85299100	3.43579700	-2.62691200
C	-4.56605900	3.00748200	0.28016200
C	-5.87988500	2.70122800	-0.07987600
C	-6.27566600	1.37850400	-0.32082300
C	-5.31846600	0.38047300	-0.18595200
C	-3.97798800	0.66988100	0.17601800
C	-3.60626300	1.99550700	0.40347800
N	-5.49602000	-0.99285500	-0.37121400
C	-4.31899800	-1.67937900	-0.12541000
C	-3.25867000	-0.62003400	0.22018100
O	-4.18445500	-2.89067200	-0.14866300
H	-4.28235300	4.04063900	0.45955300
H	-6.61344200	3.49741400	-0.17644800
H	-7.29827000	1.14479300	-0.59924400
H	-2.58419900	2.21934000	0.67418100
C	-6.74179900	-1.63907000	-0.72881400
H	-7.51704400	-1.43548600	0.01884000
H	-7.09392900	-1.29751600	-1.70903300
H	-6.55441400	-2.71343800	-0.76763400

N	-2.19365300	-1.07738900	0.84075600
C	-1.17074800	-0.32190200	1.31925500
O	-0.92142700	0.87340900	1.08939700
O	-0.29321800	-0.95826500	2.12775700
C	-0.43504500	-2.33934000	2.65164800
C	-1.71320800	-2.45780200	3.48610600
H	-1.72445700	-3.42599800	3.99972300
H	-1.74928600	-1.67085000	4.24852200
H	-2.60576900	-2.38929000	2.86225100
C	0.79460800	-2.46662400	3.55575100
H	1.71916300	-2.36536500	2.97755700
H	0.78422700	-1.69989200	4.33810000
H	0.80221300	-3.44916800	4.03938200
C	-0.37208800	-3.36978800	1.52175500
H	-0.30412100	-4.37468500	1.95516000
H	-1.25559900	-3.32079100	0.88462900
H	0.52013700	-3.20932900	0.90682000

**b-Boc-O-anti-S**

C	-2.34956600	1.12503900	-0.55221700
C	-3.70586800	0.47231600	-0.83315800
C	-3.90654800	-0.93592600	-0.66327600
C	-4.78011700	1.24253700	-1.22814200
C	-2.89123100	-1.83481300	-0.25477400
C	-5.22898600	-1.44058900	-0.90200700
C	-6.03644600	0.63458300	-1.45748900
H	-4.66516700	2.31225000	-1.36640100
C	-3.16361400	-3.18112500	-0.05306500
H	-1.87724200	-1.49606300	-0.08350700
C	-5.47306600	-2.82899400	-0.70726700
H	-6.87787100	1.24809100	-1.77739200
C	-4.47816200	-3.67635200	-0.28896400
H	-6.47914000	-3.19232500	-0.89518300
H	-4.66584100	-4.73464100	-0.13349400
C	-2.08582600	1.14997400	0.96605800
H	-2.05632800	0.10718600	1.28270000
C	-3.09954800	1.91371000	1.84266300
C	-0.30394800	1.07288700	2.65377100
C	-0.65926000	3.19449800	1.43502000
C	-2.36610600	2.44261800	3.09488700
H	-3.54363300	2.74652200	1.28713200
H	-3.90892700	1.23136800	2.11604900
C	-1.45060100	1.33459900	3.65900100
H	-0.11235800	0.01298800	2.47576000



H	0.63129500	1.55190000	2.94940200
C	-1.48428500	3.62898400	2.66300200
H	-1.06329300	3.57327400	0.49922200
H	0.39321800	3.46817700	1.50679600
H	-3.08847000	2.75937700	3.85250200
H	-1.02645400	1.63915600	4.62071600
H	-2.10167900	4.49306600	2.39741700
H	-0.82869100	3.93495900	3.48561100
O	-2.24150700	-4.06652600	0.36461100
N	-6.26891600	-0.65388000	-1.29915900
N	-0.69507000	1.68211500	1.32331000
H	-1.35751600	-3.61985100	0.47139700
H	-1.55920800	0.51401700	-1.01489600
O	-2.26489200	2.44913000	-1.05755500
C	-1.92257500	2.51445800	-2.44218100
H	-2.67190700	2.01712400	-3.07019600
H	-1.88419700	3.57463900	-2.70390900
H	-0.94053300	2.05881000	-2.62782300
C	0.99821800	-1.50379300	-1.21885200
H	1.18419700	-1.62261500	-2.27640400
H	0.01616900	1.41349400	0.61874700
H	0.59748100	-0.58146400	-0.82833900
N	0.56587500	-2.63661500	-0.58453900
O	0.01411000	-2.52068000	0.57487900
O	0.74443900	-3.76798100	-1.08846600
H	-2.02447900	0.41822500	3.83207100
C	3.25725800	-1.01579600	3.08386400
C	3.62540300	-2.36259500	3.15873200
C	3.81098400	-3.13106900	2.00307600
C	3.60797000	-2.51353600	0.77261300
C	3.20415200	-1.16135200	0.67973600
C	3.04379700	-0.40843400	1.84007300
N	3.79532200	-3.05694200	-0.49973800
C	3.58623700	-2.10396400	-1.48405300
C	3.11244000	-0.83601200	-0.75985100
O	3.75500500	-2.26233600	-2.67937700
H	3.13633800	-0.43747100	3.99563300
H	3.78039200	-2.82496200	4.12999200
H	4.11233300	-4.17147100	2.06771000
H	2.75769200	0.63515900	1.77461300
C	4.13166500	-4.43744500	-0.78118900
H	5.09307700	-4.70681100	-0.32917700
H	3.35086200	-5.10695800	-0.40618000
H	4.20281600	-4.54152700	-1.86488600

N	3.20451300	0.30952100	-1.40146900
C	2.70061100	1.48126200	-0.95078400
O	1.69239100	1.65810700	-0.23692600
O	3.41211300	2.50074300	-1.48231600
C	3.08620100	3.91609500	-1.28433100
C	4.16030900	4.62051100	-2.11903700
H	4.04092200	5.70740100	-2.05377800
H	5.16156100	4.35960200	-1.76062600
H	4.08742300	4.32671100	-3.17138100
C	3.23401800	4.29149200	0.19331800
H	2.50168300	3.77067900	0.81300600
H	4.23662700	4.03459600	0.55275900
H	3.09428300	5.37097600	0.32090800
C	1.69326300	4.23103600	-1.84060700
H	1.51861800	5.31288200	-1.81060300
H	1.62066700	3.90679900	-2.88481500
H	0.90930800	3.73486700	-1.26620700

### 3.3 *MODE c*

#### TS2-c-gau1-OS-R

C	3.15110100	0.37702800	1.21857600
C	4.40589500	-0.34982700	0.73059500
C	4.31748800	-1.40232200	-0.23570400
C	5.65286600	-0.00314200	1.20718200
C	3.09773700	-1.85530300	-0.79282100
C	5.54548900	-2.02176000	-0.64511000
C	6.80023400	-0.68272600	0.73415600
H	5.75767000	0.77761500	1.95316200
C	3.07501600	-2.89171400	-1.71274300
H	2.15684400	-1.38652800	-0.53264300
C	5.48994600	-3.07454000	-1.60073300
H	7.78226700	-0.40433900	1.11486600
C	4.29400000	-3.50200200	-2.12248300
H	6.42901500	-3.53073100	-1.89993200
H	4.25042000	-4.30975400	-2.84709200
C	2.74897500	1.47346800	0.20405200
H	2.81285200	1.02150700	-0.78780200
C	3.59361000	2.77013500	0.26692300
C	0.86393100	2.59981300	-0.93866500
C	1.00055000	2.74715200	1.52416500
C	2.66922200	3.99269300	0.10496500
H	4.11847100	2.82983800	1.22405000

H	4.34662000	2.74750700	-0.52633700
C	1.80351200	3.80676700	-1.15534600
H	0.90442400	1.86934800	-1.74841100
H	-0.17546600	2.89368600	-0.78918300
C	1.74707300	4.08864200	1.33735700
H	1.35044300	2.19789600	2.39632000
H	-0.08474500	2.84686800	1.56817200
H	3.27226500	4.90161400	0.01710600
H	1.20872400	4.70536500	-1.34816900
H	2.33642700	4.30934100	2.23306800
H	1.03116300	4.90734900	1.20651100
O	1.93434300	-3.35549400	-2.25901900
N	6.76453400	-1.65440700	-0.15715600
N	1.27926300	1.87122100	0.32279000
H	1.15195400	-2.95397200	-1.80169500
H	2.32668900	-0.34756400	1.28015000
O	3.33270500	0.97595700	2.49423100
C	3.26423100	0.05145200	3.57665000
H	4.05042600	-0.71125300	3.51399200
H	3.40195400	0.63263800	4.49195800
H	2.28573200	-0.44882800	3.61176300
C	-1.39510800	-1.50156400	0.86884300
H	-1.69089400	-2.45767900	1.27756300
H	0.69754800	1.00912900	0.35860600
H	-1.30962600	-0.62465900	1.49335800
N	-0.46303700	-1.58290400	-0.12401000
O	0.13583600	-0.52452100	-0.51320500
O	-0.24992600	-2.68569600	-0.70492600
H	2.44203100	3.64420600	-2.03019100
C	-5.19277200	-0.60190900	3.25257700
C	-5.78449200	-1.86001700	3.10883800
C	-5.52572000	-2.66199100	1.98943900
C	-4.65960600	-2.16391500	1.02111900
C	-4.04918300	-0.89618000	1.15530700
C	-4.31613400	-0.11328400	2.27526200
N	-4.27099900	-2.77224900	-0.17736600
C	-3.45244400	-1.93191600	-0.91987000
C	-3.21486200	-0.68479800	-0.05837600
O	-3.03237100	-2.15187700	-2.04014600
H	-5.40910900	0.00008800	4.13042800
H	-6.45954600	-2.22857600	3.87673100
H	-5.99262900	-3.63586900	1.88138600
H	-3.83730600	0.85268600	2.38850900
C	-4.71851600	-4.06732500	-0.64627500

H	-5.80729100	-4.08532800	-0.77453800
H	-4.24099000	-4.24865700	-1.61065800
H	-4.42891800	-4.85822900	0.05475000
N	-2.91181800	0.42770500	-0.70452400
C	-2.53114700	1.56060800	-0.06532800
O	-1.96584700	1.63686600	1.03497600
O	-2.66804600	2.73198000	-0.74492300
C	-3.41427200	2.91795100	-2.00413700
C	-2.70779300	2.21301400	-3.16591600
H	-3.23515000	2.42982600	-4.10244500
H	-1.67920300	2.57787000	-3.26997500
H	-2.68400700	1.13241700	-3.01777900
C	-3.36037300	4.43816500	-2.18742600
H	-3.84403200	4.94988300	-1.34832900
H	-2.32328400	4.78610300	-2.24901800
H	-3.87376300	4.72795100	-3.11057100
C	-4.86690000	2.45902300	-1.84277500
H	-5.45048700	2.77144700	-2.71644400
H	-4.93804700	1.37327800	-1.75508600
H	-5.31793200	2.91517200	-0.95397800

**TS2-c-gau2-OS-R**

C	3.35574500	-0.18965200	1.30220200
C	4.49628000	-0.67648600	0.40933300
C	4.21696500	-1.18256000	-0.89983100
C	5.81035700	-0.62694200	0.82092300
C	2.91042800	-1.27600600	-1.43612400
C	5.32976900	-1.59396700	-1.70279700
C	6.83456600	-1.07318700	-0.04956800
H	6.06422400	-0.25377100	1.80769300
C	2.69714500	-1.73711000	-2.72326500
H	2.04838900	-0.97485600	-0.85718400
C	5.07686200	-2.08046600	-3.01624100
H	7.87134600	-1.03585000	0.28258600
C	3.80060200	-2.14889100	-3.52021100
H	5.93083800	-2.39021700	-3.61121000
H	3.60909800	-2.51193700	-4.52546400
C	2.84818700	1.18733500	0.80460600
H	2.84158200	1.14944400	-0.28533300
C	3.65125600	2.41972700	1.28623100
C	0.83210900	2.51443200	0.27628800
C	1.18736500	1.77350300	2.60928200
C	2.66935600	3.55659500	1.63911000

H	4.24954800	2.16105700	2.16386500
H	4.33833200	2.73109500	0.49353600
C	1.69807600	3.78136600	0.46327600
H	0.84315100	2.12716900	-0.74330600
H	-0.21132400	2.64548700	0.56466400
C	1.85930000	3.13908600	2.88215200
H	1.63038100	0.96891800	3.19412400
H	0.10943700	1.78634800	2.78095900
H	3.22664500	4.47482900	1.84762000
H	1.05394900	4.64425000	0.66089000
H	2.51654600	3.05817500	3.75363500
H	1.10351300	3.89814600	3.10970700
O	1.46489200	-1.81830600	-3.27448000
N	6.62068800	-1.53739200	-1.26545700
N	1.38204200	1.41529000	1.15658800
H	0.80034600	-1.44743900	-2.65050700
H	2.52550200	-0.90637600	1.21967400
O	3.72798300	-0.07958800	2.66802100
C	3.72295000	-1.32244700	3.36757400
H	4.44737100	-2.03185900	2.94834400
H	3.99930600	-1.09771200	4.40090400
H	2.72499500	-1.78298200	3.35246500
C	-1.59236100	-2.10485700	-0.42337700
H	-1.66712500	-2.48625100	-1.43408700
H	0.83197000	0.54406900	0.95336600
H	-1.62561300	-2.81604100	0.39336600
N	-0.57728800	-1.18343600	-0.28441500
O	-0.11317600	-0.93044600	0.87336300
O	-0.18522900	-0.53533200	-1.29817300
H	2.25968600	3.99768800	-0.45164700
C	-3.55843200	-0.17328100	3.41889700
C	-4.35899800	-1.24764800	3.80810200
C	-4.77344800	-2.20964900	2.87771600
C	-4.36050900	-2.05596300	1.55844700
C	-3.55080500	-0.97622700	1.14318300
C	-3.14642800	-0.03448800	2.08520700
N	-4.66252500	-2.89499600	0.47753100
C	-4.10086600	-2.42894200	-0.69453900
C	-3.31145500	-1.13521800	-0.33916500
O	-4.20387400	-2.95552000	-1.78705000
H	-3.24913300	0.56418400	4.15468600
H	-4.67084200	-1.34426500	4.84493600
H	-5.40013400	-3.04308100	3.17919900
H	-2.53177800	0.79619300	1.76820500

C	-5.49584300	-4.07828800	0.54662000
H	-6.50514000	-3.82476500	0.89085900
H	-5.55384800	-4.49754700	-0.45904700
H	-5.06451900	-4.82258600	1.22593000
N	-3.38688800	-0.21505300	-1.31272900
C	-3.03147000	1.08561300	-1.12934300
O	-2.33532800	1.59878900	-0.24482700
O	-3.56899600	1.80977200	-2.15568500
C	-3.42864200	3.25796900	-2.25486900
C	-4.24093200	3.58694300	-3.51265300
H	-4.22543500	4.66512500	-3.70767900
H	-3.82746500	3.07100400	-4.38598800
H	-5.28310400	3.27164500	-3.39359500
C	-1.96015600	3.64723000	-2.46170800
H	-1.36847700	3.43832400	-1.56916100
H	-1.53443500	3.08881800	-3.30333100
H	-1.88481700	4.71691000	-2.69137500
C	-4.04312900	3.94962300	-1.03160700
H	-4.04120200	5.03650100	-1.17669500
H	-5.08224100	3.62838600	-0.89511800
H	-3.48495200	3.71506300	-0.12355800

**TS2-c-anti-OS-R**

C	-3.88263900	0.11834200	1.01834400
C	-4.50390000	1.44374700	0.57781800
C	-3.70409600	2.42495900	-0.08923100
C	-5.83522600	1.72630900	0.79313200
C	-2.33295500	2.24003800	-0.38265800
C	-4.34320900	3.64369900	-0.48621900
C	-6.36586500	2.96689400	0.36227800
H	-6.47590600	1.00973900	1.29653400
C	-1.60815600	3.20666900	-1.05730100
H	-1.82126200	1.32919200	-0.10554300
C	-3.56667100	4.62917700	-1.15854300
H	-7.41784400	3.18766900	0.53890100
C	-2.23789800	4.42278100	-1.44160800
H	-4.06399200	5.55045100	-1.44692200
H	-1.64913000	5.17224400	-1.96188700
C	-3.68750200	-0.80874600	-0.20857800
H	-3.34250700	-0.18234600	-1.03223200
C	-4.93525700	-1.61802000	-0.63943900
C	-2.11800300	-2.33592500	-1.35109400
C	-2.91091900	-2.92765000	0.91339200
C	-4.50422000	-3.04624000	-1.02837900

