Supporting Information

Hydrosilylative Reduction of Carbon Dioxide by Homoleptic Lanthanum Aryloxide Catalyst with High Activity and Selectivity

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General Procedures: All experiments were carried out under a dry Argon atmosphere using standard Schlenk techniques or in a glovebox. Solvents (including deuterated solvents used for NMR) were dried and distilled prior to use. NMR spectra were recorded on a Bruker 400 MHz spectrometer. Chemical shifts were reported as δ units with reference to the residual solvent resonance or an external standard. Coupling constants J are given in Hz. Elemental analysis data was recorded on a Carlo-Erba EA-1110 instrument. Fourier transform infrared spectroscopy was measured with a Bruker VERTEX70. $B(C_6F_5)_3$ was purchased from Strem and sublimed for three times prior to use. Silanes were purchased from TCI and dried prior to use. $RE(OAr)_3$ [Ar = 2,6-*t*Bu_2-C_6H_3, RE = La (**4a**), Y (**4b**), Sc (**4c**); Ar = 2,6-*i*Pr_2-C_6H_3, RE = La (**5**)][1,2] were synthesized by following the literature procedures. Methane was detected by Agilent 7890B gas chromatograph, equipped with a molecular sieve and two prepack q columns to analyze the gas product (Argon as the carrier gas). The following operating conditions were used: carrier gas: N_2, initial flow rate: 1.0 mL/min, injection temperature of 250 °C, column temperature program: 100 °C (8 min); detector temperature of TCD was 220 °C.

$$V_{CH_4}\% = \frac{A_i}{A_s} \times 10.3\% \qquad V_{H_2}\% = \frac{A_i}{A_s} \times 1.0\%$$

$$n_{CH_4} = \frac{PV}{RT} \times V_{CH_4}\% \qquad n_{H_2} = \frac{PV}{RT} \times V_{H_2}\%$$

A_i: the peak area of CH_4 (H_2)

A_s: the peak area of standard gas with V_{CH_4}% (V_{H_2}%) equals to 10.3% (1.0%)

P: total pressure of Parr autoclave (KPa)

V: total volume of Parr autoclave (L)

T: the temperature when detected the gaseous products (K)

R: 8.314 J/(mol·K)

Computational details: All DFT calculations were performed with Gaussian 09.[3] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[4] Si and La atoms were treated with a Stuttgart effective core potential[5] augmented with a polarization function (ζ_d = 0.284 for Si and ζ_f = 1.000 for La).[6] For B, F, O, C and H atoms, Pople's double-ζ basis set 6-31G(d,p) was used.[7] Calculations of vibrational frequencies were systematically done in order to characterize the nature of stationary points. Analytical frequency calculations at 298.15 K and 1 atm were systematically done in order to characterize the nature of stationary points. IRC calculations were carried out in order to confirm the connectivity between reactant(s), transition state and product(s).

References

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[7] (a) P. C. Hariharan, J. A. Pople, *Theor. Chem. Acc.* **1973**, *28*, 213-222; (b) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* **1972**, *56*, 2257-2261.

General procedures for the catalytic hydrosilylation of CO_2

In the presence of 1 bar CO_2: In a glove box, an oven-dried J-Young NMR tube was charged with $RE(OAr)_3$, $B(C_6F_5)_3$, silane, mesitylene, and 0.5 mL of C_6D_6. The tube was sealed and removed from the glove box. The mixture was degassed by a freeze-pump-thaw cycle and charged with 1 bar CO_2 at room temperature. The reaction was monitored by NMR spectroscopy. Conversion of silane was determined by ^1H NMR with mesitylene as an internal standard. TON was determined by ^1H NMR based on mol of silane reacted per mol of metal catalyst. *Note*: Stock solutions were used for the measurement of $RE(OAr)_3$ and $B(C_6F_5)_3$.

In the presence of 5 bar CO_2: In a glove box, a stainless steel Parr reactor containing a stir bar was charged with $La(OAr)_3$, $B(C_6F_5)_3$, silane, mesitylene, and 0.5 mL of C_6D_6. The reactor was taken out of the glove box, charged with 5 bar CO_2 and then sealed. The reaction mixture was allowed to stir at room temperature for desired time. Afterwards, the excess CO_2 was released and the reaction mixture was subjected to NMR spectroscopy. Conversion of silane were determined by ^1H NMR with mesitylene as an internal standard. TON was determined by ^1H NMR based on mol of silane reacted per mol of metal catalyst. *Note*: Stock solutions were used for the measurement of $La(OAr)_3$ and $B(C_6F_5)_3$.

NMR spectra of CO_2 hydrosilylation reactions

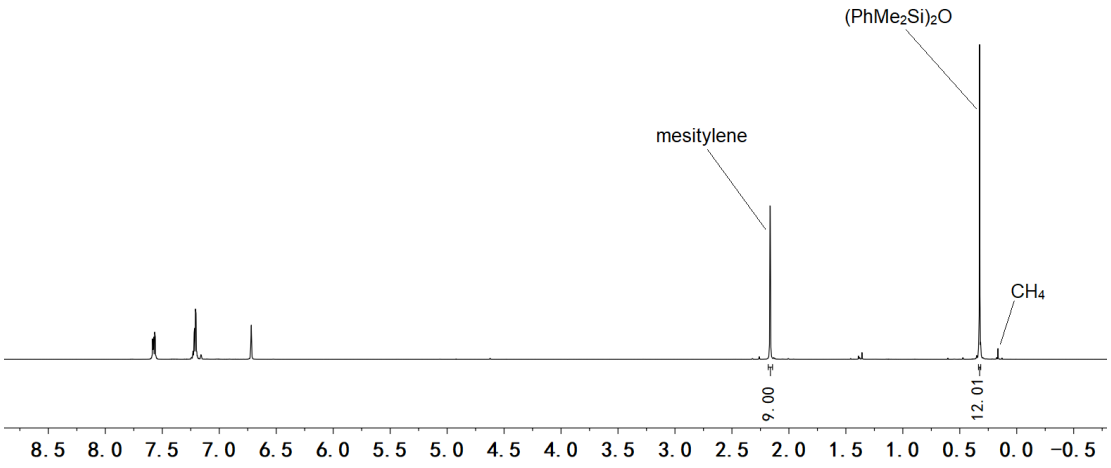


Fig. S1. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), $PhMe_2SiH$ (68.2 mg, 0.5 mmol), mesitylene (30.1 mg, 0.25 mmol)] (table 1, entry 1)

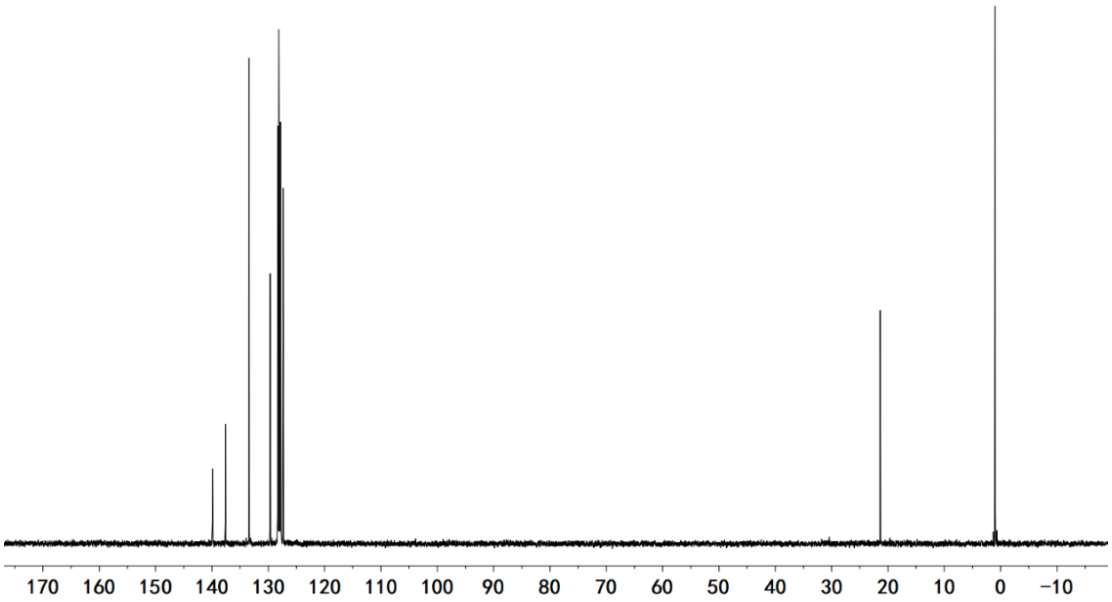


Fig. S2. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), $PhMe_2SiH$ (68.2 mg, 0.5 mmol), mesitylene (30.1 mg, 0.25 mmol)] (table 1, entry 1)

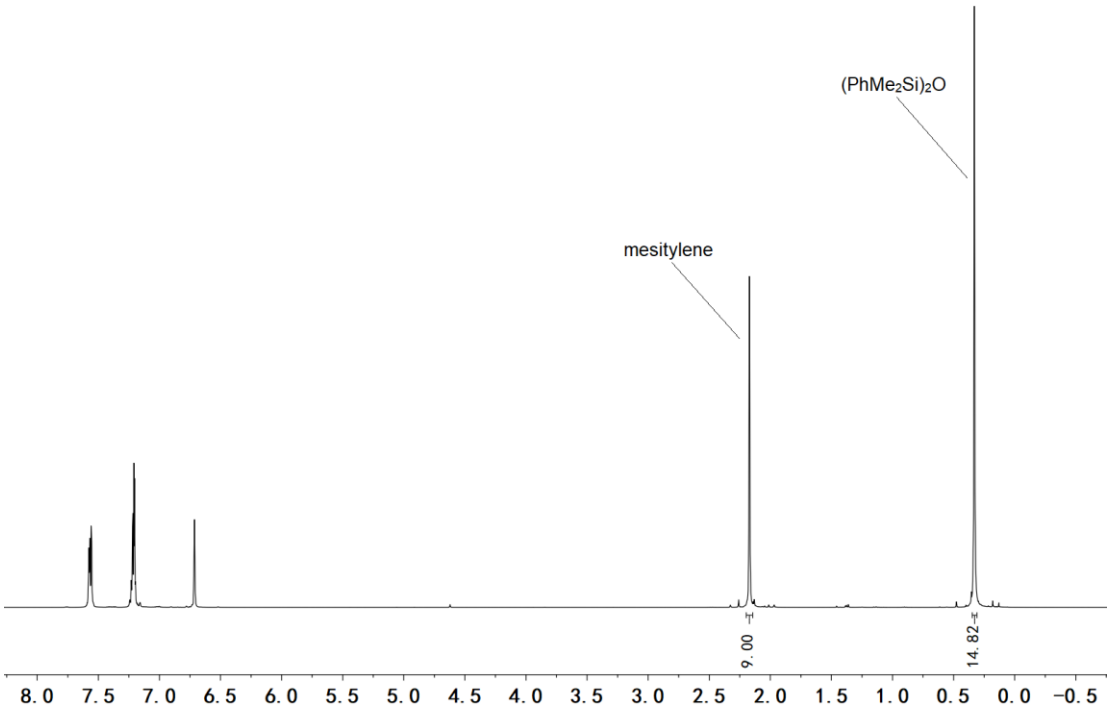


Fig. S3. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), $PhMe_2SiH$ (340.8 mg, 2.5 mmol), mesitylene (120.2 mg, 1.0 mmol)] (table 1, entry 2)

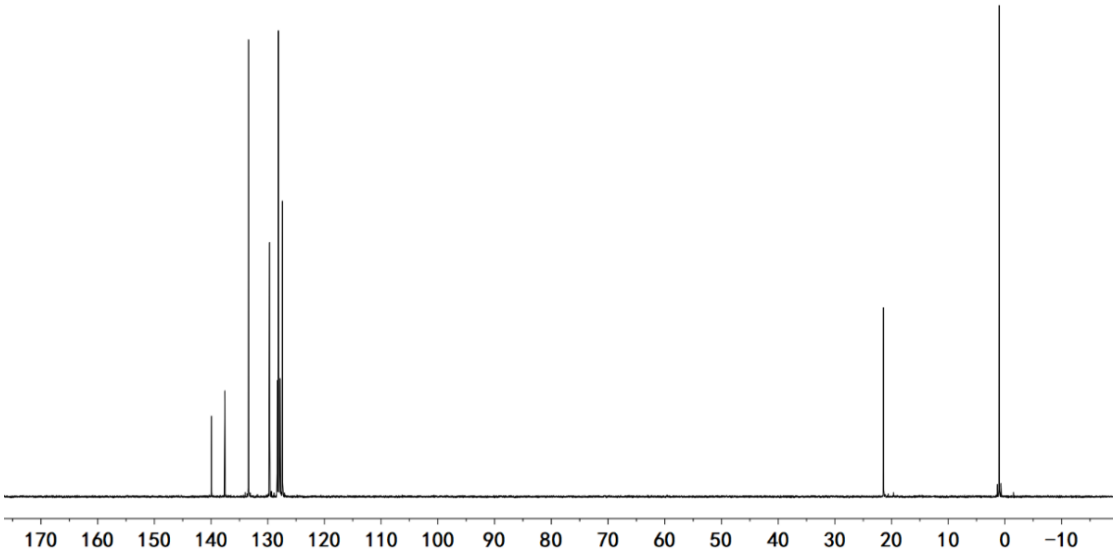


Fig. S4. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), $PhMe_2SiH$ (340.8 mg, 2.5 mmol), mesitylene (120.2 mg, 1.0 mmol)] (table 1, entry 2)

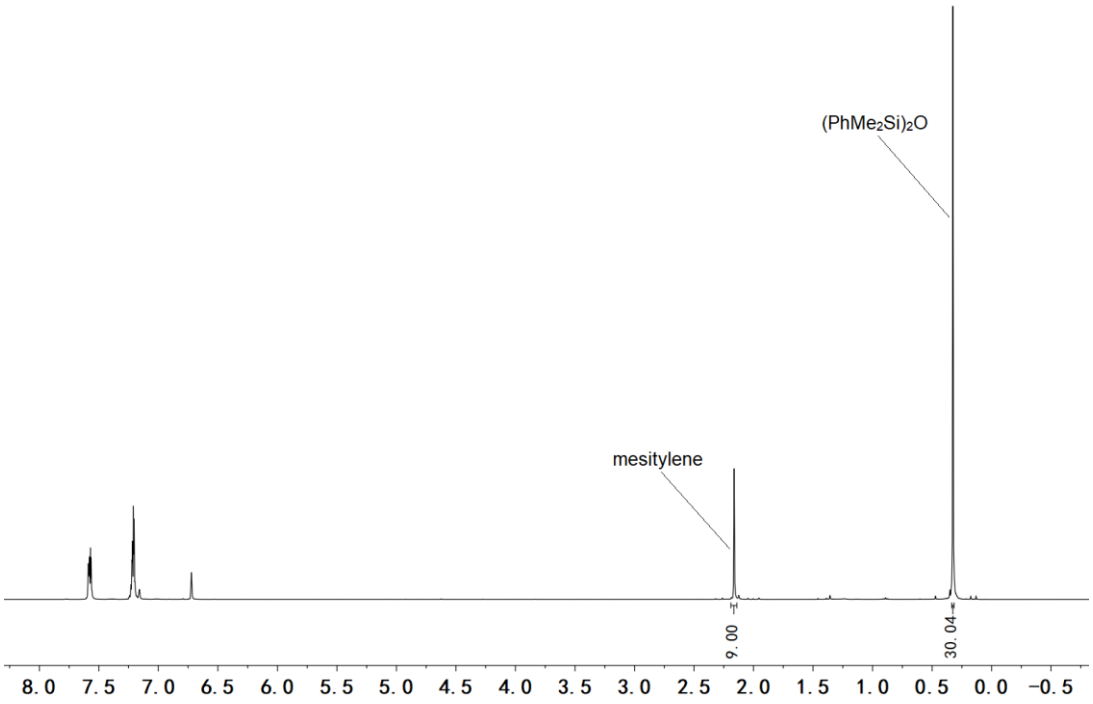


Fig. S5. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5.0 μmol), $PhMe_2SiH$ (340.8 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 1, entry 3)

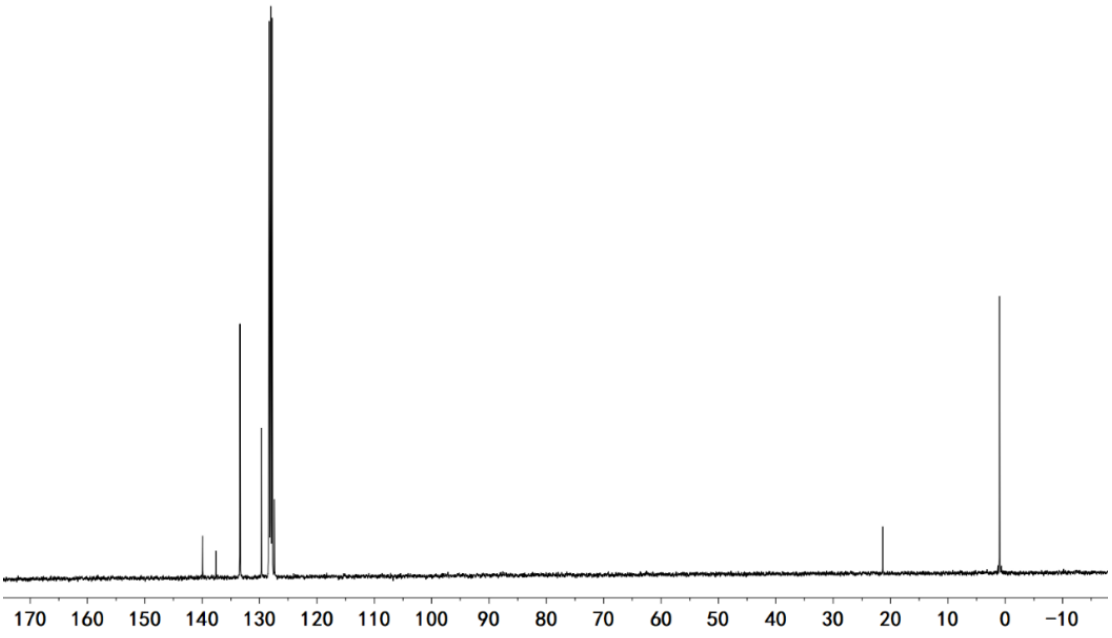


Fig. S6. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K) [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5.0 μmol), $PhMe_2SiH$ (340.8 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 1, entry 3)

