

**Calix[4]pyrroles as macrocyclic organocatalysts
for the synthesis of cyclic carbonates from epoxides and carbon dioxide**

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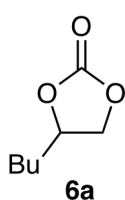
[A] General methods.

NMR spectra were measured on a JEOL JNM-ECS400 spectrometer, and chemical shifts are reported as the delta scale in ppm using a solvent residual peak as an internal reference ($\delta = 7.26$ ppm (CDCl_3)). Column chromatography was carried out using Fuji Silysia BW-127 ZH (100–270 mesh), and thin layer chromatography (TLC) was performed on Merck silica gel 60 F₂₅₄. Macrocycles **1** and **4** were prepared according to the literature,¹ while macrocycles **2** and **3** were purchased.

[B] Coupling reaction of epoxide with CO₂.

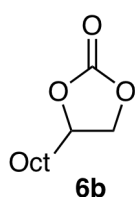
General procedure. A 30 mL stainless autoclave or 5 mL flask was charged with epoxide **5**, catalyst (amount indicated in the tables), and then CO₂ (initial pressure indicated in the tables). The mixture was stirred at a constant temperature for a reaction time. The reactor was then cooled in an ice bath, and excess CO₂ was released carefully. The yield was determined by using 2-methoxynaphthalene as an internal standard, or the product was purified by silica gel column chromatography (hexane/EtOAc (3:1) for **6a–d** and **6i–k**, hexane/EtOAc (1:1) for **6e–g**, and CHCl₃ for **6h**). Cyclic carbonates **6** were characterized according to the literature.^{2,3,4}

4-Butyl-1,3-dioxolan-2-one (**6a**).²



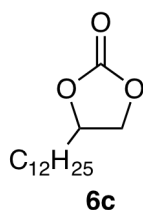
1.41 g (98% yield) (Table 3, entry 1, 15 h); ¹H NMR (CDCl_3 , 400 MHz) δ 4.73–4.66 (m, 1H, OCH), 4.52 (t, $J = 8.2$ Hz, 1H, OCH₂), 4.07 (t, $J = 7.8$ Hz, 1H, OCH₂), 1.86–1.76 (m, 1H, CH₂), 1.73–1.64 (m, 1H, CH₂), 1.50–1.30 (m, 4H, CH₂), 0.93 ppm (t, $J = 6.6$ Hz, 3H, CH₃).

4-Octyl-1,3-dioxolan-2-one (**6b**).²



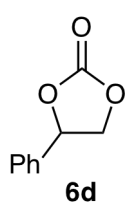
1.94 g (97% yield) (Table 3, entry 2, 15 h); ¹H NMR (CDCl_3 , 400 MHz) δ 4.73–4.66 (m, 1H, OCH), 4.52 (t, $J = 8.2$ Hz, 1H, OCH₂), 4.06 (dd, $J = 7.2, 8.0$ Hz, 1H, OCH₂), 1.84–1.77 (m, 1H, CH₂), 1.72–1.63 (m, 1H, CH₂), 1.51–1.20 (m, 12H, CH₂), 0.88 ppm (t, $J = 7.0$ Hz, 3H, CH₃).

4-Dodecyl-1,3-dioxolan-2-one (**6c**).²



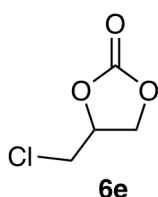
2.31 g (90% yield) (Table 3, entry 3, 24 h); ¹H NMR (CDCl_3 , 400 MHz) δ 4.73–4.66 (m, 1H, OCH), 4.52 (t, $J = 8.0$ Hz, 1H, OCH₂), 4.06 (dd, $J = 7.6, 8.2$ Hz, 1H, OCH₂), 1.84–1.76 (m, 1H, CH₂), 1.70–1.64 (m, 1H, CH₂), 1.47–1.24 (m, 20H, CH₂), 0.88 ppm (t, $J = 6.8$ Hz, 3H, CH₃).

4-Phenyl-1,3-dioxolan-2-one (6d).²



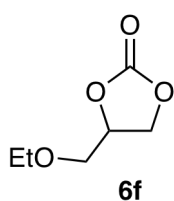
1.61 g (98% yield) (Table 3, entry 4, 15 h); ¹H NMR (CDCl₃, 400 MHz) δ 7.48–7.41 (m, 3H, Ph), 7.39–7.35 (m, 2H, Ph), 5.68 (t, *J* = 8.0 Hz, 1H, OCH), 4.80 (t, *J* = 8.4 Hz, 1H, OCH₂), 4.35 ppm (t, *J* = 8.2 Hz, 1H, OCH₂).

4-(Chloromethyl)-1,3-dioxolan-2-one (6e).²



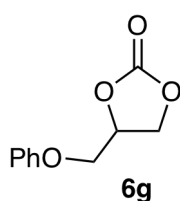
1.27 g (93% yield) (Table 3, entry 5, 15 h); ¹H NMR (CDCl₃, 400 MHz) δ 4.98–4.92 (m, 1H, OCH), 4.59 (t, *J* = 8.6 Hz, 1H, OCH₂), 4.43 (dd, *J* = 6.4, 8.8 Hz, 1H, OCH₂), 3.77 (dd, *J* = 6.0, 11.8 Hz, 1H, CH₂Cl), 3.73 ppm (dd, *J* = 4.0, 11.6 Hz, 1H, CH₂Cl).

4-(Ethoxymethyl)-1,3-dioxolan-2-one (6f).²



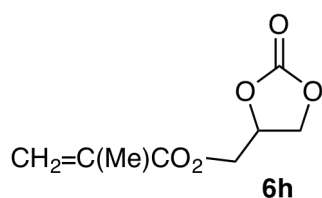
1.40 g (96% yield) (Table 3, entry 6, 15 h); ¹H NMR (CDCl₃, 400 MHz) δ 4.81–4.77 (m, 1H, OCH), 4.49 (t, *J* = 8.4 Hz, 1H, OCH₂), 4.39 (dd, *J* = 6.8, 8.4 Hz, 1H, OCH₂), 3.67 (dd, *J* = 3.6, 10.8 Hz, 1H, CH₂OEt), 3.61 (dd, *J* = 4.4, 10.2 Hz, 1H, CH₂OEt), 3.57 (q, *J* = 6.9 Hz, 2H, CH₂), 1.20 ppm (t, *J* = 7.0 Hz, 3H, CH₃).

4-(Phenoxymethyl)-1,3-dioxolan-2-one (6g).²



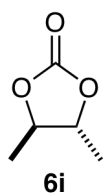
1.91 g (98% yield) (Table 3, entry 7, 15 h); ¹H NMR (CDCl₃, 400 MHz) δ 7.31 (t, *J* = 8.0 Hz, 2H, Ph), 7.02 (t, *J* = 7.4 Hz, 1H, Ph), 6.92 (d, *J* = 8.0 Hz, 2H, Ph), 5.04–4.98 (m, 1H, OCH), 4.61 (t, *J* = 8.6 Hz, 1H, OCH₂), 4.53 (dd, *J* = 6.0, 12.0 Hz, 1H, OCH₂), 4.24 (dd, *J* = 4.4, 10.4 Hz, 1H, CH₂), 4.17 ppm (dd, *J* = 4.0, 10.6 Hz, 1H, CH₂).

(2-Oxo-1,3-dioxolan-4-yl)methyl methacrylate (6h).³



1.78 g (95% yield) (Table 3, entry 8, 15 h); ¹H NMR (CDCl₃, 400 MHz) δ 6.17–6.16 (m, 1H, C=CH₂), 5.67–5.66 (m, 1H, C=CH₂), 5.00–4.95 (m, 1H, OCH), 4.58 (t, *J* = 8.8 Hz, 1H, OCH₂), 4.44 (dd, *J* = 3.2, 12.8 Hz, 1H, OCH₂), 4.37–4.32 (m, 2H, OCHCH₂O), 1.96 ppm (t, *J* = 1.4 Hz, 3H, CH₃).

***trans*-4,5-Dimethyl-1,3-dioxolan-2-one (6i).**⁴



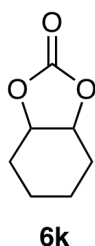
559 mg (48% yield) (Table 3, entry 9, cat. 3 mol%, 48 h); ¹H NMR (CDCl₃, 400 MHz) δ 4.35–4.28 (m, 2H, OCH), 1.43 ppm (dd, *J* = 1.0, 5.8 Hz, 6H, CH₃).

4,5-Trimethylene-1,3-dioxolan-2-one (6j).⁴



907 mg (71% yield) (Table 3, entry 10, cat. 3 mol%, 48 h); ¹H NMR (CDCl₃, 400 MHz) δ 5.12–5.09 (m, 2H, OCH), 2.18–2.13 (m, 2H, CH₂), 1.84–1.62 ppm (m, 4H, CH₂).

4,5-Tetramethylene-1,3-dioxolan-2-one (6k).⁴



1.12 g (79% yield) (Table 3, entry 11, cat. 3 mol%, 48 h); ¹H NMR (CDCl₃, 400 MHz) δ 4.70–4.65 (m, 2H, OCH), 1.93–1.86 (m, 4H, CH₂), 1.63–1.57 (m, 2H, CH₂), 1.46–1.39 ppm (m, 2H, CH₂).

References

- 1 (a) C. J. Borman, R. Custelcean, B. P. Hay, N. L. Bill, J. L. Sessler and B. A. Moyer, *Chem. Commun.*, 2011, **47**, 7611. (b) Y. Han, G.-L. Wang, J.-J. Sun, J. Sun and C.-G. Yan, *Tetrahedron*, 2013, **69**, 10604. (c) S. Dey, K. Pal and S. Sarkar, *Tetrahedron Lett.*, 2008, **49**, 960. (d) T. Ema, D. Tanida and T. Sakai, *Org. Lett.*, 2006, **8**, 3773.
- 2 C. Maeda, S. Sasaki and T. Ema, *ChemCatChem*, 2017, **9**, 946.
- 3 J. Steinbauer, A. Spannenberg and T. Werner, *Green Chem.*, 2017, **19**, 3769.
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[C] Time course of the reaction of 5a with CO₂ in the presence or absence of 1a.

To investigate the effect of calix[4]pyrrole **1a** on the reaction under the conditions of Table 3 (entry 1), we monitored the time course of the reaction of **5a** with CO₂ in the presence or absence of **1a**. As shown below (Fig. S1), the reaction with **1a** (red) was much faster than that without **1a** (blue). The former reached 95% in 9 h, whereas the latter reached only 42% in 9 h, and the latter did not reach 80% even after 48 h (not shown). The addition of **1a** is highly beneficial, and it has been confirmed again that this is cooperative catalysis driven by **1a** and TBAI.