H	-5.65776500	-1.65920100	0.17961900
H	-5.41542600	-1.11445600	-1.48365600
C	-3.34668700	-2.96757400	-2.04378100
H	-1.68249800	-1.50279600	-1.90492900
H	-1.32512900	-3.05959800	-1.15280000
C	-4.01282300	-3.77675700	0.23767600
H	-3.24633100	-2.47843300	1.84682000
H	-1.99247900	-3.48755800	1.09973200
H	-5.35169600	-3.58318900	-1.46487000
H	-3.08985600	-3.96546500	-2.41288600
H	-4.84206800	-3.92493500	0.93636000
H	-3.62553300	-4.76680500	-0.02588600
O	-0.30420500	3.04646200	-1.37603600
N	-5.66265100	3.89833100	-0.25238700
N	-2.53802100	-1.79079600	-0.00637600
H	-0.00955000	2.14588700	-1.10665900
H	-2.89056300	0.32938500	1.44486200
O	-4.66123200	-0.56201600	1.99117700
C	-4.50176500	-0.05349200	3.31469600
H	-4.81753000	0.99421500	3.39104200
H	-5.13575600	-0.66614700	3.96062900
H	-3.45810100	-0.13624600	3.64967300
C	1.70027000	0.36882200	1.05883900
H	2.12917700	1.22190300	0.54691300
H	-1.70152800	-1.29830400	0.40285400
H	1.75435700	0.30719300	2.13812500
N	0.47887200	-0.01027100	0.55820600
O	-0.27673800	-0.77342400	1.25020200
O	0.13957100	0.30661800	-0.62564000
H	-3.64632200	-2.36780900	-2.90971000
C	2.83335200	-1.39049700	-3.19396000
C	2.32932800	-2.69036400	-3.13582600
C	2.11193300	-3.32789400	-1.90561200
C	2.41666200	-2.62053600	-0.74697900
C	2.93534600	-1.30905500	-0.78829600
C	3.13680400	-0.68986300	-2.01711200
N	2.28925400	-3.05959500	0.57946700
C	2.71949600	-2.09420900	1.47163900
C	3.18909500	-0.88500300	0.62956100
O	2.72528000	-2.20181300	2.68373600
H	2.98973200	-0.91255900	-4.15688100
H	2.10198700	-3.22399000	-4.05519900
H	1.73282100	-4.34456700	-1.86401700
H	3.51881000	0.32323600	-2.05060400

C	1.81928900	-4.36553900	0.98585200
H	2.47136800	-5.15673000	0.59721100
H	1.83076300	-4.39316400	2.07678600
H	0.79780800	-4.54619700	0.63000200
N	4.28600000	-0.29199700	1.12061200
C	4.82598700	0.79065200	0.49891600
O	4.25558200	1.58051200	-0.26626100
O	6.11098300	0.94865400	0.91199200
C	6.93135900	2.08191800	0.48051800
C	8.26035800	1.81985300	1.19604000
H	8.98409800	2.60659500	0.95621100
H	8.11794600	1.79961900	2.28187500
H	8.68166300	0.85655500	0.88855100
C	6.31796400	3.40222300	0.96103200
H	5.36778700	3.60144300	0.46251100
H	6.14656100	3.37042100	2.04331100
H	7.00519100	4.23043100	0.75111500
C	7.13144900	2.05573900	-1.03914500
H	7.85845600	2.82285600	-1.33083900
H	7.52265200	1.08137400	-1.35437700
H	6.19407100	2.24367900	-1.56556600

**TS2-c-gau2-OS-S**

C	-3.48094700	0.89134500	-0.81454700
C	-4.62632000	-0.08494800	-0.54715200
C	-4.34712500	-1.43665300	-0.16935400
C	-5.94484800	0.30361900	-0.64435400
C	-3.03617400	-1.94638800	-0.02047300
C	-5.46230700	-2.29984900	0.08123600
C	-6.97273100	-0.63368100	-0.37764600
H	-6.19948600	1.31843700	-0.93161100
C	-2.81802100	-3.25234400	0.38083600
H	-2.17038200	-1.32305600	-0.19657400
C	-5.20608900	-3.64581200	0.46688300
H	-8.01337900	-0.32193400	-0.45875500
C	-3.92306900	-4.11517600	0.61735500
H	-6.06249400	-4.28868600	0.64744000
H	-3.72901800	-5.13949200	0.92114800
C	-2.85285000	1.35617000	0.52417100
H	-2.80711900	0.48141700	1.17435500
C	-3.58393000	2.51746900	1.24086200
C	-0.72563900	1.76748900	1.71968200
C	-1.23505800	3.10333800	-0.29971600
C	-2.54093100	3.49993400	1.81124700



H	-4.23855200	3.04097000	0.53927000
H	-4.20941600	2.10936800	2.04052400
C	-1.50947900	2.72065900	2.65028600
H	-0.71530900	0.73256900	2.06582500
H	0.30775200	2.07100600	1.54456000
C	-1.81407500	4.18702700	0.63856700
H	-1.76519000	3.05107100	-1.24958000
H	-0.16865400	3.22773000	-0.49166100
H	-3.04161600	4.24976400	2.43123500
H	-0.81606300	3.41175600	3.14020100
H	-2.50944000	4.82285700	0.08156100
H	-1.01360200	4.83098600	1.01828300
O	-1.57530200	-3.75640400	0.56244400
N	-6.75796400	-1.88701900	-0.02749300
N	-1.39076600	1.75468000	0.36044600
H	-0.91466300	-3.03574600	0.44407500
H	-2.70338300	0.36077900	-1.38387400
O	-3.89170800	2.02990500	-1.55684600
C	-3.99959300	1.79009600	-2.95880200
H	-4.74658100	1.01895100	-3.18495700
H	-4.31160600	2.73397900	-3.41283300
H	-3.03350500	1.48523300	-3.38554600
C	1.52531400	-1.70328500	-1.40302300
H	1.55117500	-2.74593400	-1.10875800
H	-0.88260600	1.04418900	-0.22122200
H	1.60927900	-1.47017400	-2.45693700
N	0.50961100	-1.00648600	-0.78632200
O	0.11903500	0.08070500	-1.30946000
O	0.03681900	-1.39808500	0.32572200
H	-2.01720500	2.15540900	3.43941400
C	3.33470500	-1.92232500	2.96132500
C	4.08214100	-3.09188200	2.81972200
C	4.51910800	-3.51956900	1.55894800
C	4.18235500	-2.73936400	0.45821200
C	3.43111400	-1.55067300	0.58047900
C	3.00033300	-1.14694300	1.84123700
N	4.51512700	-2.98044700	-0.88226000
C	4.02659600	-1.98909300	-1.70910900
C	3.27068100	-0.97539700	-0.80289300
O	4.16321800	-1.94158400	-2.91789600
H	3.00355900	-1.60886000	3.94751100
H	4.33260100	-3.68418200	3.69597100
H	5.10263600	-4.42819500	1.44924600
H	2.42155900	-0.23912800	1.94121600

C	5.29416400	-4.10477100	-1.35970200
H	6.29607700	-4.10225300	-0.91545100
H	4.80066100	-5.05359900	-1.11980300
H	5.38084000	-4.00705800	-2.44306400
N	3.44801800	0.29113400	-1.20472700
C	3.16896000	1.36815200	-0.42479600
O	2.37585200	1.47759400	0.51842800
O	3.91351300	2.41884200	-0.88520800
C	3.98436700	3.69756100	-0.18580600
C	4.99932100	4.48138700	-1.02513700
H	5.15910400	5.47879500	-0.60068000
H	5.96106400	3.95847600	-1.05431600
H	4.64321400	4.59642000	-2.05470200
C	4.51166900	3.50167800	1.24094100
H	3.80859000	2.92687900	1.84688200
H	5.47062900	2.97123700	1.22234900
H	4.67247200	4.47550100	1.71839600
C	2.62663000	4.40927200	-0.20307100
H	2.73452600	5.43188700	0.17821300
H	2.24240400	4.46975200	-1.22797700
H	1.90188200	3.87978800	0.41721600

**TS2-c-anti-OS-S**

C	-3.44668500	0.03446300	-1.42451800
C	-4.47299500	-1.02244800	-1.01776100
C	-4.16221700	-1.96884700	0.00960900
C	-5.71775700	-1.08455600	-1.60585700
C	-2.92422300	-1.99605900	0.69444100
C	-5.17230500	-2.92240000	0.35938300
C	-6.64159900	-2.07268500	-1.18649500
H	-5.99134900	-0.38747400	-2.39107300
C	-2.68428200	-2.91504200	1.70126300
H	-2.14072400	-1.28803000	0.46163000
C	-4.88817200	-3.86902000	1.38359000
H	-7.62310100	-2.11917000	-1.65674700
C	-3.68194800	-3.86989800	2.04143000
H	-5.66250500	-4.58859500	1.63232200
H	-3.46869500	-4.58774000	2.82766300
C	-3.39393700	1.15484300	-0.35489500
H	-3.46103700	0.66843600	0.61928800
C	-4.47659900	2.25397200	-0.48426100
C	-1.89688700	2.58916000	0.99112700
C	-1.82934100	2.78973200	-1.46978100
C	-3.83832900	3.63056800	-0.21020300

H	-4.90737600	2.23941200	-1.48853200
H	-5.28203900	2.05167600	0.22819500
C	-3.07544100	3.57950700	1.12796000
H	-1.86493200	1.83610300	1.78060300
H	-0.92573300	3.08691100	0.95592500
C	-2.84363900	3.95092200	-1.34435500
H	-1.97305900	2.21037400	-2.38033900
H	-0.78978500	3.11917600	-1.41805200
H	-4.61741500	4.39771800	-0.16897800
H	-2.69592800	4.57182100	1.39189600
H	-3.37756400	4.07610000	-2.29153200
H	-2.32361100	4.89178300	-1.13476000
O	-1.52309400	-2.95093900	2.39240300
N	-6.39506300	-2.96183100	-0.24397900
N	-2.03223400	1.84056800	-0.31377600
H	-0.94802000	-2.20391500	2.10635300
H	-2.45665700	-0.44313800	-1.46434000
O	-3.72296400	0.61775800	-2.68909800
C	-3.32778500	-0.19255700	-3.79502500
H	-3.86413400	-1.14921500	-3.81273700
H	-3.57520800	0.37235100	-4.69732100
H	-2.24657600	-0.38963300	-3.77741200
C	1.71468600	-1.20950500	0.37299500
H	1.80676300	-2.00827700	1.09827100
H	-1.26571800	1.11992800	-0.33852500
H	2.08068300	-1.35494100	-0.63599500
N	0.49621000	-0.57409200	0.41911800
O	0.12473400	0.11893900	-0.58344100
O	-0.20817600	-0.58188100	1.47991500
H	-3.74816000	3.26391800	1.93249000
C	2.70983800	3.26450900	-0.88833100
C	2.24308800	3.99188300	0.20847500
C	2.09380000	3.38804500	1.46630300
C	2.43362200	2.04325000	1.58441400
C	2.91751000	1.29727000	0.48815300
C	3.04731900	1.90877000	-0.75379100
N	2.38563200	1.25117600	2.73908900
C	2.84964600	-0.02793300	2.48963900
C	3.23165100	-0.08251500	0.99230600
O	2.92913800	-0.92518600	3.30719100
H	2.81945700	3.75106400	-1.85357700
H	1.99596900	5.04448500	0.09445400
H	1.74550800	3.95921600	2.32141800
H	3.40247500	1.33267200	-1.59961700

C	1.90767700	1.68639500	4.03407300
H	2.49288500	2.53678600	4.40230200
H	0.85057100	1.97382000	3.98577900
H	2.01963900	0.84801700	4.72348600
N	4.33013700	-0.80994500	0.74393400
C	4.78247900	-0.97118000	-0.52789300
O	4.13253900	-0.86307700	-1.57763800
O	6.08244400	-1.36685800	-0.49358700
C	6.81795800	-1.72435900	-1.70787600
C	8.19938400	-2.09672000	-1.16044100
H	8.86436100	-2.40197800	-1.97580900
H	8.65437300	-1.24403900	-0.64462600
H	8.12300600	-2.92419200	-0.44688500
C	6.92551200	-0.51899600	-2.64940500
H	5.94909000	-0.24410500	-3.05211000
H	7.34115200	0.34395800	-2.11615500
H	7.59610400	-0.75599900	-3.48404800
C	6.16881800	-2.93433600	-2.38955900
H	6.79750900	-3.27583200	-3.22041200
H	6.06654700	-3.76254400	-1.67891500
H	5.18040500	-2.68349000	-2.77850300

**TS2-c-anti-SS-S**

C	-3.53475500	-0.18056600	0.55265600
C	-3.96704100	1.28344400	0.46236700
C	-3.07761900	2.26535400	-0.07719300
C	-5.22227400	1.69027000	0.86084900
C	-1.76894700	1.96448500	-0.52078600
C	-3.56150200	3.60995700	-0.18482500
C	-5.59306500	3.05051300	0.72550600
H	-5.92543600	0.97785200	1.27991800
C	-0.96773400	2.94073000	-1.08522100
H	-1.36475100	0.96388400	-0.44122500
C	-2.70331400	4.59609400	-0.74711500
H	-6.58484300	3.36732900	1.04596800
C	-1.44339900	4.27634000	-1.19342400
H	-3.08184400	5.61145300	-0.81810000
H	-0.79256700	5.02771000	-1.63042200
C	-3.61865800	-0.82888900	-0.85072300
H	-3.18540100	-0.11583000	-1.55349700
C	-5.04401200	-1.23443300	-1.30293200
C	-2.52931300	-2.36014300	-2.45834100
C	-3.28441900	-3.26675100	-0.28906100
C	-4.98576900	-2.59934900	-2.01764700
H	-5.70708500	-1.30061400	-0.43632000

H	-5.44200900	-0.46363300	-1.96941700
C	-3.91155800	-2.54952000	-3.12128800
H	-1.95447000	-1.53146100	-2.87584100
H	-1.91128300	-3.25908800	-2.49830200
C	-4.59926100	-3.68229000	-0.98991900
H	-3.44075100	-2.98351800	0.75019100
H	-2.51068100	-4.03540900	-0.33797300
H	-5.96199300	-2.83026000	-2.45407200
H	-3.91755300	-3.47511300	-3.70543500
H	-5.39182400	-3.79807300	-0.24414000
H	-4.47709800	-4.64887800	-1.49022400
O	0.27698700	2.68084600	-1.54891200
N	-4.80913400	3.98346800	0.22065700
N	-2.72182000	-2.05382100	-0.98945400
H	0.48160900	1.73033600	-1.42112800
H	-2.48758900	-0.21524900	0.88838400
O	-4.32968100	-0.93260700	1.45818300
C	-3.98053700	-0.73312700	2.82587200
H	-4.11314400	0.31122300	3.13423000
H	-4.64766700	-1.36747400	3.41500100
H	-2.93908800	-1.02909700	3.01715500
C	2.06608600	-1.54600700	-0.96882300
H	2.34507100	-2.59166800	-0.97953100
H	-1.75574900	-1.87458800	-0.61729700
H	2.57143200	-0.84518400	-1.62099800
N	0.70582800	-1.35196600	-0.92184700
O	0.19233600	-0.26650300	-1.32750800
O	-0.03855400	-2.24268400	-0.39133800
H	-4.12013600	-1.72610000	-3.81222300
C	1.52641200	2.36657300	1.70136900
C	0.70252000	1.88702900	2.72044900
C	0.65767200	0.52021100	3.03151500
C	1.46447700	-0.33883500	2.29274300
C	2.30100300	0.12898400	1.25626500
C	2.32810100	1.48708300	0.95777200
N	1.60838600	-1.72418500	2.45481900
C	2.53610200	-2.23971300	1.57030300
C	3.04733100	-1.05583000	0.71812400
O	2.86703400	-3.40887800	1.49086800
H	1.54287100	3.42773600	1.47221100
H	0.08449900	2.57954200	3.28596900
H	0.02747800	0.15159500	3.83514600
H	2.96024700	1.84960500	0.15614400
C	0.87537900	-2.53447300	3.40186800