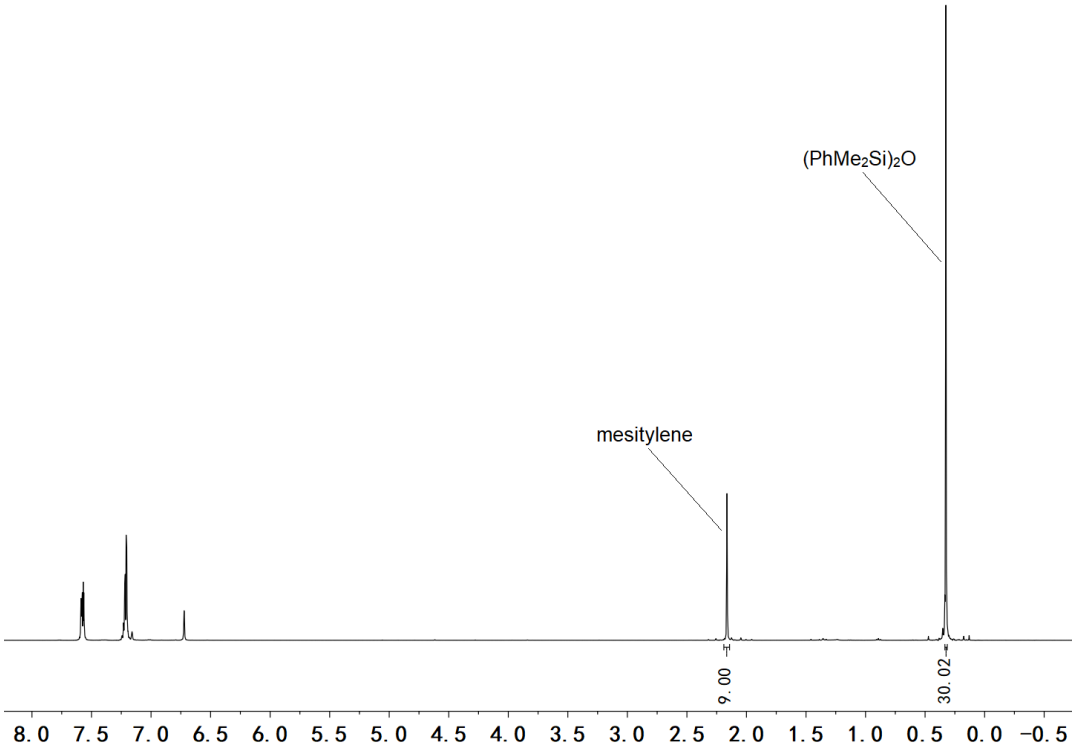


Fig. S7. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), $PhMe_2SiH$ (340.8 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 1, entry 4)

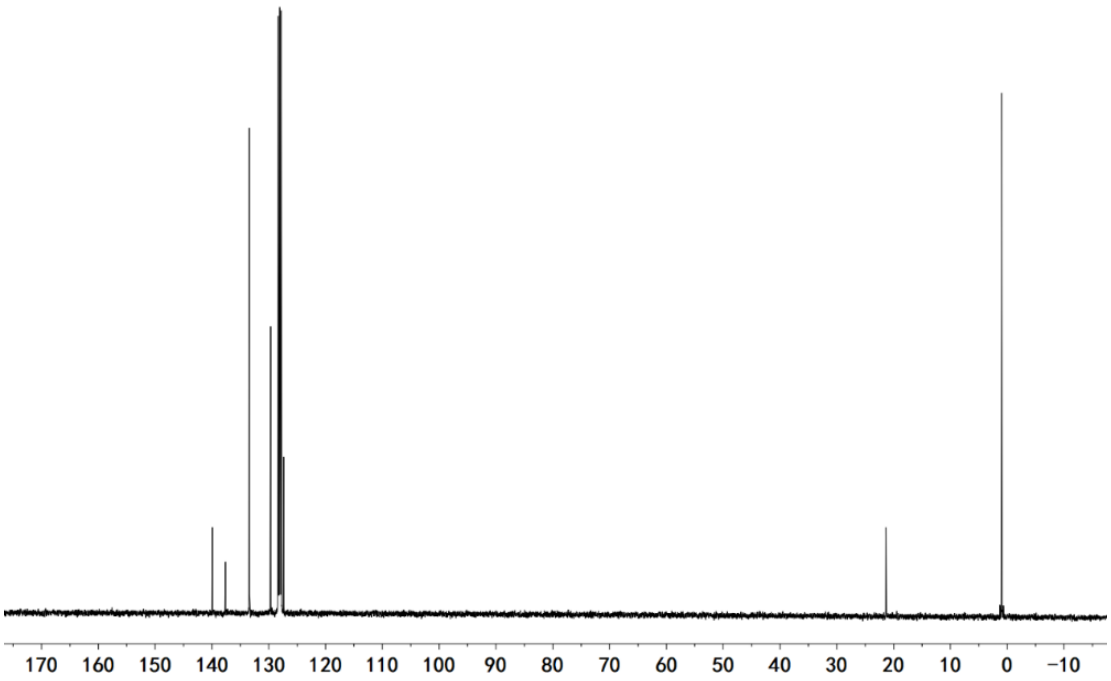


Fig. S8. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), $PhMe_2SiH$ (340.8 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 1, entry 4)

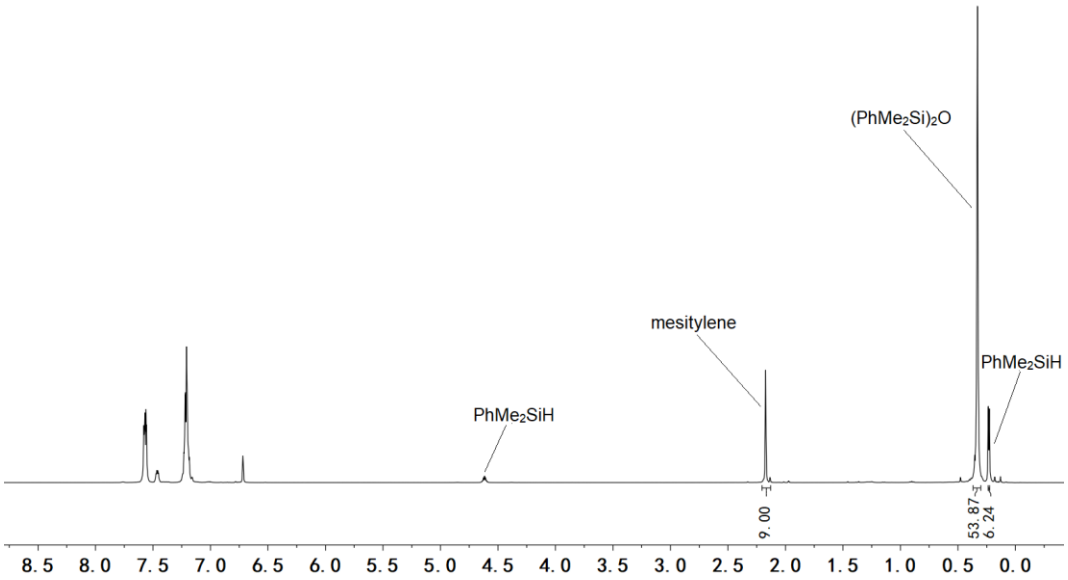


Fig. S9. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), $PhMe_2SiH$ (1.02 g, 7.5 mmol), mesitylene (90.2 mg, 0.75 mmol)] (Table 1, entry 5)

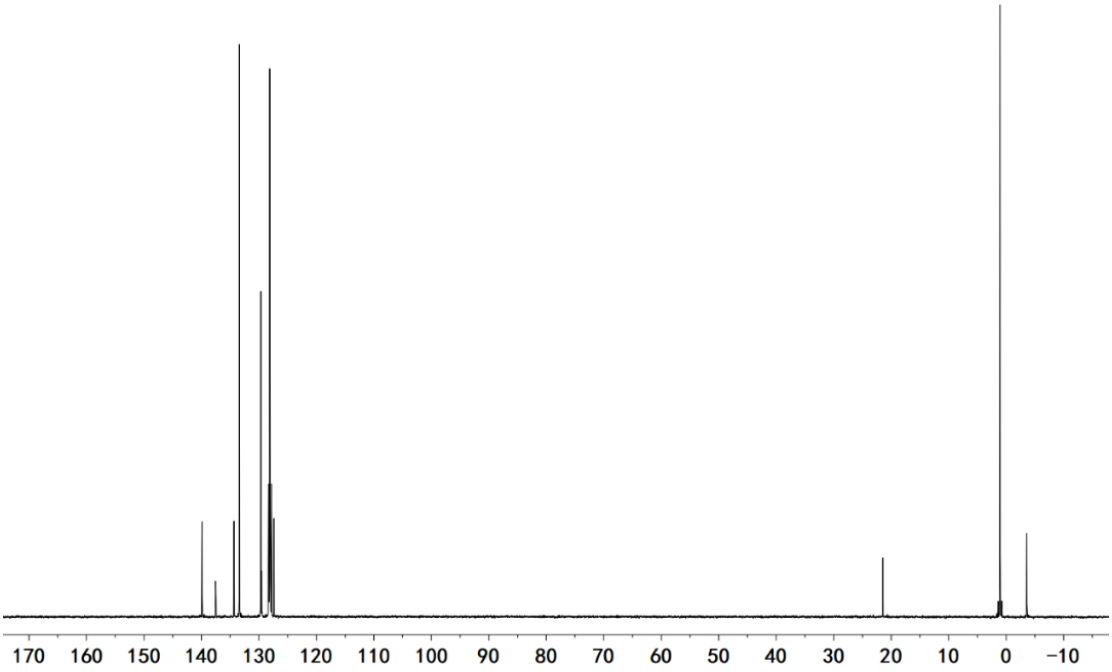


Fig. S10. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), $PhMe_2SiH$ (1.02 g, 7.5 mmol), mesitylene (90.2 mg, 0.75 mmol)] (Table 1, entry 5)

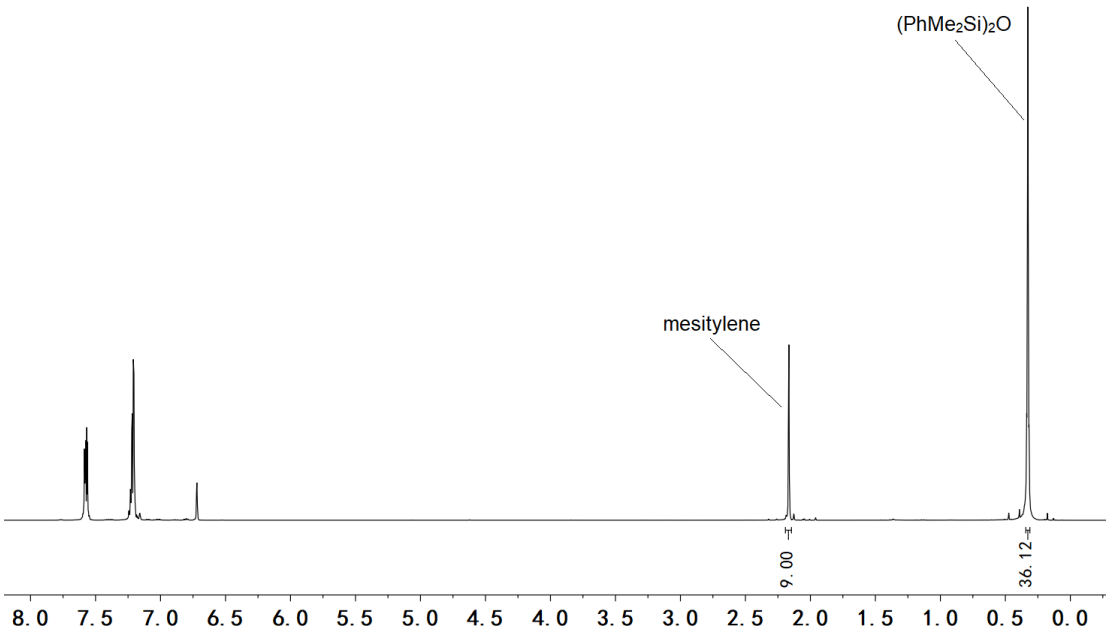


Fig. S11. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (10.2 mg, 20 μmol), $PhMe_2SiH$ (2.04 g, 15.0 mmol), mesitylene (300.5 mg, 2.5 mmol)] (table 1, entry 6)

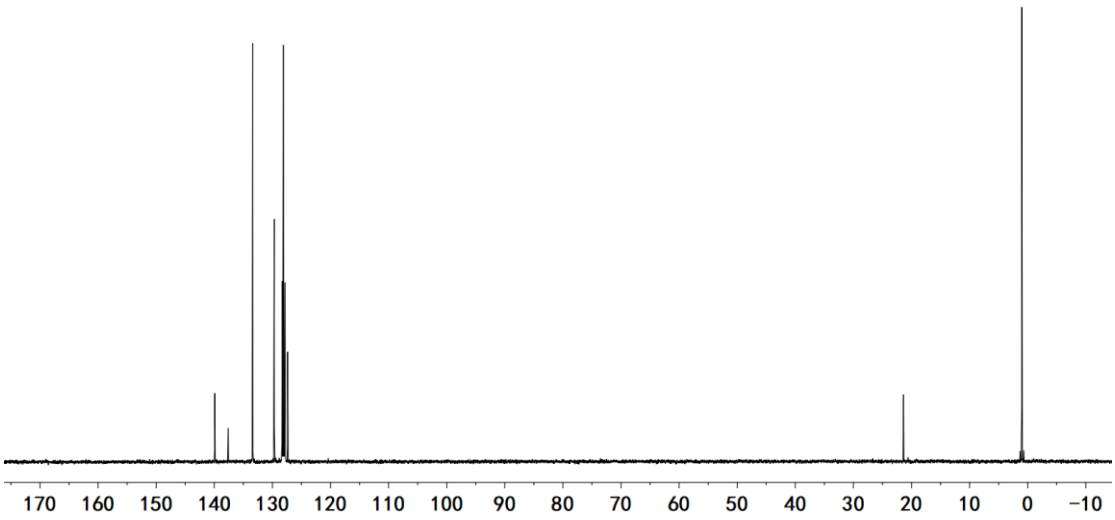


Fig. S12. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (10.2 mg, 20 μmol), $PhMe_2SiH$ (2.04 g, 15.0 mmol), mesitylene (300.5 mg, 2.5 mmol)] (table 1, entry 6)

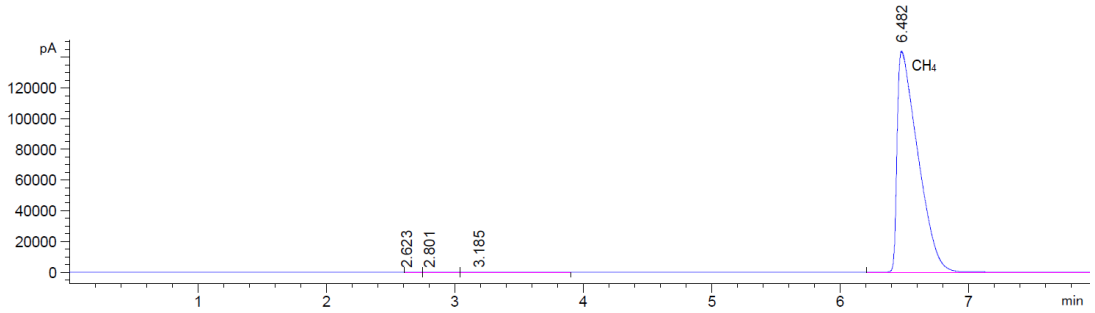


Fig. S13. Gas chromatography (GC) traces of gaseous products. (table 1, entry 6)

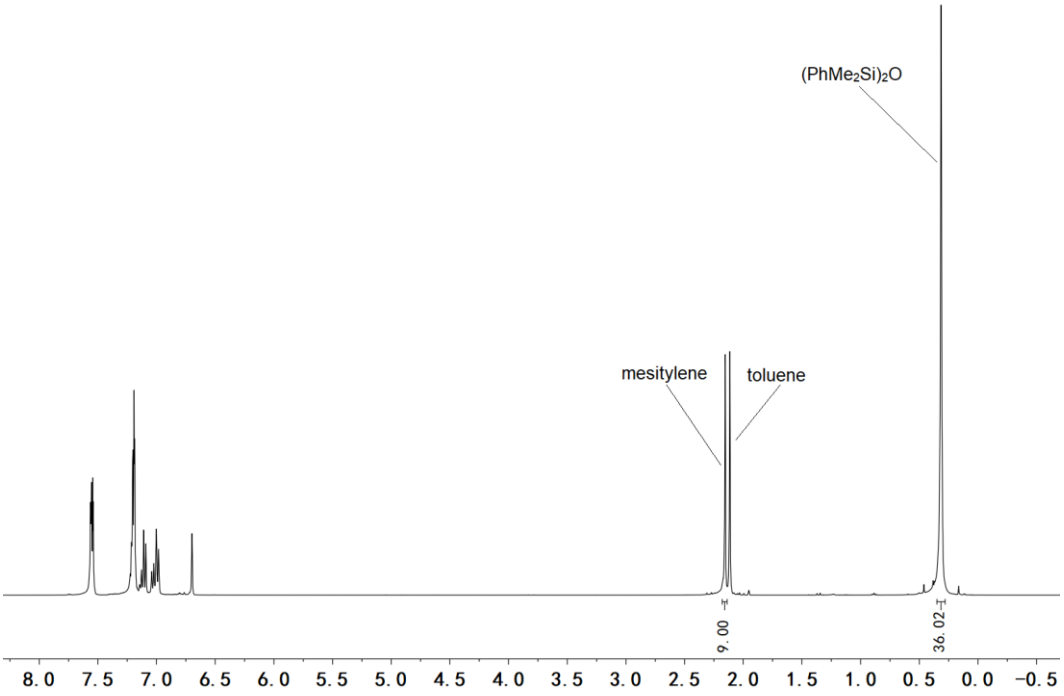


Fig. S14. **^{1}H NMR** (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (10.2 mg, 20 μmol), $PhMe_2SiH$ (2.04 g, 15.0 mmol), mesitylene (300.5 mg, 2.5 mmol)] (table 1, entry 6, in toluene)

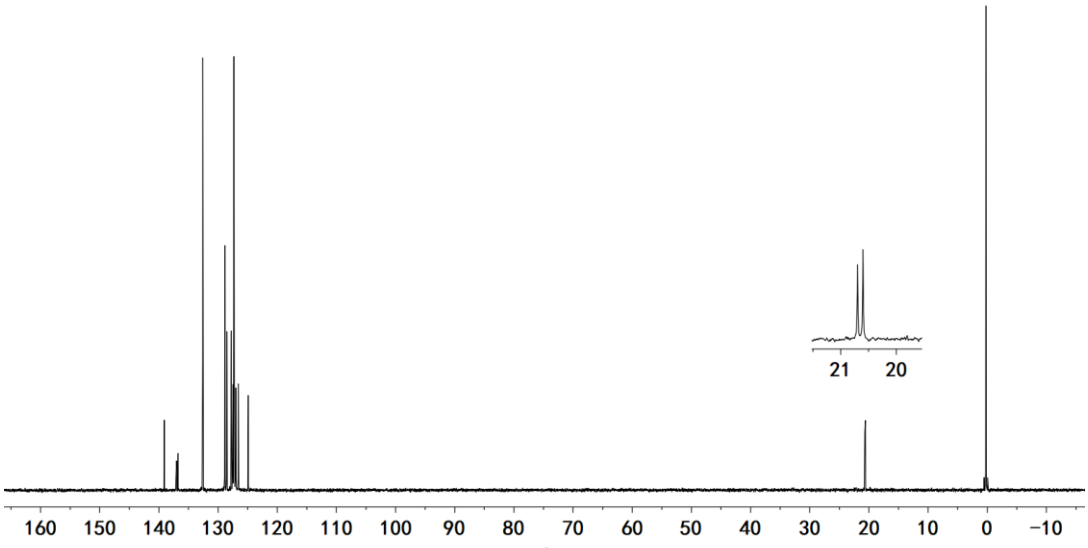


Fig. S15. $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (10.2 mg, 20 μmol), $PhMe_2SiH$ (2.04 g, 15.0 mmol), mesitylene (300.5 mg, 2.5 mmol)] (table 1, entry 6, in toluene)

General procedure for reduction of CO_2 with isolated product

In a glove box, a stainless steel Parr reactor containing a stir bar was charged with $La(OAr)_3$ (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (10.2 mg, 20 μmol), $PhMe_2SiH$ (5.11 g *or* 6.81 g), and 0.5 mL of C_6D_6 or solvent-free. The reactor was taken out of the glove box, charged with 5 bar CO_2 and then sealed. The reaction mixture was allowed to stir at room temperature for desired time. Afterwards, all volatiles were completely removed in vacuum over 2 h at 25 ℃, and then 1 h at 60 ℃. $(PhMe_2Si)_2O$ was remaining as a single product, which was confirmed by ^1H and $^{13}C\{^1H\}$ NMR spectroscopy. Yield: 5.26 g, 98% (table 1, entry 7); 5.21 g, 97% (table 1, entry 7, neat conditions); 6.94 g, 97% (table 1, entry 8). *Note*: Stock solutions were used for the measurement of $La(OAr)_3$ and $B(C_6F_5)_3$.