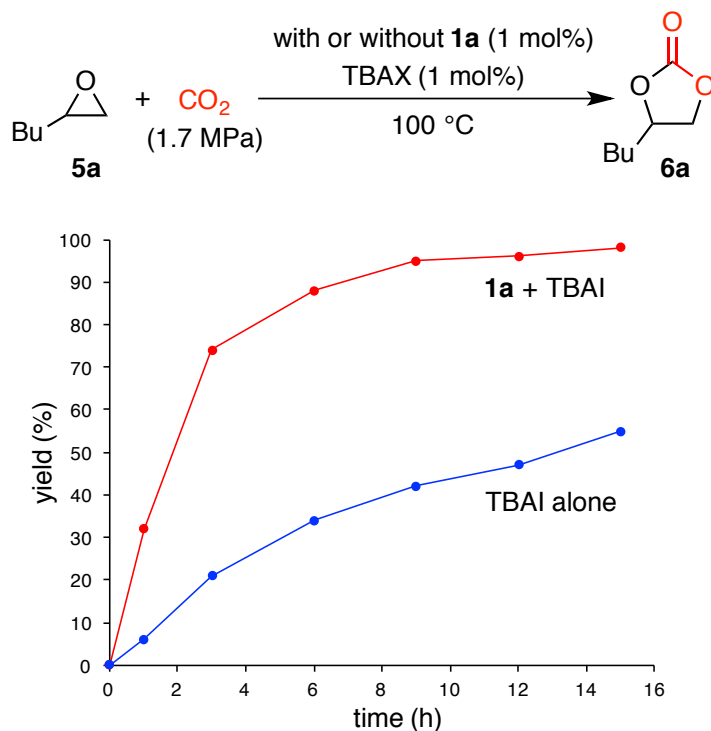
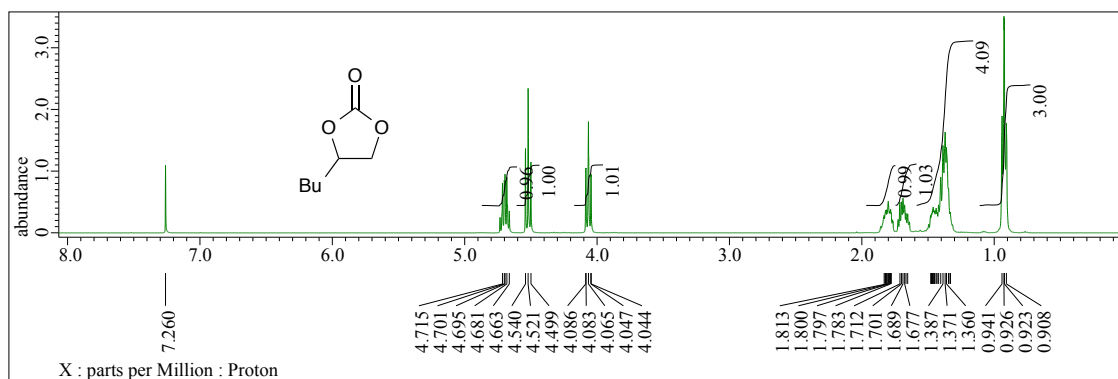
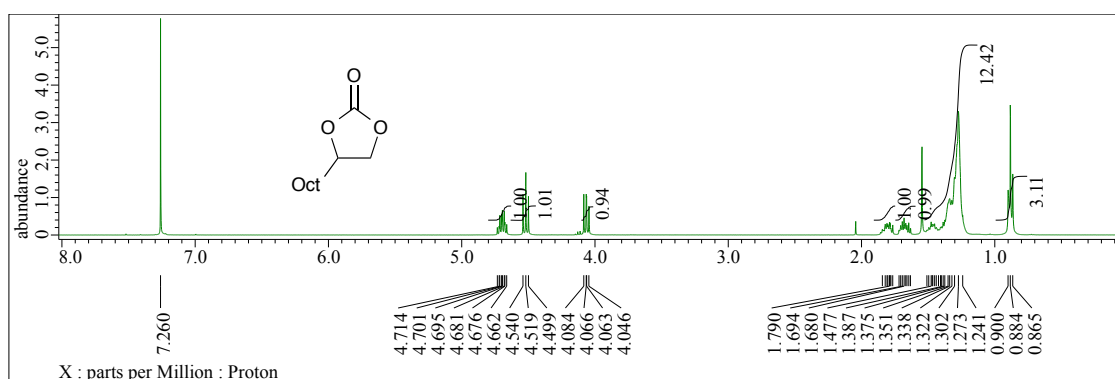


Fig. S1. Time course of the reaction of **5a** with CO₂ in the presence or absence of **1a**.

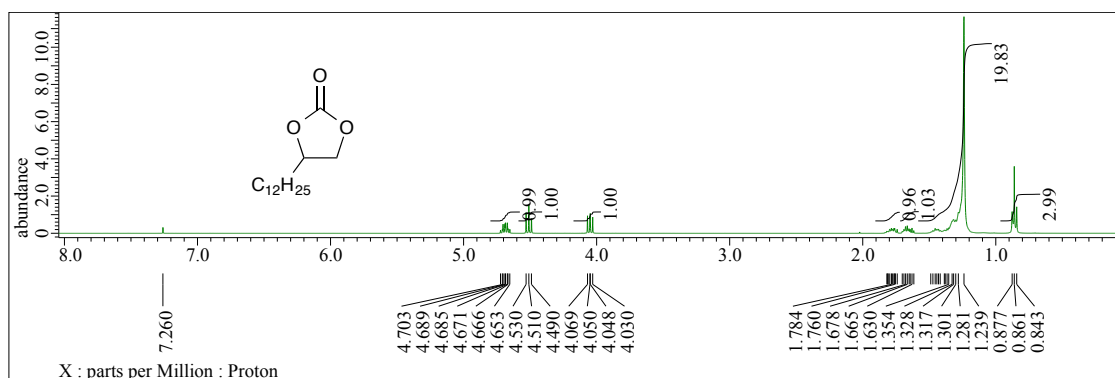
[D] ^1H NMR spectra.



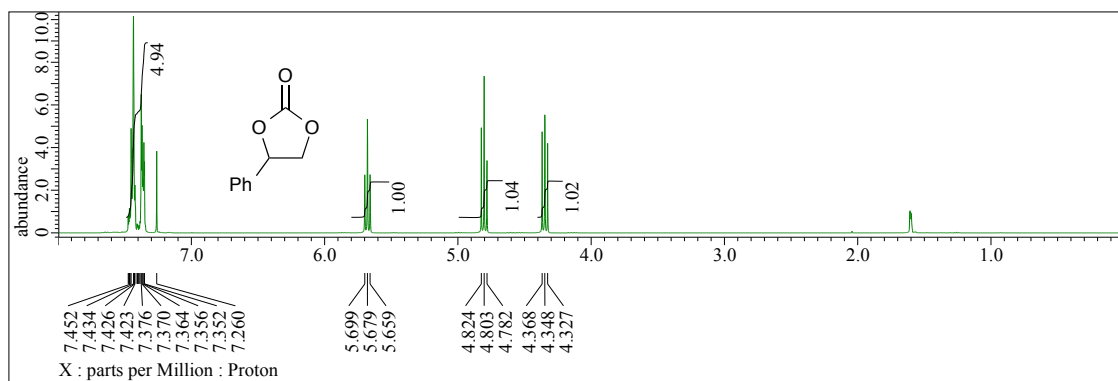
^1H NMR spectrum of **6a** in CDCl_3 .



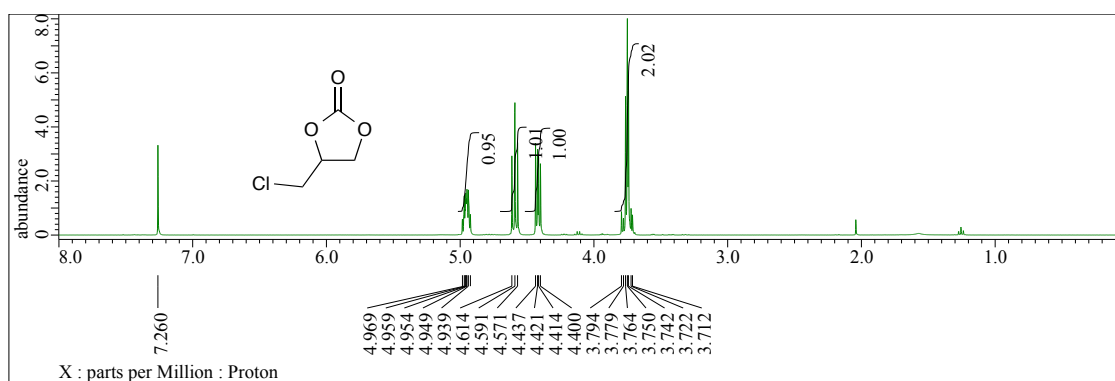
^1H NMR spectrum of **6b** in CDCl_3 .



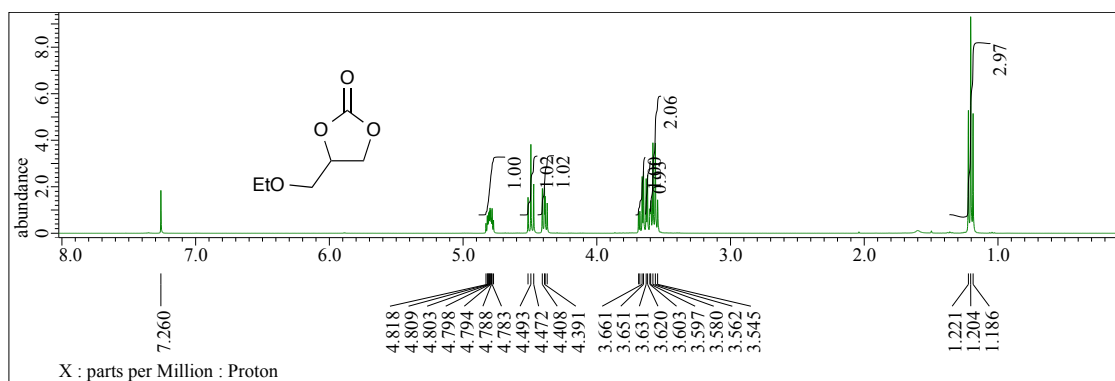
^1H NMR spectrum of **6c** in CDCl_3 .



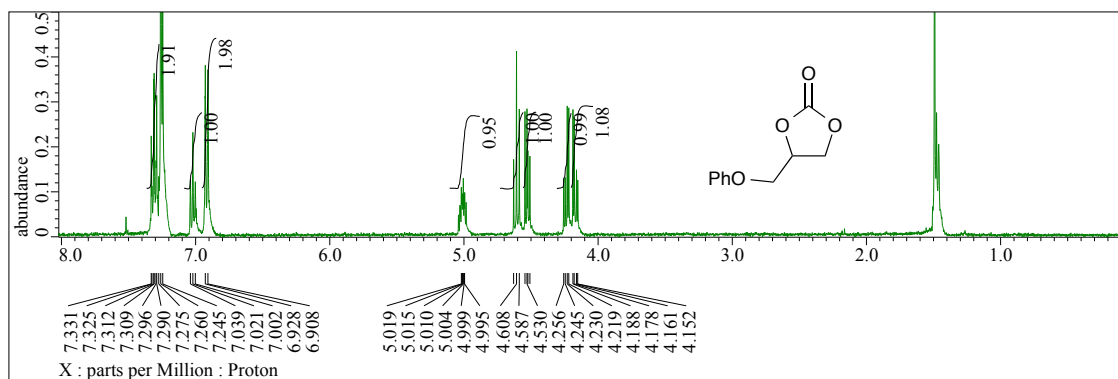
¹H NMR spectrum of **6d** in CDCl₃.