H	1.03260300	-2.17857000	4.42645500
H	-0.19905900	-2.52083600	3.18101500
H	1.24627800	-3.55717700	3.31510100
N	4.34325700	-1.13615000	0.39599900
C	4.92662200	-0.18562600	-0.38236000
O	4.36911100	0.57828700	-1.18234100
O	6.27619100	-0.24531100	-0.22484700
C	7.18617400	0.59024100	-1.00996300
C	8.56196400	0.16328100	-0.48818700
H	9.35488800	0.71812600	-1.00178900
H	8.64628500	0.35636500	0.58680500
H	8.72466700	-0.90686800	-0.65622900
C	6.94328300	2.07567000	-0.71798100
H	5.96948700	2.39800000	-1.09058200
H	6.98610500	2.26310500	0.36126800
H	7.72095900	2.68171500	-1.19781400
C	7.05716100	0.26625500	-2.50292900
H	7.83208600	0.79718200	-3.06850600
H	7.19089400	-0.80847800	-2.67210800
H	6.07889100	0.56202400	-2.88548700

### 3.4 TS2s involving Z-ketimine

#### a'-N-gau1-syn-R

C	-2.96790300	-0.30196100	-0.73444100
C	-3.51653100	-1.12019100	0.43372700
C	-2.70573800	-1.42254900	1.57535200
C	-4.83523200	-1.52716900	0.43666100
C	-1.32466500	-1.11189400	1.67683600
C	-3.35976900	-2.07372700	2.67726000
C	-5.36479600	-2.19319500	1.56485400
H	-5.46882900	-1.33365600	-0.42252800
C	-0.60797000	-1.42457100	2.82575900
H	-0.79375500	-0.64918600	0.85146200
C	-2.60572000	-2.34852800	3.85160300
H	-6.40668900	-2.51155500	1.56125700
C	-1.27476900	-2.02952700	3.93048800
H	-3.11974100	-2.83122900	4.67755600
H	-0.69172100	-2.25141000	4.81938400
C	-3.06680300	1.19998100	-0.37374500
H	-2.66471200	1.30154100	0.63668000
C	-4.49034700	1.80621400	-0.45659900
C	-1.96918600	3.40655100	-0.52884200

C	-2.65720500	2.28811300	-2.61540000
C	-4.41198200	3.21683500	-1.07343100
H	-5.13265100	1.17186900	-1.07319700
H	-4.92535000	1.84567300	0.54623900
C	-3.36023500	4.04381400	-0.31010900
H	-1.42696600	3.22008000	0.39897200
H	-1.32199900	3.99736800	-1.17686000
C	-3.97648000	3.09161700	-2.54684300
H	-2.79370800	1.30161000	-3.05420600
H	-1.86499800	2.81295700	-3.15330000
H	-5.39090900	3.70220900	-1.01251100
H	-3.35265700	5.07916900	-0.66642600
H	-4.74925100	2.57988200	-3.12907100
H	-3.84209100	4.08661000	-2.98463700
O	0.70279600	-1.17684300	2.97480900
N	-4.67071800	-2.44693000	2.65752200
N	-2.14136500	2.07120900	-1.21404500
H	1.14410800	-1.00920000	2.08685400
H	-1.91030500	-0.55077500	-0.89152800
O	-3.68130000	-0.52800400	-1.94397900
C	-3.32131900	-1.74265200	-2.59721700
H	-3.51768500	-2.61864500	-1.96663500
H	-3.93465700	-1.80683100	-3.49969700
H	-2.25965800	-1.73942900	-2.88230000
C	2.48095000	1.03392800	-1.60591200
H	2.55128200	0.10711600	-2.15460900
H	-1.19458900	1.60734300	-1.28275200
H	3.21706600	1.81451600	-1.74751100
N	1.20468000	1.51202100	-1.46172100
O	0.99346100	2.71581900	-1.16799200
O	0.23298300	0.68007800	-1.53303700
H	-3.60621400	4.06939600	0.75688800
C	2.16087200	3.18764900	2.54665300
C	3.45745500	3.70581900	2.53258500
C	4.49147700	3.06815300	1.83024200
C	4.17752600	1.90206400	1.14273200
C	2.87140900	1.37694800	1.13606200
C	1.85894900	2.01449600	1.84041200
N	5.02929700	1.06900500	0.40362200
C	4.35923500	-0.04689800	-0.07529300
C	2.87255900	0.14632600	0.31008200
O	4.88285300	-0.98489000	-0.65060500
H	1.38235300	3.69435300	3.10962200
H	3.67855800	4.61616500	3.08352800

H	5.49982200	3.46965900	1.83779900
H	0.85820000	1.59631700	1.85909500
C	6.45901200	1.25691700	0.26000300
H	6.67901100	2.19279800	-0.26611600
H	6.95104400	1.27454500	1.23943000
H	6.84555300	0.41745100	-0.31998200
N	2.01777100	-0.83859600	0.56235700
C	2.02233700	-2.07583300	-0.06375200
O	1.74449400	-3.10062100	0.54169600
O	2.24090500	-2.01378300	-1.39981500
C	2.28679200	-3.22862700	-2.22865800
C	2.61241600	-2.67653800	-3.61924300
H	2.65880400	-3.49329100	-4.34812900
H	1.84261500	-1.96895400	-3.94736800
H	3.57890300	-2.16185700	-3.61703200
C	0.91689700	-3.91533600	-2.23349600
H	0.66923000	-4.31066900	-1.24708800
H	0.13688900	-3.20532600	-2.53307800
H	0.91884300	-4.74060900	-2.95528900
C	3.40463700	-4.15809400	-1.74677800
H	3.53281400	-4.98112400	-2.45977900
H	4.34750000	-3.60635600	-1.67892300
H	3.17409900	-4.57833000	-0.76628400

**a'-N-gau1-syn-R-Boc-rotator**

C	2.94811100	-0.04048100	-0.77808100
C	3.42874800	1.03073400	0.19987700
C	2.54630600	1.59547400	1.17693800
C	4.74896100	1.43232100	0.19569200
C	1.15793800	1.30832800	1.25782600
C	3.13045500	2.50131900	2.12733400
C	5.20837700	2.35554000	1.16190500
H	5.43671900	1.03985900	-0.54589800
C	0.36919500	1.88767000	2.24471700
H	0.68145800	0.64839400	0.54008600
C	2.30158900	3.05269300	3.14304200
H	6.25192300	2.66833100	1.15323300
C	0.96513000	2.75342800	3.20753900
H	2.76405600	3.72814600	3.85688900
H	0.32609800	3.18301300	3.97338100
C	3.00490000	-1.41905000	-0.07454600
H	2.54172600	-1.28535900	0.90581300
C	4.42188000	-2.02865500	0.07260500
C	1.88267500	-3.59886400	0.21073100



C	2.71034500	-2.99204300	-2.02705500
C	4.35666500	-3.54342400	-0.20826100
H	5.11034200	-1.55377600	-0.63140600
H	4.79452000	-1.83800300	1.08303300
C	3.24753100	-4.16913600	0.65927200
H	1.28609000	-3.20442900	1.03455500
H	1.26855400	-4.32194600	-0.32555200
C	4.01156300	-3.75892400	-1.69594900
H	2.88639200	-2.13500400	-2.67435800
H	1.94228800	-3.62598000	-2.47520400
H	5.32163200	-4.00526500	0.02175500
H	3.24542000	-5.25899800	0.55440100
H	4.82566100	-3.39397800	-2.33024400
H	3.89026100	-4.82784400	-1.90249900
O	-0.95123500	1.67336600	2.36435600
N	4.44385200	2.86575200	2.10775500
N	2.11797200	-2.45747000	-0.74791500
H	-1.34128100	1.29963200	1.51692100
H	1.90708800	0.16344500	-1.05911300
O	3.74133300	-0.09823200	-1.95658800
C	3.43010700	0.92115100	-2.90359800
H	3.59823600	1.92467500	-2.49246400
H	4.09694800	0.76851400	-3.75614900
H	2.38702000	0.84434300	-3.24137300
C	-2.39075100	-1.48844700	-1.76557400
H	-2.38287400	-0.63442500	-2.42867200
H	1.18308400	-2.01298200	-0.97714200
H	-3.13543600	-2.26886200	-1.84611800
N	-1.16072200	-1.93958200	-1.38898200
O	-1.00650000	-3.08438200	-0.88861500
O	-0.16324200	-1.13304600	-1.47550800
H	3.42851700	-3.94547300	1.71630000
C	-2.38335500	-2.74910200	2.80374700
C	-3.65282900	-3.33090300	2.77358900
C	-4.63338400	-2.89984300	1.86733900
C	-4.29611500	-1.87244900	0.99451000
C	-3.01474100	-1.28570100	1.00473300
C	-2.05464200	-1.72016600	1.91035300
N	-5.09901500	-1.24923200	0.03160100
C	-4.42314300	-0.21085800	-0.59672400
C	-2.98048700	-0.24682600	-0.04358800
O	-4.91660400	0.57440100	-1.38468300
H	-1.64775100	-3.09421400	3.52454800
H	-3.89519000	-4.12899700	3.47036100

H	-5.62144600	-3.34892200	1.86079100
H	-1.07645900	-1.25161000	1.93886300
C	-6.49969200	-1.53877200	-0.19844500
H	-6.63343200	-2.57008400	-0.54419800
H	-7.08440200	-1.39126400	0.71721400
H	-6.85736600	-0.85095700	-0.96643500
N	-2.17437700	0.80158300	0.03617300
C	-2.10771800	1.74876200	-0.97513200
O	-2.19271300	1.54901100	-2.17907400
O	-1.81955300	2.94800100	-0.41494600
C	-1.59996000	4.14954800	-1.23252700
C	-1.33101200	5.22563300	-0.17739300
H	-1.15456800	6.19316700	-0.65986500
H	-2.18741500	5.32766900	0.49774300
H	-0.45055000	4.97289500	0.42287400
C	-2.86321100	4.48473600	-2.03195000
H	-3.08057600	3.71319400	-2.77235600
H	-3.72515300	4.57969100	-1.36181900
H	-2.72911300	5.44173400	-2.54980600
C	-0.37374000	3.96229000	-2.13252500
H	-0.13204600	4.90938600	-2.62907000
H	0.49467600	3.66230000	-1.53483000
H	-0.55367300	3.20379400	-2.89656900

**a'-N-gau2-syn-R**

C	3.19175900	0.17685300	0.25826400
C	3.53061100	-1.05654100	-0.58301000
C	2.52025300	-1.89622300	-1.16099500
C	4.85542000	-1.37058200	-0.81478000
C	1.12345700	-1.72985500	-0.96161200
C	2.98212000	-2.98464600	-1.98156100
C	5.19181400	-2.47184900	-1.63248600
H	5.64459800	-0.78235700	-0.35880600
C	0.21466800	-2.60827400	-1.53717300
H	0.73378400	-0.92155600	-0.35630900
C	2.02220300	-3.84380700	-2.58300800
H	6.23989900	-2.70753000	-1.81405000
C	0.67975000	-3.66549400	-2.37071800
H	2.39341700	-4.65344800	-3.20442300
H	-0.05592000	-4.32860300	-2.81639300
C	3.12716100	1.43596400	-0.64558000
H	2.59386500	1.14574600	-1.55271200
C	4.49749000	2.08656200	-0.98462400
C	2.05358700	3.62409000	-1.06116200

C	2.77780500	3.09773600	1.23359400
C	4.50181300	3.56354900	-0.53640400
H	5.29999700	1.55159500	-0.47413000
H	4.68316800	2.01698800	-2.06102800
C	3.40642900	4.33125200	-1.29880700
H	1.66104200	3.15074500	-1.96343600
H	1.27894200	4.27913000	-0.66125800
C	4.20395900	3.63384000	0.97470300
H	2.75551800	2.31210400	1.98687000
H	2.07429100	3.88045700	1.52610800
H	5.48216100	4.00388100	-0.74273600
H	3.36031100	5.36876800	-0.95066100
H	4.93173500	3.03089300	1.52437400
H	4.28507800	4.66615600	1.33003900
O	-1.11948800	-2.53204000	-1.36933100
N	4.29905700	-3.25119500	-2.21023700
N	2.23782000	2.51958100	-0.04678000
H	-1.40993100	-1.88090500	-0.66215100
H	2.20900400	0.03640400	0.72767600
O	4.16074200	0.41851900	1.27199400
C	4.08082100	-0.47341100	2.37852500
H	4.24189300	-1.51543000	2.07563700
H	4.87277700	-0.17990700	3.07281800
H	3.11012900	-0.39208100	2.88802200
C	-2.02499100	1.40668600	-1.34388000
H	-2.71036300	2.13358900	-1.75922300
H	1.28377400	2.08939800	0.10513900
H	-1.71934200	0.55437500	-1.93218600
N	-1.02523300	1.95249100	-0.58716800
O	-0.07156400	1.17145900	-0.22435500
O	-1.06521800	3.13960900	-0.19123000
H	3.63136800	4.35737200	-2.36992700
C	-5.49464600	-1.19455300	-2.73246600
C	-6.49352100	-0.23049200	-2.56297700
C	-6.37963500	0.77845100	-1.59638300
C	-5.23164300	0.79377300	-0.80940900
C	-4.21097800	-0.16311300	-0.98475200
C	-4.34286400	-1.16860100	-1.93546500
N	-4.89590200	1.67304400	0.22394800
C	-3.67071300	1.34224500	0.80029600
C	-3.16673700	0.10480100	0.02809700
O	-3.11734100	1.96763800	1.68335600
H	-5.61284900	-1.96904800	-3.48469700
H	-7.38222200	-0.26230000	-3.18783700

H	-7.16618200	1.51482200	-1.46408900
H	-3.55993200	-1.91161700	-2.05814300
C	-5.67810700	2.82146300	0.63035600
H	-5.80316900	3.52571600	-0.20087900
H	-6.66742200	2.51447400	0.98905700
H	-5.13920700	3.31497400	1.44093800
N	-2.33222300	-0.82693300	0.45832500
C	-2.05117400	-0.99980900	1.80040100
O	-2.76691900	-0.69582100	2.74314400
O	-0.89718400	-1.71458100	1.91613100
C	-0.50565900	-2.30800300	3.20049200
C	0.75237700	-3.10298600	2.83955500
H	1.14901600	-3.60666600	3.72798600
H	0.52824200	-3.86240500	2.08304900
H	1.53165500	-2.44585100	2.44042400
C	-1.59596600	-3.25790600	3.71078600
H	-2.50318800	-2.71569700	3.98057200
H	-1.84331800	-4.00026200	2.94335800
H	-1.23178400	-3.79354100	4.59522600
C	-0.17880700	-1.20772700	4.21604500
H	0.23309800	-1.65207300	5.12988200
H	0.56986000	-0.51905000	3.80605300
H	-1.07093700	-0.63480900	4.47438900

**a'-O-gau2-syn-R**

C	3.32205400	-0.18937800	1.17905000
C	4.16248700	-1.05755500	0.24550500
C	3.55667200	-1.78514600	-0.82968100
C	5.53049600	-1.13336200	0.40190600
C	2.16033700	-1.80315900	-1.09190800
C	4.43750700	-2.52669800	-1.68686800
C	6.29975100	-1.91037000	-0.49426400
H	6.01694000	-0.60071700	1.21210600
C	1.65548000	-2.50944900	-2.17301600
H	1.46226400	-1.27589300	-0.44942300
C	3.88237300	-3.24635900	-2.78080800
H	7.37977500	-1.96877200	-0.36397200
C	2.53298400	-3.23715400	-3.02418000
H	4.56624600	-3.80052100	-3.41671900
H	2.10470700	-3.78130700	-3.86061200
C	2.95322200	1.13353500	0.46789900
H	2.61159900	0.86206200	-0.53285900
C	4.07327500	2.19512500	0.37455500
C	1.12663500	2.73609700	0.08218500

