Supplementary Information

Insights into the promotion mechanism of multiple electrophilic sites in CO_2 cycloaddition via simulation and experiment

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Characterization instrument

Fourier transform infrared (FT-IR) spectra of the samples were performed at room temperature using an IRT Racer-100 with KBr as the standard. Thermogravimetric and Differential Thermal Analysis (TG-DTA) tests were carried out using a TG-DTA8122 thermal analyzer in an N_2 atmosphere with a heating rate of 10 °C/min (25 to 600 °C). The ^{13}C NMR spectra were determined using a Bruker Avance III-500 MHz spectrometer. Inductively coupled plasma optical emission spectroscopy (ICP-OES) was performed on Optima 5300DV (Pekin-Elmer). X-ray photoelectron spectroscopy (XPS) analysis was carried out on a Thermo Scientific Nexsa spectrometer, and the C 1s peak was at 284.5 eV. Scanning electron microscopy (SEM) images and energy dispersive spectroscopy (EDS) mapping images of the as-synthesized catalyst were investigated using a JSM-IT800 field emission electron microscope with an acceleration voltage of 0.01-30 kV. The strength and content of acid/base sites on the catalyst were determined by performing temperature programmed desorption of ammonia (NH_3-TPD) and CO_2 (CO_2-TPD) using a BeL-II. After the catalyst was pretreated at 50 ℃ in a helium atmosphere for 60 min, the catalyst was then adsorbed with 10% NH_3/He (or 10% CO_2/He) at 50 ℃ for 60 min. The samples were then purged in a He atmosphere at 50 ℃ for 60 min and desorbed from 50 to 200℃ with a heating rate of 5 ℃/min, followed by a 1 h hold to finish desorption. The product yield and selectivity were determined using a Gas Chromatograph (GC-2010) equipped with an FID detector and an HP-FFAP capillary column (30 m × 0.53 mm). The DFT calculation details are presented in the Supplementary Material.

Computation details

All structures were optimized and characterized in ideal gas phase model at B3LYP [1]-D3 [2]/BSI level, BSI representing a basis set with SDD [3] for Sn, Br, MWB46 for Sn and 6-31G(d,p) for C, H, O, N and Sn atoms. Harmonic frequency analysis calculations at the same level were performed to verify the optimized geometries to be minima (no imaginary frequency) or transition states (TSs, having unique one imaginary frequency). The energies were further improved by M06 [4]/BSII//B3LYP-D3/BSI single-point calculations, BSII denotes a basis set with SDD for Sn, Br, MWB46 for Sn and 6-311++G(d,p) for C, H, O, N and Sn atoms. When necessary, intrinsic reaction coordinate (IRC) calculations [5] were carried out at the B3LYP-D3/BSI level to verify a TS correctly connecting with its nearby minima. All DFT calculations were carried out using Gaussian 09 program [6]. Selected computed structures are illustrated using the CYLview [7] .

1. Supporting Figures

2. Supporting Tables

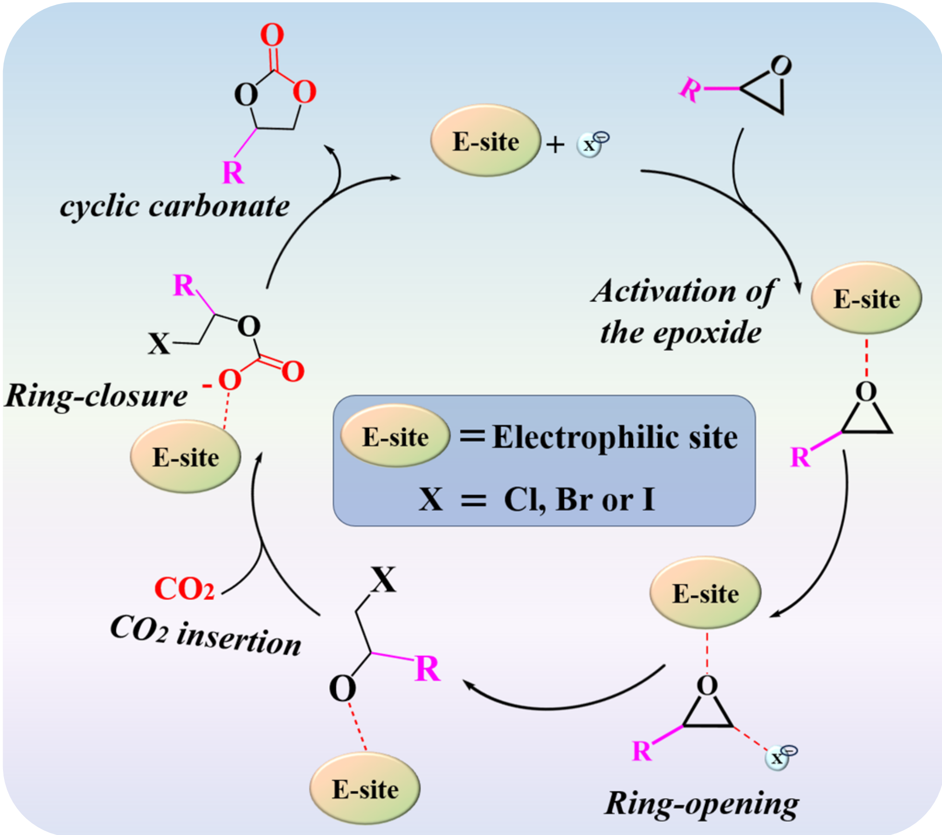

Fig. S1. The most commonly proposed mechanism for the formation of cyclic carbonates from CO_2 and epoxides.