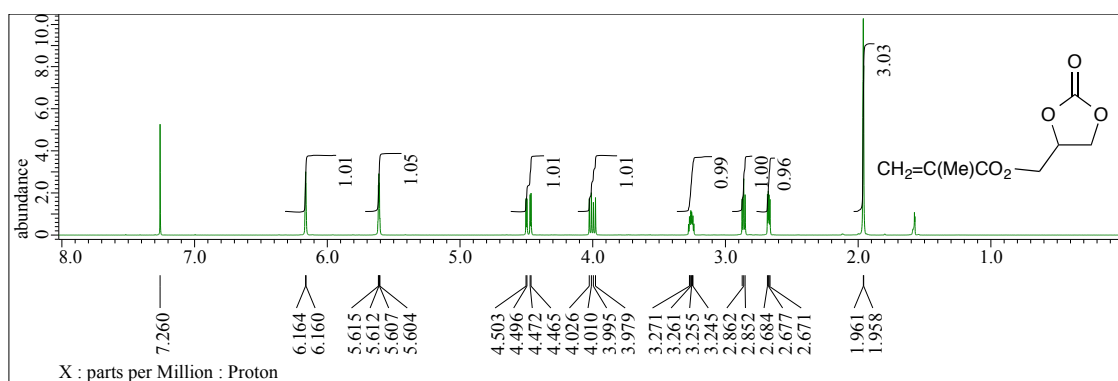
¹H NMR spectrum of **6e** in CDCl₃.



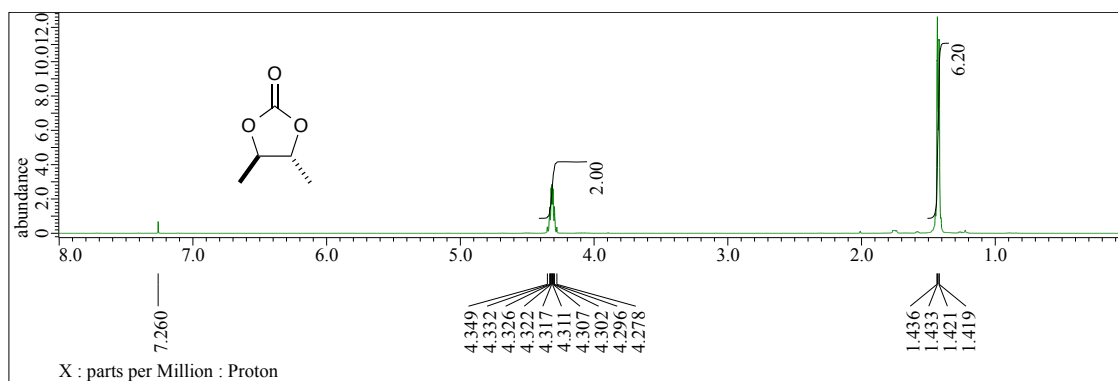
¹H NMR spectrum of **6f** in CDCl₃.



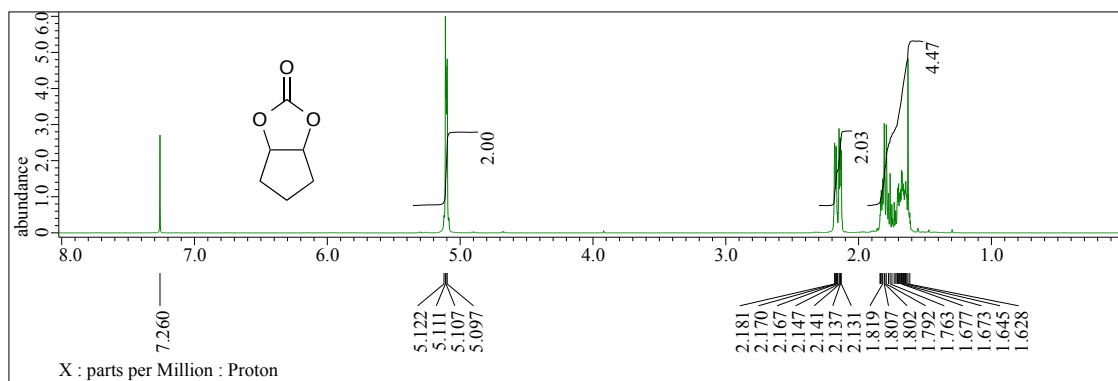
^1H NMR spectrum of **6g** in CDCl_3 .



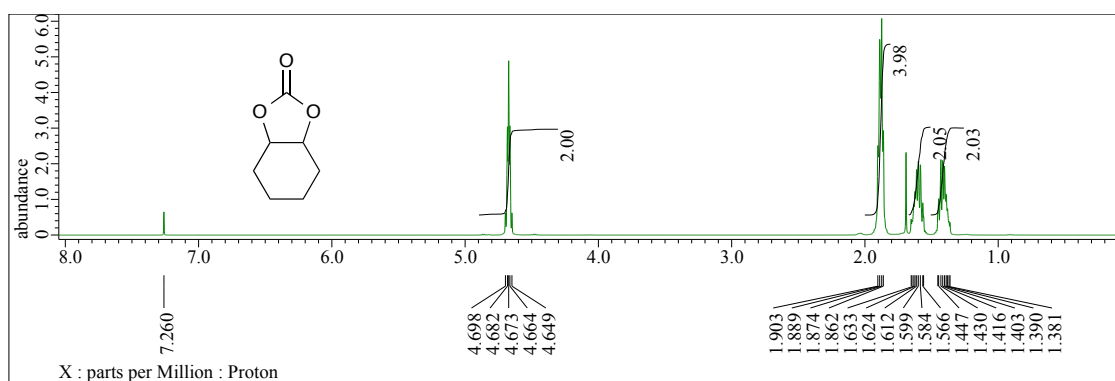
^1H NMR spectrum of **6h** in CDCl_3 .



^1H NMR spectrum of **6i** in CDCl_3 .



^1H NMR spectrum of **6j** in CDCl_3 .



^1H NMR spectrum of **6k** in CDCl_3 .

[E] DFT calculations.

DFT calculations were performed with Gaussian 16 at the B3LYP/6-31G(d) level for the H, C, N, and O atoms and at the B3LYP/LanL2DZ level for the I atom. The harmonic frequency and normal mode were calculated to verify the transition-state structures.

< Reference >

Gaussian 16, revision A.03

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

Cartesian coordinates of reactant **R**.

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C	-0.707614	3.155482	0.699818
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H	3.350104	-0.795321	2.737700
H	4.668911	0.219367	3.328971
H	4.654067	-2.861998	3.287799
H	4.464045	-1.843516	4.721398
H	6.011698	-1.873188	3.860654
H	8.997818	2.293338	-0.706839
H	9.026147	1.207590	0.675930
H	8.724246	4.271782	0.843911
H	10.189227	3.352281	1.218741
H	8.752049	3.177973	2.236683
H	-0.617700	0.470150	-3.980243
H	-2.240852	-0.393831	-3.819239
H	-1.940105	-0.543303	-1.327761
H	-0.311525	0.304596	-1.449443

Cartesian coordinates of transition state **II_TS**.

C	-1.328528	-1.455405	3.458073
C	-0.504111	-0.299676	3.607881
C	-1.199766	0.786476	3.102808
N	-2.416576	0.307586	2.674041
C	-2.513582	-1.053965	2.868332

C	-5.698437	-0.112824	-0.240422
C	-5.542763	-0.401856	1.144714
C	-4.432349	-1.215390	1.286633
N	-3.914211	-1.408890	0.019535
C	-4.680572	-0.753024	-0.926438
C	-3.797663	-1.801436	2.537369
C	-1.577207	1.510954	-3.581867
C	-2.320899	0.305997	-3.741211
C	-3.249416	0.242819	-2.717177
N	-3.085405	1.387422	-1.965496
C	-2.059785	2.163345	-2.460024
C	-4.357498	-0.758084	-2.412248
C	-2.625712	3.801132	1.813598
C	-2.856200	4.134420	0.450051
C	-1.916573	3.464177	-0.315119
N	-1.131419	2.730782	0.556533
C	-1.548326	2.932430	1.858802
C	-0.871768	2.271269	3.049900
C	-1.683036	3.490900	-1.818990
C	-3.935635	-2.170938	-2.876708
C	-5.624894	-0.343846	-3.204721
C	-4.779974	-1.640040	3.726203
C	-3.506704	-3.307802	2.351570
C	0.661151	2.459435	2.964666
C	-1.372808	2.938242	4.356142
C	-2.547062	4.611983	-2.450184
C	-0.195398	3.800401	-2.111463
H	-1.073904	-2.467518	3.740466
H	0.484398	-0.271784	4.047492
H	-3.115290	0.865601	2.199445
H	-6.488462	0.476566	-0.684530
H	-6.192345	-0.071125	1.942952
H	-3.088093	-1.963612	-0.184948
H	-0.770785	1.852784	-4.217239
H	-2.181962	-0.435837	-4.515877
H	-3.597887	1.584038	-1.114856
H	-3.175086	4.178421	2.664864
H	-3.612225	4.811537	0.077839
H	-0.386206	2.074174	0.280695

H	-3.013352	-2.511861	-2.395959
H	-3.765016	-2.178619	-3.958929
H	-4.730188	-2.891914	-2.655805
H	-5.944008	0.671388	-2.947762
H	-5.408163	-0.361245	-4.277616
H	-6.454344	-1.030549	-3.000841
H	-4.996905	-0.586067	3.928634
H	-4.333749	-2.067788	4.629561
H	-5.725542	-2.155680	3.523245
H	-2.777075	-3.496874	1.558496
H	-3.105979	-3.733883	3.278366
H	-4.433544	-3.838671	2.108900
H	1.065553	1.961033	2.078833
H	0.906799	3.526697	2.918858
H	1.150059	2.036425	3.850014
H	-2.451774	2.803223	4.480781
H	-1.156064	4.012906	4.357186
H	-0.878769	2.477646	5.217660
H	-3.614262	4.424420	-2.294710
H	-2.369739	4.648102	-3.529798
H	-2.300873	5.589485	-2.019290
H	-0.019031	3.860878	-3.191525
H	0.078976	4.763611	-1.667032
H	0.457106	3.023829	-1.699683
N	4.627193	0.356606	-0.481229
C	3.741173	0.157649	-1.730825
C	3.918713	-0.122689	0.801228
C	5.967792	-0.330771	-0.693284
C	4.886461	1.862069	-0.345629
C	7.042561	-0.082664	0.368236
C	3.666854	2.784039	-0.304235
C	3.972853	-1.616953	1.127922
C	3.568617	-1.259737	-2.285164
C	4.112381	4.206820	0.080411
C	2.951130	5.205912	0.075856
C	2.911178	-1.195817	-3.678340
C	2.574069	-2.589369	-4.218560
C	3.267529	-1.880374	2.473213
C	3.171354	-3.376046	2.791744