C	2.07270800	2.56294400	2.35290800
C	3.44450900	3.59749500	0.52750100
H	4.81587200	2.03424600	1.16171300
H	4.58261200	2.09696500	-0.58868700
C	2.22149100	3.71393000	-0.40594300
H	0.71449200	2.11571800	-0.71585600
H	0.29509800	3.22970800	0.58545600
C	2.96740000	3.76694400	1.98386400
H	2.57514500	1.86091900	3.01632300
H	1.11548800	2.85008200	2.79114900
H	4.18296700	4.36599500	0.28032000
H	1.83099100	4.73649300	-0.39925400
H	3.82275800	3.81237900	2.66550700
H	2.41401800	4.70639500	2.09089600
O	0.34260500	-2.55474200	-2.48501700
N	5.78837100	-2.58020200	-1.50817000
N	1.73824800	1.79974300	1.09477800
H	-0.19641600	-2.01768600	-1.85058300
H	2.38983200	-0.72154600	1.41064100
O	3.99300200	0.11258100	2.39516500
C	3.90665900	-0.92531800	3.36881000
H	4.36462000	-1.85766000	3.01455600
H	4.45025100	-0.57290100	4.24916900
H	2.86142500	-1.12340800	3.64465700
C	-2.20941500	-0.43530700	2.31364400
H	-1.98356300	-1.46219200	2.57446400
H	1.02809100	1.06193100	1.34658300
H	-2.97006200	0.08753200	2.87673300
N	-1.09141700	0.33670100	2.09038100
O	-1.21716100	1.57902500	2.00292800
O	0.03162100	-0.23301700	1.85602300
H	2.51121500	3.48347900	-1.43685600
C	-6.43099000	-1.97272700	2.01062000
C	-6.15109200	-3.29232400	1.64427200
C	-4.98000300	-3.62240300	0.94707600
C	-4.10145200	-2.58852800	0.64190300
C	-4.36419500	-1.26226000	1.01967800
C	-5.53438900	-0.94318300	1.69304600
N	-2.88040800	-2.65774500	-0.05692300
C	-2.31209600	-1.41133700	-0.19441300
C	-3.24598900	-0.41213900	0.51853700
O	-1.23867300	-1.15957200	-0.73843800
H	-7.35042300	-1.74348900	2.54176000
H	-6.85459900	-4.08129700	1.89617400

H	-4.77710000	-4.64745700	0.65362000
H	-5.74418600	0.08830000	1.96206300
C	-2.30927500	-3.89611300	-0.55274900
H	-2.10916700	-4.58591800	0.27512900
H	-2.99464200	-4.37622700	-1.25958100
H	-1.37379600	-3.67499900	-1.06558000
N	-3.43223500	0.85252100	0.17616500
C	-3.07019800	1.34665400	-1.04543800
O	-3.05167000	0.72912900	-2.10852600
O	-2.86343600	2.69500400	-0.95688300
C	-2.85521600	3.53388500	-2.15449100
C	-2.71595700	4.94619800	-1.57713500
H	-2.69987700	5.68952100	-2.38215200
H	-3.55419900	5.17629700	-0.91060000
H	-1.78845300	5.04224000	-1.00131200
C	-4.18509000	3.40167600	-2.90723400
H	-4.30142200	2.40162000	-3.32868800
H	-5.02534300	3.59778400	-2.23102300
H	-4.22810600	4.13353800	-3.72241400
C	-1.65806100	3.20331400	-3.05410400
H	-1.61787100	3.90329500	-3.89758100
H	-0.71972900	3.30013800	-2.49477800
H	-1.73140300	2.18578600	-3.44049200

**a'-O-anti-R**

C	-3.43194200	0.27022000	0.66667100
C	-3.57838600	1.79304900	0.64652900
C	-2.46650700	2.66085700	0.38783400
C	-4.82068400	2.36110900	0.84894200
C	-1.12389400	2.22405600	0.23708200
C	-2.75503600	4.06700700	0.29115600
C	-4.98311100	3.76109900	0.75124900
H	-5.67565200	1.73825400	1.08956900
C	-0.10399700	3.13596800	0.00610200
H	-0.86098700	1.17554400	0.30446900
C	-1.69052400	4.96743500	0.01099900
H	-5.96781200	4.20073300	0.90569500
C	-0.40227300	4.52067600	-0.13183200
H	-1.93403300	6.02271600	-0.06843000
H	0.41706300	5.20591700	-0.32737500
C	-3.70763600	-0.29661600	-0.74976900
H	-3.17370300	0.34925800	-1.44993100
C	-5.20535400	-0.42284200	-1.14100200
C	-3.11964300	-2.02293200	-2.42348700

C	-3.68930000	-2.75320400	-0.13830800
C	-5.49586100	-1.85212500	-1.64229000
H	-5.83748200	-0.20866800	-0.27689100
H	-5.44462600	0.30934300	-1.91810900
C	-4.59726200	-2.16279200	-2.85331600
H	-2.59209900	-1.23229800	-2.96060300
H	-2.54558600	-2.94476800	-2.53095700
C	-5.18658000	-2.85423500	-0.51229300
H	-3.53965100	-2.49995500	0.90937600
H	-3.12886600	-3.66211700	-0.36737100
H	-6.54918600	-1.93057600	-1.92866500
H	-4.79056700	-3.17703800	-3.21755200
H	-5.80328600	-2.62979000	0.36313000
H	-5.42644400	-3.87274500	-0.83464500
O	1.19441400	2.78845500	-0.11031700
N	-4.00043600	4.59247400	0.46540400
N	-3.05787700	-1.65941700	-0.95814200
H	1.35734500	1.88070100	0.24611200
H	-2.40288100	0.00901800	0.94728800
O	-4.33017300	-0.35040200	1.57902700
C	-3.96495000	-0.18449200	2.94591700
H	-3.96363700	0.87163300	3.24255900
H	-4.71288100	-0.72019400	3.53608700
H	-2.97178000	-0.61128600	3.14898800
C	1.63385300	-1.13356500	-1.55508500
H	2.17011200	-1.71375000	-2.29476400
H	-2.03363600	-1.55815300	-0.73104000
H	1.61417700	-0.05739400	-1.66946100
N	0.36847700	-1.65049900	-1.29730000
O	-0.49468300	-0.87192400	-0.75769500
O	0.10688400	-2.85766800	-1.48661400
H	-4.81736900	-1.47375600	-3.67502100
C	3.66047200	-5.03187900	0.09706600
C	2.88263200	-5.29478100	1.22815200
C	2.16770600	-4.27552400	1.87342100
C	2.25182900	-2.99570500	1.33640800
C	3.01754100	-2.72230000	0.19345100
C	3.73903000	-3.73291700	-0.42377600
N	1.65417500	-1.80900600	1.80523300
C	2.00177400	-0.72702300	1.03120600
C	2.95052800	-1.25462300	-0.07370800
O	1.54093300	0.40072300	1.18482400
H	4.21180400	-5.83830900	-0.37802200
H	2.83398700	-6.30566900	1.62406100

H	1.57912900	-4.48297100	2.76164200
H	4.35349600	-3.51149500	-1.29187100
C	0.73301400	-1.73558600	2.92073000
H	-0.14965400	-2.35928900	2.73609600
H	1.21803900	-2.07015400	3.84429000
H	0.42657200	-0.69456300	3.03161000
N	4.01992500	-0.62746800	-0.55919000
C	4.45299000	0.57106300	-0.05905100
O	4.42891600	0.93357900	1.11486000
O	5.04484300	1.28384100	-1.06110300
C	5.73816500	2.54494000	-0.79414500
C	6.20229600	2.97264400	-2.19026300
H	6.75824400	3.91515800	-2.13537900
H	6.85485600	2.21170900	-2.63228900
H	5.34459800	3.11672800	-2.85649700
C	6.94675200	2.30317200	0.11776900
H	6.62962000	1.97733400	1.11003100
H	7.60217600	1.53641800	-0.31179000
H	7.52859800	3.22704700	0.22078700
C	4.77611200	3.58641700	-0.21040800
H	5.26662200	4.56703500	-0.18093700
H	3.87800900	3.67058600	-0.83180500
H	4.46793500	3.31496900	0.80002000

**b'-N-gaul-syn-R**

C	2.21764800	-1.31142800	-0.40402400
C	3.52065100	-0.51445600	-0.51801200
C	3.53836800	0.90434400	-0.72696200
C	4.73191000	-1.17554500	-0.42585000
C	2.38598100	1.70045300	-0.95895400
C	4.83339000	1.53666200	-0.73834800
C	5.94273500	-0.45233300	-0.45988300
H	4.76765000	-2.25482500	-0.33110700
C	2.50323000	3.06224200	-1.20367100
H	1.39581200	1.26235400	-1.01743300
C	4.91095000	2.94179500	-0.94301600
H	6.89005100	-0.98253600	-0.36781100
C	3.78398600	3.68608200	-1.16980900
H	5.89792000	3.39495400	-0.93517500
H	3.83710000	4.75602400	-1.34831200
C	1.99701300	-1.77205100	1.05974700
H	2.16522600	-0.89556100	1.68945100
C	2.86823100	-2.96680000	1.52735400
C	0.30861700	-2.15254600	2.84390200



C	0.16673300	-3.49187200	0.77983500
C	2.03209700	-3.91257700	2.41134400
H	3.23633700	-3.52084000	0.66039200
H	3.73401400	-2.58786100	2.07688100
C	1.33572400	-3.09174500	3.50986100
H	0.36695600	-1.11668500	3.17213200
H	-0.72041400	-2.49427700	2.97884500
C	0.95791300	-4.58537100	1.53474200
H	0.40802900	-3.46632600	-0.27987800
H	-0.91363200	-3.58843600	0.90097200
H	2.68284500	-4.67145300	2.85620300
H	0.82675400	-3.74978800	4.22159700
H	1.42646400	-5.26080000	0.81185700
H	0.28631000	-5.18674900	2.15714600
O	1.46156900	3.86189500	-1.48219000
N	6.00481700	0.85859700	-0.59050200
N	0.54058600	-2.14066900	1.34478800
H	0.59512300	3.35797800	-1.54768200
H	1.37276900	-0.67188600	-0.68425600
O	2.21713400	-2.46712000	-1.24102500
C	2.18690400	-2.16487400	-2.63515700
H	3.10575100	-1.66105500	-2.95972700
H	2.10073800	-3.12160000	-3.15712700
H	1.32715900	-1.53082200	-2.89166800
C	-2.76038500	1.57776000	-1.93157600
H	-3.40256700	2.39227100	-1.63001800
H	-0.08995400	-1.40117800	0.94273400
H	-3.09876600	0.80059800	-2.59766500
N	-1.43781700	1.86018900	-1.98842900
O	-0.61550200	1.01734500	-2.44934800
O	-1.02107000	2.97916300	-1.51862900
H	2.07477000	-2.51243900	4.07399200
C	-2.35689400	-2.96283600	-2.67895700
C	-3.73913000	-3.13028100	-2.81125400
C	-4.64533300	-2.36648300	-2.06075900
C	-4.12100300	-1.43927300	-1.16756900
C	-2.72856100	-1.27043200	-1.01315800
C	-1.84274300	-2.02141000	-1.77934000
N	-4.80214400	-0.55596800	-0.32759000
C	-3.91983300	0.19455700	0.44455100
C	-2.50808500	-0.21758800	-0.01831300
O	-4.25214600	0.91978500	1.36521000
H	-1.68002300	-3.55782800	-3.28492100
H	-4.12541700	-3.86314300	-3.51448400

H	-5.71608500	-2.49719100	-2.17982800
H	-0.77433300	-1.86275400	-1.68982200
C	-6.24142000	-0.48588900	-0.17700000
H	-6.71836000	-0.19347000	-1.11925200
H	-6.64878900	-1.45120900	0.14558200
H	-6.45644000	0.26550400	0.58429100
N	-1.36406400	-0.02044200	0.57937000
C	-1.12936500	1.00475400	1.50994900
O	-0.34188900	0.82802000	2.43499100
O	-1.74101900	2.14408500	1.21907500
C	-1.58231500	3.36754700	2.03812600
C	-2.50680000	4.35664100	1.32702000
H	-2.45150800	5.33618200	1.81458000
H	-2.21068700	4.46103000	0.27961100
H	-3.54442300	4.00820200	1.36369400
C	-0.12878000	3.84254700	1.98238000
H	0.54244900	3.12986900	2.46652600
H	0.19035000	3.98304600	0.94516300
H	-0.04183600	4.80472100	2.50065700
C	-2.06379800	3.10014800	3.46634200
H	-2.10713700	4.04631900	4.01811400
H	-3.06853400	2.66559300	3.44999900
H	-1.39373900	2.42025400	3.99638900

**a'-N-gau1-syn-S**

C	-2.90635500	-0.79659900	-0.45408300
C	-3.27330200	-1.10708200	0.99643800
C	-2.34129600	-0.91766700	2.06783100
C	-4.53251800	-1.58785100	1.29603800
C	-1.00854400	-0.45037400	1.89997700
C	-2.80189200	-1.25625700	3.38686900
C	-4.88220900	-1.86964200	2.63460300
H	-5.24906700	-1.76811100	0.50181500
C	-0.14118000	-0.37540000	2.98500200
H	-0.63986200	-0.15425300	0.92278600
C	-1.90170600	-1.12619000	4.48079500
H	-5.88020300	-2.24103600	2.86481800
C	-0.61226300	-0.70737200	4.28989600
H	-2.27201400	-1.38471200	5.46850300
H	0.08540900	-0.62459300	5.11792600
C	-3.19018100	0.69260300	-0.75771500
H	-2.78285700	1.26589100	0.07836000
C	-4.67872800	1.05373000	-0.99604300
C	-2.40563600	2.69816700	-1.96656500

C	-2.90857200	0.67028800	-3.27006900
C	-4.79445500	1.97247400	-2.22826400
H	-5.26105000	0.14479400	-1.16543300
H	-5.08142300	1.54737500	-0.10656400
C	-3.86959300	3.19157200	-2.04411800
H	-1.88906200	3.02858900	-1.06316500
H	-1.80900300	3.00185900	-2.82916700
C	-4.35172400	1.18718500	-3.47883400
H	-2.85161100	-0.41438900	-3.22583100
H	-2.21361400	1.02994700	-4.03200900
H	-5.83113700	2.30329000	-2.34449800
H	-3.98481200	3.88877400	-2.88035800
H	-5.02637900	0.34239500	-3.64919200
H	-4.40143300	1.83053400	-4.36385500
O	1.14526300	-0.01015400	2.90642600
N	-4.05706700	-1.71495800	3.65191800
N	-2.39086200	1.18991100	-1.95378200
H	1.46342000	0.14822200	1.96808100
H	-1.83532300	-0.97899600	-0.60917900
O	-3.64226700	-1.59179600	-1.37653300
C	-3.14610700	-2.92404100	-1.50419500
H	-3.24357500	-3.48461200	-0.56571900
H	-3.75460800	-3.40898700	-2.27214200
H	-2.09416000	-2.92528000	-1.81812700
C	2.12524500	-0.11504000	-2.39238400
H	2.48044300	-0.92418800	-3.01654600
H	-1.37792600	0.90135300	-1.83302600
H	2.55663000	0.87507400	-2.44196800
N	0.77793500	-0.13040000	-2.17242900
O	0.26199800	0.89120100	-1.59165300
O	0.07065300	-1.13866300	-2.43698100
H	-4.13703700	3.73332300	-1.13070500
C	1.52072800	-4.00484500	0.19927600
C	2.61647100	-4.69318400	-0.32514800
C	3.73476200	-4.00918400	-0.82405600
C	3.71352500	-2.62046900	-0.77810000
C	2.61094000	-1.91062900	-0.26133800
C	1.51105600	-2.60333900	0.22977400
N	4.70961600	-1.72659800	-1.18524600
C	4.35309500	-0.41039900	-0.92080100
C	2.89902100	-0.46273900	-0.38168400
O	5.08807000	0.54901800	-1.05924500
H	0.67005400	-4.55677400	0.58842400
H	2.61132400	-5.77984800	-0.34370600

H	4.58820500	-4.54957700	-1.22088000
H	0.66325900	-2.07051400	0.64405600
C	6.01826000	-2.10798700	-1.67600100
H	6.54407100	-2.73078100	-0.94258900
H	5.93581600	-2.66115300	-2.61849200
H	6.58773100	-1.19223400	-1.84245300
N	2.35405800	0.43299300	0.43381500
C	2.59617700	1.78969300	0.27182300
O	2.86772300	2.38528900	-0.76039600
O	2.38878500	2.39419100	1.47030700
C	2.48449600	3.84871700	1.62590400
C	2.18078500	4.04505000	3.11375100
H	2.20069000	5.11035600	3.36862000
H	1.19167400	3.64613400	3.36294000
H	2.92167300	3.52735400	3.73231700
C	1.42427400	4.54543200	0.76526400
H	1.61534600	4.38782600	-0.29759100
H	0.42611400	4.16030500	1.00597600
H	1.42954200	5.62268800	0.96916500
C	3.90298100	4.32900200	1.29960500
H	3.99863800	5.39405300	1.54160800
H	4.63735400	3.77824200	1.89836000
H	4.13785800	4.18659900	0.24342300