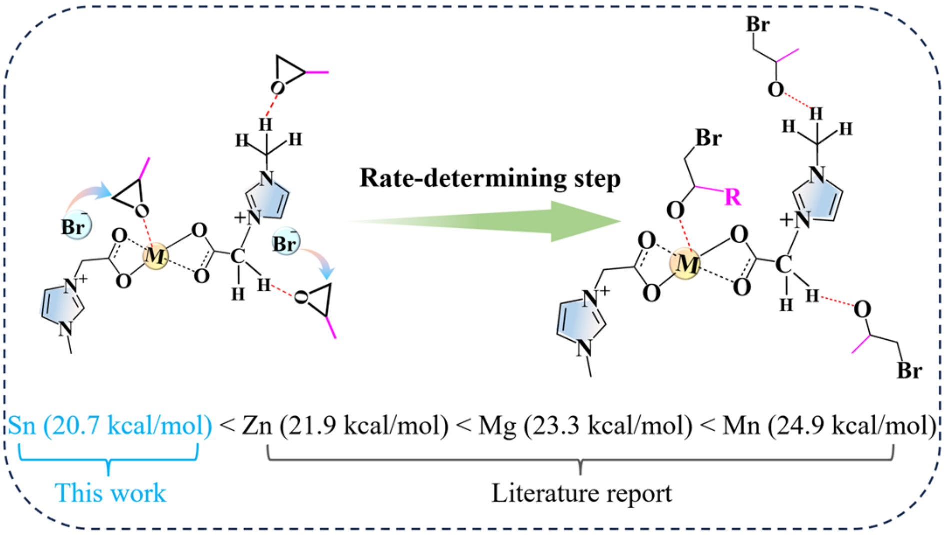

Fig. S2. The rate-determining step in the cycloaddition reaction process of PO and CO_2

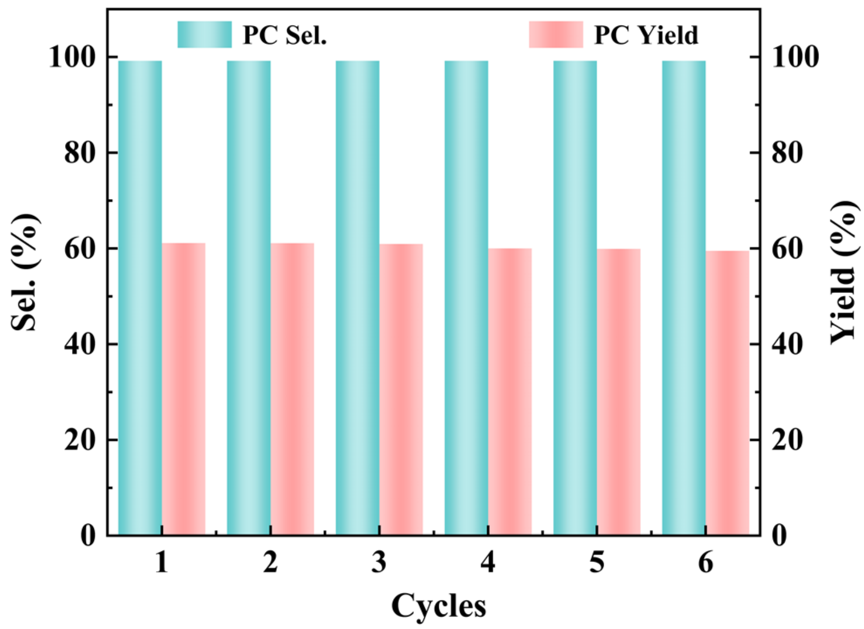

Fig. S3. Recyclability studies for the cycloaddition of CO_2 and PO catalyzed by $[EIMBr\text{-}COO]_2Sn$ (Weakened reaction condition: 0.14 mol PO, 4.76×10^{-4} mol catalyst, 2.4 MPa CO_2, 90 ℃, 2 h).