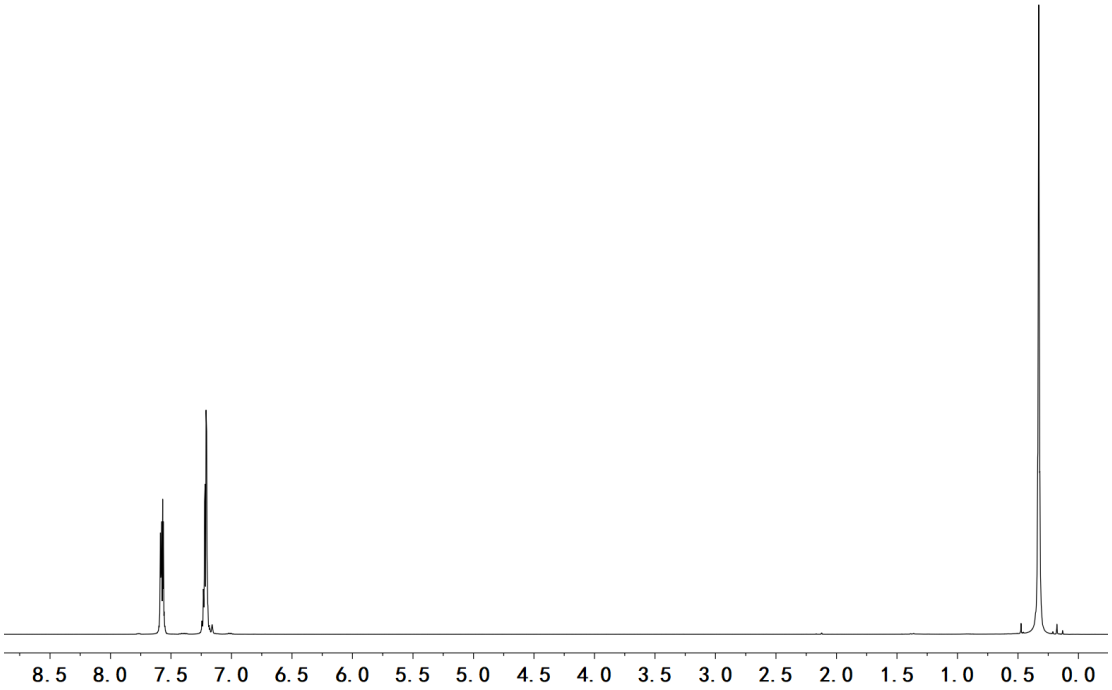


Fig. S16. ^1H NMR (400 MHz, C_6D_6, 298 K) of $(PhMe_2Si)_2O$.

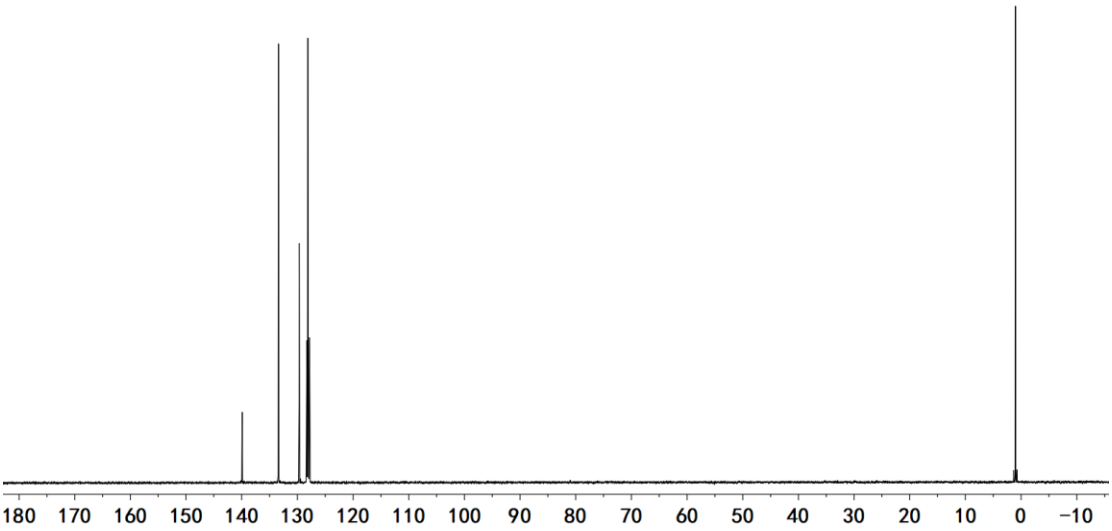


Fig. S17. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K) of $(PhMe_2Si)_2O$.

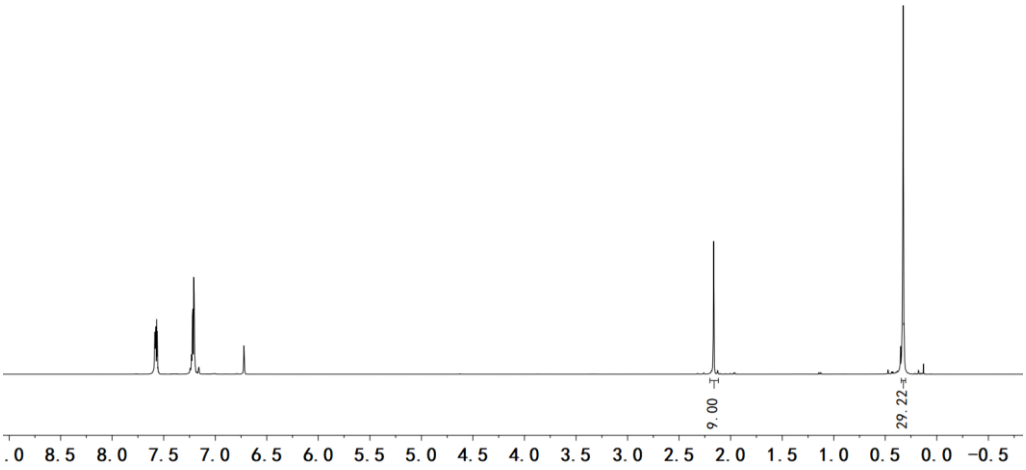


Fig. S18. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**5** (1.7 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), $PhMe_2SiH$ (340.8 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 1, entry 9)

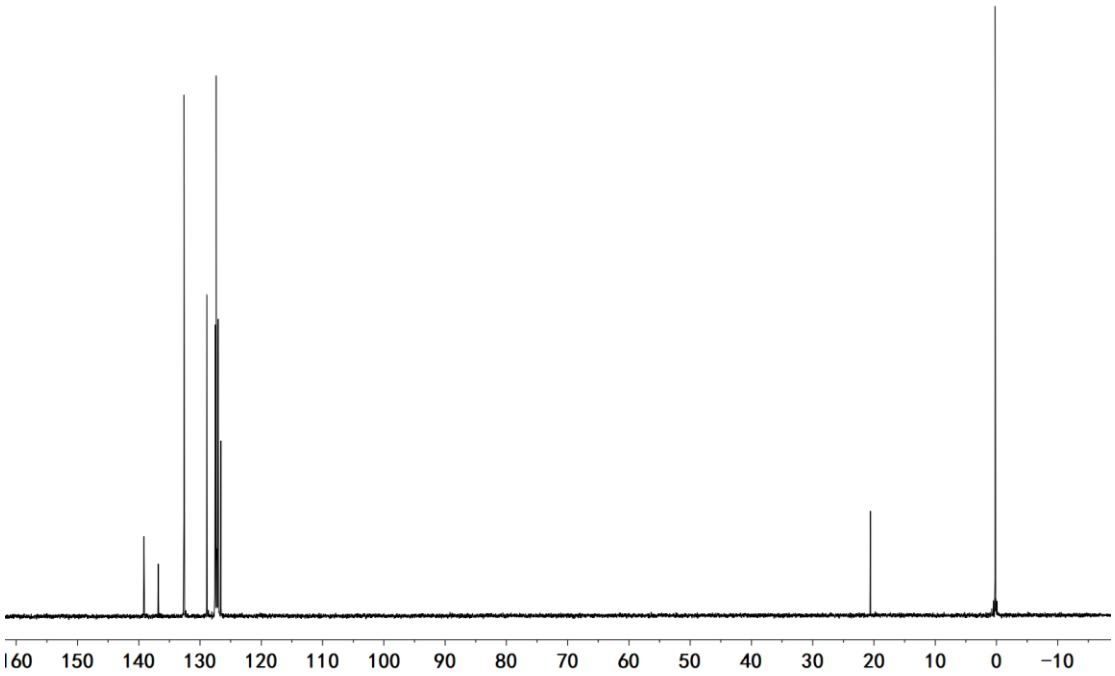


Fig. S19. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K). [**5** (1.7 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), $PhMe_2SiH$ (340.8 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 1, entry 9)

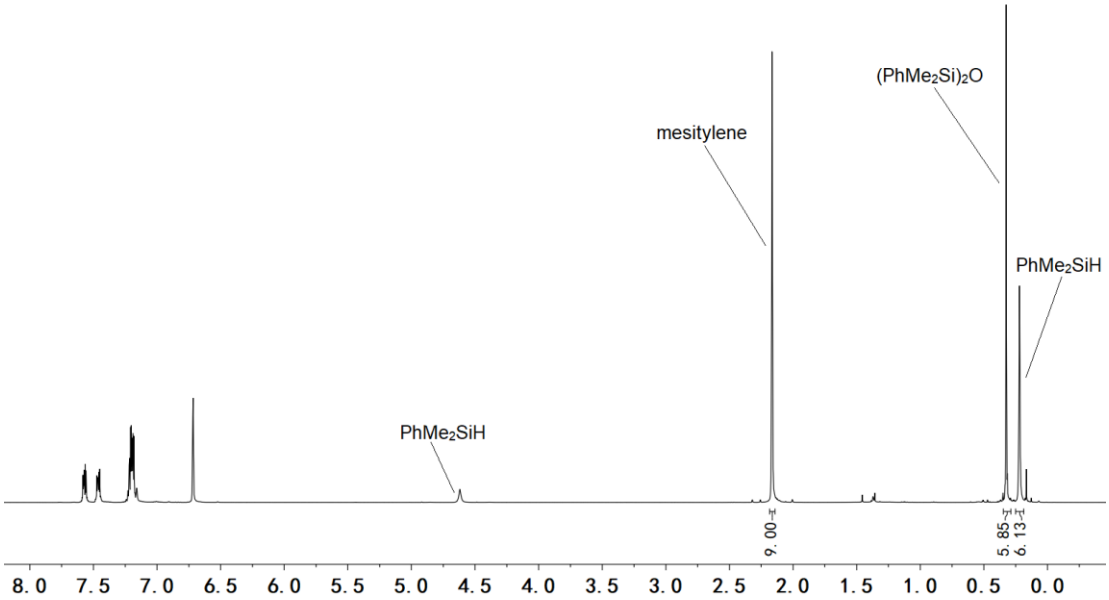


Fig. S20. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4b** (1.8 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), $PhMe_2SiH$ (68.2 mg, 0.5 mmol), mesitylene (30.1 mg, 0.25 mmol)] (table 1, entry 10)

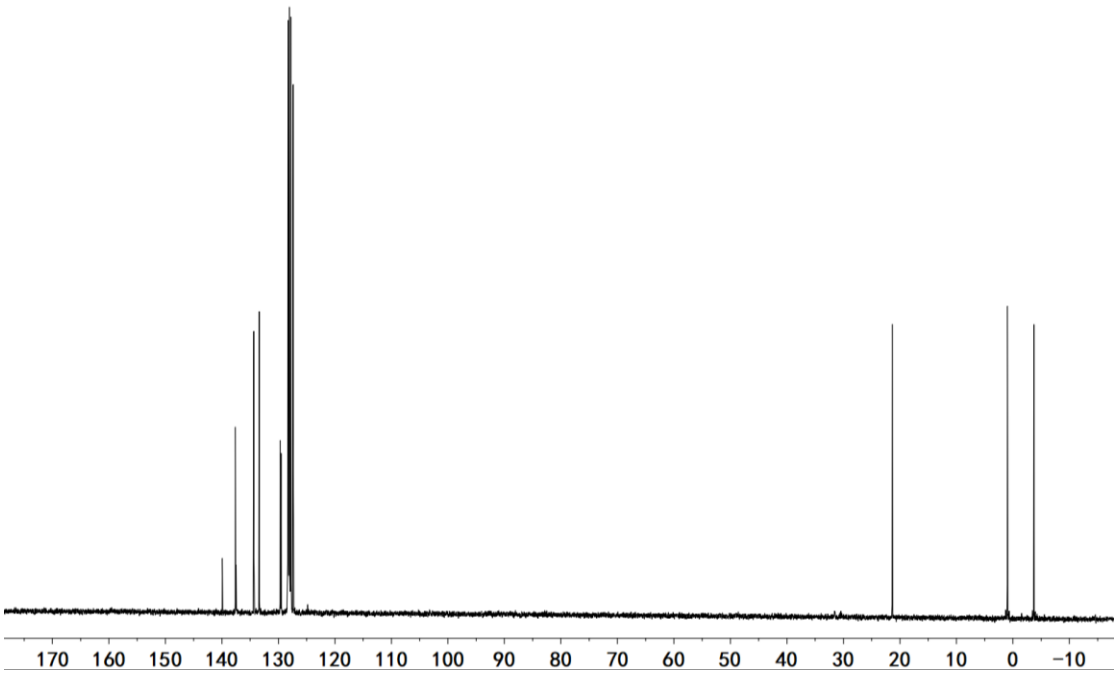


Fig. S21. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K). [**4b** (1.8 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), $PhMe_2SiH$ (68.2 mg, 0.5 mmol), mesitylene (30.1 mg, 0.25 mmol)] (table 1, entry 10)

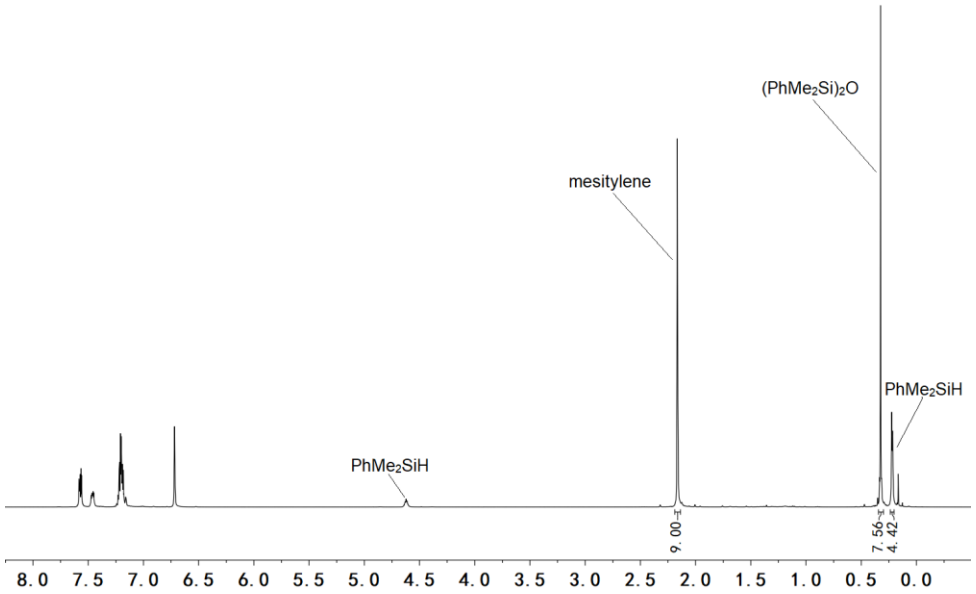


Fig. S22. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4c** (1.7 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), $PhMe_2SiH$ (68.2 mg, 0.5 mmol), mesitylene (30.1 mg, 0.25 mmol)] (table 1, entry 11)

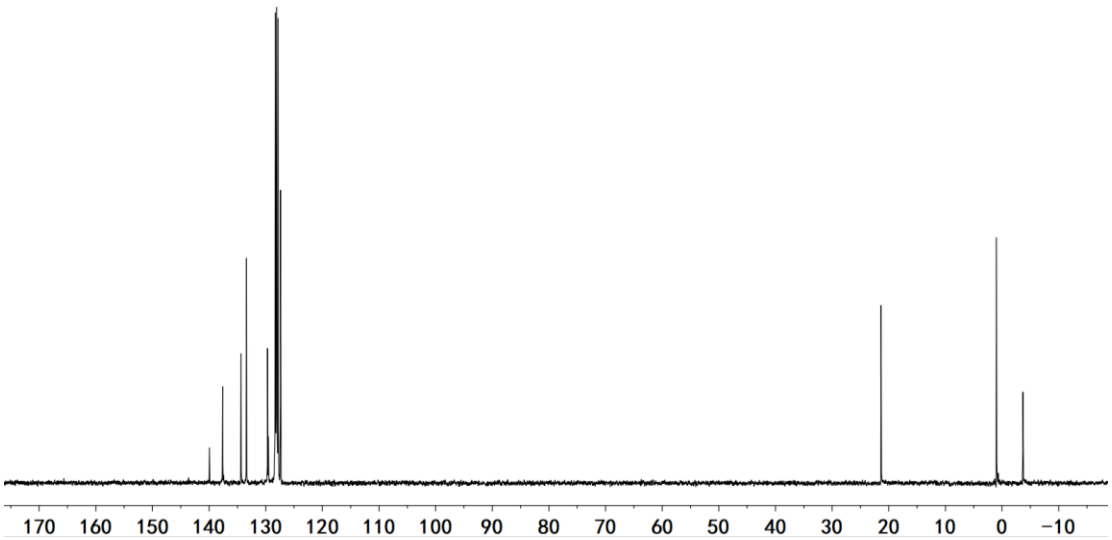


Fig. S23. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K). [**4c** (1.7 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), $PhMe_2SiH$ (68.2 mg, 0.5 mmol), mesitylene (30.1 mg, 0.25 mmol)] (table 1, entry 11)

Table S1. Optimization of the ratio of **4a** and $B(C_6F_5)_3$ in the tandem hydrosilylation of CO_2.[a]

Entry	Cat.	La/B	Time (h)	Conv. (%)	TON	TOF (h^{-1})
1	**4a**	1:2	2	36	3600	1800
2	**4a**	1:5	2	53	5300	2650
3	**4a**	1:6	2	78	7800	3900
4	**4a**	1:8	2	87	8700	4350
5	**4a**	1:10	2	15	1500	750

[a]Conditions: **4a** (2.5 μmol), $PhMe_2SiH$ (25.0 mmol), 5 bar CO_2, C_6D_6 (0.5 mL). Conversions were determined by ^1H NMR with mesitylene as an internal standard. TONs were determined by ^1H NMR based on mol of siloxane formed per mol of metal catalyst.