**a'-N-gau2-syn-S**

C	3.37948900	0.02065900	-1.05477900
C	3.88808000	1.23432900	-0.27598200
C	2.98641600	2.20982100	0.26091900
C	5.24271500	1.42598200	-0.09699400
C	1.57435700	2.12247900	0.16495100
C	3.57370800	3.33949100	0.92704800
C	5.70902900	2.56700900	0.59515600
H	5.95406500	0.71548500	-0.50446700
C	0.76567300	3.10759300	0.71230200
H	1.09504100	1.27687700	-0.31399000
C	2.71607100	4.34763600	1.44632200
H	6.78026100	2.70925200	0.73450700
C	1.35223100	4.24106300	1.34215100
H	3.17990400	5.19886200	1.93602200
H	0.69307300	5.00269500	1.74827400
C	2.93691600	-1.10813300	-0.09366400
H	2.28207100	-0.65390000	0.65325300
C	4.08830100	-1.89459600	0.58025800
C	1.31762600	-2.94674400	0.26168600

C	2.75861100	-3.03417900	-1.73287500
C	3.77197800	-3.40351000	0.54181400
H	5.03018800	-1.70526200	0.05812200
H	4.20529100	-1.55196300	1.61283400
C	2.37536100	-3.64799200	1.14432400
H	0.67818200	-2.26020800	0.81797900
H	0.68578100	-3.64674200	-0.28778700
C	3.77411400	-3.87752600	-0.92548000
H	3.24321600	-2.40387300	-2.47472600
H	1.99105100	-3.63871100	-2.22035400
H	4.52899000	-3.95251500	1.11055900
H	2.16617600	-4.72152600	1.19703900
H	4.77393700	-3.76524700	-1.35683100
H	3.51251600	-4.93995300	-0.97610800
O	-0.58166500	3.05785000	0.68306300
N	4.91835700	3.50013400	1.08761800
N	2.02640300	-2.11963100	-0.78635400
H	-0.90632900	2.14724100	0.41692200
H	2.50628700	0.32668900	-1.64602900
O	4.37185100	-0.49755800	-1.93636100
C	4.52008300	0.25336800	-3.13762400
H	4.83629800	1.28510900	-2.93930800
H	5.29239600	-0.24822600	-3.72678000
H	3.58363000	0.27393500	-3.71362600
C	-1.97327400	-0.18800200	-2.48235500
H	-1.71840000	0.82312700	-2.76770400
H	1.29199500	-1.57864300	-1.30722800
H	-2.76024600	-0.69658300	-3.02608000
N	-0.85941700	-0.97561200	-2.26738800
O	-0.91094300	-2.22286200	-2.32174900
O	0.19987300	-0.37628200	-1.88975200
H	2.33455500	-3.25782100	2.16692400
C	-4.74198300	3.32173000	-1.63229800
C	-5.93823300	2.63895100	-1.87018400
C	-6.03926700	1.25431900	-1.67526500
C	-4.90229400	0.57813900	-1.24394500
C	-3.68646900	1.25362400	-1.02052900
C	-3.60295300	2.62804600	-1.20151300
N	-4.75943800	-0.78532300	-0.94775200
C	-3.48502700	-1.06882300	-0.47973300
C	-2.69661400	0.25034000	-0.54844100
O	-3.08034700	-2.16281600	-0.12588800
H	-4.69449000	4.39674600	-1.77969000
H	-6.81342600	3.18923100	-2.20525900

H	-6.97633200	0.73420300	-1.84767600
H	-2.67295300	3.15351900	-1.00253000
C	-5.79895800	-1.78454500	-1.08485400
H	-6.65835400	-1.54638700	-0.44734600
H	-6.13684700	-1.85873000	-2.12497700
H	-5.37739300	-2.74226600	-0.77474900
N	-1.67125600	0.54527100	0.24510600
C	-1.33647500	-0.18635500	1.36431400
O	-0.18456000	-0.44341100	1.70581600
O	-2.42364700	-0.43421600	2.13866600
C	-2.33350700	-1.15180100	3.41959500
C	-3.80272400	-1.26807800	3.83566700
H	-3.88267000	-1.76556800	4.80841900
H	-4.26294500	-0.27730100	3.91613600
H	-4.36866800	-1.85211400	3.10219700
C	-1.55138900	-0.30795500	4.43087700
H	-0.51595300	-0.17336200	4.11216300
H	-2.01355800	0.67886500	4.54754000
H	-1.55565200	-0.80218400	5.40959600
C	-1.72436500	-2.54439600	3.22732100
H	-1.87699900	-3.13875800	4.13590900
H	-2.21146500	-3.05729000	2.39189200
H	-0.65262800	-2.48785100	3.02885100

**a'-O-gau2-syn-S**

C	2.66908000	-0.21398400	-0.65830100
C	3.33868600	0.91240800	0.13181300
C	2.77338600	1.42186800	1.34549900
C	4.54760400	1.42619400	-0.29103900
C	1.50595200	1.03547400	1.85485500
C	3.55079400	2.38898800	2.06953200
C	5.21519900	2.39683500	0.49006400
H	4.98874200	1.08603500	-1.22180700
C	1.02037500	1.58793700	3.03042000
H	0.87617000	0.33655400	1.31541800
C	3.04139200	2.89624800	3.29640900
H	6.17164900	2.79308900	0.15046800
C	1.81419600	2.50689800	3.77010800
H	3.65091300	3.61595300	3.83467100
H	1.41101200	2.90791600	4.69530700
C	3.07859400	-1.56551000	-0.02615300
H	2.89518600	-1.47606500	1.04719000
C	4.53973400	-2.00627500	-0.29182500
C	2.33801800	-3.85455100	0.51847300

C	2.44445200	-3.19487200	-1.85392200
C	4.57678000	-3.52365500	-0.56260000
H	4.94035200	-1.47072800	-1.15645900
H	5.15762500	-1.75148200	0.57409000
C	3.82975200	-4.25827700	0.56731000
H	1.95470800	-3.51637700	1.48324700
H	1.69350300	-4.65871800	0.15715500
C	3.86439200	-3.80550700	-1.89971400
H	2.33424100	-2.33231400	-2.50536100
H	1.65917800	-3.91559200	-2.08798600
H	5.61491000	-3.86602100	-0.61122100
H	3.92398700	-5.34254600	0.45021800
H	4.42767100	-3.36376800	-2.72784200
H	3.81387000	-4.88542900	-2.07837100
O	-0.20095100	1.29865300	3.53215400
N	4.75706100	2.85676200	1.63781300
N	2.16785300	-2.71058200	-0.45067800
H	-0.75020300	0.86348100	2.83695600
H	1.57770800	-0.11407500	-0.59778500
O	3.05572000	-0.21658900	-2.02432700
C	2.31828100	0.71628800	-2.81991000
H	2.52685800	1.75108100	-2.51865900
H	2.65298100	0.57310400	-3.85097400
H	1.24143500	0.52621600	-2.74605600
C	-2.47472000	-1.88553700	-0.99365800
H	-2.86558600	-1.90240500	-2.00406600
H	1.16385000	-2.40422100	-0.38033500
H	-2.89371200	-2.59811400	-0.29414000
N	-1.08094400	-1.96453800	-0.99012800
O	-0.49840900	-2.21898400	0.11513300
O	-0.41891300	-1.78487800	-2.03101500
H	4.26428600	-3.99639600	1.53782400
C	-6.92067000	-1.58927200	-0.45619100
C	-6.97424400	-2.02079700	0.87177000
C	-5.89048000	-1.83542400	1.74307500
C	-4.75793100	-1.21219300	1.23159200
C	-4.68794800	-0.78350200	-0.10324100
C	-5.76828000	-0.96313100	-0.95338300
N	-3.56219300	-0.88475500	1.89859500
C	-2.70909900	-0.18157100	1.07617200
C	-3.34764100	-0.15692400	-0.32765600
O	-1.66678300	0.35997500	1.43062900
H	-7.77859300	-1.73583100	-1.10616300
H	-7.87430300	-2.50175200	1.24536900

H	-5.94547100	-2.15851400	2.77788500
H	-5.71762600	-0.61076800	-1.97966300
C	-3.31631400	-1.13764300	3.30484600
H	-4.00918000	-0.56697400	3.93421700
H	-3.43051900	-2.20460900	3.52404400
H	-2.29445500	-0.83554500	3.53640500
N	-3.27395800	0.87878800	-1.15599100
C	-2.11476700	1.55796500	-1.40067800
O	-0.97764600	1.09901900	-1.48817000
O	-2.43025700	2.86181300	-1.66032700
C	-1.41667500	3.84495100	-2.03536700
C	-2.23691600	5.12942100	-2.19400800
H	-1.58609300	5.96706600	-2.46886300
H	-2.99769500	5.01256100	-2.97379600
H	-2.74552300	5.38126500	-1.25702100
C	-0.76444800	3.46493200	-3.37014400
H	-0.18330200	2.54615100	-3.27614800
H	-1.53050800	3.31572800	-4.13998800
H	-0.10002500	4.27054400	-3.70523500
C	-0.38632800	4.01129700	-0.91257000
H	0.29935900	4.83248400	-1.15282600
H	-0.88843500	4.25462400	0.03085800
H	0.19298000	3.09811300	-0.76991400

**a'-O-anti-S**

C	-3.02064400	-0.05463300	-0.99319200
C	-3.75277800	-1.14712500	-0.21473100
C	-3.11156300	-1.89184000	0.82829900
C	-5.07964000	-1.40935500	-0.49059300
C	-1.74259800	-1.75626200	1.19173400
C	-3.92965000	-2.83616000	1.53936300
C	-5.78256900	-2.37271800	0.26601100
H	-5.58370800	-0.88008800	-1.29211500
C	-1.20795300	-2.52025000	2.21921200
H	-1.09011900	-1.06940600	0.66128400
C	-3.34965600	-3.58869200	2.59723500
H	-6.83017800	-2.57245900	0.04413400
C	-2.03061100	-3.43581600	2.93366100
H	-3.98914300	-4.29238900	3.12158200
H	-1.57830300	-4.01328800	3.73419700
C	-3.09781500	1.27706000	-0.20662200
H	-2.82269700	1.04274200	0.82452300
C	-4.46230300	2.00914200	-0.24844200
C	-1.85946200	3.31705800	0.42289400



C	-2.34977900	2.94142600	-1.95992700
C	-4.22404900	3.52701600	-0.39310700
H	-5.05627300	1.65017000	-1.09323200
H	-5.01970500	1.79002900	0.66705300
C	-3.22549400	3.99349300	0.68453100
H	-1.46051000	2.81036100	1.30440900
H	-1.09880500	4.00734300	0.05413900
C	-3.62110800	3.80430900	-1.78437500
H	-2.48605200	2.14726400	-2.69106000
H	-1.46310500	3.52162000	-2.22174100
H	-5.17271300	4.06093700	-0.28216500
H	-3.11168800	5.08189800	0.65667600
H	-4.34527200	3.55728100	-2.56695700
H	-3.38023700	4.86790400	-1.88545700
O	0.08002800	-2.45918400	2.61790800
N	-5.24357700	-3.05908800	1.25413400
N	-2.02927200	2.26973800	-0.64703700
H	0.63672000	-1.89677000	2.02535000
H	-1.96412700	-0.33075100	-1.09967800
O	-3.57413600	0.15094500	-2.28725000
C	-3.16406900	-0.82427500	-3.24381500
H	-3.48301300	-1.83468600	-2.95869700
H	-3.64073500	-0.55281200	-4.18912600
H	-2.07259300	-0.81797700	-3.37401900
C	2.38996100	0.76185700	-1.52940300
H	2.24196600	-0.27119700	-1.81197600
H	-1.11466600	1.75180400	-0.74914200
H	3.05682600	1.36597000	-2.13254100
N	1.18848800	1.41561700	-1.28045600
O	1.10153400	2.66363100	-1.31861200
O	0.18530400	0.70775800	-0.90984800
H	-3.59665200	3.73077500	1.68073100
C	4.83874300	4.03404300	0.62489400
C	3.97868300	4.36168100	1.67637200
C	3.02873200	3.44598300	2.15154000
C	2.97050400	2.20447600	1.52836800
C	3.81695000	1.86935000	0.46386400
C	4.76388100	2.77526800	0.01218400
N	2.14342400	1.10437300	1.84359300
C	2.42342400	0.02202300	1.04449200
C	3.50957200	0.46747100	0.03265900
O	1.91135100	-1.08999200	1.14041800
H	5.57434200	4.75702800	0.28399900
H	4.04895100	5.33994700	2.14443600

H	2.37554400	3.70083900	2.98018100
H	5.43804800	2.50154000	-0.79438800
C	1.21807400	1.08164900	2.95921100
H	1.73436200	1.35327000	3.88646400
H	0.39108400	1.78239700	2.79595000
H	0.81791300	0.07310500	3.06173800
N	4.54632100	-0.31054100	-0.30494200
C	4.49250700	-1.65593100	-0.54126000
O	5.38766700	-2.42648400	-0.21665600
O	3.40603000	-2.04653300	-1.28746800
C	3.17667800	-3.45139400	-1.64037300
C	1.83884400	-3.40132600	-2.38545800
H	1.54178200	-4.40770600	-2.70164500
H	1.05134800	-2.99614100	-1.74066700
H	1.91320700	-2.77127200	-3.27926900
C	3.04716000	-4.31093600	-0.37760800
H	3.99457300	-4.36346100	0.16105400
H	2.28745000	-3.89321300	0.29110800
H	2.74242600	-5.32811000	-0.65157300
C	4.28765100	-3.95363600	-2.56920700
H	4.04682600	-4.96117100	-2.92927500
H	4.38344900	-3.29625300	-3.44156700
H	5.24582200	-3.98463600	-2.04817200

**b'-N-gaul-syn-S**

C	-2.08131000	1.33431500	-0.28158300
C	-3.53037300	0.86675200	-0.45416200
C	-3.86842700	-0.51369200	-0.63147500
C	-4.55840700	1.78698400	-0.38695800
C	-2.91414300	-1.54559800	-0.81459200
C	-5.26811900	-0.84310500	-0.64530000
C	-5.90172900	1.35218000	-0.43561400
H	-4.34054100	2.84561800	-0.29454700
C	-3.31784300	-2.85972700	-1.01131000
H	-1.85740200	-1.32222400	-0.90528300
C	-5.64557200	-2.20603000	-0.79902600
H	-6.70559100	2.08507400	-0.37343100
C	-4.70421800	-3.18806900	-0.97236200
H	-6.70700300	-2.43629600	-0.79405800
H	-4.99054200	-4.22644700	-1.11171300
C	-1.70996800	1.25904400	1.21857400
H	-1.89013700	0.22476700	1.52186100
C	-2.47724400	2.23016000	2.15003000
C	0.11937700	0.88865200	2.84253000

C	0.17498600	2.92933700	1.46885500
C	-1.54417500	2.70863000	3.28017400
H	-2.83407200	3.09418200	1.58225100
H	-3.35371200	1.71764400	2.55567600
C	-0.83245200	1.49128300	3.89879200
H	0.03882400	-0.19542600	2.76457800
H	1.16630800	1.14145600	3.02391100
C	-0.48112000	3.64214700	2.67060700
H	-0.16446600	3.32135100	0.51348000
H	1.26379000	2.94672200	1.49356700
H	-2.12226900	3.23884300	4.04279400
H	-0.25873000	1.78595600	4.78323100
H	-0.94117200	4.57649100	2.33353300
H	0.27085000	3.90138600	3.42420600
O	-2.46535500	-3.86855500	-1.24994800
N	-6.25889600	0.08625800	-0.53783300
N	-0.21874900	1.46655700	1.48516800
H	-1.52161200	-3.54842900	-1.34743000
H	-1.40221600	0.67037400	-0.83386100
O	-1.89610600	2.67015300	-0.73421400
C	-1.78296400	2.77193800	-2.15348400
H	-2.68717500	2.40950100	-2.65855400
H	-1.64837800	3.83260200	-2.38021800
H	-0.91664900	2.20630600	-2.52308500
C	2.03014300	-2.23987700	-2.04792300
H	2.57126500	-3.17214300	-1.96370900
H	0.37270100	0.96167100	0.77430900
H	2.38573200	-1.41060000	-2.64064400
N	0.68102500	-2.33578900	-1.92869900
O	-0.04856400	-1.34051500	-2.19356200
O	0.17640800	-3.41851400	-1.46110600
H	-1.56847900	0.74652200	4.22033300
C	0.44772200	-3.41951800	2.20166900
C	1.55172200	-4.19820200	2.55427000
C	2.83174600	-3.92130100	2.05011600
C	2.96820100	-2.83213500	1.19927400
C	1.86801400	-2.01591800	0.85681700
C	0.60018700	-2.32674800	1.33657100
N	4.12501000	-2.36947600	0.56046500
C	3.85973100	-1.24028100	-0.19742900
C	2.35990700	-0.96551000	-0.04554200
O	4.68828500	-0.56900100	-0.79114500
H	-0.53764300	-3.67329700	2.58117600
H	1.42062800	-5.04508500	3.22238000