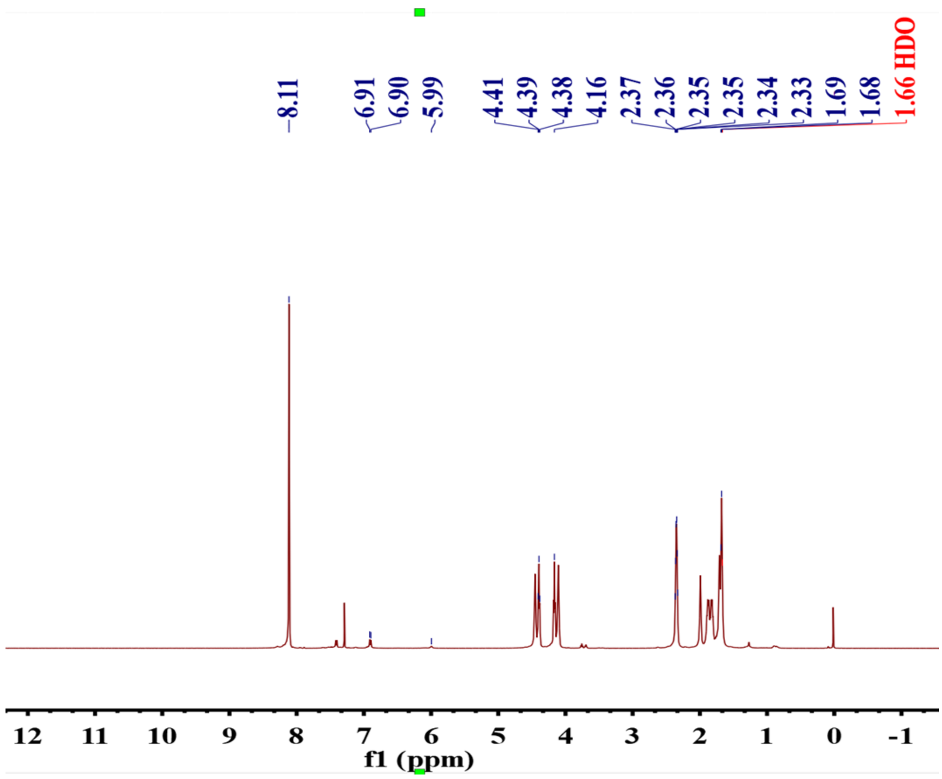

Fig. S4. ^1H NMR spectrum of recycled $[EIMBr\text{-}COO]_2Sn$

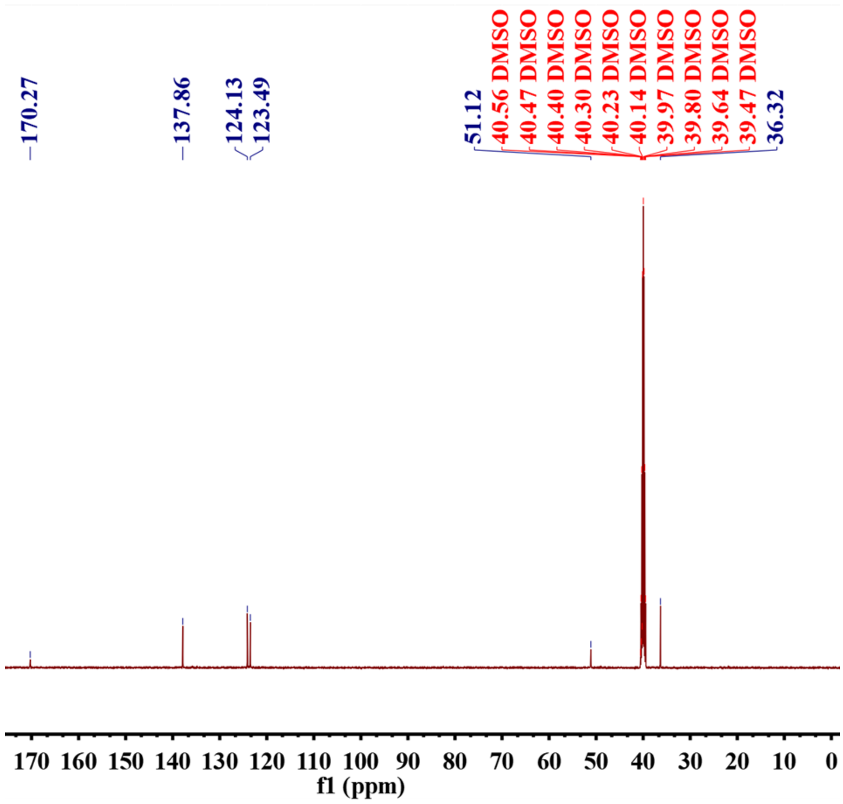

Fig. S5. ^{13}C NMR spectrum of recycled $[EIMBr\text{-}COO]_2Sn$

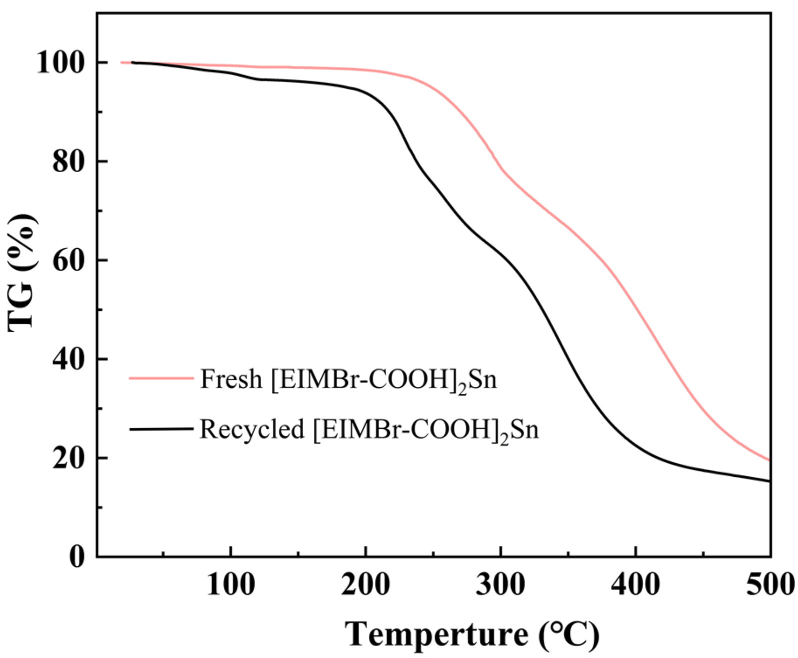

Fig. S6. TG curves of fresh and recycled $[EIMBr\text{-}COO]_2Sn$

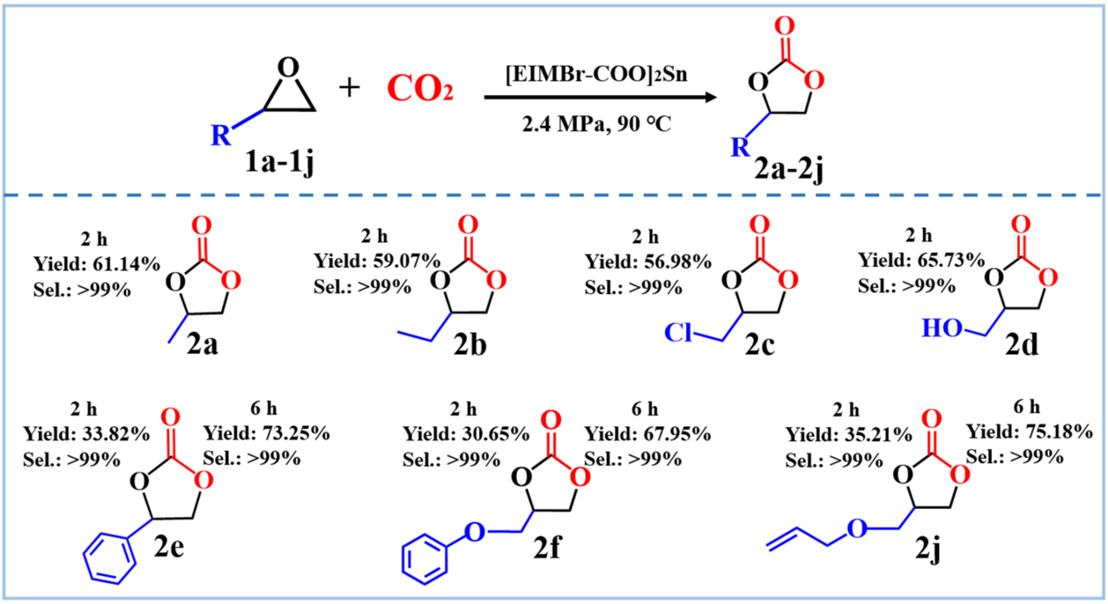

Fig. S7. Catalytic performance of $[EIMBr\text{-}COO]_2Sn$ for the cycloaddition of CO2 with various epoxides. Weakened reaction condition: epoxides (0.14 mol), $[EIMBr\text{-}COO]_2Sn$ (4.76×10^{-4} mol), 90 °C, 2.4 MPa CO_2.

Table S1 Comparison of the activation energies of PO and CO_2 reactions catalyzed by different catalysts.

Entry	Catalyst	*Ea* kJ/mol	Ref.
1	DTAB-IL	43.93	[8]
2	PAN-PD-BrOH	30.26	[9]
3	PIL-DVB-IV	77.74	[10]
4	Zn-NPCIH	30.80	[11]
5	[bmim]Br	57.40	[12]
6	$[P_{4,4,4,2}NH_2][Br]$-DEG	56.23	[13]
7	Mim/$ZnBr_2$	41.10	[14]
8	Multi-hydroxyl ILs	37.20	[15]
9	$[EIMBr\text{-}COO]_2Sn$	26.23	This work

Table S2 Calculation atomic coordinates of [ECOOHIM]Br

[ECOOHIM]Br	q(N)	q(N+1)	q(N-1)	f^-	f^+	△f
1(C)	-0.0067	-0.0551	0.0527	0.0593	0.0484	-0.0109
2(C)	-0.0051	-0.0392	0.0551	0.0602	0.0341	-0.0261
3(C)	0.1006	-0.0079	0.11	0.0094	0.1085	0.0991
4(N)	0.0067	-0.0447	0.0435	0.0369	0.0513	0.0145

5(H)	0.0721	0.0375	0.1041	0.032	0.0346	0.0026
6(H)	0.066	0.0428	0.0944	0.0284	0.0233	-0.0051
7(H)	0.0772	0.0307	0.0989	0.0217	0.0465	0.0247
8(N)	0.0025	-0.0365	0.0386	0.0361	0.039	0.0029
9(C)	-0.0109	-0.0364	0.0058	0.0167	0.0255	0.0089
10(H)	0.0459	0.0235	0.0567	0.0108	0.0225	0.0117
11(H)	0.0508	0.0216	0.0735	0.0228	0.0292	0.0064
12(H)	0.0527	0.0266	0.0765	0.0238	0.0262	0.0024