C	8.256611	-0.996448	0.123591
C	9.383472	-0.757405	1.133482
C	0.089337	-0.104566	-1.026839
C	0.425132	-0.976026	0.086394
O	0.874115	0.795433	-0.260504
I	-0.401890	-3.601967	-0.607144
H	4.204161	0.791666	-2.494731
H	2.766815	0.573770	-1.455698
H	4.379057	0.439789	1.617985
H	2.882448	0.207775	0.693518
H	6.319706	0.001429	-1.675350
H	5.760456	-1.397097	-0.763862
H	5.534317	2.127394	-1.187781
H	5.466971	1.980741	0.570967
H	6.646788	-0.274577	1.372877
H	7.376756	0.960617	0.350194
H	2.920651	2.426595	0.410771
H	3.168238	2.810234	-1.278021
H	5.006968	-1.974303	1.204678
H	3.487631	-2.212703	0.349318
H	2.932773	-1.862317	-1.630353
H	4.525501	-1.784436	-2.385393
H	4.894632	4.550003	-0.612226
H	4.573522	4.184490	1.078031
H	2.506877	5.292444	-0.921881
H	3.292076	6.201433	0.379677
H	2.157494	4.894953	0.764267
H	3.585767	-0.673150	-4.371954
H	1.994008	-0.596246	-3.624646
H	3.472115	-3.215382	-4.294286
H	2.130556	-2.520256	-5.217471
H	1.856599	-3.098892	-3.565740
H	2.259548	-1.448871	2.453326
H	3.814207	-1.359472	3.272456
H	2.558659	-3.895494	2.046614
H	2.706841	-3.533045	3.770715
H	4.162345	-3.847089	2.812171
H	8.635414	-0.834448	-0.894974
H	7.936623	-2.046165	0.170091

H	9.750927	0.274444	1.083363
H	10.230716	-1.422761	0.938235
H	9.043760	-0.942244	2.159421
H	0.497616	-0.371352	-2.006968
H	-0.964216	0.163266	-1.121848
H	-0.154830	-0.953973	0.998887
H	1.397221	-1.434185	0.120474

Cartesian coordinates of intermediate **II**.

C	-2.079495	-1.644289	3.380977
C	-0.962133	-0.775039	3.557707
C	-1.315945	0.473726	3.075646
N	-2.616254	0.372126	2.636108
C	-3.096614	-0.910320	2.798343
C	-6.011299	0.715916	-0.387439
C	-5.970072	0.406825	1.002354
C	-4.984664	-0.543315	1.198019
N	-4.432983	-0.803816	-0.042950
C	-5.050442	-0.049185	-1.023466
C	-4.534647	-1.265073	2.456790
C	-1.275373	1.141667	-3.511796
C	-2.325157	0.193101	-3.682540
C	-3.294503	0.460305	-2.732900
N	-2.852733	1.549890	-2.012547
C	-1.618525	1.969076	-2.457348
C	-4.669021	-0.144452	-2.491141
C	-1.903195	3.668769	1.759055
C	-2.011103	4.047178	0.393124
C	-1.172093	3.221665	-0.339324
N	-0.566765	2.351880	0.548295
C	-1.000326	2.618561	1.833404
C	-0.573405	1.802992	3.046102
C	-0.933878	3.181020	-1.842935
C	-4.680292	-1.622516	-2.948241
C	-5.710902	0.633017	-3.335221
C	-5.446789	-0.844386	3.636744
C	-4.666437	-2.794688	2.263164
C	0.947650	1.537586	3.024908
C	-0.916722	2.587994	4.338304

C	-1.521777	4.460711	-2.491042
C	0.578146	3.131249	-2.150845
H	-2.125247	-2.691045	3.648728
H	-0.007768	-1.041227	3.992061
H	-3.107711	1.116904	2.158103
H	-6.689814	1.406752	-0.867785
H	-6.611609	0.820284	1.767752
H	-3.638503	-1.411098	-0.200630
H	-0.366307	1.200167	-4.095151
H	-2.358511	-0.598992	-4.418262
H	-3.317737	1.924391	-1.195543
H	-2.413819	4.131125	2.592724
H	-2.617976	4.850486	-0.001326
H	0.117820	1.598654	0.290584
H	-3.931980	-2.219568	-2.417710
H	-4.460996	-1.693790	-4.019209
H	-5.667308	-2.063546	-2.772317
H	-5.724699	1.694573	-3.067964
H	-5.450879	0.559323	-4.395768
H	-6.718103	0.225121	-3.190251
H	-5.380862	0.232028	3.825694
H	-5.131691	-1.364702	4.546572
H	-6.493858	-1.096893	3.433071
H	-4.013607	-3.161946	1.465219
H	-4.397445	-3.323847	3.184150
H	-5.700841	-3.051597	2.011730
H	1.224369	0.958106	2.139078
H	1.492444	2.489344	3.021647
H	1.250880	0.981803	3.920248
H	-1.994425	2.755187	4.431007
H	-0.414290	3.562368	4.349154
H	-0.594360	2.014703	5.213844
H	-2.604624	4.523228	-2.343253
H	-1.334806	4.444369	-3.569808
H	-1.063147	5.361748	-2.067027
H	0.749162	3.114429	-3.233741
H	1.067265	4.024658	-1.745704
H	1.033170	2.241182	-1.706086
N	4.787139	0.303898	-0.373743

C	3.927781	0.290583	-1.656432
C	4.076710	-0.442904	0.777089
C	6.170298	-0.246544	-0.671780
C	4.948661	1.769123	0.047605
C	7.206937	-0.138251	0.449838
C	3.673417	2.603444	0.171433
C	4.259512	-1.959798	0.861532
C	3.915469	-0.990089	-2.491803
C	3.988069	3.914742	0.914476
C	2.798000	4.879570	0.941114
C	3.104250	-0.752553	-3.779986
C	2.986140	-2.017510	-4.635794
C	3.658420	-2.472479	2.184374
C	3.711141	-3.999079	2.300189
C	8.483364	-0.913520	0.079993
C	9.572055	-0.799292	1.151782
C	0.412453	-0.616493	-0.750407
C	0.295007	-1.800200	0.208015
O	1.234552	0.331939	-0.162279
I	-0.979815	-3.473337	-0.629497
H	4.317787	1.115494	-2.262281
H	2.906415	0.515277	-1.310725
H	4.454118	0.013665	1.695969
H	3.008163	-0.200974	0.653911
H	6.518852	0.287353	-1.562038
H	6.037213	-1.290802	-0.950920
H	5.624165	2.216616	-0.689519
H	5.471210	1.745523	1.005862
H	6.803595	-0.536533	1.388665
H	7.470684	0.908737	0.636022
H	2.885418	2.055232	0.693786
H	3.274153	2.833334	-0.820660
H	5.314770	-2.257276	0.827903
H	3.759868	-2.458854	0.024770
H	3.453291	-1.809624	-1.932838
H	4.924893	-1.313189	-2.775099
H	4.850065	4.411675	0.444381
H	4.294907	3.679672	1.943765
H	2.523347	5.195546	-0.071593

H	3.038328	5.779210	1.518388
H	1.914400	4.413008	1.389441
H	3.581097	0.046846	-4.364920
H	2.102346	-0.393434	-3.516021
H	3.972933	-2.399499	-4.926565
H	2.422379	-1.816621	-5.552893
H	2.462759	-2.812853	-4.092832
H	2.619865	-2.131307	2.269975
H	4.202961	-2.018923	3.024662
H	3.128486	-4.477284	1.504321
H	3.298528	-4.332543	3.258143
H	4.741314	-4.370800	2.232177
H	8.871272	-0.541485	-0.878421
H	8.233182	-1.971341	-0.079338
H	9.871163	0.244373	1.305301
H	10.465600	-1.363327	0.864668
H	9.224464	-1.192080	2.114682
H	0.794885	-0.990828	-1.722686
H	-0.602972	-0.239195	-0.962788
H	-0.194392	-1.548028	1.148051
H	1.249208	-2.295020	0.389052

Cartesian coordinates of intermediate **II**·CO₂.

C	-2.761571	-3.512748	-0.245550
C	-1.520572	-3.517087	0.458196
C	-1.613655	-2.593226	1.485313
N	-2.879315	-2.056903	1.420160
C	-3.590679	-2.590249	0.366340
C	-5.930439	1.298542	1.166631
C	-6.041097	-0.107218	1.366449
C	-5.267401	-0.735635	0.408011
N	-4.691970	0.263907	-0.354970
C	-5.090196	1.511837	0.088612
C	-5.042366	-2.210895	0.122563
C	-1.041046	3.848697	-0.141987
C	-2.215972	3.812837	-0.947445
C	-3.174886	3.088412	-0.262851
N	-2.603127	2.705432	0.931838
C	-1.299694	3.140703	1.018602

C	-4.636958	2.802511	-0.573045
C	-1.549217	-0.232083	4.082394
C	-1.504541	1.185341	3.984451
C	-0.789387	1.504873	2.841014
N	-0.407460	0.317748	2.244340
C	-0.860272	-0.749362	2.996024
C	-0.647238	-2.201268	2.594556
C	-0.460500	2.872046	2.259146
C	-4.841425	2.716697	-2.104375
C	-5.496621	3.974255	-0.033334
C	-5.943527	-3.052563	1.061126
C	-5.431807	-2.532248	-1.339986
C	0.803232	-2.427645	2.113195
C	-0.905858	-3.115170	3.819990
C	-0.766620	3.966548	3.312874
C	1.038617	2.950461	1.893814
H	-3.010703	-4.117192	-1.106936
H	-0.661477	-4.135551	0.234620
H	-3.199513	-1.297483	2.007752
H	-6.434268	2.065781	1.737496
H	-6.643300	-0.600079	2.116627
H	-4.021445	0.103594	-1.096339
H	-0.111907	4.344068	-0.389789
H	-2.338108	4.265565	-1.922129
H	-3.046412	2.099992	1.610760
H	-2.012766	-0.803852	4.874623
H	-1.928611	1.888304	4.688120
H	0.122672	0.234469	1.343069
H	-4.222738	1.935268	-2.556658
H	-4.572013	3.665965	-2.580133
H	-5.891834	2.507182	-2.333480
H	-5.364633	4.098034	1.046353
H	-5.188025	4.907036	-0.515555
H	-6.560834	3.807314	-0.236575
H	-5.698506	-2.873752	2.113121
H	-5.790592	-4.116936	0.857460
H	-7.002332	-2.814430	0.906632
H	-4.802287	-1.995963	-2.056694
H	-5.324559	-3.604225	-1.539644