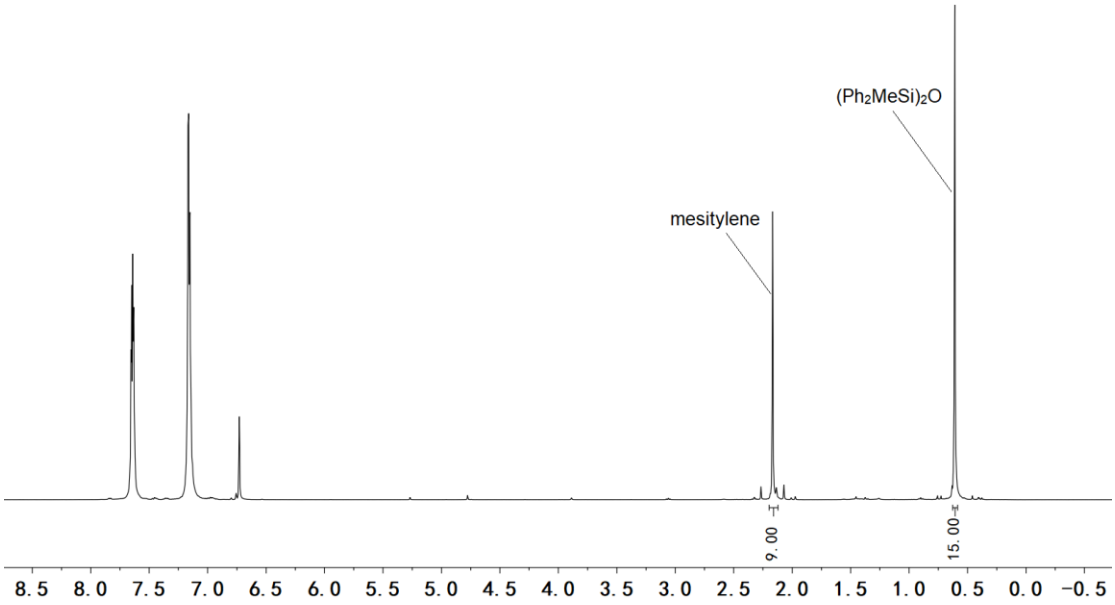


Fig. S24. ^1H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), Ph_2MeSiH (495.8 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 2, entry 1)

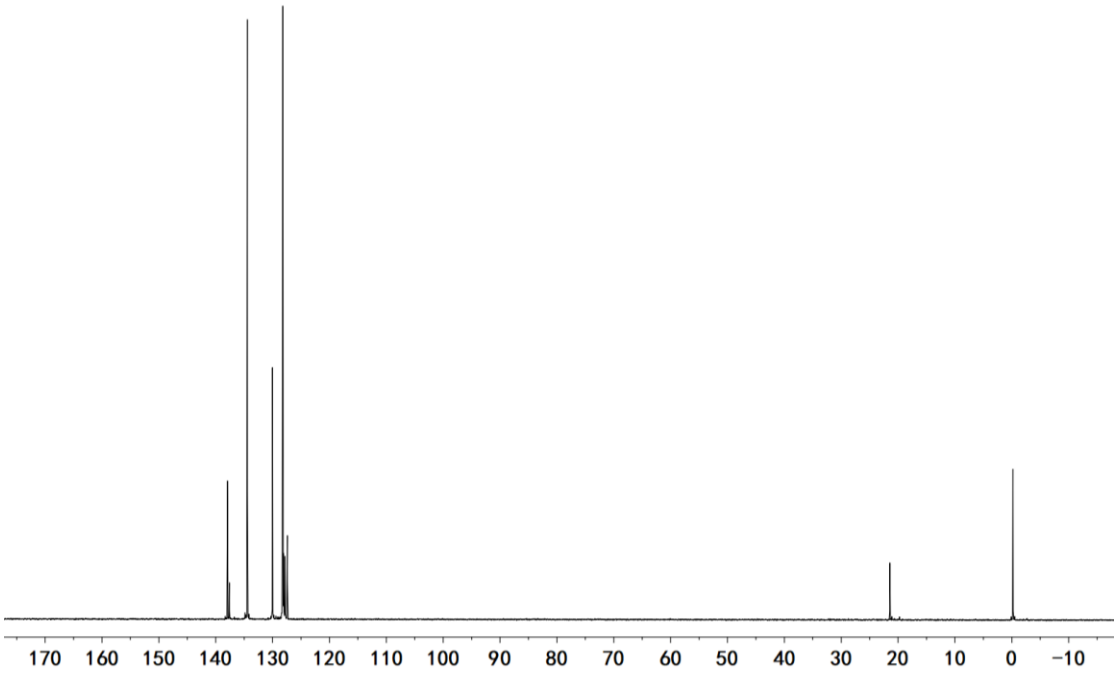


Fig. S25. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), Ph_2MeSiH (495.8 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 2, entry 1)

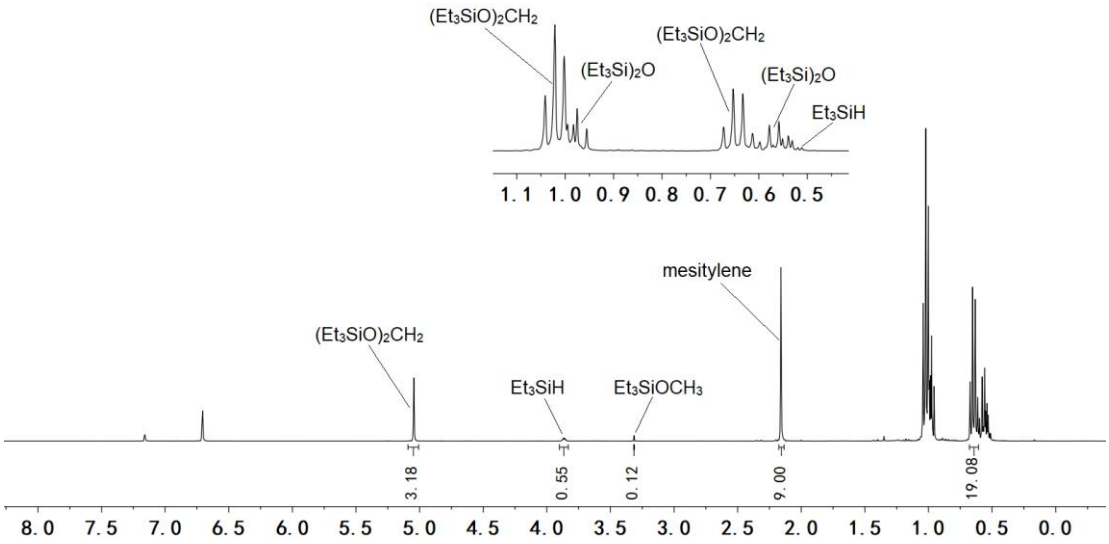


Fig. S26. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), Et_3SiH (290.7 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 2, entry 2)

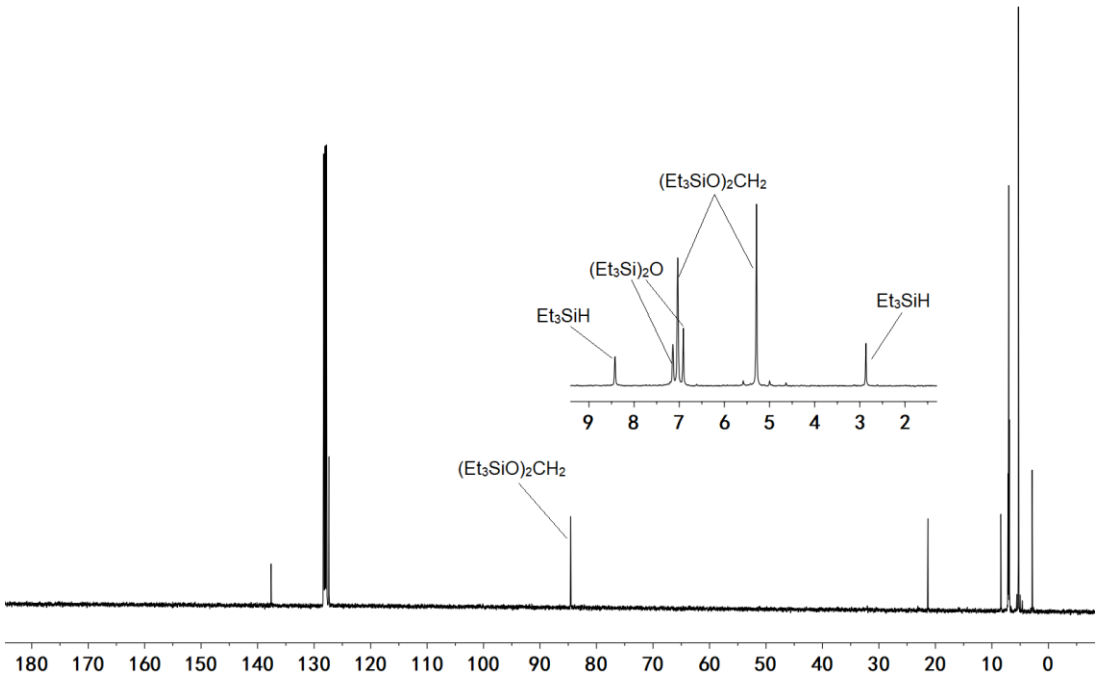


Fig. S27. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), Et_3SiH (290.7 mg, 2.5 mmol), mesitylene (60.1 mg, 0.5 mmol)] (table 2, entry 2)

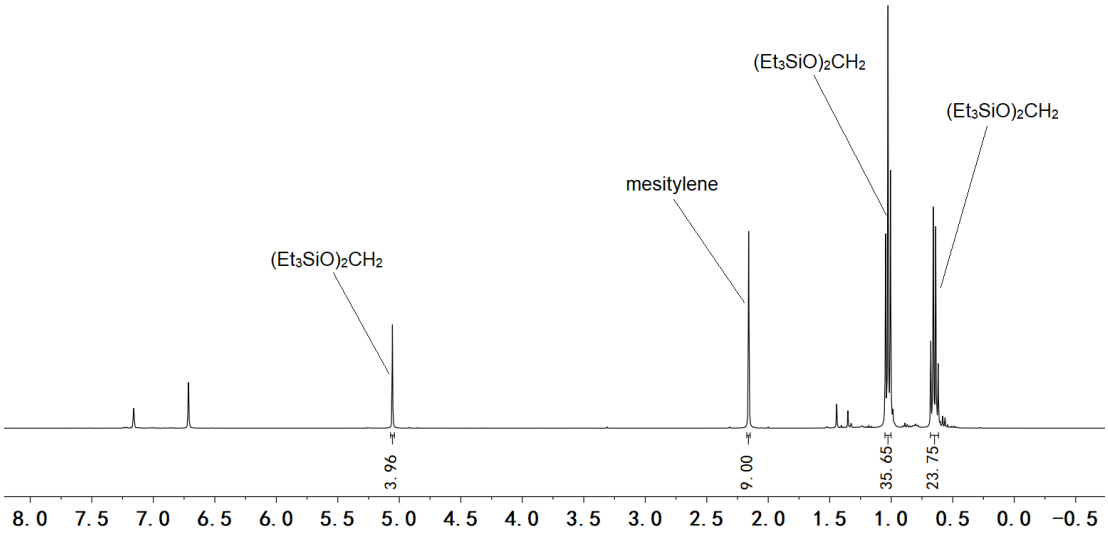


Fig. S28. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), Et_3SiH (29.1 mg, 0.25 mmol), mesitylene (7.5 mg, 0.0625 mmol)] (table 2, entry 3)

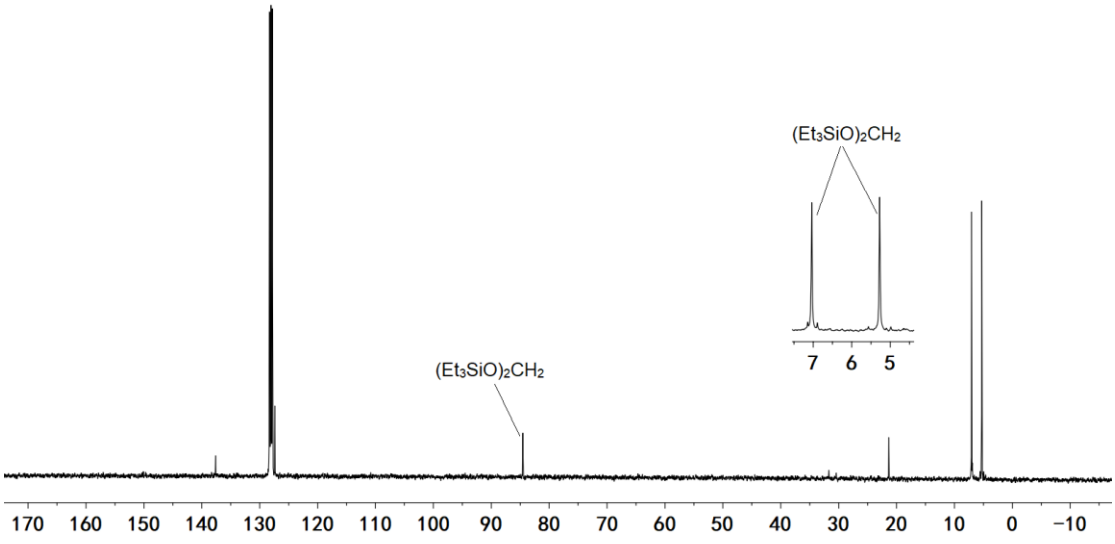


Fig. S29. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (1.3 mg, 2.5 μmol), Et_3SiH (29.1 mg, 0.25 mmol), mesitylene (7.5 mg, 0.0625 mmol)] (table 2, entry 3)

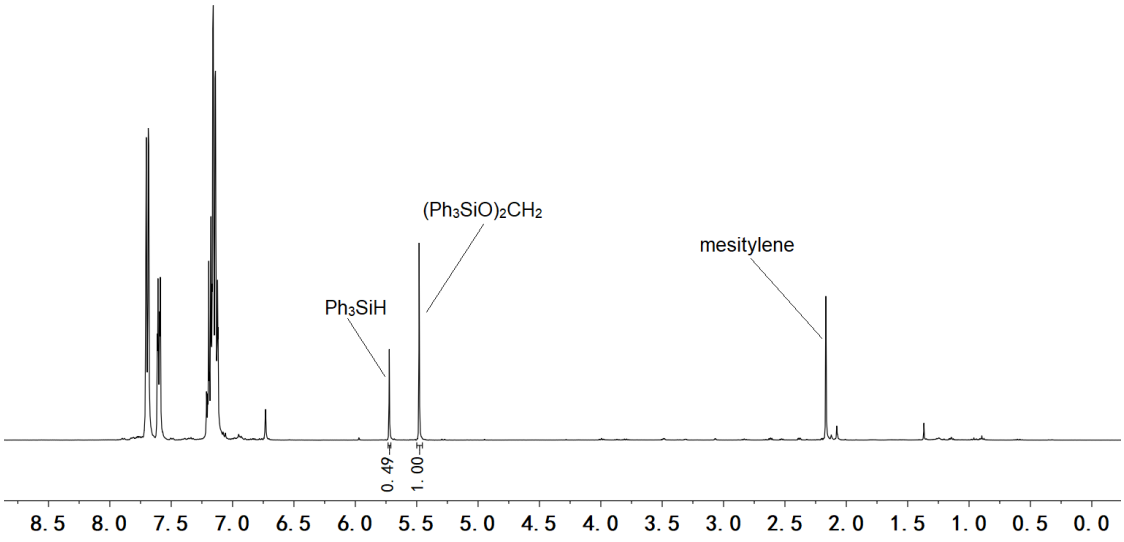


Fig. S30. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), Ph_3SiH (651.0 mg, 2.5 mmol)] (table 2, entry 4) (Conversion was determined with Ph_3SiH as an internal standard)

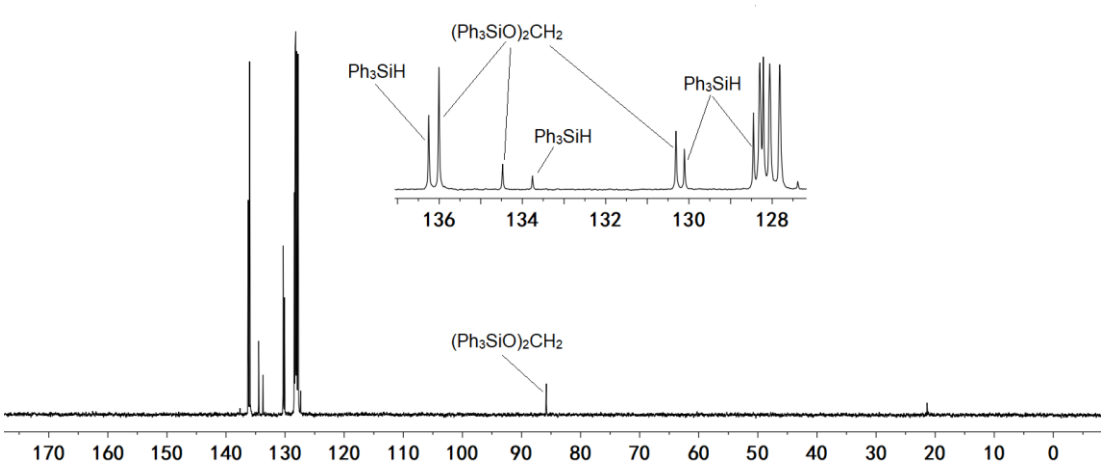
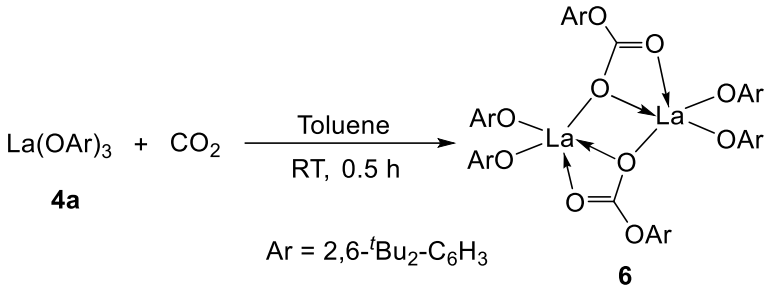


Fig. S31. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K). [**4a** (1.9 mg, 2.5 μmol), $B(C_6F_5)_3$ (2.6 mg, 5 μmol), Ph_3SiH (651.0 mg, 2.5 mmol)] (table 2, entry 4)

Preparation of complex 6



Scheme S1.