13(C)	0.0151	-0.0154	0.0238	0.0088	0.0305	0.0217
14(H)	0.0531	0.0123	0.0606	0.0075	0.0409	0.0334
15(H)	0.0633	0.0167	0.0774	0.0141	0.0465	0.0325
16(C)	0.2214	0.1408	0.2273	0.0058	0.0806	0.0748
17(O)	-0.2607	-0.3471	-0.239	0.0218	0.0864	0.0646
18(Br)	-0.5751	-0.7171	-0.0254	0.5498	0.142	-0.4077
19(O)	-0.1649	-0.2158	-0.1477	0.0172	0.0509	0.0337
20(H)	0.196	0.1629	0.213	0.017	0.0332	0.0161

Table S3 Calculation atomic coordinates of $[EIMBr\text{-}COO]_2Sn$

$[EIMBr\text{-}COO]_2Sn$	q(N)	q(N+1)	q(N-1)	f^-	f^+	△f
1(C)	0.0067	-0.0017	0.0158	0.0084	0.0090	-0.0006
2(C)	-0.0062	-0.0067	0.0170	0.0005	0.0233	-0.0227
3(C)	0.0889	0.0842	0.1047	0.0046	0.0158	-0.0112
4(N)	0.0323	0.0318	0.0346	0.0005	0.0023	-0.0018
5(H)	0.0699	0.0599	0.0872	0.0100	0.0173	-0.0072
6(H)	0.0688	0.0656	0.0843	0.0032	0.0155	-0.0123
7(H)	0.0436	0.0467	0.0734	-0.0031	0.0298	-0.0328
8(N)	0.0208	0.0203	0.0318	0.0005	0.0110	-0.0106
9(C)	-0.0137	-0.0226	0.0007	0.0089	0.0144	-0.0055
10(H)	0.0565	0.0363	0.0666	0.0203	0.0101	0.0101
11(H)	0.0530	0.0448	0.0644	0.0082	0.0114	-0.0032
12(H)	0.0330	0.0320	0.0543	0.0009	0.0213	-0.0204
13(C)	0.0214	0.0082	0.0243	0.0132	0.0029	0.0104
14(H)	0.0524	0.0563	0.0614	-0.0039	0.0090	-0.0128
15(H)	0.0652	0.0521	0.0721	0.0131	0.0069	0.0061
16(C)	0.2028	0.1754	0.1985	0.0274	-0.0042	0.0316
17(O)	-0.2650	-0.2972	-0.2607	0.0322	0.0042	0.0280
18(O)	-0.2504	-0.2928	-0.2597	0.0425	-0.0094	0.0518
19(C)	0.0033	-0.0073	0.0158	0.0106	0.0124	-0.0019
20(C)	-0.0017	-0.0069	0.0170	0.0052	0.0187	-0.0135
21(C)	0.0952	0.0840	0.1047	0.0113	0.0095	0.0018
22(N)	0.0234	0.0283	0.0345	-0.0049	0.0111	-0.0160
23(H)	0.0611	0.0516	0.0872	0.0094	0.0261	-0.0167