H	-6.476099	-2.254841	-1.518297
H	1.016231	-1.825756	1.224106
H	1.505932	-2.158817	2.911354
H	0.953198	-3.487070	1.872609
H	-1.939349	-3.030486	4.170175
H	-0.238068	-2.855995	4.650074
H	-0.735794	-4.160639	3.542185
H	-1.828435	3.978666	3.578650
H	-0.515975	4.950673	2.903516
H	-0.183762	3.805735	4.227455
H	1.291552	3.951010	1.522040
H	1.650250	2.754553	2.782605
H	1.278895	2.215081	1.120533
N	4.321055	0.304708	-0.572587
C	3.557792	1.393161	-1.347286
C	5.825960	0.363346	-0.792841
C	3.924557	0.420760	0.903131
C	3.779251	-1.045008	-1.080028
C	4.441721	-0.673398	1.839849
C	4.031574	-1.377484	-2.552378
C	6.646616	1.317136	0.082137
C	3.891630	2.857075	-1.064981
C	3.560503	-2.812664	-2.852521
C	3.750093	-3.196266	-4.323487
C	2.922034	3.759871	-1.850918
C	3.202303	5.249973	-1.632294
C	8.118728	1.310706	-0.366165
C	9.000463	2.212999	0.503304
C	4.160872	-0.280496	3.301451
C	4.590338	-1.364706	4.294621
H	2.509477	1.171402	-1.103238
H	3.741530	1.184729	-2.402577
H	6.196045	-0.655560	-0.648357
H	5.965346	0.612230	-1.848052
H	2.830834	0.431580	0.883980
H	4.281447	1.396457	1.234830
H	2.704009	-0.994584	-0.857495
H	4.248758	-1.804680	-0.453702
H	5.519464	-0.843364	1.714413

H	3.943881	-1.625644	1.632579
H	5.095812	-1.297058	-2.809439
H	3.487808	-0.691963	-3.211604
H	6.595218	1.011670	1.132709
H	6.260921	2.338593	0.030645
H	4.917658	3.099582	-1.368262
H	3.799203	3.091168	0.001528
H	2.500613	-2.907151	-2.582186
H	4.109092	-3.515876	-2.211664
H	3.178451	-2.532937	-4.983018
H	3.410268	-4.220781	-4.508710
H	4.804890	-3.135579	-4.618920
H	1.892552	3.526941	-1.553215
H	2.994391	3.526302	-2.922258
H	3.100575	5.521844	-0.574679
H	2.500371	5.867508	-2.202569
H	4.217546	5.518463	-1.950347
H	8.182474	1.634543	-1.414198
H	8.505824	0.282575	-0.337922
H	8.658275	3.254174	0.470172
H	10.040543	2.192738	0.161230
H	8.987328	1.890884	1.551293
H	3.088796	-0.077040	3.418461
H	4.681731	0.659194	3.533972
H	4.051849	-2.302320	4.113304
H	4.383528	-1.056469	5.324928
H	5.664229	-1.575976	4.217188
C	0.033452	0.410146	-1.131294
C	-0.270004	-0.883179	-1.885522
O	0.996250	0.121178	-0.176503
I	-1.788796	-0.582807	-3.535341
H	0.358359	1.177672	-1.865303
H	-0.907543	0.795292	-0.699895
H	-0.717678	-1.652301	-1.257242
H	0.596901	-1.273874	-2.420450
C	3.027870	-5.036790	0.604996
O	2.128616	-5.780018	0.640503
O	3.936685	-4.297707	0.566369

Cartesian coordinates of transition state **I2_TS**.

C	3.327238	3.158562	-1.261361
C	2.298476	3.607973	-0.380680
C	2.483299	2.983259	0.839476
N	3.603315	2.190126	0.711682
C	4.124312	2.270319	-0.562386
C	5.920460	-1.626769	1.041545
C	6.273659	-0.271118	0.780687
C	5.470394	0.188661	-0.247364
N	4.642526	-0.860280	-0.601483
C	4.906287	-1.977169	0.169231
C	5.409002	1.544132	-0.932283
C	0.445128	-3.205715	0.631315
C	1.534775	-3.644909	-0.177168
C	2.695605	-3.121454	0.359729
N	2.325436	-2.394845	1.472574
C	0.959020	-2.420419	1.647782
C	4.159058	-3.287010	-0.017755
C	2.379099	1.217950	3.909415
C	1.968580	-0.130620	4.101829
C	1.022659	-0.425017	3.135235
N	0.856464	0.710929	2.363116
C	1.676938	1.723222	2.829576
C	1.756792	3.090940	2.172325
C	0.313599	-1.736455	2.844572
C	4.272953	-3.759386	-1.486157
C	4.793593	-4.369228	0.891391
C	6.616386	2.399426	-0.471010
C	5.494954	1.373012	-2.466960
C	0.338541	3.656433	1.962611
C	2.542878	4.061162	3.089718
C	0.434618	-2.670998	4.075363
C	-1.183393	-1.487814	2.567520
H	3.459295	3.455073	-2.292943
H	1.505048	4.299053	-0.629205
H	3.927834	1.546289	1.421749
H	6.378633	-2.276585	1.773934
H	7.048741	0.293797	1.279301
H	3.909516	-0.804861	-1.298075

H	-0.599118	-3.440491	0.476762
H	1.467140	-4.261627	-1.062509
H	2.952939	-1.815134	2.015612
H	3.093710	1.761585	4.511527
H	2.314660	-0.800390	4.876904
H	0.213500	0.790933	1.564868
H	3.804981	-3.053013	-2.178750
H	3.781056	-4.729834	-1.616520
H	5.326778	-3.870686	-1.762110
H	4.725113	-4.092203	1.948418
H	4.262720	-5.317090	0.758192
H	5.850052	-4.520761	0.641581
H	6.590025	2.574791	0.609319
H	6.585326	3.374079	-0.967902
H	7.563953	1.907430	-0.719625
H	4.643774	0.812312	-2.865596
H	5.506405	2.351047	-2.960358
H	6.416486	0.845308	-2.734990
H	-0.263903	2.987935	1.345607
H	-0.162682	3.778592	2.929383
H	0.379012	4.638003	1.476773
H	3.573800	3.725186	3.241135
H	2.060641	4.150751	4.070094
H	2.581490	5.051823	2.625311
H	1.479208	-2.916716	4.290380
H	-0.091441	-3.610557	3.875998
H	-0.000815	-2.203767	4.966309
H	-1.696992	-2.440940	2.390437
H	-1.648257	-1.011385	3.438474
H	-1.323242	-0.838833	1.696827
N	-4.791132	-0.035740	-0.435949
C	-4.230665	-1.346046	-1.009148
C	-6.310376	-0.030992	-0.391305
C	-4.157880	0.241649	0.939279
C	-4.335904	1.098656	-1.373539
C	-4.663883	1.483650	1.672932
C	-4.644116	0.938170	-2.863296
C	-7.006682	-1.020467	0.543823
C	-4.047901	-2.543599	-0.072754

C	-4.193283	2.197372	-3.627724
C	-4.432398	2.079616	-5.136233
C	-3.647647	-3.781393	-0.897316
C	-3.425409	-5.019873	-0.022823
C	-8.513892	-0.716051	0.611730
C	-9.273139	-1.706170	1.500701
C	-3.863526	1.667758	2.975543
C	-4.310224	2.902950	3.763334
H	-3.255665	-1.086626	-1.425488
H	-4.894496	-1.609622	-1.836847
H	-6.590182	0.988999	-0.118164
H	-6.645906	-0.197485	-1.417234
H	-3.078024	0.339461	0.732588
H	-4.342145	-0.645741	1.544644
H	-3.260767	1.174303	-1.192338
H	-4.808304	2.005395	-0.992472
H	-5.732371	1.403272	1.917239
H	-4.525021	2.382306	1.065571
H	-5.716421	0.784147	-3.041971
H	-4.118700	0.071945	-3.279298
H	-6.584633	-0.968660	1.553855
H	-6.870130	-2.047213	0.188916
H	-4.957319	-2.769613	0.492117
H	-3.257278	-2.333153	0.652846
H	-3.128296	2.375636	-3.436496
H	-4.731622	3.071985	-3.236590
H	-3.871329	1.239221	-5.561379
H	-4.109525	2.988975	-5.653659
H	-5.494576	1.924495	-5.363406
H	-2.731486	-3.560575	-1.460562
H	-4.427665	-3.993661	-1.642369
H	-2.618367	-4.856993	0.700494
H	-3.151182	-5.885316	-0.635090
H	-4.331658	-5.280089	0.537946
H	-8.936999	-0.734246	-0.402293
H	-8.661347	0.305207	0.988821
H	-9.176285	-2.732221	1.126421
H	-10.340305	-1.463323	1.535080
H	-8.893396	-1.688528	2.529110

H	-2.800333	1.753226	2.724431
H	-3.969064	0.771229	3.602825
H	-4.169115	3.816029	3.173454
H	-3.728516	3.009363	4.685207
H	-5.369938	2.841736	4.042468
C	-0.836292	0.168119	-1.111470
C	0.655931	0.402051	-1.329053
O	-1.259559	0.909853	-0.026678
I	1.389166	-0.590261	-3.226953
H	-1.354650	0.439185	-2.060113
H	-0.986872	-0.926808	-0.984701
H	1.274094	-0.043023	-0.550541
H	0.907152	1.449061	-1.477849
C	-1.759737	3.241546	-0.776208
O	-1.133471	3.204879	-1.768404
O	-2.467737	3.506972	0.125256

Cartesian coordinates of intermediate **I2**.

C	1.018499	2.879237	-2.715632
C	0.850463	3.618592	-1.508508
C	1.824723	3.197077	-0.616573
N	2.571445	2.249322	-1.272169
C	2.087822	2.017045	-2.535162
C	5.492628	-1.208322	-2.260808
C	5.073978	-0.082856	-3.019732
C	3.719915	0.098385	-2.799723
N	3.314133	-0.890793	-1.915870
C	4.388286	-1.701584	-1.588562
C	2.747481	1.038493	-3.493718
C	2.269595	-2.882687	2.404286
C	2.632055	-3.575852	1.215177
C	3.511250	-2.775164	0.510277
N	3.707133	-1.640654	1.265979
C	2.937384	-1.671559	2.405665
C	4.234415	-2.994499	-0.801892
C	4.109345	2.857963	2.339124
C	4.315713	1.675405	3.098122
C	3.293111	0.793241	2.798141
N	2.472758	1.415881	1.869388

C	2.963433	2.683035	1.584533
C	2.198448	3.707621	0.762177
C	2.965509	-0.552176	3.427499
C	3.430702	-4.002907	-1.662318
C	5.633855	-3.595774	-0.517251
C	3.508300	1.854629	-4.568828
C	1.658427	0.192983	-4.203957
C	0.911095	4.094610	1.534673
C	3.063347	4.983533	0.595424
C	4.029654	-0.882791	4.504592
C	1.580758	-0.465198	4.116509
H	0.437745	2.985984	-3.622878
H	0.135534	4.413316	-1.335837
H	3.303035	1.700912	-0.841451
H	6.488096	-1.628994	-2.240215
H	5.693874	0.506525	-3.680644
H	2.414273	-0.893112	-1.422062
H	1.586981	-3.232424	3.166812
H	2.273565	-4.548475	0.907294
H	4.234440	-0.835209	0.959873
H	4.720290	3.749088	2.370122
H	5.112830	1.504515	3.807616
H	1.766176	0.921901	1.307195
H	2.419759	-3.630210	-1.851573
H	3.353102	-4.972176	-1.155968
H	3.934060	-4.158208	-2.622410
H	6.251166	-2.904527	0.066229
H	5.524251	-4.520621	0.057628
H	6.162539	-3.828882	-1.448758
H	4.291448	2.470410	-4.114943
H	2.813723	2.523436	-5.086949
H	3.970895	1.191897	-5.308696
H	1.089941	-0.400257	-3.482101
H	0.958401	0.838725	-4.747267
H	2.124058	-0.490289	-4.922705
H	0.279685	3.213286	1.686257
H	1.171270	4.502414	2.517265
H	0.334210	4.852415	0.990036
H	3.998937	4.755910	0.075107