Stoichiometric CO_2 (4.9 mL, 0.2 mmol) was slowly added to a solution of $La(OAr)_3$ **4a** (151 mg, 0.2 mmol) in toluene (2 mL) using an injector at room temperature. The reaction mixture was stirred for 30 minutes and then all volatiles were removed in vacuo. The residue was washed with hexane (3×2 mL) to eventually give complex **6** as a white crystalline solid (128 mg, 80%). Crystals of **6** suitable for analysis by single crystal X-ray diffraction were obtained by a saturated toluene solution at room temperature.

Elemental Analysis: calcd. for $C_{86}H_{126}O_{10}La_2$: C, 64.65; H, 7.95. Found: C, 64.97; H, 8.29.

IR (KBr, cm^{-1}): ν = 1638 (C=O).

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 7.23 (4H, *m*), 6.81 (2H, *p*) (each m, O*Ar*), 7.08 (2H, *m*), 6.92 (1H, *p*) (each m, O*Ar*'), 1.55 (s, 36H, C(CH_3)$_3$), 1.28 (s, 18H, C(CH_3)$_3$').

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 162.1 (*i*), 137.1 (*o*), 125.0 (*m*), 118.0 (*p*) (O*Ar*), 160.8 (*i*), 142.0 (*o*), 126.9 (*m*), 126.3 (*p*) (O*Ar*'), 149.6 (*C*=O), 35.8 (*C*(CH$_3$)$_3$'), 34.5 (*C*(CH$_3$)$_3$), 32.0 (C(*C*H$_3$)$_3$'), 31.8 (C(*C*H$_3$)$_3$).

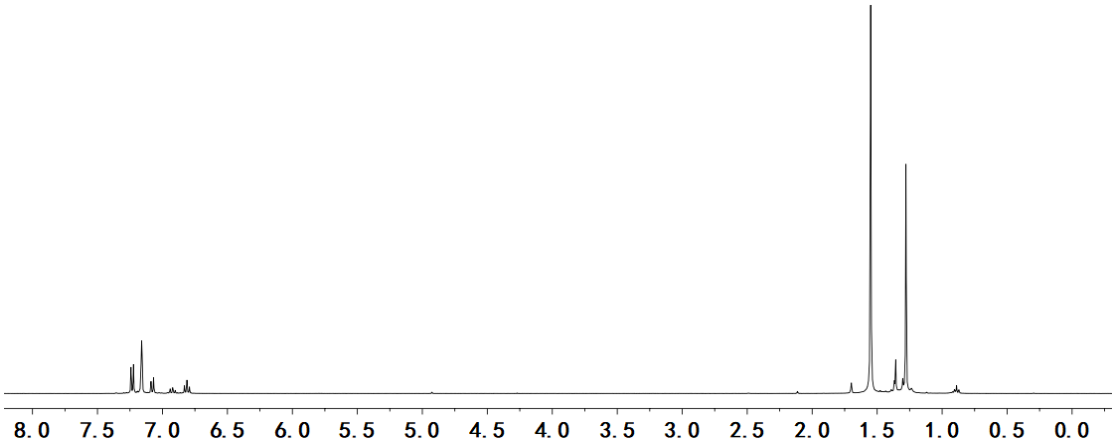


Fig. S32. ^{1}H NMR (400 MHz, C_6D_6, 298 K).

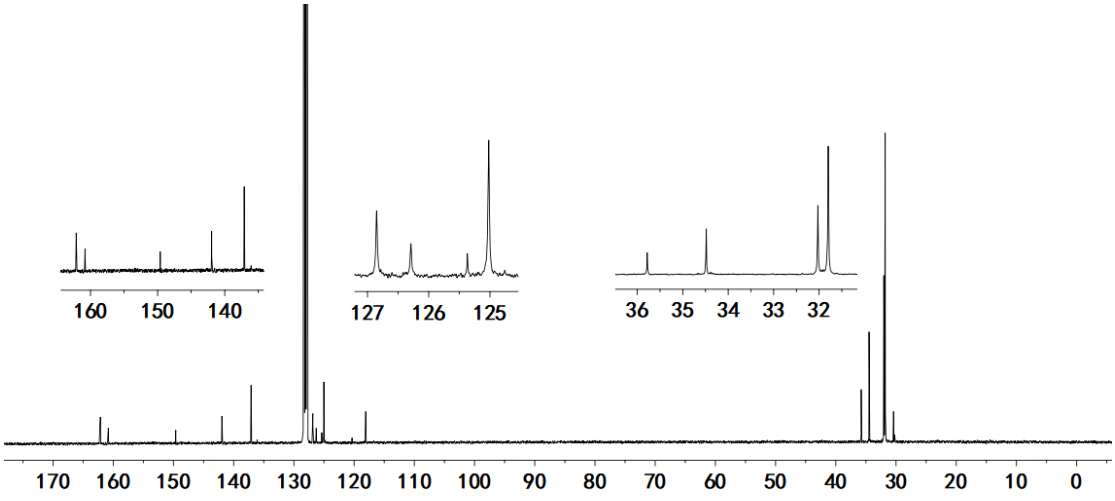


Fig. S33. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K).

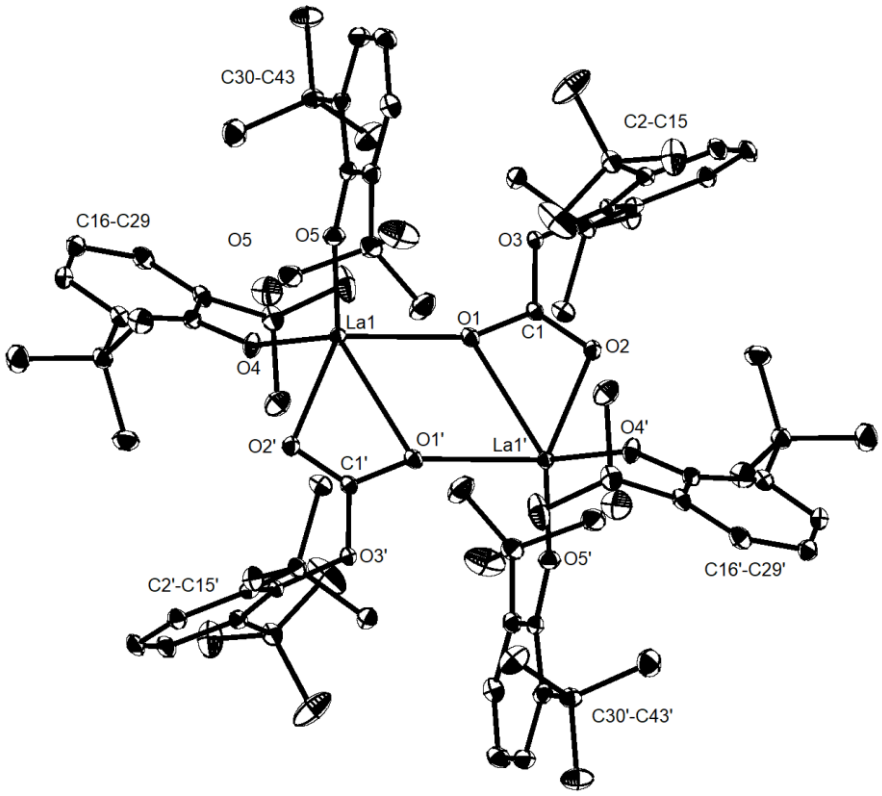


Fig. S34. Molecular structure of complex **6**.

X-ray crystal structure analysis of complex 6: formula $2(C_{43}H_{63}LaO_5)$, M = 1597.69 gmol^{-1}, colourless, 0.15 x 0.10 x 0.08 mm, Triclinic, space group *P-1*, a = 12.4626(13), b = 13.1639(14), c = 13.6063(15) Å, β = 75.396(3)°, V = 2002.6(4) Å^3, ρ_{calc} = 1.325 gcm^{-3}, μ = 1.108 mm^{-1}, empirical absorption correction (0.851 ≤ T ≤ 0.917), Z = 1, λ = 0.71073 Å, T = 120(2) K, 66337 reflections collected (-16 ≤ h ≤ 16, -17 ≤ k ≤ 17, -17 ≤ l ≤ 17), 9231 independent (R_{int} = 0.0559) and 8135 observed reflections [I>2σ(I)], 460 refined parameters, the final R_1 was 0.0297 (I > 2σ(I)) and wR_2 was 0.0913 (all data). max. (min.) residual electron density 1.868 (-0.818) e.Å^{-3}, hydrogen atoms were placed in calculated positions and refined using a riding model.

Hydrosilylation of CO_2 (5 bar) with $PhMe_2SiH$ Catalyzed by 6/$B(C_6F_5)_3$

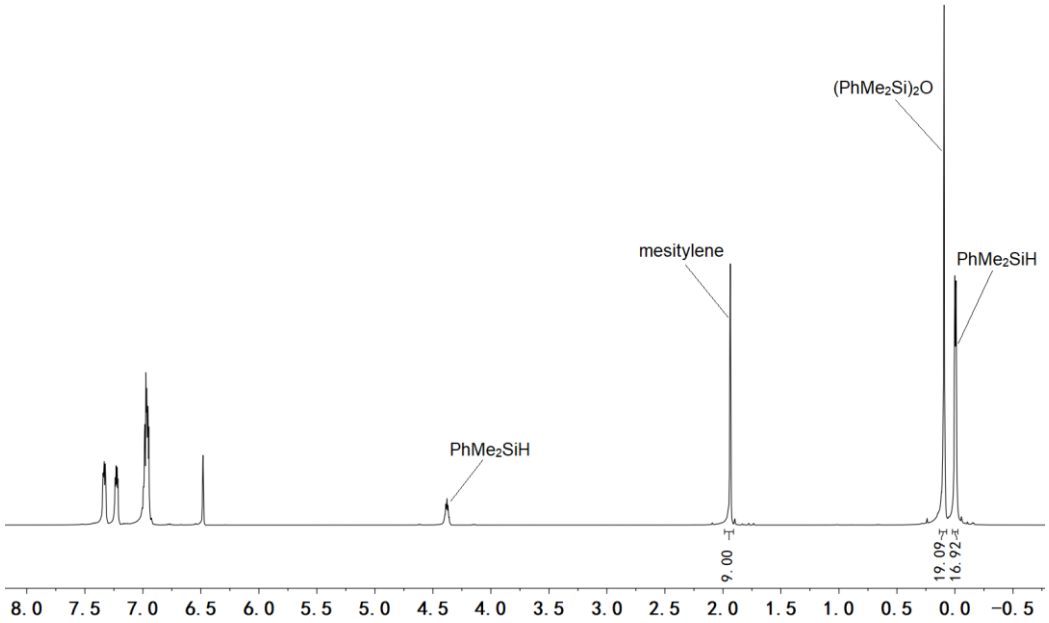


Fig. S35. ^{1}H NMR (400 MHz, C_6D_6, 298 K). [**6** (2.0 mg, 1.25 μmol), $B(C_6F_5)_3$ (10.2 mg, 20 μmol), $PhMe_2SiH$ (2.04 g, 15.0 mmol), mesitylene (300.5 mg, 2.5 mmol)]

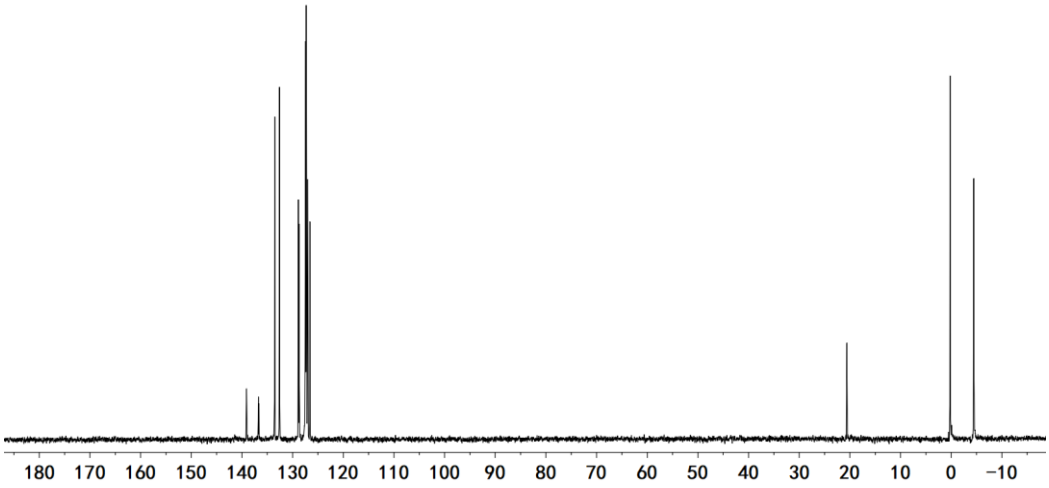


Fig. S36. $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6, 298 K). [**6** (2.0 mg, 1.25 μmol), $B(C_6F_5)_3$ (10.2 mg, 20 μmol), $PhMe_2SiH$ (2.04 g, 15.0 mmol), mesitylene (300.5 mg, 2.5 mmol)]

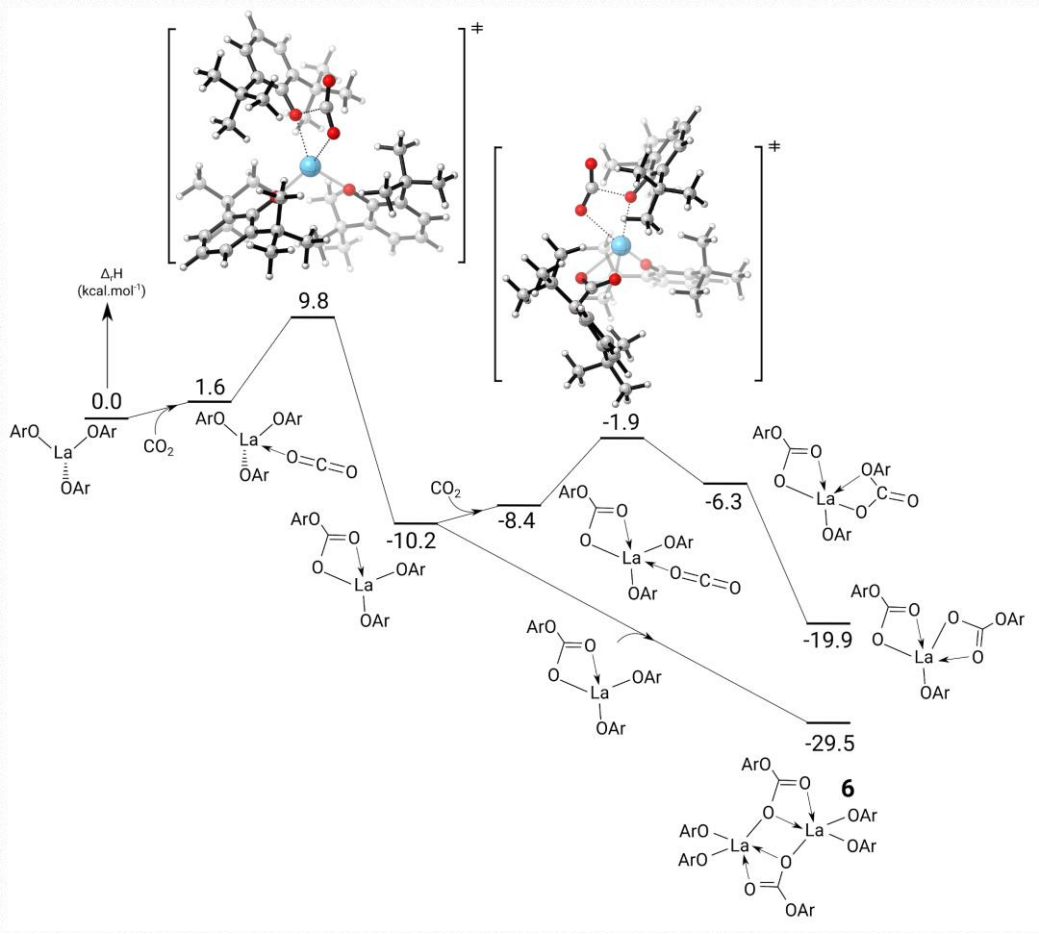


Fig. S37. Computed enthalpy profile for the reaction of CO_2 with $La(OAr)_3$ at room temperature.

Note: The reaction of CO_2 with $La(OAr)_3$ started from the coordination of CO_2 molecule to La center, which yielded the monomeric La carbonate. Although the second CO_2 molecule insertion into remaining La-O bond is exothermic by 9.7 kcal/mol, the dimerization reaction of the monomeric carbonate is more favorable to generate complex **6** by 19.3 kcal/mol.

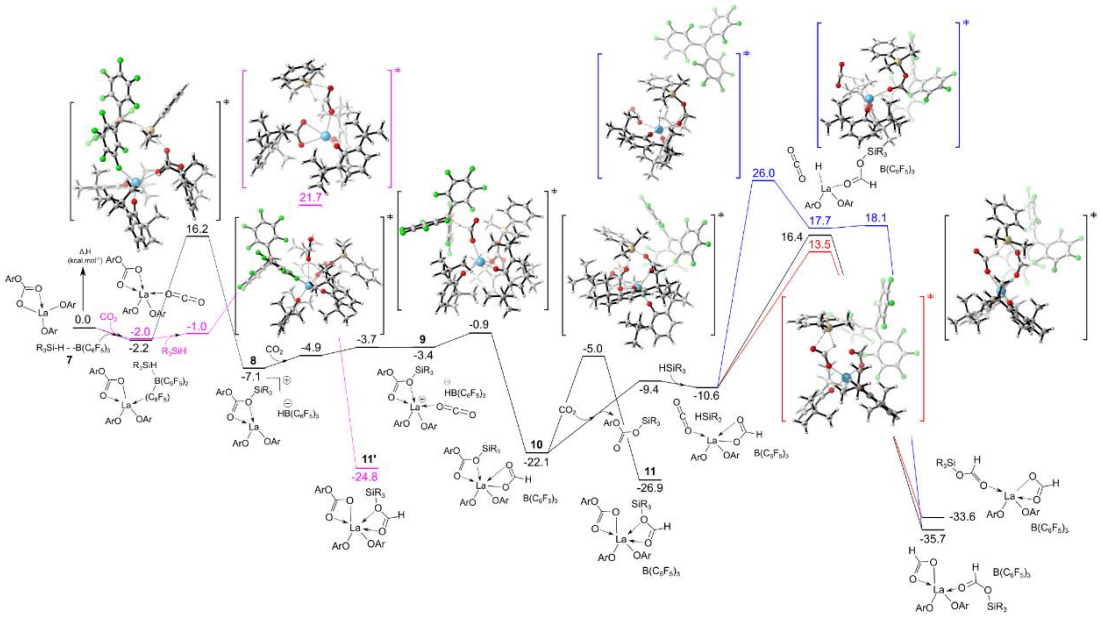


Fig. S38. Computed enthalpy profile and possible reaction pathways for catalytic hydrosilylation of CO_2 at room temperature

Note: As for the pink pathway, it starts with the coordination of CO_2 to the monomeric carbonate, resulting in the formation of CO_2-coordination intermediate. This process is favored by 2.0 kcal/mol relative to the monomeric carbonate. The next step of the reaction is the cleavage of Si-H bond to give product **11′**, with the associated barrier of 21.7 kcal/mol. In other three pathways, second CO_2 activation were considered after the formation of **10** with elease of $ArOC(O)OSiR_3$ ligand. All of these pathways were found to be higher in energy compared with the pathway for formation of **11**.