24(H)	0.0527	0.0547	0.0843	-0.0020	0.0316	-0.0337
25(H)	0.0808	0.0542	0.0732	0.0266	-0.0076	0.0342
26(N)	0.0164	0.0244	0.0318	-0.0080	0.0154	-0.0234
27(C)	-0.0046	-0.0204	0.0008	0.0157	0.0054	0.0103
28(H)	0.0569	0.0451	0.0666	0.0118	0.0097	0.0021
29(H)	0.0610	0.0364	0.0644	0.0246	0.0035	0.0211
30(H)	0.0503	0.0374	0.0543	0.0129	0.0040	0.0088
31(C)	0.0200	0.0047	0.0243	0.0153	0.0043	0.0109
32(H)	0.0505	0.0468	0.0613	0.0037	0.0108	-0.0072
33(H)	0.0700	0.0526	0.0721	0.0174	0.0021	0.0153
34(C)	0.2019	0.1785	0.1986	0.0234	-0.0033	0.0267
35(O)	-0.2515	-0.2896	-0.2607	0.0381	-0.0093	0.0473
36(O)	-0.2710	-0.3222	-0.2598	0.0512	0.0112	0.0400
37(Br)	-0.6006	-0.6652	-0.2909	0.0647	0.3096	-0.2450
38(Br)	-0.6235	-0.6557	-0.2907	0.0321	0.3328	-0.3007
39(Sn)	0.6295	0.1761	0.6405	0.4534	0.0110	0.4425

Cartesian Coordinates in Å, SCF Energies and Free Energies (in a.u.) at 298.15 K and 1 atm for the Optimized Structures [BSI= 6-31G(d,p), BSII=6-311++G(d,p)

Cat-Sn
B3LYP-D3/BSI SCF energy in gas: -1017.153197 a.u.
M06/BSII SCF energy in gas: -1016.675417 a.u.
M06/BSII free energy in gas: -1016.444153 a.u.

C	1.36310600	-0.07198900	2.76092400
C	0.01230300	0.10142500	2.72642200
C	0.95786900	1.83686500	1.70479400
N	1.92769900	1.02431700	2.12745900
H	1.96897200	-0.89129300	3.11357700
H	-0.79478900	-0.52248900	3.06693600
H	1.06381600	2.72367600	1.07206800
N	-0.22214000	1.29598400	2.05050900
C	3.35925900	1.24637600	1.90896900
H	3.47465100	2.08050100	1.21613900
H	3.84186800	1.48605100	2.85909400
H	3.78205700	0.32941700	1.48986900
C	-1.50731900	1.91761000	1.70745200
H	-1.30444100	2.75237400	1.02824000

H	-1.99373600	2.28483600	2.61737600
C	-2.44459200	0.94245200	1.01057800
O	-2.52225400	-0.26818400	1.43789400
O	-3.12519200	1.30957100	0.02444000
C	2.06494000	0.71472000	-1.86150600
C	0.87662300	0.18705500	-1.46372300
C	2.25153300	-1.48841100	-1.93706800
N	2.90329400	-0.34612900	-2.17329600
H	2.33848500	1.75416000	-1.96327200
H	-0.03694700	0.69247600	-1.20782900
H	2.66708400	-2.47714700	-2.02756700
N	0.99897100	-1.19886200	-1.54899500
C	4.34190900	-0.26763700	-2.41660000
H	4.62464600	-0.97650200	-3.19675700
H	4.58718800	0.74320800	-2.74200300
H	4.86309600	-0.51466500	-1.48670000
C	0.16432200	-2.21942500	-0.91524100
H	0.56204700	-2.39765800	0.09281000
H	0.26585100	-3.15802200	-1.46674000
C	-1.30659700	-1.88879800	-0.80578400
O	-1.79287700	-0.84160500	-1.36392200
O	-2.03473700	-2.63924400	-0.10987700
Br	3.36037100	-2.23243700	0.81420900
Br	0.44731400	3.73305600	-0.95776300
Sn	-3.74866500	-0.96807000	-0.30108400

1a
B3LYP-D3/BSI SCF energy in gas: -193.1173659 a.u.
M06/BSII SCF energy in gas: -193.0331465 a.u.
M06/BSII free energy in gas: -192.9738755 a.u.

C	-0.15151400	-0.04047400	0.49121500
C	1.04341600	0.61582000	-0.06025800
H	-0.15703000	-0.25614800	1.56301100
H	1.87322200	0.88381800	0.59523800
H	0.94944300	1.22676500	-0.95966600
C	-1.50953600	0.10094900	-0.14909200
H	-2.08045600	-0.82836200	-0.05120100
H	-2.08211000	0.90317900	0.32957500
H	-1.40790200	0.32851000	-1.21412700
O	0.82632900	-0.78944200	-0.24425200

IM1-Sn
B3LYP-D3/BSI SCF energy in gas: -1210.301438 a.u.
M06/BSII SCF energy in gas: -1209.746597 a.u.
M06/BSII free energy in gas: -1209.438285 a.u.