H	3.305992	5.427890	1.567345
H	2.517399	5.724208	0.002663
H	5.029822	-0.951703	4.064328
H	3.797056	-1.849386	4.961784
H	4.048139	-0.119666	5.291644
H	1.364347	-1.390112	4.663596
H	1.568494	0.364533	4.832152
H	0.786732	-0.318266	3.378422
N	-3.560179	1.981640	0.489091
C	-4.719073	1.029826	0.815388
C	-2.508747	1.309403	-0.414368
C	-4.115197	3.256331	-0.135016
C	-2.875175	2.358765	1.816360
C	-3.116097	4.379982	-0.414859
C	-2.546941	1.221316	2.784939
C	-3.006646	0.810000	-1.770602
C	-5.905377	0.948149	-0.152265
C	-1.870288	1.800945	4.043171
C	-1.779461	0.767985	5.171188
C	-6.853201	-0.181726	0.291268
C	-8.102187	-0.275613	-0.590926
C	-1.834220	0.333199	-2.645920
C	-3.827782	5.565318	-1.091702
C	-2.874557	6.729180	-1.382179
C	-2.311798	-0.150083	-4.019095
H	-5.097312	1.350563	1.789455
H	-4.259225	0.048408	0.947906
H	-1.711653	2.044390	-0.546605
H	-2.085681	0.485245	0.169263
H	-4.893205	3.607415	0.550773
H	-4.603536	2.960956	-1.063254
H	-1.961344	2.885867	1.538960
H	-3.552636	3.076299	2.292594
H	-2.307927	4.029006	-1.065456
H	-2.649259	4.729333	0.512489
H	-1.884750	0.481746	2.319914
H	-3.462601	0.705477	3.096641
H	-3.547859	1.595667	-2.315208
H	-3.703089	-0.026336	-1.637598

H	-5.583795	0.760071	-1.179419
H	-6.460875	1.893373	-0.156975
H	-2.429156	2.678863	4.401041
H	-0.864526	2.155140	3.784819
H	-2.777976	0.451600	5.497791
H	-1.258584	1.182690	6.040876
H	-1.233481	-0.123082	4.845970
H	-7.152957	-0.020463	1.336127
H	-6.314020	-1.137900	0.269124
H	-8.684538	0.653171	-0.558984
H	-8.753855	-1.090032	-0.258264
H	-7.836055	-0.468607	-1.636858
H	-1.297136	-0.474358	-2.137262
H	-1.110096	1.147106	-2.762874
H	-4.649526	5.914643	-0.450892
H	-4.289988	5.226499	-2.029137
H	-2.423731	7.113229	-0.459543
H	-3.403824	7.557426	-1.864901
H	-2.060516	6.419263	-2.047661
H	-1.465403	-0.483177	-4.628151
H	-3.008626	-0.993348	-3.929128
H	-2.826209	0.647523	-4.570810
C	0.074560	-1.027985	0.203308
C	-0.748862	-3.262689	-0.200201
C	-2.154408	-3.067825	-0.747490
O	0.995131	-0.233279	-0.087767
O	-0.835211	-0.936439	1.060944
O	0.068673	-2.176162	-0.626142
I	-3.498401	-4.742572	-0.193018
H	-0.293762	-4.168296	-0.610312
H	-0.767087	-3.322051	0.889358
H	-2.179543	-3.038485	-1.836356
H	-2.615861	-2.183867	-0.314850

Cartesian coordinates of transition state **P_TS**.

C	1.022527	3.026878	-2.197891
C	0.838347	3.548470	-0.883808
C	1.894981	3.108651	-0.102580
N	2.704605	2.361867	-0.924234

C	2.185580	2.274969	-2.193294
C	5.649795	-0.881263	-2.476277
C	5.239671	0.361415	-3.031907
C	3.883336	0.504514	-2.798887
N	3.468611	-0.624756	-2.109753
C	4.538119	-1.481352	-1.912421
C	2.915075	1.556070	-3.316048
C	2.438880	-3.225628	1.875191
C	2.749840	-3.717171	0.574995
C	3.664441	-2.852196	0.003251
N	3.927461	-1.877669	0.940747
C	3.170747	-2.069286	2.074785
C	4.370563	-2.879406	-1.337112
C	4.271622	2.434323	2.716607
C	4.545247	1.155606	3.273335
C	3.545782	0.290915	2.864616
N	2.675113	1.019876	2.070365
C	3.108978	2.333875	1.974076
C	2.281212	3.433247	1.328187
C	3.279124	-1.149318	3.274917
C	3.543859	-3.733506	-2.331510
C	5.763125	-3.536346	-1.164937
C	3.698278	2.609356	-4.140100
C	1.884455	0.873488	-4.251682
C	0.997146	3.647084	2.169916
C	3.089325	4.756218	1.333753
C	4.431180	-1.642454	4.186461
C	1.956885	-1.210806	4.080667
H	0.389943	3.207215	-3.057241
H	0.047667	4.214057	-0.561187
H	3.516015	1.846336	-0.611249
H	6.645320	-1.300329	-2.516901
H	5.867642	1.055979	-3.571982
H	2.570466	-0.710471	-1.627851
H	1.750681	-3.670646	2.580728
H	2.342741	-4.605214	0.111286
H	4.491801	-1.057700	0.766708
H	4.851565	3.333286	2.871195
H	5.371402	0.907753	3.924560

H	1.969204	0.596236	1.460731
H	2.532622	-3.332048	-2.446672
H	3.464207	-4.769270	-1.981628
H	4.031920	-3.740583	-3.311580
H	6.396037	-2.954802	-0.486346
H	5.645287	-4.539173	-0.742860
H	6.279580	-3.624990	-2.127585
H	4.445537	3.117358	-3.521904
H	3.007243	3.366261	-4.524137
H	4.209214	2.141795	-4.989180
H	1.299047	0.122683	-3.712663
H	1.192207	1.610603	-4.675407
H	2.402859	0.376903	-5.078743
H	0.393391	2.733858	2.187802
H	1.263575	3.903119	3.200737
H	0.388563	4.463472	1.761244
H	4.020452	4.648912	0.768576
H	3.338020	5.063305	2.355856
H	2.499058	5.551013	0.866989
H	5.392507	-1.607683	3.663466
H	4.245175	-2.679743	4.481059
H	4.507605	-1.031492	5.093456
H	1.788320	-2.221338	4.470092
H	2.003074	-0.520807	4.930084
H	1.102958	-0.945277	3.449907
N	-3.650175	1.771243	0.488453
C	-4.776347	0.748408	0.737885
C	-2.558641	1.212823	-0.439268
C	-4.256904	3.055795	-0.067103
C	-3.000221	2.097964	1.844712
C	-3.311045	4.239298	-0.277743
C	-2.579791	0.920166	2.726934
C	-3.012921	0.755826	-1.826144
C	-5.952746	0.684846	-0.242109
C	-2.059244	1.451288	4.077043
C	-1.719395	0.317676	5.049940
C	-6.876054	-0.485403	0.148758
C	-8.104679	-0.580030	-0.761182
C	-1.806224	0.377376	-2.704684

C	-4.081705	5.431834	-0.873365
C	-3.183257	6.652309	-1.098515
C	-2.237110	-0.028645	-4.117896
H	-5.168553	0.988414	1.729640
H	-4.286843	-0.225020	0.802886
H	-1.800808	1.995432	-0.520802
H	-2.095253	0.390839	0.108467
H	-5.052714	3.330591	0.632280
H	-4.728260	2.790622	-1.012770
H	-2.130905	2.718313	1.620233
H	-3.735701	2.716797	2.369918
H	-2.494695	3.969845	-0.956672
H	-2.852700	4.551362	0.667076
H	-1.799188	0.320002	2.246867
H	-3.428981	0.256879	2.925026
H	-3.578716	1.547282	-2.335065
H	-3.674374	-0.114401	-1.747760
H	-5.616651	0.542103	-1.272276
H	-6.528750	1.617442	-0.214508
H	-2.815095	2.108904	4.531060
H	-1.168563	2.070109	3.909424
H	-2.602745	-0.293859	5.270436
H	-1.344298	0.717753	5.997914
H	-0.949232	-0.340606	4.635150
H	-7.200074	-0.361452	1.191859
H	-6.311452	-1.425321	0.103402
H	-8.710347	0.333951	-0.719068
H	-8.741795	-1.418709	-0.462992
H	-7.811655	-0.743044	-1.804923
H	-1.254714	-0.448187	-2.241434
H	-1.106732	1.220175	-2.750367
H	-4.910312	5.703223	-0.204626
H	-4.539159	5.131264	-1.825881
H	-2.740725	6.999313	-0.157369
H	-3.753668	7.483712	-1.525436
H	-2.363022	6.420419	-1.787674
H	-1.365495	-0.292742	-4.725473
H	-2.904511	-0.898474	-4.097654
H	-2.764535	0.787614	-4.628157

C	0.274783	-1.175124	0.053702
C	-0.874721	-3.139713	-0.501926
C	-1.960806	-2.522333	0.352193
O	1.199343	-0.375896	-0.126914
O	-0.570205	-1.203261	1.019306
O	0.061493	-2.132369	-0.915919
I	-4.108650	-3.986248	-0.306599
H	-1.271969	-3.570985	-1.418601
H	-0.347570	-3.913404	0.065263
H	-2.524177	-1.692314	-0.033297
H	-2.120445	-2.817273	1.374245

Cartesian coordinates of product **P**.