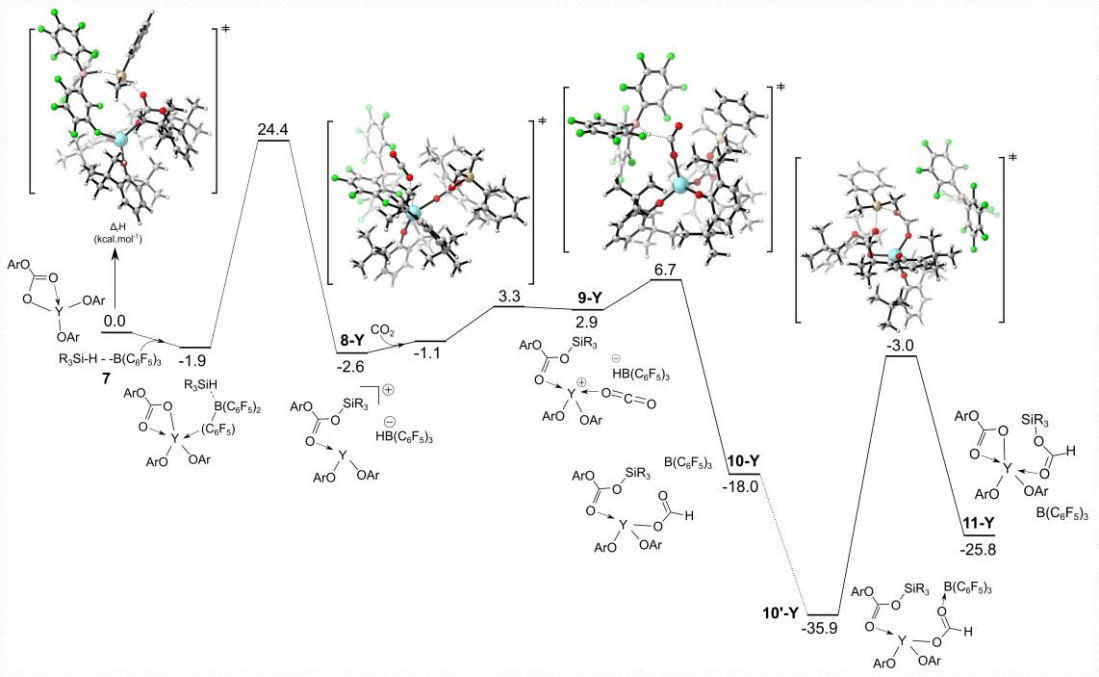


Fig. S39. Computed enthalpy profile for catalytic hydrosilylation of CO_2 with $Y(OAr)_3$ at room temperature.

Cartesian coordinates:

3

CO_2

O	11.76597	3.97222	-1.45343
C	10.64054	4.27624	-1.52148
O	9.51504	4.57985	-1.58956

24

$OCHOSiMe_2Ph$

C	-3.33362	2.54861	3.90524
C	-2.87367	3.59181	3.08727
C	-3.50635	4.84168	3.19286
C	-4.55937	5.04491	4.08216
C	-5.00169	3.99522	4.88689
C	-4.38733	2.74742	4.79681
Si	-1.45469	3.36877	1.86863
C	0.01384	4.45350	2.31097
O	-1.03354	1.68565	2.12706
C	-0.04711	1.12254	1.43327
O	0.63173	1.67093	0.59631
C	-2.02694	3.60306	0.09476
H	-3.17684	5.67467	2.57347
H	-5.03458	6.02015	4.14784
H	-5.82293	4.15045	5.58157
H	-4.72901	1.92656	5.42196
H	-2.86139	1.57238	3.84196
H	-0.27684	5.50920	2.28694

H	0.37194	4.22768	3.31962
H	0.83113	4.29863	1.60258
H	0.08035	0.06581	1.72157
H	-2.42858	4.61307	-0.04004
H	-1.19534	3.46060	-0.59946
H	-2.82049	2.89177	-0.15217

21

$PhMe_2Si$-H

C	12.02554	11.48978	4.72485
C	12.92041	10.75341	3.93321
C	14.29079	10.85922	4.22433
C	14.75004	11.66640	5.26303
C	13.84211	12.38914	6.03718
C	12.47807	12.29976	5.76653
Si	12.29662	9.65126	2.52454
C	12.71843	7.83459	2.85462
C	13.02463	10.20147	0.86500
H	15.01607	10.30336	3.63244
H	14.19768	13.01947	6.84804
H	11.76589	12.86090	6.36612
H	10.95790	11.43006	4.52462
H	13.80141	7.68895	2.92403
H	12.27264	7.49577	3.79448
H	12.34370	7.19542	2.04842
H	14.11761	10.13542	0.87223
H	12.65509	9.57013	0.05033

H	12.75192	11.23782	0.64478
H	10.80384	9.80993	2.48465
H	15.81521	11.73256	5.46960
34			
$B(C_6F_5)_3$			
B	8.34821	9.65598	2.09025
C	8.44211	11.21705	2.00195
C	8.61524	8.78299	0.81723
C	7.99099	8.96776	3.45126
C	7.05087	9.50981	4.33804
C	6.71690	8.90882	5.54498
C	7.35175	7.72584	5.91398
C	8.30083	7.15370	5.07119
C	8.59382	7.77110	3.86188
F	6.40358	10.63771	4.02707
F	5.80301	9.44974	6.34816
F	7.05241	7.14422	7.06810
F	8.91348	6.02716	5.42964
F	9.52129	7.18652	3.09657
C	7.99539	11.92908	0.88042
C	8.06354	13.31336	0.78832
C	8.61800	14.03805	1.83996
C	9.08581	13.37500	2.97136
C	8.98127	11.99152	3.03819
F	7.44423	11.28306	-0.15246
F	7.60831	13.95014	-0.28882

F	8.70053	15.35992	1.76398
F	9.62387	14.06914	3.97215
F	9.45663	11.40423	4.14132
C	7.87411	7.62770	0.53474
C	8.09090	6.84873	-0.59474
C	9.10089	7.20679	-1.48376
C	9.87232	8.34001	-1.24040
C	9.61259	9.10747	-0.11221
F	6.88517	7.24600	1.34979
F	7.34862	5.76949	-0.83356
F	9.32802	6.46837	-2.56217
F	10.84379	8.67564	-2.08674
F	10.39005	10.17826	0.07979

55

$PhMe_2Si$-H-B_R_3

Si	12.02377	9.25959	3.01552
C	12.90243	8.84699	1.40447
C	12.60163	10.88880	3.75140
C	12.05411	7.83773	4.24558
C	13.28825	11.82600	2.96051
C	13.75576	13.01999	3.50548
C	13.54536	13.29895	4.85510
C	12.86752	12.38131	5.65697
C	12.40030	11.18876	5.10961
H	13.45985	11.62692	1.90653
H	14.28263	13.73219	2.87664

H	13.90863	14.23016	5.28128
H	12.70128	12.59511	6.70917
H	11.86868	10.49031	5.74898
H	13.09457	7.59227	4.48426
H	11.53899	8.08720	5.17533
H	11.58191	6.95289	3.81200
H	13.98517	8.85250	1.56955
H	12.61319	7.85246	1.05751
H	12.66884	9.57134	0.62086
H	10.49858	9.44119	2.63131
B	9.01295	9.61123	2.20022
C	8.92640	11.19687	2.36711
C	9.10758	9.01368	0.71947
C	8.32321	8.69260	3.31353
C	7.37036	7.71232	3.02276
C	6.76601	6.92674	4.00158
C	7.11276	7.10363	5.33576
C	8.05327	8.07130	5.67560
C	8.61703	8.84384	4.66998
F	6.96877	7.49494	1.76392
F	5.85758	6.00984	3.66844
F	6.55039	6.35585	6.28062
F	8.39855	8.25090	6.95189
F	9.51074	9.77374	5.05513
C	7.95664	11.85134	3.13135
C	7.90307	13.23675	3.26250

C	8.84770	14.02525	2.61643
C	9.83064	13.41996	1.83941
C	9.83865	12.03745	1.72442
F	7.00025	11.16262	3.76753
F	6.95186	13.81119	3.99966
F	8.81180	15.34929	2.73723
F	10.74112	14.16594	1.21254
F	10.80195	11.50217	0.95184
C	8.60430	9.66273	-0.41095
C	8.67186	9.11886	-1.69140
C	9.26552	7.87634	-1.87989
C	9.77604	7.18831	-0.78330
C	9.67184	7.75970	0.47727
F	7.99856	10.85198	-0.30761
F	8.17024	9.77913	-2.73520
F	9.34415	7.34765	-3.09756
F	10.35158	5.99622	-0.94931
F	10.17110	7.04503	1.50429

224

dimer

La	5.95089	7.30599	1.82705
C	9.23648	5.76832	1.64407
O	8.17180	6.44745	1.70746
O	9.90606	5.55248	0.60505
C	10.81179	4.50219	2.91327
O	9.62857	5.26045	2.83257

C	11.99355	5.17509	3.28747
O	4.93998	5.97095	3.21867
C	13.14616	3.05147	2.99926
H	14.07236	2.48372	2.99778
O	5.66529	9.35499	2.49112
C	13.16544	4.40837	3.28847
H	14.11211	4.87296	3.53374
C	10.72446	3.10556	2.74002
C	11.93879	2.40753	2.76984
H	11.94414	1.33589	2.61745
C	12.02176	6.62846	3.81061
C	11.13832	6.71225	5.07307
H	10.09653	6.47004	4.85514
H	11.17421	7.72603	5.48860
H	11.49724	6.02117	5.84277
C	11.54363	7.66149	2.77429
H	12.07910	7.54809	1.82760
H	11.74313	8.67124	3.15047
H	10.47200	7.60400	2.58236
C	13.44422	7.04833	4.22183
H	14.13726	7.05181	3.37349
H	13.85627	6.40506	5.00550
H	13.41116	8.06681	4.62133
C	8.55563	2.61498	3.91151
H	8.31464	3.67455	4.00792
H	9.09584	2.30223	4.81125

H	7.61344	2.05705	3.87236
C	9.39122	2.32912	2.64699
C	8.56978	2.68166	1.39274
H	9.17535	2.61355	0.48427
H	8.12016	3.67427	1.45045
H	7.74097	1.97288	1.29321
C	9.63210	0.80953	2.59692
H	8.66376	0.29969	2.59160
H	10.18444	0.44999	3.47084
H	10.16751	0.50212	1.69232
C	3.89718	12.42405	3.39441
H	2.90589	12.86003	3.35657
C	4.10414	11.13592	2.89114
C	5.42199	10.59703	2.96274
C	4.92479	13.17450	3.94763
H	4.73072	14.17246	4.33059
C	6.20256	12.63728	4.00557
H	6.99448	13.23640	4.43937
C	6.48931	11.35662	3.52422
C	2.91893	10.35764	2.28641
C	2.63795	9.07898	3.09678
H	1.79622	8.52803	2.66173
H	2.37891	9.32779	4.13095
H	3.49621	8.40612	3.14048
C	3.19005	10.02433	0.80834
H	4.11412	9.46239	0.66247

H	3.28372	10.94184	0.21955
H	2.36525	9.44086	0.38382
C	1.61307	11.17245	2.30981
H	1.69449	12.10030	1.73413
H	1.29995	11.42319	3.32860
H	0.81243	10.57610	1.85934
C	7.92704	10.81193	3.61864
C	8.48044	10.50802	2.21369
H	7.86276	9.78802	1.67471
H	9.49877	10.10886	2.27937
H	8.51385	11.42246	1.61237
C	8.89761	11.82449	4.25244
H	9.89974	11.38361	4.29203
H	8.61345	12.08269	5.27775
H	8.96875	12.74879	3.66966
C	7.96451	9.55884	4.51262
H	7.26715	8.79062	4.17531
H	7.68276	9.81589	5.53898
H	8.97113	9.12733	4.53502
C	4.30808	5.04138	3.96677
C	4.49172	5.02002	5.37998
C	3.82634	4.02864	6.10801
H	3.94703	3.98592	7.18382
C	3.00602	3.08778	5.50110
H	2.50379	2.33161	6.09789
C	2.83123	3.12636	4.12543

H	2.18380	2.38962	3.66410
C	3.46412	4.08563	3.33026
C	5.37806	6.04089	6.11958
C	4.84364	7.46992	5.90856
H	4.84741	7.76518	4.85950
H	5.45443	8.19062	6.46404
H	3.81395	7.55028	6.27269
C	6.84023	5.92738	5.64917
H	7.24852	4.94534	5.90907
H	7.45851	6.68928	6.13766
H	6.94048	6.04621	4.56903
C	5.39569	5.80418	7.64050
H	5.79306	4.81781	7.90237
H	4.40122	5.90725	8.08718
H	6.04369	6.55246	8.10929
C	3.23160	4.09328	1.80924
C	4.56147	3.85945	1.06596
H	4.91582	2.83852	1.23974
H	5.35569	4.52153	1.41914
H	4.43925	3.99520	-0.01377
C	2.56384	5.41643	1.38543
H	3.12527	6.29375	1.71360
H	1.57096	5.49803	1.83970
H	2.44060	5.46270	0.29772
C	2.28407	2.97124	1.34910
H	2.16430	3.02470	0.26139

H	1.28848	3.06531	1.79456
H	2.67701	1.97763	1.58759
La	9.57719	5.50105	-1.83603
C	6.34534	7.14924	-1.64505
O	7.38472	6.43186	-1.70099
O	5.66277	7.36833	-0.61459
C	4.86051	8.51924	-2.92402
O	5.99830	7.69576	-2.82981
C	3.64397	7.91579	-3.30451
O	10.59275	6.70352	-3.33931
C	2.62216	10.11149	-3.06548
H	1.73341	10.73583	-3.08830
O	9.79590	3.42663	-2.45023
C	2.52258	8.75412	-3.33489
H	1.55221	8.34618	-3.58776
C	5.03033	9.90956	-2.76144
C	3.86291	10.68168	-2.82064
H	3.92127	11.75334	-2.67947
C	3.53031	6.45642	-3.79611
C	4.40386	6.29242	-5.05735
H	5.45708	6.48968	-4.84823
H	4.31729	5.26964	-5.44232
H	4.07720	6.97722	-5.84677
C	3.95462	5.42556	-2.73315
H	3.48521	5.63573	-1.76854
H	3.64098	4.42451	-3.04972

H	5.03569	5.38592	-2.59483
C	2.08456	6.10952	-4.19427
H	1.39497	6.16518	-3.34487
H	1.70726	6.75671	-4.99209
H	2.05872	5.08218	-4.57098
C	7.25623	10.25857	-3.88094
H	7.44017	9.18660	-3.96594
H	6.75756	10.59408	-4.79633
H	8.22641	10.76442	-3.82105
C	6.40573	10.60225	-2.64086
C	7.16683	10.20860	-1.36079
H	6.53904	10.32359	-0.47250
H	7.55138	9.18800	-1.39567
H	8.03631	10.86350	-1.24163
C	6.25838	12.13414	-2.60337
H	7.25570	12.58364	-2.56949
H	5.75597	12.52326	-3.49463
H	5.71527	12.47779	-1.71654
C	11.33193	0.21414	-3.27594
H	12.29439	-0.28320	-3.25496
C	11.22995	1.53964	-2.84193
C	9.94500	2.15561	-2.88226
C	10.23533	-0.49757	-3.74090
H	10.34853	-1.52686	-4.06951
C	8.99493	0.12175	-3.78917
H	8.15012	-0.44468	-4.16297

C	8.81206	1.44373	-3.37295
C	12.49211	2.27937	-2.35730
C	12.78486	3.48793	-3.26607
H	13.67979	4.01889	-2.92132
H	12.96447	3.15863	-4.29461
H	11.95875	4.20000	-3.29942
C	12.33819	2.71677	-0.89001
H	11.46212	3.34603	-0.72495
H	12.22666	1.84325	-0.24038
H	13.22306	3.26934	-0.55449
C	13.74678	1.38881	-2.40829
H	13.65344	0.50590	-1.76722
H	13.97670	1.05573	-3.42562
H	14.60709	1.96442	-2.05007
C	7.41505	2.08506	-3.46454
C	6.91200	2.48208	-2.06422
H	7.59275	3.17040	-1.56041
H	5.92662	2.95622	-2.12879
H	6.82016	1.59580	-1.42800
C	6.36336	1.12046	-4.04103
H	5.39589	1.63212	-4.08981
H	6.61419	0.79664	-5.05628
H	6.23211	0.23074	-3.41645
C	7.44831	3.30108	-4.40983
H	8.21049	4.02793	-4.12364
H	7.68377	2.98226	-5.43040

H	6.47593	3.80514	-4.42776
C	11.38017	7.54405	-4.04270
C	11.29069	7.58136	-5.46328
C	12.13356	8.46664	-6.14307
H	12.09208	8.51858	-7.22469
C	13.03274	9.29112	-5.47978
H	13.67383	9.96540	-6.04065
C	13.10338	9.24705	-4.09458
H	13.80799	9.89825	-3.58934
C	12.29192	8.38974	-3.34756
C	10.31058	6.69386	-6.25438
C	10.62210	5.20363	-6.02201
H	10.52466	4.91983	-4.97409
H	9.93897	4.57775	-6.60779
H	11.64455	4.97152	-6.33796
C	8.85732	7.01183	-5.85295
H	8.61022	8.04980	-6.09926
H	8.16178	6.36188	-6.39689
H	8.68997	6.87464	-4.78369
C	10.40877	6.93031	-7.77161
H	10.17268	7.96361	-8.04720
H	11.40136	6.68502	-8.16396
H	9.68687	6.28274	-8.28058
C	12.38761	8.37172	-1.81338
C	11.03136	8.78249	-1.20027
H	10.85223	9.84862	-1.37165

H	10.18891	8.26235	-1.66419
H	11.01183	8.60861	-0.11912
C	12.84689	6.98012	-1.33064
H	12.28767	6.16549	-1.79839
H	13.89164	6.81229	-1.61139
H	12.77160	6.88577	-0.24232
C	13.42090	9.37225	-1.26760
H	13.43312	9.31858	-0.17329
H	14.43367	9.15019	-1.61897
H	13.17850	10.40363	-1.54312

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Monomer

C	14.55292	2.39069	1.24917
O	13.68896	2.61004	0.34547
O	15.77356	2.16841	0.99334
C	15.00994	2.21171	3.55964
O	14.09081	2.40154	2.51053
C	15.57704	3.36187	4.14220
C	16.88264	1.85142	5.53319
H	17.64834	1.70588	6.29017
C	16.54453	3.13551	5.12909
H	17.04220	3.97506	5.59800
C	15.22966	0.89896	4.02048
C	16.20977	0.75558	5.01082
H	16.45137	-0.22949	5.38986
C	15.10913	4.79875	3.81953