C	5.11198100	-2.01775000	0.29391600
C	4.02848400	-2.67639000	0.79349900
C	3.43073100	-0.57887600	0.39586500

N	4.71615700	-0.71269700	0.04656400
H	6.11162000	-2.35971500	0.08037500
H	3.87816000	-3.70892400	1.05613500
H	2.85800000	0.34249900	0.27110200
N	2.99657500	-1.75740900	0.86173900
C	5.54975900	0.35689400	-0.51321000
H	6.34378000	0.60849800	0.19357100
H	5.98643000	0.01233900	-1.45273900
H	4.91694500	1.22906800	-0.69687800
C	1.61302700	-2.04606900	1.24469000
H	1.03766000	-1.12135000	1.19778900
H	1.59334100	-2.41259300	2.27528600
C	0.97348600	-3.12337000	0.32098700
O	1.71082700	-3.83019300	-0.35945300
O	-0.30855800	-3.17254400	0.40938700
C	0.29099100	3.90523800	1.51054600
C	0.13713900	3.02262800	2.53525100
C	-1.32570100	2.49565600	0.95393000
N	-0.64017500	3.56613400	0.54643100
H	1.00542600	4.69586100	1.35733700
H	0.66261000	2.92675400	3.47104200
H	-2.10013700	1.97702500	0.38616300
N	-0.87175100	2.14600300	2.16631000
C	-0.75941600	4.18082700	-0.77788600
H	-1.59024500	3.70961500	-1.30348100
H	-0.95181100	5.24948800	-0.66456600
H	0.17799900	4.00811700	-1.31318900
C	-1.37762800	1.01778400	2.94780400
H	-2.32986100	1.27793500	3.41470400
H	-0.65651000	0.80675000	3.74126100
C	-1.60071000	-0.26204300	2.12154400
O	-1.00913400	-0.32848500	0.97582800
O	-2.33983000	-1.12799900	2.59104400
Sn	-2.12130900	-1.96450600	-0.10982300
Br	-3.61582200	0.60026900	-0.88768500
Br	2.46659300	2.51389000	-0.71202200
C	-0.00900200	0.07346900	-2.00301500
C	0.60526700	-1.21616700	-2.34713700
H	0.21342700	0.48167800	-1.02104900
H	1.28222300	-1.72289000	-1.66733000
H	0.72150800	-1.48670500	-3.39470900
C	-0.45194700	1.05936100	-3.04245000
H	-1.39040600	1.52347800	-2.72890900
H	0.32392400	1.82446700	-3.14622500
H	-0.61571200	0.56936500	-4.00610800
O	-0.79009400	-1.17108300	-1.93205700

TS1-Sn

B3LYP-D3/BSI SCF energy in gas: -1210.272788 a.u.

M06/BSII SCF energy in gas: -1209.705958 a.u.

M06/BSII free energy in gas: -1209.397023 a.u.

C	-6.03766800	0.44867600	0.74708200
C	-5.13979200	1.22030600	1.42342400
C	-4.07924200	-0.57924200	0.69883500
N	-5.35058100	-0.66842600	0.30008800
H	-7.08638400	0.59445200	0.54476300
H	-5.25181100	2.17765200	1.90576100
H	-3.29435700	-1.28658000	0.42691300
N	-3.93180300	0.54910300	1.40234400
C	-5.88910000	-1.77229400	-0.50271600
H	-6.57421800	-2.37073500	0.10145300
H	-6.41581400	-1.36054700	-1.36522000
H	-5.05359200	-2.38712000	-0.84411800
C	-2.62103800	1.09101900	1.75387200
H	-1.99015600	0.28244900	2.12599300
H	-2.73727600	1.83347700	2.54574100
C	-1.95522500	1.72621700	0.50436000
O	-2.62930500	1.91530100	-0.50628900
O	-0.70624100	1.95463400	0.69528700
C	0.40094700	-1.67362600	2.18275400
C	0.89706300	-0.44277300	2.49824500
C	2.44427800	-1.51900100	1.32722200
N	1.38398800	-2.32664800	1.45426500
H	-0.54729800	-2.14073400	2.39343800
H	0.46065500	0.39637000	3.01476600
H	3.38369600	-1.69893500	0.76857100
N	2.17105600	-0.37259400	1.95995900
C	1.29428500	-3.67891200	0.89750800
H	2.18298300	-3.85662200	0.29171500
H	1.25333900	-4.40868800	1.70946500
H	0.39790400	-3.75048500	0.27757800
C	3.03372100	0.81948100	1.94343700
H	3.97417500	0.52997200	1.45668800
H	3.20934900	1.15202300	2.96670700
C	2.34442800	1.92886800	1.13638700
O	1.97163700	1.51196600	-0.04182300
O	2.16325900	3.04558700	1.60379200
Sn	0.50741800	2.69596700	-1.04066900
Br	5.29427600	-1.23248600	-0.28302700
Br	-1.98331900	-2.74329100	-0.95743400
C	0.31906300	-0.41029400	-1.43076800
C	-1.03565800	-0.55036000	-1.97923100
H	0.34689100	-0.30667000	-0.34471900
H	-1.85518700	-0.00628300	-1.53680900
H	-1.14382400	-0.88263100	-3.00428200
C	1.42296500	-1.29156000	-1.96444100
H	2.39929700	-0.93285300	-1.62502600
H	1.27891900	-2.32001500	-1.62156400
H	1.40815200	-1.28796200	-3.05817800

O	0.21282300	0.84941800	-2.11502600

IM2-Sn
B3LYP-D3/BSI SCF energy in gas: -1210.313007 a.u.
M06/BSII SCF energy in gas: -1209.753489 a.u.
M06/BSII free energy in gas: -1209.441551 a.u.