H	3.68122200	-4.54252500	2.31541800
H	-0.26106900	-1.74235700	1.03054100
C	5.44205200	-2.96101200	0.68058600
H	5.44101500	-3.99384000	0.31393600
H	6.12815100	-2.36492400	0.07667900
H	5.78008600	-2.95316400	1.72313400
N	1.80554000	0.20940700	-0.22862800
C	2.37757200	1.11093000	-1.14152900
O	2.48868500	0.92673000	-2.33833300
O	2.66074100	2.27482000	-0.50818600
C	3.28557200	3.40359800	-1.23320600
C	3.47946200	4.44909300	-0.13209700
H	3.98440300	5.33171100	-0.53886300
H	2.51823700	4.77100000	0.28338800
H	4.09327800	4.04781500	0.68151000
C	2.33971800	3.93016500	-2.31617500
H	2.18805300	3.19115800	-3.10430800
H	1.36584500	4.19266700	-1.88626900
H	2.76367100	4.83681900	-2.76341900
C	4.64080700	2.97469100	-1.80249200
H	5.15145100	3.84899700	-2.22225000
H	5.27300700	2.55484700	-1.01320600
H	4.52696400	2.22657300	-2.58803100

**b'-N-gau2-syn-S**

C	-2.93853300	0.47100000	-0.49399100
C	-3.94999600	-0.59157100	-0.06211400
C	-3.52383200	-1.83453500	0.50638900
C	-5.30471400	-0.35003500	-0.16156800
C	-2.16688600	-2.23187200	0.60483000
C	-4.54800600	-2.71719200	0.99032300
C	-6.22887100	-1.30212500	0.32804600
H	-5.66466600	0.56714500	-0.61546000
C	-1.82660200	-3.46025800	1.15318900
H	-1.37232600	-1.60952900	0.20841100
C	-4.16079700	-3.94884300	1.58710600
H	-7.29694200	-1.10166600	0.24991300
C	-2.84033500	-4.31252300	1.67323700
H	-4.94884900	-4.59853100	1.95652100
H	-2.54231400	-5.26177100	2.10861800
C	-2.52299300	1.28647900	0.75492400
H	-2.31841400	0.56342500	1.54683800
C	-3.56208100	2.34143200	1.22517100

C	-0.76415800	2.60763200	1.89060000
C	-1.23527200	3.08934600	-0.47928000
C	-2.91391700	3.73891300	1.27448500
H	-4.40806900	2.35817000	0.53533900
H	-3.94519000	2.06612100	2.21282000
C	-1.75346200	3.72745200	2.28467800
H	-0.73960500	1.79411200	2.61614500
H	0.25652300	2.96711800	1.74814300
C	-2.35943000	4.08449000	-0.12003600
H	-1.38518300	2.60244100	-1.43838400
H	-0.24362200	3.54694400	-0.46916100
H	-3.66329600	4.47837000	1.57277100
H	-1.24643900	4.69800900	2.28903900
H	-3.15846400	4.02057200	-0.86363000
H	-1.96947700	5.10766700	-0.13245300
O	-0.55471800	-3.90389100	1.21880000
N	-5.87970800	-2.43774700	0.90046400
N	-1.18728200	2.00024600	0.57087700
H	0.00671300	-3.36143900	0.60270000
H	-2.04249700	-0.00691700	-0.91034900
O	-3.47451400	1.36328600	-1.46118900
C	-3.46194000	0.82924600	-2.78597000
H	-4.08384500	-0.07202000	-2.86389200
H	-3.87714700	1.60345300	-3.43680500
H	-2.43931300	0.59141900	-3.10309800
C	2.70294000	-2.10073000	0.12023700
H	2.30728800	-2.45972600	1.06035700
H	-0.44508700	1.30566000	0.30359000
H	3.75508100	-2.23487200	-0.09292000
N	1.88390900	-2.32851200	-0.96580000
O	2.32772600	-2.21937000	-2.12457700
O	0.64217200	-2.52220100	-0.76061300
H	-2.12798200	3.55129600	3.29816100
C	1.83253000	0.00734800	4.12012600
C	3.16921200	0.22106500	4.47000800
C	4.16062600	0.38304700	3.49248300
C	3.76878500	0.33061600	2.15746300
C	2.42433400	0.13175900	1.79119900
C	1.45464000	-0.03948300	2.77122700
N	4.55943500	0.43639400	1.01267800
C	3.80750300	0.29777000	-0.15639000
C	2.34160700	0.14244000	0.31211700
O	4.29107200	0.28008600	-1.27303500
H	1.08609400	-0.13487400	4.89637300

H	3.45153100	0.25421300	5.51890300
H	5.19795600	0.53847000	3.77175200
H	0.42543600	-0.24251900	2.49016900
C	6.00430000	0.53881800	1.00862100
H	6.33136100	1.45989300	1.50450700
H	6.46139800	-0.31949300	1.51562600
H	6.32868300	0.55543300	-0.03286300
N	1.21049900	0.49375100	-0.28568500
C	1.07920400	0.90939300	-1.60673100
O	0.04537500	0.70089600	-2.23732800
O	2.07605200	1.70531900	-2.03336100
C	2.25118700	2.05047400	-3.45937100
C	3.58643500	2.79828000	-3.45834800
H	3.84775700	3.10266800	-4.47794900
H	3.52671800	3.70012100	-2.83790700
H	4.38036200	2.15910600	-3.06335300
C	1.12039700	2.96897100	-3.93164700
H	0.16226800	2.44703300	-3.93702800
H	1.04223200	3.85160300	-3.28542100
H	1.33427600	3.31869000	-4.94858900
C	2.34688000	0.76784000	-4.28824900
H	2.63446800	1.01479900	-5.31687300
H	3.10142200	0.10200400	-3.86038500
H	1.39226100	0.23802800	-4.31499300

**b'-O-anti-S**

C	-2.31863400	-1.27146800	0.91747000
C	-3.78903300	-0.87589500	0.76191300
C	-4.18036200	0.28083600	0.01327000
C	-4.77869000	-1.63386700	1.35357100
C	-3.26486800	1.14853700	-0.63274700
C	-5.58609700	0.55934800	-0.07440900
C	-6.13570900	-1.26592200	1.20251700
H	-4.51886300	-2.50425600	1.94631400
C	-3.71107600	2.24844400	-1.34934600
H	-2.20022200	0.95318600	-0.61188400
C	-6.01060500	1.69899600	-0.81234400
H	-6.91041600	-1.87140900	1.67180200
C	-5.10550400	2.52198800	-1.43433900
H	-7.07792000	1.89318300	-0.86557500
H	-5.42752500	3.39112700	-2.00026900
C	-1.82300200	-2.03326000	-0.33455000
H	-2.12415500	-1.44537600	-1.20354000
C	-2.32911800	-3.49264600	-0.45846900

C	0.09946900	-2.45456300	-1.83868300
C	0.33896100	-3.01928500	0.55012300
C	-1.17271400	-4.40850700	-0.90528400
H	-2.71697900	-3.83674900	0.50394300
H	-3.15080600	-3.52876100	-1.18020600
C	-0.52775600	-3.82591600	-2.17694300
H	-0.23801700	-1.64975700	-2.49059700
H	1.18928400	-2.46291900	-1.84123400
C	-0.11484000	-4.45803200	0.21402900
H	0.02351200	-2.70519800	1.54140400
H	1.41207200	-2.86210300	0.44819700
H	-1.55536600	-5.41449900	-1.10350500
H	0.24434500	-4.50207200	-2.55841700
H	-0.53442600	-4.93120500	1.10759600
H	0.74027800	-5.06341400	-0.10595100
O	-2.88561600	3.10085100	-1.98981000
N	-6.54016000	-0.21471300	0.51662800
N	-0.29856300	-2.06338000	-0.43170800
H	-1.93687900	2.83334900	-1.89529800
H	-1.70856600	-0.36551000	1.01819000
O	-2.11637600	-2.09565300	2.05996100
C	-2.01060200	-1.36710400	3.28017400
H	-2.89520700	-0.74297600	3.46105300
H	-1.93150200	-2.10818600	4.08015800
H	-1.11323800	-0.73388600	3.28560600
C	1.78625500	1.51413500	-1.76227600
H	2.11354700	0.50744800	-1.98342900
H	0.08442000	-1.11932000	-0.24218400
H	2.30026500	2.35967200	-2.19814500
N	0.40930900	1.64436000	-1.78777600
O	-0.11240400	2.79560400	-1.84994600
O	-0.31106500	0.61345000	-1.66630400
H	-1.28214500	-3.71740300	-2.96375400
C	3.69445100	5.23040800	0.24884800
C	2.53718200	5.72245100	0.86152300
C	1.48788600	4.87011000	1.23269700
C	1.63876100	3.51562200	0.95846000
C	2.78327400	3.01431700	0.32333900
C	3.82508200	3.86309800	-0.02420800
N	0.77019600	2.45235800	1.27104400
C	1.29608100	1.24064900	0.88774300
C	2.62484300	1.54602700	0.16475500
O	0.77196400	0.14720300	1.10234700
H	4.49644300	5.91354100	-0.01553300

H	2.44768400	6.78634100	1.06349800
H	0.59843600	5.25969700	1.71704800
H	4.71918500	3.46183300	-0.49259100
C	-0.49951500	2.62009100	1.95141900
H	-0.35619700	3.17531300	2.88474800
H	-1.21196100	3.15976000	1.31857500
H	-0.89839900	1.63264300	2.18361600
N	3.71250100	0.78142500	0.15666500
C	3.72077600	-0.55478600	-0.07960900
O	2.91005000	-1.22219800	-0.73874000
O	4.86284700	-1.07970600	0.44389600
C	5.36557300	-2.40628400	0.08582400
C	6.68857100	-2.47618600	0.85576500
H	7.19667500	-3.42655200	0.65841200
H	7.35362100	-1.65919600	0.55669100
H	6.51411800	-2.39584100	1.93437300
C	5.61856200	-2.48367700	-1.42385600
H	4.68511500	-2.39121400	-1.98317400
H	6.29741100	-1.68343800	-1.73968800
H	6.08396900	-3.44335400	-1.67764400
C	4.41773900	-3.51118400	0.56601600
H	4.91651500	-4.48500100	0.49431100
H	4.14247900	-3.34914500	1.61437100
H	3.50918000	-3.54394700	-0.03685700

#### ***4. STEP3 (protonation of product) for model catalyst***

##### **Si-IM3-model**

C	3.45928400	0.10157700	-0.84285900
C	3.40001800	1.52396600	-0.28921800
C	2.39795200	1.92362700	0.65364400
C	4.33363600	2.46493900	-0.67178600
C	1.36491700	1.06586600	1.11648800
C	2.44232700	3.27468500	1.13294100
C	4.29144000	3.76938200	-0.12830500
H	5.09654300	2.20574200	-1.39784400
C	0.41254900	1.52987600	2.00319100
H	1.30125600	0.04231600	0.76346100
C	1.45175100	3.70990000	2.05536400
H	5.03919800	4.50083500	-0.43400600
C	0.45843400	2.86355000	2.48374800
H	1.50834100	4.73543200	2.40788300
H	-0.30207900	3.19163300	3.18590000



C	4.16035400	-0.85467500	0.15486200
H	3.73615600	-0.60594100	1.13374500
C	5.71026100	-0.69801000	0.22730100
C	4.13378400	-3.02644900	1.15311300
C	4.51847300	-2.86583600	-1.20481200
C	6.32686400	-2.10763100	0.35672200
H	6.09664800	-0.21430700	-0.67602900
H	5.99280000	-0.07113200	1.08146300
C	5.64230700	-2.85786600	1.51757900
H	3.48879100	-2.68140300	1.96963800
H	3.88898700	-4.07900300	0.96954200
C	6.05753800	-2.87724800	-0.95131300
H	4.27589900	-2.29100900	-2.09901300
H	4.13402300	-3.88260300	-1.34715600
H	7.40517700	-2.02885800	0.53767800
H	6.11895900	-3.83377100	1.67322300
H	6.59173500	-2.40420500	-1.78461800
H	6.43800200	-3.90364600	-0.86696900
O	-0.61186800	0.75049800	2.45884900
N	3.38957000	4.17704400	0.74268100
N	3.78231100	-2.27310800	-0.06694500
H	-2.27991600	0.50284200	1.05437700
H	2.43865700	-0.27692900	-0.98580100
O	4.13644300	0.06434500	-2.09764300
C	3.31880600	0.45813000	-3.19059600
H	2.98909300	1.50306800	-3.10478200
H	3.92533400	0.35201200	-4.09471700
H	2.42909100	-0.18242800	-3.27584000
C	-2.29092200	-1.21832600	-1.59784000
H	-2.84050400	-0.57386000	-2.28294900
H	-2.28950300	-2.25325300	-1.93353100
N	-0.86199100	-0.75936800	-1.63251700
O	-0.65476900	0.44935700	-1.54884800
O	0.00978600	-1.61959400	-1.74548500
H	5.76010100	-2.29260800	2.45116700
C	-6.51037100	-2.49984700	-0.77540500
C	-6.35503900	-3.67481800	-0.03871900
C	-5.15341000	-3.96002500	0.62348500
C	-4.12873000	-3.02890300	0.51511600
C	-4.26791400	-1.84242400	-0.22048000
C	-5.46047400	-1.57492500	-0.87976400
N	-2.84515300	-3.09046800	1.09937700
C	-2.12288900	-1.97384800	0.82129700
C	-2.93529000	-1.09752700	-0.17872300

O	-1.01115400	-1.70266600	1.27112300
H	-7.45137600	-2.29806800	-1.27863600
H	-7.17575100	-4.38358600	0.02773300
H	-5.03332200	-4.87318000	1.19706000
H	-5.57454300	-0.66097700	-1.45060300
C	-2.37626900	-4.15790900	1.96707400
H	-3.00671900	-4.23024500	2.85943900
H	-2.39447000	-5.11295900	1.43265100
H	-1.35282500	-3.92588000	2.26310500
N	-2.96127300	0.25842000	0.33946100
C	-3.47990800	1.31225900	-0.37430800
O	-4.13344700	1.18945600	-1.40322100
O	-3.17442000	2.46038900	0.24873000
C	-3.58269800	3.77441100	-0.29717000
C	-2.98612800	4.75004600	0.71834600
H	-3.22682900	5.77949900	0.43265300
H	-3.39219700	4.56659100	1.71890800
H	-1.89703600	4.64885700	0.76342200
C	-5.10981000	3.87687500	-0.31655800
H	-5.54872900	3.17723900	-1.03049600
H	-5.52089300	3.67174000	0.67834100
H	-5.40366000	4.89372800	-0.60052700
C	-2.96038500	3.98185900	-1.67996100
H	-3.14340900	5.01053200	-2.01016200
H	-1.87694700	3.82519700	-1.63905600
H	-3.38634900	3.29953000	-2.41781300
H	-0.52931300	-0.15693000	2.09199000

**Si-product**

H	-0.66367700	0.88237000	1.32878700
C	0.63646500	1.07470600	-1.44944500
H	-0.05023400	0.51230900	-2.08202600
H	1.60737300	1.19626100	-1.92567700
N	0.05654000	2.45383500	-1.31169300
O	-1.13494300	2.53764600	-1.01645800
O	0.80281800	3.40878800	-1.51017600
C	2.40084600	-3.04591800	-1.06316000
C	3.63375500	-2.82520300	-0.44763200
C	3.89164000	-1.64037300	0.25519700
C	2.87256000	-0.69765400	0.31984200
C	1.62586200	-0.90522900	-0.29458000
C	1.38572000	-2.07939000	-0.99490900
N	2.89487500	0.54840600	0.97504600
C	1.68649000	1.18284700	0.86954600