C	13.60708	4.92486	4.15065
H	13.00189	4.24256	3.55053
H	13.26709	5.94717	3.94877
H	13.42246	4.71051	5.20851
C	15.34727	5.19539	2.34799
H	16.35690	4.93255	2.02126
H	15.22974	6.27918	2.23913
H	14.62362	4.73762	1.67123
C	15.85563	5.83196	4.68172
H	16.93007	5.84967	4.46890
H	15.71542	5.65660	5.75309
H	15.46162	6.82879	4.46017
C	12.90311	-0.04580	3.88254
H	12.52878	0.82555	3.34183
H	12.75522	0.12422	4.95415
H	12.29743	-0.91185	3.59168
C	14.39020	-0.31784	3.57147
C	14.55121	-0.64411	2.07305
H	15.60380	-0.66097	1.77686
H	14.01503	0.06082	1.43584
H	14.12522	-1.63209	1.86732
C	14.79160	-1.58608	4.34567
H	14.13761	-2.40860	4.03965
H	14.67802	-1.46376	5.42755
H	15.82217	-1.89202	4.13549
La	15.33911	2.30167	-1.41879

O	16.20791	4.08076	-2.33535
O	14.97189	0.42091	-2.45567
C	16.16618	-2.69187	-3.94395
H	17.09217	-3.18200	-4.22196
C	16.20125	-1.41507	-3.37700
C	14.96484	-0.80328	-3.02282
C	14.96965	-3.35801	-4.16900
H	14.96919	-4.35027	-4.61116
C	13.77244	-2.74283	-3.82856
H	12.84854	-3.27687	-4.01735
C	13.72730	-1.46858	-3.25459
C	17.54829	-0.69714	-3.17509
C	17.58706	0.58920	-4.02410
H	18.52349	1.13520	-3.86575
H	17.51889	0.33908	-5.08769
H	16.75152	1.26086	-3.81192
C	17.79145	-0.39992	-1.68014
H	16.92135	0.05010	-1.19206
H	17.98262	-1.32813	-1.13205
H	18.66060	0.25402	-1.54269
C	18.74557	-1.54826	-3.63381
H	18.81521	-2.49153	-3.08253
H	18.70046	-1.77516	-4.70369
H	19.67290	-0.99303	-3.45497
C	12.36888	-0.83510	-2.89598
C	12.27046	-0.59384	-1.37764

H	13.05422	0.07061	-1.01340
H	11.30333	-0.14504	-1.12293
H	12.35734	-1.54074	-0.83472
C	11.18491	-1.74432	-3.26996
H	10.24979	-1.24066	-3.00241
H	11.14850	-1.95504	-4.34395
H	11.20823	-2.69703	-2.73055
C	12.16786	0.48173	-3.67112
H	12.97569	1.19009	-3.48269
H	12.14181	0.29143	-4.74935
H	11.21885	0.95115	-3.38621
C	16.51375	5.22576	-2.97961
C	15.55825	5.80923	-3.85987
C	15.90168	6.99750	-4.51038
H	15.19443	7.46381	-5.18661
C	17.13448	7.60543	-4.31814
H	17.37751	8.52825	-4.83718
C	18.05492	7.02380	-3.45651
H	19.01203	7.51387	-3.31982
C	17.78229	5.83742	-2.76872
C	14.18683	5.15774	-4.11456
C	14.37458	3.77034	-4.76041
H	15.03097	3.11637	-4.18002
H	13.41091	3.26767	-4.89806
H	14.84323	3.87290	-5.74442
C	13.37283	5.07088	-2.80606

H	13.07032	6.07089	-2.47898
H	12.46224	4.47676	-2.94622
H	13.94608	4.65385	-1.97282
C	13.32057	5.96804	-5.09519
H	13.11452	6.97725	-4.72443
H	13.78538	6.05039	-6.08284
H	12.35737	5.46315	-5.22714
C	18.83612	5.23807	-1.81796
C	18.28790	5.18595	-0.37898
H	18.06795	6.19583	-0.01726
H	17.36708	4.60498	-0.31436
H	19.02544	4.73688	0.29669
C	19.24951	3.83175	-2.29274
H	18.39029	3.16418	-2.37098
H	19.71689	3.88256	-3.28195
H	19.97366	3.39014	-1.59773
C	20.12306	6.07921	-1.76722
H	20.83351	5.60634	-1.08055
H	20.60981	6.14948	-2.74560
H	19.93790	7.09373	-1.39938

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Monomer - $PhMe_2Si$-H-B_R_3 coordination

C	24.86641	8.46738	-1.83698
C	24.04686	9.04258	-0.82225
C	24.59932	9.94022	0.13729
C	25.96844	10.21502	0.06231

C	26.78287	9.64987	-0.90830
C	26.22623	8.79122	-1.84501
O	22.73158	8.73241	-0.76960
La	20.62817	8.23613	-0.58545
O	20.58369	7.21053	1.67342
C	20.18710	6.09690	1.22893
O	19.81110	5.92557	0.03138
Si	15.74798	4.09092	-1.13882
C	15.31082	5.55935	-0.06321
C	23.75098	10.60867	1.23712
C	24.57836	11.56914	2.11102
C	24.30113	7.53238	-2.92270
C	23.25345	8.28480	-3.76542
F	20.37273	6.73519	-2.90029
C	19.57686	6.03861	-3.75245
C	18.21069	5.96581	-3.53609
C	17.33658	5.28130	-4.38180
C	17.94303	4.68404	-5.48935
C	19.31458	4.73346	-5.73477
C	20.14515	5.41595	-4.85570
B	15.74728	5.25704	-4.09784
C	14.88808	4.09396	-4.79547
C	15.25685	2.75556	-4.64855
C	14.55109	1.68950	-5.18606
C	13.41107	1.95070	-5.93975
C	13.00788	3.26596	-6.13418

C	13.74217	4.30523	-5.56589
F	16.36253	2.45128	-3.93947
F	14.95270	0.43163	-4.99257
F	12.71538	0.94863	-6.47167
F	11.92209	3.52518	-6.86428
F	13.29469	5.54265	-5.81679
F	17.74143	6.60688	-2.44775
F	21.45622	5.47499	-5.07473
F	19.83373	4.13899	-6.80703
F	17.21545	4.03731	-6.40484
C	15.05436	6.70009	-3.95117
C	15.53439	7.85458	-4.57194
C	14.92772	9.10094	-4.44124
C	13.78338	9.22907	-3.66315
C	13.25760	8.10369	-3.03536
C	13.89001	6.87954	-3.20460
F	16.62298	7.80980	-5.35596
F	13.32491	5.81945	-2.59188
F	12.15560	8.20693	-2.28911
F	13.19108	10.41124	-3.52479
F	15.43797	10.16751	-5.05778
O	19.32934	9.91278	-1.09145
C	18.56723	11.01445	-1.27806
C	17.67514	11.43446	-0.24945
C	16.92007	12.59172	-0.45947
C	17.01000	13.32160	-1.63553

C	17.86676	12.88885	-2.63722
C	18.65787	11.74431	-2.49837
C	17.50285	10.63897	1.05612
C	16.46306	11.26878	2.00041
C	19.59059	11.32448	-3.64973
C	19.46974	12.25505	-4.87039
C	16.98365	9.22499	0.72998
C	18.82418	10.59557	1.84814
C	21.05973	11.39574	-3.19452
C	19.22588	9.91356	-4.14973
O	20.15852	4.99801	2.01573
C	20.64271	5.10479	3.33341
C	19.71510	5.36348	4.36130
C	20.24800	5.54899	5.64288
C	21.60950	5.43654	5.88601
C	22.46844	5.05490	4.86491
C	22.01008	4.84672	3.55807
C	18.18626	5.34730	4.15080
C	17.43527	5.54222	5.47954
C	22.95192	4.24445	2.49190
C	24.35900	4.00008	3.06537
C	17.76825	3.97152	3.58999
C	17.70801	6.46215	3.20276
C	22.38835	2.87442	2.05784
C	23.12912	5.14037	1.25118
C	17.50005	3.46129	-0.95484

C	14.44939	2.74746	-1.18631
C	14.82526	1.40588	-1.37669
C	13.87430	0.38862	-1.35783
C	12.53030	0.69612	-1.14924
C	12.13863	2.02129	-0.95958
C	13.08963	3.03805	-0.97859
C	22.63216	11.46462	0.61248
C	23.17619	9.54655	2.19292
C	23.70528	6.26153	-2.28775
C	25.38047	7.05141	-3.90864
H	15.73172	4.80673	-2.74609
H	21.99768	5.60523	6.88659
H	19.58965	5.78110	6.47076
H	23.51610	4.90873	5.09525
H	18.23607	3.77095	2.62397
H	16.67953	3.93579	3.46134
H	18.04869	3.16896	4.28009
H	18.13187	7.42972	3.48498
H	16.61590	6.54241	3.25409
H	17.96399	6.26425	2.16113
H	17.62354	6.52671	5.92091
H	17.69367	4.77549	6.21667
H	16.35902	5.46809	5.29344
H	21.39805	2.97124	1.60748
H	22.31387	2.19597	2.91425
H	23.05439	2.41384	1.31902

H	23.35061	6.17548	1.52486
H	22.25264	5.11968	0.60078
H	23.96618	4.76816	0.65148
H	24.97797	3.52828	2.29590
H	24.34407	3.32753	3.92887
H	24.85405	4.93265	3.35658
H	26.41742	10.89156	0.77972
H	27.84358	9.88273	-0.93852
H	26.87255	8.36511	-2.60326
H	22.02365	11.93153	1.39525
H	23.06153	12.26388	-0.00057
H	21.96886	10.89087	-0.03701
H	22.59445	8.77965	1.68081
H	23.98777	9.03234	2.71886
H	22.53247	10.01324	2.94762
H	25.38397	11.05441	2.64493
H	25.01506	12.38650	1.52774
H	23.92240	12.01758	2.86485
H	22.98119	6.49494	-1.50575
H	23.21496	5.64313	-3.04656
H	24.49675	5.66537	-1.82204
H	24.91648	6.39654	-4.65427
H	25.84690	7.88249	-4.44733
H	26.16802	6.47602	-3.41085
H	22.46174	8.71417	-3.15042
H	23.72735	9.11452	-4.30021

H	22.80034	7.61736	-4.50532
H	17.91949	13.46365	-3.55372
H	16.41142	14.21747	-1.77382
H	16.23962	12.93418	0.31119
H	21.27199	10.73440	-2.35299
H	21.73038	11.12280	-4.01685
H	21.31106	12.41365	-2.87880
H	18.22774	9.91135	-4.59666
H	19.93853	9.58313	-4.91479
H	19.22036	9.18233	-3.34006
H	18.45426	12.26925	-5.27939
H	19.76612	13.28338	-4.63838
H	20.13694	11.89380	-5.66042
H	15.99962	9.29107	0.25374
H	17.63870	8.69405	0.03549
H	16.88030	8.62922	1.64242
H	19.66874	10.27445	1.23536
H	19.07529	11.59535	2.21725
H	18.74609	9.92454	2.71034
H	16.38707	10.65989	2.90802
H	16.74624	12.28060	2.30796
H	15.46696	11.31147	1.54799
H	12.76655	4.06466	-0.83689
H	11.09172	2.26279	-0.79916
H	11.78759	-0.09686	-1.13593
H	14.18142	-0.64227	-1.50858

H	15.86719	1.15090	-1.54672
H	14.29648	5.91469	-0.25026
H	15.39246	5.26095	0.98753
H	16.01123	6.37804	-0.24151
H	17.82357	2.91940	-1.84615
H	18.19931	4.27726	-0.75147
H	17.53209	2.77025	-0.10459

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Monomer - $PhMe_2Si$-H-B_R_3 coord TS

C	24.64083	8.13816	-1.35238
C	23.68581	8.70590	-0.46028
C	24.10367	9.48326	0.65650
C	25.47736	9.62468	0.87709
C	26.42095	9.04807	0.03991
C	25.99615	8.32463	-1.06453
O	22.36083	8.50564	-0.67865
La	20.25111	8.07854	-0.75911
O	19.61832	6.28170	0.62527
C	18.96326	5.29482	1.12982
O	17.87295	4.85765	0.75951
Si	16.43866	4.55630	-1.29540
C	15.80477	6.19531	-0.64150
C	23.10897	10.18890	1.59754
C	23.81900	10.97370	2.71595
C	24.23637	7.36413	-2.62061
C	23.42423	8.28307	-3.55290

F	20.47776	6.97178	-3.29655
C	19.66156	6.31544	-4.17134
C	18.31393	6.21235	-3.88963
C	17.39713	5.50960	-4.66462
C	17.95606	4.95514	-5.82012
C	19.31022	5.05258	-6.15331
C	20.18585	5.73210	-5.31504
B	15.83813	5.35466	-4.21136
C	15.01186	4.17087	-4.94484
C	15.36175	2.83170	-4.77618
C	14.68042	1.76641	-5.34942
C	13.58654	2.02863	-6.16681
C	13.20807	3.34612	-6.39152
C	13.92009	4.38198	-5.78998
F	16.43405	2.51494	-4.02110
F	15.06983	0.50741	-5.13429
F	12.91541	1.02786	-6.73398
F	12.17034	3.61146	-7.18761
F	13.50468	5.62203	-6.08778
F	17.92644	6.82796	-2.74041
F	21.48287	5.81747	-5.59833
F	19.77118	4.49107	-7.26845
F	17.20100	4.28967	-6.69699
C	15.03686	6.75061	-4.06341
C	15.42531	7.95911	-4.64093
C	14.70433	9.14258	-4.50436

C	13.52236	9.14557	-3.77480
C	13.07988	7.96030	-3.19531
C	13.83243	6.80464	-3.36016
F	16.54070	8.04137	-5.38865
F	13.35279	5.68709	-2.78115
F	11.94576	7.94417	-2.49125
F	12.81994	10.26697	-3.63144
F	15.14356	10.26896	-5.07132
O	19.07622	9.88453	-0.92107
C	18.40216	11.05243	-1.09401
C	17.53110	11.52472	-0.07015
C	16.86140	12.73365	-0.28430
C	17.02025	13.46809	-1.44918
C	17.86498	12.99111	-2.43937
C	18.56906	11.79097	-2.30148
C	17.30527	10.76841	1.25225
C	16.29681	11.47911	2.17326
C	19.47754	11.32143	-3.45362
C	19.47052	12.29701	-4.64530
C	16.72624	9.36924	0.97944
C	18.62333	10.68012	2.04103
C	20.94191	11.23324	-2.98883
C	18.97706	9.97442	-4.00490
O	19.50786	4.62370	2.18942
C	20.68765	5.02170	2.82011
C	20.57601	5.86284	3.94841

C	21.77791	6.26268	4.54616
C	23.00633	5.81189	4.08183
C	23.06072	4.88109	3.05385
C	21.90118	4.42519	2.41379
C	19.22461	6.21980	4.60646
C	19.42483	7.10156	5.85188
C	21.97638	3.22906	1.43957
C	23.42044	2.72059	1.28369
C	18.54070	4.91621	5.07045
C	18.27528	6.98741	3.66689
C	21.14148	2.06586	2.01742
C	21.47134	3.56698	0.02683
C	18.13298	3.91607	-1.80414
C	15.29797	3.15400	-0.80243
C	15.65038	1.81127	-1.02186
C	14.80518	0.77573	-0.63213
C	13.58970	1.06376	-0.01248
C	13.22181	2.38907	0.21490
C	14.06791	3.42292	-0.17814
C	22.27856	11.21912	0.80885
C	22.20808	9.16684	2.31232
C	23.44594	6.09574	-2.25100
C	25.45134	6.88620	-3.43589
H	15.92444	4.89224	-2.94432
H	23.92371	6.15012	4.55562
H	21.75946	6.92914	5.39918

H	24.02663	4.49001	2.76010
H	18.33311	4.25157	4.22972
H	17.58989	5.14959	5.56356
H	19.17072	4.38115	5.78870
H	18.79152	7.81389	3.17128
H	17.45038	7.41080	4.25114
H	17.82352	6.34669	2.90915
H	19.87506	8.06985	5.60670
H	20.04332	6.61349	6.61171
H	18.44896	7.29925	6.30683
H	20.08851	2.33568	2.11923
H	21.51811	1.77083	3.00230
H	21.20964	1.19432	1.35592
H	21.97485	4.45237	-0.37054
H	20.39561	3.73144	0.00261
H	21.68294	2.73048	-0.64895
H	23.41989	1.85104	0.61873
H	23.85286	2.40143	2.23728
H	24.07981	3.47334	0.83807
H	25.82561	10.20365	1.72389
H	27.48138	9.17278	0.23989
H	26.74510	7.89739	-1.72051
H	21.58287	11.74232	1.47361
H	22.93701	11.96672	0.35458
H	21.69840	10.76658	0.00347
H	21.66484	8.51670	1.62054

H	22.80174	8.49658	2.93937
H	21.47693	9.67380	2.95130
H	24.42355	10.32506	3.35848
H	24.46156	11.76598	2.31877
H	23.06476	11.45215	3.34949
H	22.59395	6.32118	-1.60712
H	23.07983	5.59050	-3.15119
H	24.08474	5.39574	-1.70280
H	25.09651	6.35605	-4.32625
H	26.07198	7.72059	-3.77823
H	26.08356	6.19244	-2.87194
H	22.56120	8.71676	-3.04810
H	24.04948	9.11307	-3.89802
H	23.07527	7.73109	-4.43189
H	17.97556	13.57287	-3.34596
H	16.48574	14.40365	-1.58631
H	16.19376	13.11658	0.47779
H	21.09132	10.53207	-2.16526
H	21.58959	10.92480	-3.81673
H	21.28963	12.20923	-2.63535
H	17.99774	10.09179	-4.47631
H	19.66913	9.58446	-4.76044
H	18.85724	9.22754	-3.21761
H	18.47129	12.41720	-5.07529
H	19.85415	13.28566	-4.37319
H	20.11976	11.89993	-5.43298

H	15.76515	9.44892	0.46120
H	17.38574	8.76743	0.35257
H	16.56187	8.82865	1.91791
H	19.40958	10.18179	1.47127
H	18.98849	11.68330	2.28458
H	18.47622	10.13669	2.98072
H	16.17784	10.89212	3.09026
H	16.63611	12.47775	2.46675
H	15.30828	11.57051	1.71174
H	13.76321	4.44875	0.00568
H	12.27534	2.61784	0.69669
H	12.92956	0.25601	0.29183
H	15.09438	-0.25573	-0.81302
H	16.58881	1.56666	-1.50957
H	16.39633	7.04410	-0.97755
H	14.77764	6.33667	-0.98110
H	15.82706	6.15493	0.44828
H	18.12322	3.52813	-2.82218
H	18.90463	4.67731	-1.70145
H	18.37601	3.10629	-1.11264

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Monomer - $PhMe_2Si$-H-B_R_3 coord product