C	-1.90642000	1.88356600	-1.98671000
C	-1.12529400	1.20421100	-2.87700200
C	0.20117600	2.03917900	-1.31603500
N	-1.05521200	2.39105900	-1.01948200
H	-2.97832300	2.00565500	-1.89858900
H	-1.37919900	0.62738500	-3.75016700
H	1.07267800	2.27246000	-0.72205000
N	0.18513200	1.32733400	-2.45164700
C	-1.46675700	3.19840400	0.13805000
H	-1.61336300	4.23455000	-0.17441500
H	-2.41040900	2.79290200	0.51400100
H	-0.68230500	3.14569000	0.89406100
C	1.33410300	0.60177300	-2.99666100
H	2.24346900	1.15426200	-2.76277500
H	1.21604500	0.54123400	-4.08086700
C	1.36742000	-0.82401800	-2.37451300
O	2.53597700	-1.14385600	-1.93989000
O	0.31911600	-1.46381000	-2.33789300
C	-4.19054200	-2.37868100	1.93487000
C	-2.86901100	-2.05626900	1.98326700
C	-3.64809900	-1.46778900	-0.00205100
N	-4.65609700	-2.02449500	0.67818500
H	-4.83310600	-2.83801800	2.66783700
H	-2.11875600	-2.21923300	2.73666900
H	-3.71406100	-1.05439300	-0.99226900
N	-2.54840500	-1.49727900	0.75701800
C	-6.05438500	-1.98333100	0.25118300
H	-6.40783900	-0.95036100	0.32773000
H	-6.13111600	-2.32379000	-0.78279800
H	-6.63538800	-2.64717600	0.89171500
C	-1.28672300	-0.85619900	0.39635000
H	-1.25258800	0.13605200	0.85486200
H	-1.25193900	-0.74013700	-0.68853900
C	-0.05075100	-1.67217500	0.79655800
O	-0.14586000	-2.77926400	1.31177900
O	1.03818100	-1.03376200	0.48907200
Br	-4.74575000	1.45330100	0.02757400
Br	2.32370400	2.97785300	1.62902000
C	3.68634200	0.59840800	0.41212600
C	3.08957500	1.05560200	1.74056600
H	2.92206600	0.73505100	-0.36846100
H	2.22347500	0.45735200	2.00848200
H	3.82307200	1.10546000	2.54386700

C	4.95088300	1.35088200	0.00927500
H	5.32462400	0.94195000	-0.93344300
H	4.76600100	2.42255300	-0.11328300
H	5.72356900	1.20894300	0.77168700
O	3.99020300	-0.75950800	0.61620300
Sn	2.78594100	-2.28389800	-0.04884700

CO_2
B3LYP-D3/BSI SCF energy in gas: -188.5777604 a.u.
M06/BSII SCF energy in gas: -188.5583831 a.u.
M06/BSII free energy in gas: -188.5674851 a.u.

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16976100
O	0.00000000	0.00000000	-1.16976100

TS2-Sn
B3LYP-D3/BSI SCF energy in gas: -1398.899742 a.u.
M06/BSII SCF energy in gas: -1398.310646 a.u.
M06/BSII free energy in gas: -1397.989931 a.u.

C	5.46326900	2.38335600	-0.22759300
C	4.69206800	2.46751500	-1.34709900
C	3.80254400	0.92976400	-0.02464300
N	4.89291800	1.41527400	0.58170400
H	6.35460600	2.91570600	0.06183700
H	4.77956700	3.09022300	-2.22244300
H	3.16273200	0.15916700	0.39517400
N	3.67041600	1.54555800	-1.20722100
C	5.38207800	1.00272400	1.90255300
H	4.77662800	0.16198700	2.25041900
H	6.42701200	0.69786900	1.81649900
H	5.29372600	1.84129300	2.59670800
C	2.53295400	1.36154200	-2.10850200
H	2.49292200	0.32620200	-2.46114700
H	2.65867100	2.02244400	-2.96679600
C	1.19055600	1.65475400	-1.40292100
O	1.15040100	1.85639900	-0.19977900
O	0.20236700	1.62723500	-2.24957700
C	-2.24169100	-3.72093400	0.83818400
C	-1.38017900	-3.91080900	-0.19752100
C	-0.28370200	-2.85120900	1.40759600
N	-1.53629400	-3.05845900	1.82924700
H	-3.28867900	-3.95074300	0.94206000
H	-1.53540800	-4.33833800	-1.17390200
H	0.52411400	-2.34727900	1.93778600
N	-0.16149700	-3.37893600	0.18315100
C	-2.09245900	-2.60037600	3.10158200
H	-1.33894800	-2.00731700	3.61938400
H	-2.96590900	-1.98170300	2.89008100

H	-2.37002200	-3.45971700	3.71605900
C	0.97974400	-3.14408800	-0.70329400
H	1.13952900	-4.02607500	-1.32644700
H	1.86692700	-2.97548800	-0.08482200
C	0.76290900	-1.91092900	-1.60383800
O	-0.32831900	-1.26739300	-1.33892300
O	1.61436900	-1.65032600	-2.44868600
Sn	-1.37587800	0.18305600	-2.56922500
Br	2.89835000	-1.72683100	2.08613000
Br	-2.77947900	3.53982400	2.25811000
C	-1.93703600	1.41973600	0.37005100
C	-3.20246400	2.08526900	0.90321800
H	-1.28067200	2.18166000	-0.06036400
H	-3.74204900	2.59465800	0.10703300
H	-3.84958400	1.38391700	1.42446600
C	-1.14025200	0.63378600	1.40603600
H	-0.33390500	0.09940900	0.90365300
H	-0.69218400	1.31414300	2.13271500
H	-1.78587000	-0.07430300	1.92718300
O	-2.39808300	0.58183800	-0.70796300
O	-3.72973200	-0.99347300	0.75261200
C	-3.37427900	-0.97945700	-0.38822700
O	-3.34137100	-1.50718000	-1.46693100

IM3-Sn
B3LYP-D3/BSI SCF energy in gas: -1398.9058 a.u.
M06/BSII SCF energy in gas: -1398.318615 a.u.
M06/BSII free energy in gas: -1397.995593 a.u.