C	0.325543	2.864301	-1.226585
C	0.321430	3.122223	0.175844
C	1.614675	2.962537	0.640563
N	2.385759	2.634651	-0.451845
C	1.622526	2.550262	-1.592903
C	5.508303	0.381856	-2.965926
C	4.783992	1.582809	-3.208766
C	3.474168	1.375317	-2.815494
N	3.397145	0.077849	-2.339841
C	4.630841	-0.542313	-2.428202
C	2.249190	2.264356	-2.946957
C	3.428413	-3.316041	1.130625
C	3.620500	-3.483190	-0.272149
C	4.297542	-2.372331	-0.742607
N	4.529967	-1.561861	0.347660
C	3.991893	-2.105314	1.492487
C	4.820951	-2.019487	-2.121652
C	4.559750	2.307713	2.860952
C	5.092856	1.012200	3.108869
C	4.150076	0.080756	2.714140
N	3.060596	0.788386	2.232804
C	3.298252	2.150542	2.317662
C	2.230425	3.186514	2.007884
C	4.151551	-1.433441	2.844146
C	4.067393	-2.855965	-3.186007
C	6.327592	-2.372207	-2.197590

C	2.660788	3.608956	-3.597638
C	1.211732	1.573004	-3.866085
C	1.127037	3.112617	3.092462
C	2.857645	4.603207	2.050857
C	5.490954	-1.890769	3.475077
C	2.997140	-1.870883	3.779584
H	-0.522189	2.920163	-1.896827
H	-0.528822	3.420325	0.774046
H	3.364569	2.384195	-0.409669
H	6.551323	0.209962	-3.191598
H	5.178189	2.486851	-3.651335
H	2.605562	-0.290103	-1.817835
H	2.943356	-4.013788	1.799969
H	3.302462	-4.328425	-0.867060
H	4.942146	-0.640067	0.298240
H	5.042112	3.248773	3.084823
H	6.053354	0.792319	3.552990
H	2.297019	0.371828	1.704754
H	2.990199	-2.667642	-3.146290
H	4.235690	-3.927738	-3.029508
H	4.428262	-2.595905	-4.186173
H	6.910319	-1.789123	-1.476829
H	6.468689	-3.433186	-1.969409
H	6.726304	-2.178473	-3.199757
H	3.395981	4.137715	-2.982348
H	1.782032	4.253123	-3.701213
H	3.093005	3.446621	-4.591424
H	0.872490	0.623298	-3.441205
H	0.334746	2.213654	-4.014840
H	1.656176	1.372395	-4.846443
H	0.640849	2.131502	3.093541
H	1.566526	3.277134	4.081250
H	0.361464	3.879985	2.926337
H	3.663269	4.702518	1.316390
H	3.267331	4.822538	3.043182
H	2.093036	5.351580	1.819913
H	6.342381	-1.602557	2.850055
H	5.497543	-2.980741	3.571398
H	5.626880	-1.452175	4.470251

H	3.018258	-2.954563	3.940800
H	3.098075	-1.379665	4.752981
H	2.021464	-1.611683	3.357331
N	-4.148616	1.143335	0.690842
C	-5.360367	0.222423	0.957146
C	-3.258586	0.606775	-0.443874
C	-4.643653	2.555515	0.419831
C	-3.300404	1.164138	1.967778
C	-3.582473	3.640828	0.232828
C	-2.780891	-0.184225	2.469441
C	-3.788501	0.708124	-1.872056
C	-6.620146	0.408332	0.109233
C	-2.085641	-0.003601	3.830543
C	-1.492863	-1.316574	4.352302
C	-7.640731	-0.681599	0.488704
C	-8.942993	-0.559438	-0.308335
C	-2.713951	0.194353	-2.847727
C	-4.239611	4.964471	-0.197038
C	-3.221422	6.099163	-0.349552
C	-3.179719	0.249160	-4.305727
H	-5.613949	0.385333	2.009255
H	-4.990802	-0.800852	0.833355
H	-2.307857	1.139113	-0.351638
H	-3.100633	-0.450292	-0.212548
H	-5.298959	2.806510	1.260368
H	-5.265963	2.493829	-0.472214
H	-2.456355	1.825523	1.764670
H	-3.930672	1.639445	2.727179
H	-2.851363	3.342624	-0.526677
H	-3.026796	3.809199	1.161927
H	-2.065698	-0.609283	1.758835
H	-3.590387	-0.913490	2.570034
H	-4.056458	1.738525	-2.140692
H	-4.677968	0.082831	-1.988326
H	-6.396863	0.318823	-0.957357
H	-7.073011	1.394948	0.268977
H	-2.804179	0.395109	4.561156
H	-1.287729	0.746734	3.740712
H	-2.270682	-2.078500	4.480294

H	-1.003587	-1.168152	5.321009
H	-0.748295	-1.712303	3.652958
H	-7.860731	-0.616722	1.563983
H	-7.186726	-1.664893	0.316880
H	-9.429835	0.409971	-0.141566
H	-9.651243	-1.342955	-0.018848
H	-8.758297	-0.661930	-1.384240
H	-2.469036	-0.840683	-2.580235
H	-1.794180	0.782524	-2.727439
H	-5.003023	5.251462	0.539594
H	-4.769830	4.814287	-1.147486
H	-2.712592	6.306245	0.599251
H	-3.710675	7.023353	-0.674703
H	-2.452928	5.846987	-1.089334
H	-2.396796	-0.115966	-4.978963
H	-4.067680	-0.375081	-4.458577
H	-3.430372	1.273411	-4.610374
C	0.733254	-1.584647	-0.122996
C	-0.250331	-3.455040	-0.992470
C	-0.339278	-3.489440	0.539711
O	1.334167	-0.534166	-0.062682
O	0.128534	-2.172613	0.925338
O	0.566596	-2.287234	-1.253654
I	-4.128825	-3.187359	-0.389246
H	-1.232328	-3.310487	-1.450358
H	0.254042	-4.321629	-1.422310
H	-1.367132	-3.610075	0.886272
H	0.327785	-4.224198	0.997406

Cartesian coordinates of transition state **II**_TS in a 1,2-alternate conformation.

C	-1.933768	0.814905	-3.575294
C	-2.126872	-0.596987	-3.558613
C	-3.290119	-0.855710	-2.855476
N	-3.787420	0.364679	-2.455252
C	-2.979974	1.400042	-2.882778
C	-3.267883	2.853721	-2.540150
C	-5.094695	0.919912	3.356559
C	-4.217282	2.038548	3.360111
C	-3.080118	1.685162	2.657437

N	-3.259078	0.382472	2.224763
C	-4.482467	-0.100901	2.650480
C	-1.841588	2.500766	2.317182
C	-6.280468	-1.985950	-1.143556
C	-6.521212	-1.818902	0.249099
C	-5.293575	-1.711807	0.882065
N	-4.325496	-1.813797	-0.094981
C	-4.908548	-1.985006	-1.334497
C	-4.071261	-2.135767	-2.592323
C	-4.955809	-1.521884	2.358139
C	-0.574830	1.605020	2.376001
C	-1.674387	3.623758	3.362874
C	-4.794572	3.074517	-2.357431
C	-2.793865	3.746847	-3.706072
C	-3.094331	-3.326300	-2.440938
C	-4.999243	-2.413592	-3.800665
C	-6.221434	-1.801368	3.193349
C	-3.868808	-2.542934	2.788961
C	-1.577782	4.376127	0.465626
C	-1.947260	4.462868	-0.907889
C	-2.557977	3.272235	-1.258728
N	-2.555351	2.479024	-0.129127
C	-1.969385	3.133810	0.934864
H	-1.115349	1.342974	-4.046596
H	-1.490868	-1.336448	-4.026703
H	-4.653681	0.452520	-1.941756
H	-6.066084	0.871261	3.828482
H	-4.405221	2.997083	3.824402
H	-2.563236	-0.167059	1.706614
H	-7.030266	-2.116260	-1.912137
H	-7.489222	-1.789255	0.729396
H	-3.311672	-1.710776	0.057494
H	-0.630716	0.780112	1.661279
H	-0.456223	1.178823	3.380331
H	0.312712	2.205994	2.142693
H	-2.514373	4.323598	3.335244
H	-1.612057	3.195059	4.368164
H	-0.756795	4.191963	3.173611
H	-5.187825	2.529980	-1.491393

H	-5.348302	2.759255	-3.249969
H	-4.992909	4.136090	-2.178915
H	-1.713983	3.662852	-3.862268
H	-3.299378	3.455584	-4.632189
H	-3.024124	4.798338	-3.504247
H	-2.422101	-3.182307	-1.590178
H	-3.656791	-4.252533	-2.281383
H	-2.482734	-3.448818	-3.342374
H	-5.700025	-1.587424	-3.959860
H	-5.577812	-3.331339	-3.644196
H	-4.401024	-2.527905	-4.710373
H	-7.031836	-1.109975	2.942988
H	-6.000774	-1.693795	4.260226
H	-6.575140	-2.820976	3.010301
H	-3.652961	-2.429019	3.857873
H	-4.223502	-3.565150	2.612041
H	-2.934567	-2.408729	2.237107
H	-1.098675	5.151835	1.047385
H	-1.802979	5.316935	-1.555461
H	-2.902207	1.529335	-0.087191
N	5.471867	0.311439	0.213833
C	5.038560	-0.410229	1.500636
C	4.308483	0.415364	-0.797289
C	6.045066	1.674581	0.579518
C	6.593466	-0.521229	-0.419309
C	6.731908	2.455320	-0.544518
C	6.277325	-1.981741	-0.743210
C	3.369283	1.617553	-0.684603
C	4.014636	0.272793	2.405323
C	7.436145	-2.605281	-1.542098
C	7.193846	-4.086394	-1.851272
C	3.836558	-0.563008	3.687576
C	2.813941	0.054003	4.646835
C	2.273108	1.520706	-1.762815
C	1.331546	2.727901	-1.739508
C	7.029189	3.895884	-0.091634
C	7.769887	4.705306	-1.160736
H	5.969892	-0.583737	2.050458
H	4.630247	-1.371295	1.181740

H	4.777641	0.420615	-1.784478
H	3.746302	-0.517633	-0.695820
H	6.750346	1.489911	1.396084
H	5.217998	2.255506	0.985123
H	7.438075	-0.457660	0.274991
H	6.872481	0.005484	-1.333486
H	6.101406	2.484042	-1.441209
H	7.673464	1.974077	-0.831667
H	5.350930	-2.066580	-1.320583
H	6.122990	-2.561037	0.172247
H	3.913181	2.559674	-0.823707
H	2.893119	1.664057	0.298938
H	3.047123	0.338041	1.898677
H	4.318452	1.289613	2.681374
H	8.374237	-2.495501	-0.979209
H	7.573120	-2.050470	-2.481002
H	7.094150	-4.672277	-0.930560
H	8.024822	-4.505464	-2.428481
H	6.274971	-4.224582	-2.431743
H	4.806137	-0.661902	4.196419
H	3.520417	-1.576252	3.409927
H	3.119346	1.057923	4.966449
H	2.702251	-0.562595	5.544754
H	1.827995	0.138672	4.176068
H	1.697249	0.599902	-1.612032
H	2.744024	1.434761	-2.752772
H	0.843676	2.846380	-0.766143
H	0.534632	2.610813	-2.478785
H	1.869001	3.658337	-1.963087
H	7.625862	3.872268	0.830724
H	6.086225	4.397904	0.163556
H	8.735324	4.248457	-1.408624
H	7.963126	5.725464	-0.813699
H	7.184049	4.772928	-2.084982
C	-0.446905	-1.259896	-0.155268
C	-0.002663	-2.361096	0.728053
O	-1.646755	-1.228165	0.534687
I	2.456041	-3.121191	0.170197
H	0.167161	-0.348070	-0.063177

H	-0.525464	-1.531927	-1.216594
H	-0.438649	-3.337796	0.561389
H	0.214393	-2.110166	1.757803

Cartesian coordinates of transition state **II_TS** in a partial cone conformation.