C	0.77902300	0.34279100	-0.08050300
O	1.34158700	2.21147400	1.42733000
H	2.22200600	-3.97304200	-1.59980300
H	4.41131500	-3.58167900	-0.50995900
H	4.85043800	-1.47255800	0.73485400
H	0.42284300	-2.24403000	-1.46452000
C	3.98932500	1.04398100	1.78949800
H	4.19146100	0.36029300	2.62154100
H	4.89622100	1.15467000	1.18602300
H	3.69627100	2.01745100	2.18493000
N	-0.47749600	0.17168900	0.62861300
C	-1.58952500	-0.39642500	0.05231300
O	-1.57405600	-1.03487400	-0.99189600
O	-2.65610500	-0.16140200	0.83471100
C	-4.00629700	-0.64687000	0.47757000
C	-4.85975000	-0.11433000	1.63004100
H	-5.90358500	-0.41605000	1.49401800
H	-4.50919200	-0.50842100	2.58998700
H	-4.81943800	0.97933600	1.67066700
C	-4.01722900	-2.17716400	0.45191900
H	-3.39750400	-2.56664900	-0.35812300
H	-3.65013400	-2.57991500	1.40267000
H	-5.04339300	-2.53373600	0.30720900
C	-4.44710200	-0.03306400	-0.85351700
H	-5.49744700	-0.28351500	-1.04127400
H	-4.35898400	1.05837200	-0.81983100
H	-3.84687500	-0.40825900	-1.68439400

**Re-product**

C	-0.63615900	1.07420300	-1.44951400
H	-1.60701500	1.19584900	-1.92582100
H	0.05040900	0.51142300	-2.08190000
N	-0.05602600	2.45328900	-1.31209700
O	1.13525700	2.53719100	-1.01606000
O	-0.80205000	3.40828000	-1.51112000
C	-2.40174800	-3.04565000	-1.06294200
C	-3.63462800	-2.82453000	-0.44747700
C	-3.89220800	-1.63962700	0.25534300
C	-2.87281900	-0.69724900	0.32007500
C	-1.62620100	-0.90518600	-0.29436600
C	-1.38633900	-2.07942300	-0.99465400
N	-2.89465100	0.54882700	0.97534400
C	-1.68621400	1.18301100	0.86950200
C	-0.77908100	0.34255800	-0.08041300

O	-1.34096700	2.21173400	1.42691000
H	-2.22314600	-3.97284100	-1.59955000
H	-4.41244300	-3.58073500	-0.50993200
H	-4.85095600	-1.47152700	0.73500100
H	-0.42342500	-2.24437600	-1.46411500
C	-3.98910000	1.04502100	1.78944100
H	-4.89574800	1.15620500	1.18568200
H	-4.19183900	0.36142700	2.62140700
H	-3.69564500	2.01835000	2.18493400
C	1.58938800	-0.39697800	0.05224500
O	1.57383400	-1.03573200	-0.99179900
O	2.65601300	-0.16135900	0.83437700
C	4.00637100	-0.64685000	0.47750500
C	4.85944300	-0.11429500	1.63023900
H	5.90328300	-0.41616100	1.49457900
H	4.81926400	0.97937700	1.67077300
H	4.50850600	-0.50827200	2.59009100
C	4.44762400	-0.03287700	-0.85337100
H	3.84797200	-0.40836300	-1.68451600
H	4.35900600	1.05851400	-0.81969900
H	5.49817500	-0.28287200	-1.04061600
C	4.01745400	-2.17715400	0.45189400
H	5.04371000	-2.53362600	0.30756600
H	3.65009900	-2.57990900	1.40254300
H	3.39804400	-2.56678400	-0.35831300
N	0.47734800	0.17101700	0.62867000
H	0.66367000	0.88164200	1.32894800

### 5. Lowest-lying transition states for real catalyst

#### *Si-ts2a-real*

C	-1.90925000	0.90117500	0.64863500
C	-2.09155700	0.50991500	2.11131800
C	-0.96094300	0.16318000	2.92127300
C	-3.33914200	0.54757300	2.69866900
C	0.36969100	0.06103000	2.43572400
C	-1.21797900	-0.06831000	4.31620600
C	-3.47690000	0.26272500	4.07588900
H	-4.21774900	0.79627700	2.11375800
C	1.41761300	-0.23460900	3.29952500
H	0.60149700	0.21240600	1.38636700
C	-0.12127300	-0.36062300	5.17303500
H	-4.46548900	0.28569900	4.53262600

C	1.15802800	-0.43256700	4.68692100
H	-0.33646800	-0.52680800	6.22443300
H	1.99861600	-0.65838500	5.33631200
C	-1.36437400	2.34717000	0.58028500
H	-0.52794400	2.37581500	1.28092300
C	-2.36878300	3.47586000	0.90942800
C	0.20608000	3.85495300	-0.55996800
C	-1.70801800	2.98149800	-1.84403300
C	-2.10810100	4.67296300	-0.02759100
H	-3.39647000	3.12812800	0.77109600
H	-2.26165600	3.76157200	1.95894100
C	-0.60368600	5.07020900	-0.01796000
H	0.99905400	3.52570200	0.11353600
H	0.65820300	4.05042100	-1.53174900
C	-2.48542000	4.26152900	-1.46479900
H	-2.35389600	2.11120500	-1.94289200
H	-1.12035900	3.08545600	-2.75780800
H	-2.71133700	5.52912000	0.28842200
H	-0.48390600	5.90292200	-0.72060300
H	-3.56208900	4.07551300	-1.53199500
H	-2.25149400	5.07293700	-2.16244500
O	2.69656900	-0.34011000	2.91021900
N	-2.46270700	-0.02129900	4.86907900
N	-0.71446900	2.67430000	-0.75421000
H	2.76931900	-0.42591400	1.91674700
H	-1.17951500	0.24166600	0.16864400
O	-3.13737800	0.84935100	-0.08233000
C	2.57310500	-0.06834200	-2.53811400
H	2.35351100	-1.12151700	-2.43661300
H	-0.14173800	1.84489000	-1.07518900
H	3.26116600	0.28653500	-3.29200900
N	1.54336500	0.78383400	-2.28009800
O	0.55851600	0.37103400	-1.56975000
O	1.58399200	1.98457800	-2.66578300
C	6.97803700	-1.38042700	-2.47070000
C	7.52468600	-0.10823400	-2.65598200
C	6.86358200	1.03875300	-2.19626700
C	5.64617000	0.86763000	-1.54832500
C	5.07371800	-0.41206900	-1.35959000
C	5.74546700	-1.54042800	-1.82523500
N	4.82594700	1.85981900	-0.99473300
C	3.72102800	1.30192800	-0.38407500
C	3.80288000	-0.20530500	-0.62071200
O	2.85928100	1.90563600	0.23802600

H	7.50719800	-2.25492000	-2.83794700
H	8.47851200	0.00026200	-3.16527900
H	7.29381300	2.02506900	-2.33767700
H	5.30503400	-2.52221700	-1.70416100
C	5.09960300	3.28154600	-1.02127400
H	4.29806300	3.78262500	-0.47656400
H	6.05715600	3.50275800	-0.53625500
H	5.12513400	3.65490600	-2.05118200
N	3.14891800	-0.97163600	0.23399100
C	3.04916800	-2.33346500	0.03466100
O	3.10996800	-2.91626400	-1.04676300
O	2.78656400	-2.93122700	1.21457600
C	2.53595200	-4.37703800	1.32106400
C	2.31486800	-4.56494800	2.82411300
H	2.10687900	-5.61735100	3.04567300
H	3.20327600	-4.26165300	3.38823600
H	1.46769700	-3.96418900	3.17118600
C	3.76217200	-5.16814400	0.85527000
H	3.92681300	-5.05461400	-0.21762200
H	4.65884900	-4.83122100	1.38796300
H	3.61759900	-6.23196600	1.07617600
C	1.27100400	-4.74760900	0.54052100
H	1.01187800	-5.79482000	0.73431800
H	0.43078500	-4.12390500	0.86678600
H	1.41112000	-4.61591700	-0.53397700
C	-0.11092300	5.53162300	1.33093000
H	-0.05647900	4.77676000	2.11652200
C	0.25728200	6.78315800	1.60887500
H	0.23339300	7.56904400	0.85540400
H	0.59894700	7.07084700	2.60011900
C	-6.70243400	1.08374100	-2.12782400
C	-5.51257900	0.98852800	-1.43050100
C	-4.85995800	-0.25585600	-1.27054900
C	-5.43826800	-1.43497900	-1.82954400
C	-6.65459900	-1.29802600	-2.53906700
C	-7.27500800	-0.07068400	-2.68906900
C	-3.61117000	-0.35755000	-0.54544000
C	-4.77477500	-2.72106500	-1.65106400
C	-3.55485600	-2.76213400	-0.91632100
C	-2.99476600	-1.55976100	-0.36766800
C	-2.89696400	-4.00087600	-0.72805500
H	-1.96597400	-4.01632800	-0.16682500
C	-3.41829800	-5.17024900	-1.24733900
C	-4.62301400	-5.13524100	-1.97367700

C	-5.28347100	-3.93479100	-2.16975900
H	-7.19311500	2.04674800	-2.23975300
H	-5.06923000	1.87336500	-0.98903900
H	-7.12106100	-2.17233900	-2.97887600
H	-8.20927600	-0.00269100	-3.23972400
H	-2.07008000	-1.64789400	0.19048000
H	-2.89982500	-6.11304500	-1.09552300
H	-5.03770000	-6.05196200	-2.38394000
H	-6.20989200	-3.93825500	-2.73380500

*Si-ts2b-real*

C	-1.68547500	-1.36574700	0.21057100
C	-2.60667100	-2.29260100	-0.57702200
C	-2.34901700	-2.56862500	-1.95880100
C	-3.68430200	-2.90555900	0.02762000
C	-1.28222200	-1.99495800	-2.69614000
C	-3.23950700	-3.48652600	-2.61282700
C	-4.49872300	-3.78886100	-0.71735900
H	-3.92180400	-2.70941000	1.06768100
C	-1.09009900	-2.31858500	-4.03253800
H	-0.58641200	-1.30202500	-2.23738400
C	-3.01464500	-3.79504500	-3.98303100
H	-5.34938300	-4.26866700	-0.23508100
C	-1.97223700	-3.23381000	-4.67535200
H	-3.69893300	-4.49081200	-4.45962000
H	-1.79740500	-3.46743300	-5.72145300
C	-0.43199800	-2.15439600	0.65483200
H	-0.07623900	-2.66362100	-0.24300500
C	-0.65243400	-3.17193000	1.79841800
C	2.01123500	-2.09297400	0.99715800
C	0.60556600	-0.64976700	2.41380900
C	0.55796700	-3.14500700	2.75129100
H	-1.55660300	-2.92198300	2.36025300
H	-0.79953400	-4.16796300	1.37377200
C	1.88523700	-3.30925500	1.95992800
H	2.16339300	-2.37705600	-0.04438800
H	2.81566900	-1.41970200	1.28891300
C	0.58776100	-1.78046800	3.46753900
H	-0.31126100	-0.06377000	2.41068100
H	1.45730900	0.02382300	2.51658800
H	0.46994500	-3.95273100	3.48394300
H	2.70472200	-3.25656900	2.68608700
H	-0.29230400	-1.67639800	4.11033600
H	1.47106400	-1.71348100	4.11155800

O	-0.09612500	-1.80762300	-4.77744300
N	-4.29396900	-4.08106100	-1.98697100
N	0.74517600	-1.26544800	1.04198400
H	0.43700400	-1.15294300	-4.24779700
H	-1.36148000	-0.53353700	-0.41979400
O	-2.32323800	-0.83020400	1.37606000
C	3.16998500	0.78510400	-2.45857900
H	4.05330500	0.37473600	-1.98977100
H	0.83332200	-0.48132500	0.35584100
H	3.26297900	1.57097400	-3.19431200
N	2.18427600	-0.12624000	-2.74184900
O	1.27762300	0.20022500	-3.57956300
O	2.13587100	-1.22559300	-2.13433500
C	4.51042800	5.11185700	-1.46881200
C	3.42106100	5.73078300	-2.08602500
C	2.17703300	5.09061400	-2.16980100
C	2.06705600	3.82290500	-1.61421200
C	3.15982100	3.17584500	-0.99347200
C	4.38957600	3.82718200	-0.92347600
N	0.92125100	3.00980300	-1.56083400
C	1.18870400	1.84875900	-0.89257400
C	2.65986400	1.85715600	-0.51838900
O	0.36566000	0.97027600	-0.61905000
H	5.46599800	5.62574900	-1.41826400
H	3.53391900	6.72421500	-2.51154700
H	1.33140500	5.57392400	-2.64832300
H	5.23919600	3.33289000	-0.46992700
C	-0.36290500	3.33595300	-2.15109500
H	-0.73404000	4.28883000	-1.75975300
H	-0.28014100	3.39834200	-3.24140700
H	-1.06368500	2.54314400	-1.88868200
N	3.00278100	1.07797900	0.49120000
C	4.31901200	0.93873900	0.85143400
O	5.30877000	1.12783000	0.14612400
O	4.37729000	0.45218900	2.12162000
C	5.66265900	0.21635300	2.79891000
C	5.22716700	-0.25445900	4.18923600
H	6.10556500	-0.45249900	4.81259600
H	4.61681000	0.50778900	4.68542500
H	4.64047100	-1.17746500	4.12409200
C	6.45627000	1.52286300	2.90622700
H	6.79704400	1.86493500	1.92758600
H	5.84248200	2.30864200	3.36124500
H	7.33345600	1.36635600	3.54428200



C	6.45248400	-0.88249400	2.08104700
H	7.35543200	-1.12215200	2.65464300
H	5.85425200	-1.79757900	1.99946700
H	6.74842000	-0.56683800	1.07942600
C	1.99488100	-4.62828000	1.23589400
H	1.33003300	-4.77566700	0.38380200
C	2.84391300	-5.60100400	1.57048200
H	2.88184200	-6.53889000	1.02192200
H	3.53701900	-5.49696900	2.40392400
C	-5.85207500	3.40786800	-1.31478900
C	-4.95847800	2.35623000	-1.24690400
C	-4.54236500	1.83215100	0.00051900
C	-5.05783600	2.39343700	1.20431300
C	-5.96987400	3.46964100	1.10201900
C	-6.36170000	3.96794100	-0.12852200
C	-3.61796000	0.73590500	0.04688600
C	-4.62052500	1.83253900	2.47745100
C	-3.70416700	0.73842800	2.49292800
C	-3.20916400	0.21333400	1.23796700
C	-3.29243700	0.18697500	3.72819100
H	-2.60635000	-0.65189000	3.72430400
C	-3.76045000	0.69483200	4.92576800
C	-4.65860700	1.77586900	4.92050100
C	-5.07789800	2.32566600	3.72233900
H	-3.26941500	0.33532100	-0.89741300
H	-6.16321400	3.79855300	-2.27986900
H	-4.56065000	1.91273800	-2.15657000
H	-6.38077200	3.92023700	1.99908000
H	-7.06624000	4.79376100	-0.17618900
H	-3.43507900	0.25919600	5.86649400
H	-5.03006500	2.18001400	5.85825300
H	-5.77546300	3.15532700	3.74755800

*Si-ts2c-real*

C	-1.93939300	0.82255000	0.57719100
C	-2.08745200	0.42925600	2.04499200
C	-0.93646600	0.20337800	2.86952800
C	-3.33681400	0.36853900	2.62798900
C	0.40080000	0.19970900	2.39154800
C	-1.18058100	0.00248800	4.27189500
C	-3.45794200	0.11015800	4.01167100
H	-4.23102300	0.52581100	2.03574900
C	1.46493300	0.04707900	3.27228100