C	5.46326900	2.38335600	-0.22759300
C	4.69206800	2.46751500	-1.34709900
C	3.80254400	0.92976400	-0.02464300
N	4.89291800	1.41527400	0.58170400
H	6.35460600	2.91570600	0.06183700
H	4.77956700	3.09022300	-2.22244300
H	3.16273200	0.15916700	0.39517400
N	3.67041600	1.54555800	-1.20722100
C	5.38207800	1.00272400	1.90255300
H	4.77662800	0.16198700	2.25041900
H	6.42701200	0.69786900	1.81649900
H	5.29372600	1.84129300	2.59670800
C	2.53295400	1.36154200	-2.10850200
H	2.49292200	0.32620200	-2.46114700
H	2.65867100	2.02244400	-2.96679600
C	1.19055600	1.65475400	-1.40292100
O	1.15040100	1.85639900	-0.19977900
O	0.20236700	1.62723500	-2.24957700
C	-2.24169100	-3.72093400	0.83818400
C	-1.38017900	-3.91080900	-0.19752100
C	-0.28370200	-2.85120900	1.40759600

N	-1.53629400	-3.05845900	1.82924700
H	-3.28867900	-3.95074300	0.94206000
H	-1.53540800	-4.33833800	-1.17390200
H	0.52411400	-2.34727900	1.93778600
N	-0.16149700	-3.37893600	0.18315100
C	-2.09245900	-2.60037600	3.10158200
H	-1.33894800	-2.00731700	3.61938400
H	-2.96590900	-1.98170300	2.89008100
H	-2.37002200	-3.45971700	3.71605900
C	0.97974400	-3.14408800	-0.70329400
H	1.13952900	-4.02607500	-1.32644700
H	1.86692700	-2.97548800	-0.08482200
C	0.76290900	-1.91092900	-1.60383800
O	-0.32831900	-1.26739300	-1.33892300
O	1.61436900	-1.65032600	-2.44868600
Sn	-1.37587800	0.18305600	-2.56922500
Br	2.89835000	-1.72683100	2.08613000
Br	-2.77947900	3.53982400	2.25811000
C	-1.93703600	1.41973600	0.37005100
C	-3.20246400	2.08526900	0.90321800
H	-1.28067200	2.18166000	-0.06036400
H	-3.74204900	2.59465800	0.10703300
H	-3.84958400	1.38391700	1.42446600
C	-1.14025200	0.63378600	1.40603600
H	-0.33390500	0.09940900	0.90365300
H	-0.69218400	1.31414300	2.13271500
H	-1.78587000	-0.07430300	1.92718300
O	-2.39808300	0.58183800	-0.70796300
O	-3.72973200	-0.99347300	0.75261200
C	-3.37427900	-0.97945700	-0.38822700
O	-3.34137100	-1.50718000	-1.46693100

TS3-Sn
B3LYP-D3/BSI SCF energy in gas: -1398.893649 a.u.
M06/BSII SCF energy in gas: -1398.296907 a.u.
M06/BSII free energy in gas: -1397.971917 a.u.

C	-2.09436200	1.71062300	-2.39666200
C	-0.87071900	1.70418400	-2.99752400
C	-0.74992700	3.02644600	-1.21905400
N	-1.99396600	2.54022000	-1.29244900
H	-3.00330100	1.16092500	-2.59945100
H	-0.49534800	1.17120700	-3.85594600
H	-0.37083600	3.64956100	-0.41771000
N	-0.04974500	2.53856000	-2.25355400
C	-3.08294200	2.84068700	-0.35099200
H	-3.74861600	3.58434700	-0.79423900
H	-3.63242500	1.91350200	-0.16993700
H	-2.64450500	3.22692800	0.57081800
C	1.38315100	2.72783400	-2.49072300

H	1.72716700	3.56025800	-1.87654300
H	1.53619000	2.94544100	-3.54833800
C	2.11439700	1.42718300	-2.11195900
O	2.37142100	1.32565100	-0.84607800
O	2.35457600	0.57204500	-2.96154700
C	-1.22759900	-3.38177900	2.01896000
C	-0.25920100	-3.53514400	1.07554500
C	-2.11901500	-2.87994000	0.05328000
N	-2.37876700	-2.97789300	1.36237100
H	-1.18307800	-3.48404700	3.09046000
H	0.79036500	-3.75102100	1.18664600
H	-2.81917600	-2.48495900	-0.68241500
N	-0.83711000	-3.21757600	-0.14317300
C	-3.66822900	-2.65885400	1.98491000
H	-4.25315800	-2.06334300	1.27919500
H	-4.19508000	-3.58149400	2.23818500
H	-3.48414200	-2.07807500	2.89056300
C	-0.16083700	-3.24010700	-1.44135400
H	-0.81867800	-2.75691800	-2.16838100
H	0.01039200	-4.27210000	-1.75191900
C	1.19351600	-2.50976000	-1.42701200
O	2.11572800	-2.94596000	-2.10153900
O	1.22789300	-1.44988200	-0.66864200
Br	-4.33640100	-0.61793900	-1.09608600
Br	-0.16834800	3.63288600	2.25044000
C	0.05238200	0.51122300	2.45472700
C	1.16068000	1.44213800	1.98751800
H	-0.41788400	0.92982500	3.34377900
H	1.87113900	1.82948300	2.70239800
H	1.24338500	1.75801600	0.96332600
C	-0.97120900	0.22116200	1.36803600
H	-1.73909600	-0.45714400	1.74005900
H	-1.45814300	1.14932600	1.07392500
H	-0.48911000	-0.23038500	0.49707400
O	0.64280300	-0.74522300	2.90787500
O	2.28346400	-0.08983800	1.55957900
C	1.75900300	-1.10271900	2.23670300
O	2.20542700	-2.23410700	2.26895600
Sn	3.23384500	-0.65412400	-0.43123000

product

B3LYP-D3/BSI SCF energy in gas: -381.7291259 a.u.
M06/BSII SCF energy in gas: -381.6112474 a.u.
M06/BSII free energy in gas: -381.5384024 a.u.

C	-1.09110200	-0.10276200	0.50463600
C	-0.57618200	1.31348600	0.18706800
H	-1.58033900	-0.15185600	1.48106200
H	-0.46804000	1.93330200	1.08413400
H	-1.18815500	1.83949900	-0.54929100

C	-1.97019700	-0.70308000	-0.58239700
H	-2.16192000	-1.75891100	-0.37679900
H	-2.92795900	-0.17455100	-0.63045500
H	-1.47714300	-0.62157800	-1.55642400
O	0.13998700	-0.85022700	0.60517600
O	0.71938400	1.07298900	-0.37636100
C	1.14274300	-0.17328600	-0.01928200
O	2.23712800	-0.60676900	-0.22786200

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