C	-2.635268	4.215671	1.363443
C	-3.427593	3.676823	2.412057
C	-3.207389	2.311894	2.452917
N	-2.298073	2.018718	1.450562
C	-1.945331	3.173360	0.772235
C	-0.956185	3.194594	-0.388243
C	-3.189098	-0.109978	-3.515570
C	-3.373046	-1.322777	3.406978
C	-3.903665	-2.330472	2.551439
C	-4.650393	-1.703131	1.571913
N	-4.593777	-0.350082	1.833455
C	-3.803395	-0.095395	2.937508
C	-3.634954	1.299333	3.505190
C	-5.513401	-2.265452	0.458413
C	-3.712527	0.034788	-4.959062
C	-2.086746	-1.200287	-3.523217
C	0.276266	2.321515	-0.033489
C	-0.463237	4.640615	-0.594350
C	-4.977554	1.748309	4.138647
C	-2.560477	1.265696	4.621978
C	-5.090707	-3.727425	0.167811
C	-6.990605	-2.271814	0.927477
C	-2.573410	2.454540	-3.708901
C	-1.938227	3.381998	-2.836055
C	-1.593346	2.704064	-1.680262
N	-1.996031	1.394232	-1.845774
C	-2.605742	1.225765	-3.072550
C	-6.363822	-1.041569	-1.712288
C	-5.706551	-0.479688	-2.839875
C	-4.342722	-0.547876	-2.617480
N	-4.164881	-1.143397	-1.380733
C	-5.391408	-1.449819	-0.817407
H	-2.579071	5.256814	1.077806
H	-4.064006	4.237858	3.082599

H	-2.069730	1.070605	1.145259
H	-2.751137	-1.486249	4.276126
H	-3.757006	-3.396956	2.652158
H	-4.958038	0.358030	1.210429
H	-4.486228	0.804611	-5.031735
H	-4.138620	-0.912909	-5.302401
H	-2.893751	0.313775	-5.630789
H	-1.652546	-1.343967	-2.530973
H	-2.501128	-2.159531	-3.854161
H	-1.279442	-0.913917	-4.207409
H	-0.000230	1.271417	0.096127
H	0.736662	2.672990	0.898267
H	1.016861	2.385330	-0.841303
H	-1.287070	5.311365	-0.853187
H	0.007301	5.016254	0.320149
H	0.267725	4.677249	-1.409630
H	-5.768793	1.818074	3.385442
H	-5.289153	1.022944	4.897261
H	-4.879557	2.727432	4.620667
H	-1.594489	0.935831	4.225955
H	-2.853121	0.585973	5.430809
H	-2.434257	2.268632	5.041355
H	-4.043515	-3.781568	-0.145565
H	-5.710697	-4.137424	-0.635810
H	-5.216913	-4.358308	1.055463
H	-7.640342	-2.726229	0.170988
H	-7.081724	-2.849779	1.852616
H	-7.349419	-1.255970	1.122572
H	-2.972772	2.672609	-4.689518
H	-1.773077	4.432544	-3.032150
H	-1.848187	0.656265	-1.155340
H	-7.431495	-1.159897	-1.588906
H	-6.185818	-0.077443	-3.721336
H	-3.279972	-1.208051	-0.869899
N	4.969831	0.439517	-0.496382
C	5.316541	-0.980009	-0.994739
C	3.920644	0.412371	0.627273
C	6.244743	1.154570	-0.068975
C	4.367669	1.208193	-1.681442

C	6.104367	2.607869	0.388973
C	3.145168	0.596876	-2.366549
C	4.355138	-0.087533	2.003664
C	6.375263	-1.782145	-0.235403
C	2.696555	1.503147	-3.529089
C	1.439818	0.977543	-4.230187
C	6.490423	-3.184843	-0.862531
C	7.549567	-4.045274	-0.166613
C	3.207647	0.121192	3.009606
C	3.562103	-0.393392	4.407981
C	7.462146	3.144478	0.877591
C	7.384188	4.605616	1.331654
C	-0.763485	-1.360585	0.950151
C	-0.055497	-1.745185	-0.279553
O	-1.641612	-0.675686	0.105775
I	2.208803	-3.159456	0.237871
H	5.647642	-0.845425	-2.028858
H	4.373093	-1.532397	-0.996223
H	3.544231	1.435849	0.698260
H	3.117113	-0.229828	0.262929
H	6.921572	1.089810	-0.927025
H	6.676115	0.558424	0.733977
H	5.186564	1.323168	-2.399115
H	4.112273	2.198582	-1.301490
H	5.376164	2.687920	1.204470
H	5.746196	3.247027	-0.425503
H	2.317422	0.494823	-1.658066
H	3.363601	-0.404247	-2.751828
H	5.248347	0.435976	2.367102
H	4.581075	-1.156584	1.960138
H	6.110066	-1.890372	0.819870
H	7.355377	-1.292052	-0.280249
H	3.517785	1.596062	-4.254202
H	2.501423	2.515310	-3.148638
H	1.599864	-0.032746	-4.625619
H	1.164225	1.626900	-5.067079
H	0.584667	0.946991	-3.547285
H	6.737891	-3.088245	-1.929181
H	5.513977	-3.681098	-0.808639

H	8.543810	-3.584779	-0.223395
H	7.612732	-5.034485	-0.631592
H	7.306414	-4.191991	0.892242
H	2.316468	-0.402823	2.643620
H	2.952281	1.189061	3.060395
H	3.769925	-1.469204	4.389491
H	2.733564	-0.226879	5.103993
H	4.445951	0.116117	4.812164
H	8.203631	3.048609	0.072492
H	7.823430	2.520211	1.706160
H	7.060898	5.259971	0.513574
H	8.361171	4.960034	1.675919
H	6.674344	4.727878	2.158090
H	-1.216315	-2.187152	1.506927
H	-0.186746	-0.721359	1.635995
H	0.509910	-0.988327	-0.802431
H	-0.473328	-2.540429	-0.881007

Cartesian coordinates of transition state **II**_TS in a cone conformation.

C	1.777063	2.879888	3.261537
C	1.553007	3.701447	2.122234
C	1.532100	2.885390	1.006465
N	1.728132	1.590498	1.455978
C	1.890335	1.570460	2.830786
C	2.105840	0.290974	3.633335
C	1.339210	3.233996	-0.464989
C	0.919173	-0.682888	3.405402
C	2.122453	0.652107	5.132823
C	0.927989	4.716259	-0.570382
C	0.185395	2.384353	-1.063107
C	5.475338	-1.361196	3.298730
C	4.565378	-0.561283	4.042394
C	3.414524	-0.410752	3.291688
N	3.617424	-1.107453	2.112123
C	4.871164	-1.691619	2.101006
C	6.971181	-0.440317	-1.785591
C	7.107810	-1.340149	-0.692147
C	5.841598	-1.627908	-0.219218
N	4.951436	-0.923617	-1.006807

C	5.623601	-0.189425	-1.966608
C	5.383800	-2.518766	0.928050
C	4.906683	0.650051	-3.016380
C	6.579234	-3.367382	1.405634
C	4.280567	-3.493354	0.436588
C	3.877582	-0.232385	-3.774084
C	5.943993	1.141499	-4.045734
C	3.467362	3.937031	-1.858640
C	4.465407	3.213309	-2.567657
C	4.200879	1.864171	-2.422071
N	3.061653	1.765256	-1.643511
C	2.604083	3.021313	-1.287617
H	1.853144	3.218993	4.284895
H	1.431551	4.775556	2.125341
H	1.802778	0.781893	0.845202
H	0.831732	-0.981899	2.357980
H	-0.024657	-0.206811	3.697524
H	1.052611	-1.592226	4.002193
H	2.934152	1.346429	5.368120
H	1.176752	1.123211	5.420318
H	2.258719	-0.251358	5.734767
H	1.702693	5.374512	-0.167314
H	0.761942	4.987589	-1.617639
H	0.004827	4.895591	-0.009070
H	0.401913	1.313599	-1.014215
H	0.027371	2.648415	-2.115407
H	-0.745043	2.568190	-0.510607
H	6.463912	-1.663057	3.614856
H	4.737079	-0.152316	5.028105
H	2.966336	-1.153993	1.335317
H	7.777558	-0.030778	-2.377602
H	8.036166	-1.732859	-0.301586
H	3.945065	-0.921163	-0.863370
H	7.401385	-2.738877	1.760008
H	6.955394	-3.985122	0.583775
H	6.272949	-4.022713	2.227241
H	3.395499	-2.965867	0.066239
H	4.664358	-4.111922	-0.382349
H	3.962903	-4.151335	1.253676

H	3.109085	-0.633219	-3.106414
H	4.383645	-1.083334	-4.243642
H	3.373270	0.352554	-4.552013
H	6.445817	0.287742	-4.511592
H	5.451857	1.727298	-4.828552
H	6.706162	1.769973	-3.575610
H	3.390510	5.013065	-1.788058
H	5.281185	3.641663	-3.132585
H	2.661888	0.893136	-1.303871
N	-5.686114	0.073823	-0.374128
C	-5.028919	-0.185893	-1.740424
C	-4.655573	0.013560	0.774033
C	-6.423137	1.405690	-0.422803
C	-6.722316	-1.035969	-0.151982
C	-7.322453	1.737402	0.771216
C	-6.219959	-2.478603	-0.221830
C	-3.895795	1.295277	1.123943
C	-4.050452	0.852777	-2.284471
C	-7.329349	-3.443696	0.233721
C	-6.898484	-4.910355	0.127599
C	-3.615523	0.439248	-3.703741
C	-2.620700	1.428223	-4.318977
C	-2.925361	1.018765	2.288804
C	-2.169603	2.276147	2.729952
C	-7.799493	3.198570	0.692840
C	-8.750484	3.566996	1.835937
C	1.122269	-1.440612	-1.390708
C	0.278001	-1.567537	-0.207006
O	1.973313	-0.791881	-0.467063
I	-2.165678	-2.762304	-0.859873
H	-5.867676	-0.311182	-2.433572
H	-4.502463	-1.137554	-1.642437
H	-5.214863	-0.318631	1.652396
H	-3.954525	-0.780652	0.498779
H	-7.012978	1.383994	-1.344688
H	-5.660203	2.174113	-0.540278
H	-7.503206	-0.866309	-0.900837
H	-7.155348	-0.843513	0.831134
H	-6.788097	1.584371	1.716512

H	-8.198958	1.080252	0.790586
H	-5.333137	-2.621069	0.404274
H	-5.918390	-2.737233	-1.241461
H	-4.582865	2.094251	1.427500
H	-3.326413	1.669897	0.268476
H	-3.159021	0.899217	-1.652029
H	-4.489562	1.856989	-2.322204
H	-8.233107	-3.280957	-0.371085
H	-7.608222	-3.215670	1.272203
H	-6.656140	-5.178174	-0.907012
H	-7.696945	-5.577279	0.469657
H	-6.008943	-5.106636	0.736255
H	-4.502318	0.359354	-4.348662
H	-3.164440	-0.559653	-3.657948
H	-3.051261	2.434029	-4.398841
H	-2.327911	1.109738	-5.324805
H	-1.709165	1.500632	-3.714919
H	-2.211816	0.240954	1.989403
H	-3.489025	0.608464	3.138900
H	-1.561676	2.689871	1.918338
H	-1.482824	2.052742	3.551482
H	-2.861866	3.056573	3.070592
H	-8.300022	3.367279	-0.270615
H	-6.927661	3.866511	0.708556
H	-9.650841	2.941438	1.822259
H	-9.069046	4.611414	1.757311
H	-8.267879	3.438166	2.811916
H	1.515065	-2.378541	-1.797824
H	0.735441	-0.799455	-2.191218
H	-0.276715	-0.708259	0.134852
H	0.476697	-2.361328	0.497856