H	0.62036700	0.30351500	1.33370900
C	-0.06806000	-0.14246300	5.14533400
H	-4.44800400	0.05436800	4.46260300
C	1.21587600	-0.10823900	4.66698000
H	-0.27433900	-0.28326100	6.20226500
H	2.06963900	-0.21970900	5.32889900
C	-1.50912000	2.30494100	0.50336200
H	-0.62644700	2.37713400	1.14133000
C	-2.56396400	3.34845400	0.93895800
C	-0.14378400	3.95277200	-0.70775500
C	-2.09339400	2.98461800	-1.86154400
C	-2.45256700	4.59291100	0.03548300
H	-3.57189900	2.93157200	0.85448300
H	-2.40750900	3.60398600	1.98980700
C	-0.98039200	5.08977000	-0.05007800
H	0.72963600	3.65965000	-0.12205600
H	0.19748700	4.22204900	-1.70944900
C	-2.91261900	4.20483200	-1.38342200
H	-2.69030100	2.07793700	-1.93000200
H	-1.60024700	3.15181800	-2.82117100
H	-3.08222000	5.39658600	0.42843100
H	-0.96880300	5.95660900	-0.72086500
H	-3.97843500	3.95559200	-1.37685300
H	-2.77978800	5.04911200	-2.06839200
O	2.75247200	0.04534900	2.89374400
N	-2.42787400	-0.04889300	4.81902700
N	-0.99219300	2.71391100	-0.86748100
H	2.84577300	-0.09953300	1.90953500
H	-1.16150700	0.23098100	0.08455600
O	-3.17396100	0.67608100	-0.13572400
C	2.36761700	-0.28310800	-2.48406300
H	2.55061500	-1.34436900	-2.39675400
H	-0.35255500	1.97571300	-1.28859800
H	2.75589600	0.29821700	-3.30820800
N	1.18668600	0.15110800	-1.97707000
O	0.56696100	-0.54273200	-1.12701300
O	0.75648300	1.31285800	-2.32273900
C	6.95315300	-0.87555800	-2.73797900
C	7.26624800	0.43408100	-3.10981400
C	6.46570900	1.51147100	-2.70836800
C	5.35090800	1.23290300	-1.92623500
C	5.01262100	-0.08741000	-1.54695400
C	5.82192800	-1.14560500	-1.95837100
N	4.43416600	2.14906300	-1.39359900

C	3.49457800	1.50695800	-0.61167500
C	3.80135900	0.01174500	-0.69441000
O	2.60529000	2.04421100	0.03262900
H	7.58729800	-1.69560700	-3.06213700
H	8.14466700	0.62673700	-3.71993500
H	6.71481300	2.52812000	-2.99526100
H	5.56342200	-2.16111500	-1.68730000
C	4.48083100	3.58280200	-1.58869500
H	3.67931300	4.02479200	-0.99519700
H	5.44127700	3.98980000	-1.25278300
H	4.33388500	3.83935900	-2.64424800
N	3.32927100	-0.73951000	0.27941000
C	3.43465500	-2.11824000	0.22445800
O	3.56393800	-2.79866000	-0.79065900
O	3.29784300	-2.61481500	1.46855900
C	3.27021400	-4.06172900	1.73639100
C	3.09676900	-4.11152500	3.25655500
H	3.06208400	-5.15149700	3.59835100
H	3.93096500	-3.60949200	3.75797700
H	2.16860300	-3.61566700	3.55942600
C	4.59904300	-4.70282500	1.32427800
H	4.73588300	-4.67579500	0.24165400
H	5.43811100	-4.18217900	1.79972300
H	4.62022800	-5.74840600	1.65254500
C	2.06999400	-4.70388100	1.03376500
H	1.97037600	-5.74707700	1.35523200
H	1.14686600	-4.17731100	1.30114000
H	2.18540600	-4.68336500	-0.05152200
C	-0.41346600	5.52694800	1.27761600
H	-0.24143300	4.74507200	2.01836600
C	-0.11679400	6.79003400	1.58697400
H	0.28131100	7.06015000	2.56190800
H	-0.26008500	7.60389500	0.87770900
C	-2.88124200	-5.29350800	-1.52817600
C	-2.44861100	-4.08801800	-1.01008000
C	-3.26615500	-2.93392100	-1.06842600
C	-4.55246700	-3.01583400	-1.67567900
C	-4.96709000	-4.26374400	-2.19665600
C	-4.15195100	-5.38018600	-2.12698900
C	-2.79263800	-1.69145500	-0.52940800
C	-5.37716900	-1.81433600	-1.72455800
C	-4.87837400	-0.59030600	-1.18509500
C	-3.55705800	-0.56533700	-0.59376600
C	-5.68281700	0.57234300	-1.22702800

H	-5.29660600	1.49194500	-0.80317100
C	-6.94480600	0.54571000	-1.79099700
C	-7.44210900	-0.65383300	-2.32870900
C	-6.67298600	-1.80328500	-2.29289300
H	-1.80535400	-1.68327700	-0.08390200
H	-2.24213300	-6.17074400	-1.47592700
H	-1.46708500	-4.00729900	-0.54976000
H	-5.93994100	-4.35982700	-2.66656100
H	-4.49684900	-6.32573700	-2.53640000
H	-7.55012500	1.44778700	-1.81441600
H	-8.43346000	-0.68226900	-2.77273600
H	-7.08408900	-2.71545500	-2.71074100

*re-ts2a-real*

C	-2.96286300	-1.02215800	-0.40944900
C	-3.43431800	-1.09249800	1.04030200
C	-2.56973400	-0.72604700	2.12239400
C	-4.72834900	-1.47564800	1.33040700
C	-1.20898600	-0.35498800	1.96672900
C	-3.13776700	-0.77117100	3.44285400
C	-5.18001100	-1.47771800	2.66869700
H	-5.40238900	-1.78754900	0.54004200
C	-0.42226800	-0.07088400	3.07585500
H	-0.73935900	-0.33657500	0.99015500
C	-2.31432200	-0.43706000	4.55268100
H	-6.20443300	-1.77497600	2.88959300
C	-0.99745900	-0.09916300	4.37960000
H	-2.76404800	-0.47329800	5.54056900
H	-0.35895200	0.14096400	5.22473200
C	-3.19162500	0.41091700	-0.94566700
H	-2.80983600	1.07447400	-0.16670000
C	-4.65312600	0.78308600	-1.31134000
C	-2.36737300	2.22178400	-2.39326400
C	-2.70723800	-0.00450100	-3.39460100
C	-4.70129500	1.38043700	-2.73235100
H	-5.28635200	-0.10606700	-1.27802500
H	-5.04890000	1.48811600	-0.57562100
C	-3.79626800	2.64062300	-2.84116100
H	-2.06466900	2.70556000	-1.46158400
H	-1.61005500	2.43986200	-3.14836200
C	-4.17878000	0.32777400	-3.72949800
H	-2.53284400	-1.06215600	-3.21293200
H	-2.01205500	0.32897100	-4.16835000
H	-5.73105200	1.65365800	-2.98114700

H	-3.76123900	2.92654700	-3.89876700
H	-4.78846900	-0.57792600	-3.66769100
H	-4.25526100	0.70624800	-4.75407000
O	0.88164600	0.23502500	3.01160100
N	-4.42711900	-1.13245700	3.69490000
N	-2.31416800	0.73612300	-2.14296500
H	1.23236500	0.22516000	2.07591800
H	-1.89357900	-1.23942200	-0.48602600
O	-3.68155000	-1.93825400	-1.24332300
C	2.14946800	-0.65950500	-2.17043100
H	2.46465100	-1.59685800	-2.60717600
H	-1.30027600	0.52113800	-1.91531600
H	2.69640100	0.25737100	-2.33217200
N	0.80449700	-0.50836900	-2.05196600
O	0.35757300	0.64936800	-1.71725700
O	0.01099900	-1.47895300	-2.18856200
C	6.60899600	-0.73132900	-0.94879700
C	6.74493100	-2.12139300	-0.92485200
C	5.65517400	-2.94815900	-0.62520100
C	4.43464800	-2.34019600	-0.35244900
C	4.27452500	-0.93434700	-0.37853200
C	5.37337700	-0.12988600	-0.68030700
N	3.23210200	-2.96990400	-0.01408600
C	2.24826600	-2.03796100	0.26081200
C	2.86053600	-0.65892300	-0.00749200
O	1.11963800	-2.28184500	0.65402900
H	7.46687200	-0.10811200	-1.18422200
H	7.70888900	-2.57451800	-1.14055600
H	5.76420800	-4.02765600	-0.60046100
H	5.25915000	0.94550300	-0.71955600
C	3.04665600	-4.40144400	0.10234400
H	3.66246500	-4.81347900	0.91061400
H	1.99435900	-4.58509400	0.32274700
H	3.30837200	-4.90227200	-0.83628600
N	2.26974200	0.36706400	0.57908000
C	2.65584500	1.66257600	0.29756300
O	3.31317200	2.04640800	-0.66678500
O	2.13213000	2.47874500	1.23821100
C	2.30818400	3.93585300	1.19109200
C	1.53958400	4.40161900	2.43032000
H	1.58955100	5.49217000	2.51994100
H	0.48652600	4.10683200	2.36740000
H	1.96285700	3.95907500	3.33811800
C	1.67382700	4.50565100	-0.08218500

H	2.20874700	4.17483100	-0.97395100
H	0.62811200	4.18668300	-0.16191100
H	1.69232600	5.60111300	-0.04611000
C	3.79249600	4.29546600	1.31237200
H	3.90360100	5.38214400	1.40404400
H	4.22466100	3.83426900	2.20772300
H	4.35411000	3.96083000	0.43836500
C	-4.30208800	3.82600100	-2.05964500
H	-4.32785000	3.71769000	-0.97444800
C	-4.71010900	4.97121600	-2.60822900
H	-4.69414000	5.13068900	-3.68525900
H	-5.07640200	5.79523100	-2.00096300
C	-0.73394700	-7.09646500	0.28290000
C	-1.00123600	-5.74096800	0.27369200
C	-2.08520900	-5.21830300	-0.47206600
C	-2.91638600	-6.10164600	-1.21861600
C	-2.61492100	-7.48354100	-1.19144700
C	-1.54810700	-7.97367700	-0.45829300
C	-2.33840200	-3.80698000	-0.46790300
C	-4.03518300	-5.53869200	-1.96495100
C	-4.27101700	-4.13065000	-1.93377400
C	-3.37869400	-3.28160900	-1.17392200
C	-5.37184500	-3.59085300	-2.63874000
H	-5.54981000	-2.52284000	-2.59402500
C	-6.22036300	-4.40381000	-3.36685700
C	-5.98963100	-5.78957200	-3.41140100
C	-4.92233300	-6.33857000	-2.72345900
H	-1.66289500	-3.18395500	0.10537900
H	0.10005000	-7.48511700	0.86130100
H	-0.38413300	-5.04873500	0.84109700
H	-3.22635200	-8.18426000	-1.74978400
H	-1.34138500	-9.04044800	-0.45506100
H	-7.06309000	-3.97236600	-3.90028200
H	-6.65203500	-6.43417000	-3.98283700
H	-4.77168900	-7.41143100	-2.76969400

*re-ts2b-real*

C	1.86218600	0.39115600	1.06131500
C	2.66696200	1.57861500	1.58093000
C	2.20062600	2.91480000	1.37038600
C	3.82405300	1.39819800	2.30926800
C	1.05960700	3.23201200	0.59629400
C	2.94863200	3.97689700	1.98055200
C	4.49318700	2.52067300	2.85237900

H	4.23237500	0.40648700	2.47062500
C	0.66771700	4.54755700	0.42097200
H	0.48524000	2.46036400	0.09899000
C	2.50132600	5.31509500	1.80196800
H	5.40442300	2.37022200	3.43006800
C	1.38933100	5.59980000	1.04712000
H	3.07720800	6.10510200	2.27488400
H	1.05420600	6.62208200	0.89860200
C	0.83665500	-0.05276700	2.13887900
H	0.45761900	0.86335600	2.59485200
C	1.37659400	-1.02795700	3.21998000
C	-1.41066300	-0.96703400	2.63452300
C	-0.11182500	-1.96469600	0.78734900
C	0.59284500	-2.35632600	3.17088900
H	2.43502100	-1.22678000	3.04492300
H	1.29520800	-0.56639500	4.20795300
C	-0.89870600	-2.11924300	3.53622000
H	-1.53132600	-0.03007100	3.18195200
H	-2.34878500	-1.19862900	2.12964900
C	0.64447200	-2.92052800	1.73680300
H	0.45599900	-1.70331700	-0.10448400
H	-1.08185200	-2.35405400	0.47785400
H	1.03531600	-3.06973600	3.87263200
H	-1.44868000	-3.03413400	3.28538100
H	1.68331600	-3.02795100	1.41552500
H	0.18119200	-3.91200300	1.70566700
O	-0.39918100	4.88169000	-0.34006500
N	4.07777000	3.76467400	2.71537200
N	-0.40979700	-0.68677100	1.53164100
H	-0.70998400	4.07442800	-0.81479400
H	1.29851000	0.68121800	0.17441700
C	-2.42967900	0.87555300	-2.35207000
H	-3.04955800	1.52643600	-2.95240900
H	-0.87869200	-0.00374100	0.90305800
H	-2.33188300	-0.16697500	-2.61923500
N	-1.28273900	1.47522000	-1.89538700
O	-0.37048200	0.76396500	-1.38237900
O	-1.19811200	2.74023000	-1.93433500
C	-7.06998100	0.99216900	-2.25868600
C	-7.19312800	2.31866400	-1.83900300
C	-6.19998300	2.92582800	-1.05865400
C	-5.09185100	2.16121700	-0.71720000
C	-4.94554200	0.82062700	-1.13847000
C	-5.94191300	0.23523200	-1.91617300

N	-3.99390900	2.55187800	0.06725900
C	-3.12310700	1.50776400	0.23566500
C	-3.65663000	0.33139000	-0.57240900
O	-2.10251100	1.53011400	0.92444700
H	-7.85138800	0.54281500	-2.86471700
H	-8.07084300	2.89481300	-2.11919900
H	-6.29859300	3.95584800	-0.73138000
H	-5.83092100	-0.78503000	-2.26125000
C	-3.79676500	3.87643200	0.62483800
H	-4.59346100	4.11896800	1.33697200
H	-2.83574300	3.88545100	1.13906900
H	-3.78388600	4.62845100	-0.17064900
N	-3.27297100	-0.86945600	-0.16488600
C	-3.61680400	-1.98844700	-0.87560900
O	-3.90285700	-2.05206400	-2.07136500
O	-3.50437800	-3.07799000	-0.06612300
C	-3.82184300	-4.43241000	-0.54527200
C	-3.62429500	-5.28546600	0.71082000
H	-3.83517900	-6.33744100	0.49104500
H	-2.59367300	-5.21278100	1.07574700
H	-4.29695300	-4.95919300	1.51140400
C	-2.84171900	-4.85512500	-1.64422400
H	-2.96051800	-4.24042600	-2.53798000
H	-1.80694200	-4.76996500	-1.29253000
H	-3.01964500	-5.90268300	-1.91385900
C	-5.27972900	-4.50624500	-1.01166800
H	-5.54598200	-5.54846400	-1.22157400
H	-5.95135500	-4.13654200	-0.22832000
H	-5.43782600	-3.91856400	-1.91724300
O	2.71076600	-0.71987600	0.74971100
C	4.25813700	0.60844700	-5.03891600
C	3.53305000	0.69499100	-3.86621900
C	3.88483700	-0.07700300	-2.73306400
C	5.00277400	-0.95735000	-2.80207600
C	5.72595500	-1.02245600	-4.01596900
C	5.36462300	-0.25836500	-5.11196200
C	3.11052100	0.02373600	-1.52949600
C	5.34201000	-1.74592200	-1.62390100
C	4.55274200	-1.62719700	-0.44011200
C	3.42490000	-0.72026600	-0.43157400
C	4.88785300	-2.38878500	0.70375700
H	4.28526200	-2.28360200	1.59827000
C	5.96688300	-3.25294000	0.69338000
C	6.74740100	-3.37843000	-0.46868800



C	6.43856000	-2.63978000	-1.59690800
H	2.25896900	0.69464700	-1.54217900
H	3.97627700	1.20694100	-5.90094600
H	2.67576600	1.35974700	-3.79612100
H	6.58229500	-1.68242000	-4.10368400
H	5.93843800	-0.33091000	-6.03182400
H	6.21111200	-3.83004500	1.58108400
H	7.59696300	-4.05582000	-0.48387200
H	7.05984700	-2.75483400	-2.47805700
C	-1.13385200	-1.82404400	4.99499600
C	-1.83558400	-2.60354700	5.81917200
H	-1.96825300	-2.35076700	6.86828900
H	-2.30650100	-3.52379100	5.47738000
H	-0.69159400	-0.90479800	5.38210500