C	18.03721	6.38319	-3.88809
C	16.94147	5.72729	-4.42508
C	17.08968	5.46014	-5.79064
C	18.21762	5.80709	-6.54037

C	19.28133	6.47054	-5.93812
C	19.16607	6.75598	-4.58797
B	15.69997	5.29766	-3.44074
C	14.57428	4.34074	-4.12367
C	13.54437	4.82690	-4.92885
C	12.53751	4.02820	-5.46095
C	12.54124	2.66292	-5.19538
C	13.55164	2.12588	-4.40799
C	14.53749	2.96669	-3.89702
F	13.49918	6.13336	-5.24061
F	11.57423	4.55231	-6.22682
F	11.58603	1.87576	-5.69718
F	13.56944	0.81150	-4.15101
F	15.48922	2.36632	-3.15144
F	16.12865	4.83233	-6.47326
F	18.28523	5.51026	-7.83766
F	20.36922	6.81711	-6.62598
F	20.16954	7.41665	-3.92819
La	20.06829	8.09779	-1.31839
F	18.06892	6.72841	-2.54936
O	19.01439	9.95231	-1.10426
C	18.58613	11.24334	-1.12809
C	18.01340	11.81771	0.04040
C	17.67349	13.17338	-0.00301
C	17.85037	13.94132	-1.14467
C	18.34168	13.34429	-2.29610

C	18.70689	11.99536	-2.32967
C	17.71180	10.99726	1.30797
C	19.00424	10.44263	1.92891
C	19.17208	11.36467	-3.65542
C	18.23756	10.19923	-4.03465
O	22.21218	8.25511	-1.14757
C	23.56042	8.23594	-0.98553
C	24.15505	9.00448	0.05546
C	25.54121	8.91772	0.22074
C	26.33321	8.12173	-0.59329
C	25.74178	7.40307	-1.62144
C	24.36408	7.44254	-1.85512
C	23.33614	9.90584	0.99876
C	22.40224	9.04057	1.86388
C	23.78225	6.68885	-3.06543
C	24.85138	5.90235	-3.84501
O	19.62460	6.34130	0.35902
C	19.38604	5.13162	0.50899
O	19.20754	4.34751	-0.50232
Si	18.65579	2.65594	-0.77797
C	16.89004	2.52550	-0.19325
C	24.22923	10.68798	1.98000
C	22.55056	10.96497	0.20226
C	23.19332	7.71855	-4.04965
C	22.73960	5.64277	-2.62461
C	19.10823	12.35665	-4.83153

C	20.64241	10.91464	-3.56611
C	17.02949	11.83838	2.40153
C	16.73642	9.85673	0.96156
O	19.31326	4.55573	1.70536
C	19.54107	5.37805	2.84671
C	18.41723	5.96081	3.46315
C	18.69213	6.84013	4.51849
C	19.98979	7.07943	4.94712
C	21.04991	6.38665	4.38021
C	20.86311	5.48873	3.32076
C	16.95696	5.59156	3.12363
C	16.57740	5.89583	1.66196
C	22.03812	4.60526	2.84297
C	22.37298	4.77520	1.34822
C	15.96044	6.36500	4.00514
C	16.75887	4.09160	3.42702
C	23.32859	4.92376	3.61905
C	21.68401	3.13287	3.13471
C	18.85448	2.56880	-2.63277
C	19.81928	1.47269	0.10219
C	19.37205	0.68430	1.17516
C	20.20760	-0.25837	1.77261
C	21.50986	-0.42921	1.30612
C	21.97321	0.34162	0.23975
C	21.13343	1.27878	-0.35717
C	15.02026	6.59509	-2.71450

C	14.98473	7.89299	-3.22068
C	14.43325	8.97446	-2.53814
C	13.86282	8.77249	-1.28747
C	13.85563	7.49275	-0.74498
C	14.42305	6.44531	-1.46327
F	15.52566	8.17216	-4.42230
F	14.45884	10.20275	-3.06879
F	13.35010	9.80027	-0.60293
F	13.32482	7.28347	0.46812
F	14.39206	5.23558	-0.86769
H	20.17245	7.77913	5.75769
H	17.87616	7.34367	5.02084
H	22.04382	6.54432	4.77843
H	17.45554	3.46736	2.86290
H	15.73793	3.78825	3.16958
H	16.91409	3.88782	4.49163
H	16.87534	6.90862	1.37948
H	15.49428	5.82332	1.53343
H	17.01242	5.19179	0.95280
H	16.00962	7.44574	3.83567
H	16.10992	6.17099	5.07194
H	14.94546	6.04339	3.75397
H	20.79227	2.81068	2.59461
H	21.51135	2.98158	4.20543
H	22.50983	2.48167	2.82928
H	22.49124	5.82700	1.07432

H	21.63022	4.31466	0.69530
H	23.32095	4.27109	1.13271
H	24.11706	4.24351	3.28293
H	23.21088	4.77637	4.69706
H	23.68133	5.94488	3.44035
H	26.02151	9.48812	1.00639
H	27.40682	8.07217	-0.43552
H	26.37531	6.80097	-2.26162
H	21.98878	11.61586	0.88059
H	23.23859	11.59259	-0.37368
H	21.84251	10.52555	-0.50003
H	21.73090	8.41753	1.26761
H	22.98968	8.36288	2.49168
H	21.79007	9.66301	2.52404
H	24.79719	10.02823	2.64417
H	24.93303	11.34641	1.46031
H	23.59550	11.31892	2.61193
H	21.95953	6.06767	-1.98969
H	22.26633	5.17500	-3.49519
H	23.22055	4.85458	-2.03599
H	24.37491	5.39163	-4.68880
H	25.62618	6.55614	-4.25715
H	25.33524	5.13828	-3.22738
H	22.48229	8.38741	-3.56336
H	23.99715	8.34257	-4.45322
H	22.69230	7.22578	-4.88941

H	18.43391	13.94609	-3.19204
H	17.58112	14.99360	-1.14466
H	17.25087	13.64595	0.87535
H	20.85467	10.29546	-2.68884
H	20.93950	10.36159	-4.46392
H	21.30365	11.78172	-3.47006
H	17.21300	10.55526	-4.17147
H	18.56069	9.73528	-4.97298
H	18.18683	9.42921	-3.26173
H	18.09109	12.72330	-5.00037
H	19.76907	13.21712	-4.68540
H	19.43152	11.84909	-5.74678
H	15.78556	10.25611	0.59678
H	17.13675	9.19774	0.18857
H	16.52578	9.25661	1.85400
H	19.56612	9.83063	1.22284
H	19.65997	11.26088	2.24451
H	18.78062	9.82654	2.80710
H	16.82672	11.19933	3.26777
H	17.66137	12.66379	2.74640
H	16.07173	12.25004	2.06780
H	18.35720	0.79810	1.54769
H	19.84076	-0.86113	2.59874
H	22.16128	-1.16587	1.76834
H	22.98539	0.20577	-0.13132
H	21.50853	1.85934	-1.19690

H	16.48551	1.56372	-0.52607
H	16.79519	2.58511	0.89263
H	16.27991	3.30880	-0.65031
H	18.60401	1.56099	-2.97809
H	18.16928	3.27006	-3.11492
H	19.87906	2.79219	-2.94341
H	16.23709	4.66268	-2.55578

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Monomer - CO_2 coord adduct

C	-3.62810	3.51871	2.15677
C	-2.62459	4.30726	1.59622
C	-2.79830	5.67891	1.77864
C	-3.86466	6.23230	2.48509
C	-4.83058	5.39821	3.03492
C	-4.71000	4.02415	2.86808
B	-1.36956	3.59627	0.82902
C	-0.00822	4.49460	0.78723
C	0.56250	5.10016	-0.33042
C	1.76654	5.80229	-0.29925
C	2.45337	5.93165	0.90131
C	1.92168	5.35540	2.04953
C	0.71645	4.66784	1.96705
F	-0.03704	5.02849	-1.53409
F	2.26384	6.35564	-1.41100
F	3.61022	6.59869	0.95257
F	2.57371	5.46489	3.21490

F	0.25323	4.14594	3.12313
F	-1.91981	6.55265	1.26337
F	-3.97375	7.55697	2.63211
F	-5.86213	5.90884	3.71226
F	-5.63704	3.20417	3.39016
F	-3.58273	2.17272	2.02249
C	-1.84259	3.03434	-0.63883
C	-1.48738	1.77794	-1.08811
C	-1.89650	1.21498	-2.28293
C	-2.72854	1.91525	-3.13767
C	-3.12430	3.19213	-2.74471
C	-2.67561	3.71744	-1.53313
F	-0.65032	0.95334	-0.34729
La	0.63925	-1.17540	-1.34343
F	-1.45091	-0.03927	-2.61394
F	-3.08201	4.95554	-1.24868
F	-3.91957	3.90159	-3.54419
F	-3.12649	1.38845	-4.29430
O	1.97058	-0.12928	-2.65516
C	3.04972	0.48300	-3.20789
C	3.06222	0.77591	-4.59845
C	4.22483	1.35052	-5.12250
C	5.32408	1.65224	-4.32961
C	5.27249	1.40312	-2.96555
C	4.14744	0.82579	-2.37204
C	1.84298	0.53586	-5.50957

C	2.10967	0.96492	-6.96249
C	4.09821	0.59799	-0.85307
C	5.37156	1.07690	-0.13528
O	0.74282	-1.90812	1.05289
C	0.38991	-2.69403	1.94313
O	-0.29363	-3.76158	1.67473
Si	-0.89966	-5.19781	2.53941
C	-2.28826	-5.71229	1.39678
O	0.22783	-3.10712	-2.20300
C	-0.11433	-4.38612	-2.48168
C	0.89728	-5.38677	-2.54407
C	0.49096	-6.71076	-2.74496
C	-0.84449	-7.05794	-2.89917
C	-1.81042	-6.06066	-2.89773
C	-1.48267	-4.71440	-2.70841
C	2.39824	-5.05730	-2.42846
C	3.28628	-6.29635	-2.64139
C	-2.57707	-3.63668	-2.82064
C	-2.23408	-2.70122	-3.99845
C	2.93570	1.40488	-0.23551
C	3.97674	-0.91010	-0.54421
C	1.46440	-0.95585	-5.55632
C	0.65980	1.38478	-5.00430
O	0.66647	-2.50845	3.23137
C	1.39506	-1.32869	3.57054
C	0.66179	-0.15392	3.82077

C	1.42745	1.01017	3.97539
C	2.81531	0.97456	3.95854
C	3.48421	-0.23960	3.86692
C	2.79316	-1.44529	3.68544
C	-0.86373	-0.11822	4.07092
C	-1.32778	1.29477	4.46407
C	3.54067	-2.79516	3.76671
C	5.04674	-2.58561	4.00439
C	-1.17038	-1.04162	5.26824
C	-1.70727	-0.54270	2.85358
C	2.99370	-3.57778	4.97901
C	3.41191	-3.65445	2.49560
C	-1.51802	-4.73982	4.24535
C	0.48708	-6.45952	2.58628
C	1.09715	-6.82477	3.79739
C	2.08298	-7.80967	3.83721
C	2.47419	-8.44913	2.66226
C	1.87630	-8.10420	1.45005
C	0.89044	-7.12042	1.41226
C	2.81033	-4.04197	-3.51214
C	2.72932	-4.52761	-1.02145
C	-2.74156	-2.86414	-1.49646
C	-3.96295	-4.23085	-3.12972
O	-5.73500	-0.03939	2.93486
C	-6.10042	0.58656	2.01808
O	-6.48454	1.17845	1.08886

H	3.37670	1.89814	4.06633
H	0.93351	1.96431	4.10160
H	4.56409	-0.24672	3.94482
H	-0.87777	-2.07530	5.07567
H	-2.24472	-1.02530	5.48345
H	-0.64309	-0.70039	6.16499
H	-1.43748	0.03598	1.96732
H	-2.76277	-0.34484	3.06115
H	-1.62830	-1.60948	2.63115
H	-1.17277	2.02241	3.66418
H	-0.82304	1.65038	5.36800
H	-2.40045	1.26482	4.67621
H	1.92928	-3.79713	4.87087
H	3.13233	-3.00837	5.90360
H	3.52544	-4.53022	5.08144
H	3.71454	-3.09818	1.60463
H	2.40547	-4.04401	2.34130
H	4.06725	-4.52766	2.58001
H	5.53007	-3.56302	4.09922
H	5.24765	-2.03126	4.92623
H	5.52829	-2.06223	3.17165
H	1.23617	-7.49582	-2.79557
H	-1.12759	-8.09575	-3.05014
H	-2.84426	-6.34089	-3.06174
H	3.88004	-3.81636	-3.43362
H	2.62680	-4.45527	-4.50925

H	2.25955	-3.10440	-3.44099
H	2.09779	-3.68408	-0.73272
H	2.57561	-5.30727	-0.26888
H	3.77626	-4.20860	-0.96737
H	3.11768	-7.06697	-1.88177
H	3.13690	-6.74413	-3.62920
H	4.33756	-5.99749	-2.57231
H	-1.78618	-2.52697	-1.08729
H	-3.39597	-1.99616	-1.62907
H	-3.18756	-3.50825	-0.73251
H	-4.69237	-3.41711	-3.20206
H	-3.97685	-4.76732	-4.08356
H	-4.30845	-4.91119	-2.34406
H	-1.23350	-2.27644	-3.91442
H	-2.26877	-3.26363	-4.93699
H	-2.95534	-1.88005	-4.07052
H	4.27641	1.57783	-6.18056
H	6.21055	2.09785	-4.77162
H	6.12597	1.67116	-2.35353
H	1.19758	-1.34557	-4.57380
H	0.60901	-1.10723	-6.22487
H	2.29895	-1.55400	-5.93700
H	0.89148	2.45151	-5.08712
H	-0.24046	1.18506	-5.59692
H	0.43621	1.17487	-3.95828
H	2.35147	2.02962	-7.04136

H	2.92050	0.38909	-7.42145
H	1.20644	0.79029	-7.55655
H	3.14688	2.47639	-0.29835
H	1.98869	1.26962	-0.76447
H	2.79699	1.15441	0.82202
H	3.30092	-1.42997	-1.23313
H	4.94173	-1.40870	-0.68262
H	3.65769	-1.07783	0.49065
H	5.27091	0.88771	0.93902
H	6.26495	0.54799	-0.48293
H	5.53241	2.15133	-0.26575
H	0.80055	-6.34145	4.72457
H	2.54098	-8.08035	4.78450
H	3.23974	-9.21972	2.69122
H	2.17256	-8.60754	0.53406
H	0.43361	-6.87217	0.45714
H	-1.99583	-5.62297	4.68423
H	-0.72266	-4.41073	4.91710
H	-2.26923	-3.94764	4.18737
H	-2.70624	-6.66644	1.73367
H	-3.08942	-4.96740	1.40679
H	-1.94309	-5.83300	0.36615
H	-1.08921	2.60757	1.47313

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Monomer - CO_2 coord TS

C	15.16798	5.61121	-4.01276

C	15.17117	5.30003	-2.62452
C	16.29290	5.60911	-1.80573
C	17.42355	6.15457	-2.41956
C	17.46093	6.41044	-3.78242
C	16.33762	6.15299	-4.55547
O	14.09006	4.70427	-2.06429
La	12.64618	3.63274	-0.90331
O	9.80886	3.94925	0.58982
C	8.77693	3.92542	1.13954
O	7.75127	3.87553	1.68242
C	16.27361	5.39257	-0.28306
C	15.14015	6.22317	0.35288
C	13.92670	5.42601	-4.90693
C	13.51165	3.94641	-4.98930
O	12.93210	3.11262	1.57524
C	12.48708	2.46561	2.52845
O	12.90090	2.61566	3.78039
C	13.88264	3.59582	4.08123
C	13.43986	4.89979	4.38126
C	14.44788	5.86277	4.52261
C	15.79231	5.52433	4.45541
C	16.17100	4.19558	4.31945
C	15.22576	3.17583	4.14460
C	11.97500	5.26614	4.70894
C	11.55644	4.45611	5.95383
C	15.66764	1.69587	4.16872

C	15.01523	1.00812	5.38583
O	11.54884	1.58332	2.37299
Si	10.78977	0.26130	3.29106
C	10.60550	0.69220	5.10230
C	11.85472	-1.24880	2.98304
C	12.37936	-2.00342	4.04445
C	13.11365	-3.16395	3.80324
C	13.33649	-3.58709	2.49406
C	12.82452	-2.84975	1.42574
C	12.08873	-1.69265	1.66934
C	9.13147	0.14411	2.43003
C	10.99518	4.99395	3.55521
C	11.83321	6.75629	5.06347
C	15.30780	0.93314	2.88230
C	17.19188	1.57068	4.34150
O	12.35664	1.70756	-1.87560
C	12.21774	0.47158	-2.40869
C	13.33941	-0.40879	-2.45859
C	13.13600	-1.70531	-2.94395
C	11.89706	-2.14296	-3.38774
C	10.82814	-1.25978	-3.38269
C	10.95032	0.05227	-2.91551
C	14.75768	0.01532	-2.03230
C	15.23746	1.20979	-2.87753
C	9.73762	0.99641	-3.01116
C	9.30824	1.46968	-1.61135

F	11.64148	6.03588	-0.19223
C	10.59442	6.68003	-0.82276
C	10.14065	7.90863	-0.38182
C	9.08125	8.40918	-1.14817
C	8.51476	7.73967	-2.23332
C	9.00798	6.49431	-2.61593
C	10.06307	5.97436	-1.88740
B	10.75623	8.61494	0.96925
C	11.98721	9.63717	0.65203
C	12.14970	10.38200	-0.51520
C	13.24263	11.20919	-0.76184
C	14.23825	11.32995	0.19937
C	14.12023	10.61887	1.38742
C	13.01139	9.80154	1.58544
F	8.54534	9.59419	-0.85307
F	7.50193	8.27559	-2.91440
F	8.48587	5.82602	-3.64443
F	10.58570	4.74623	-2.20521
F	11.22351	10.33413	-1.49064
F	13.34061	11.89082	-1.90905
F	15.29477	12.11955	-0.01400
F	15.07110	10.72610	2.32538
F	12.96858	9.15359	2.76791
C	14.79774	0.34811	-0.53236
C	15.79494	-1.10306	-2.24574
C	8.50007	0.31764	-3.62594

C	10.08470	2.17962	-3.93488
C	9.54518	9.22867	1.87851
C	9.32166	10.57534	2.16254
C	8.29963	11.02497	2.99771
C	7.43223	10.10868	3.57904
C	7.60189	8.75446	3.31474
C	8.63706	8.35596	2.47720
F	10.10210	11.52872	1.63006
F	8.14030	12.33078	3.23931
F	6.44575	10.52214	4.37996
F	6.77257	7.85567	3.86322
F	8.73785	7.02221	2.25527
C	16.13647	3.89394	0.04924
C	17.57262	5.85709	0.39869
C	12.77485	6.29353	-4.36263
C	14.17579	5.88648	-6.35402
H	16.54917	6.29630	4.55930
H	14.17725	6.89713	4.69033
H	17.22458	3.94946	4.35482
H	11.62559	3.37948	5.78295
H	10.52103	4.69454	6.22220
H	12.19146	4.70427	6.81040
H	11.34673	5.43877	2.62162
H	10.02979	5.45408	3.78238
H	10.81255	3.92684	3.40925
H	12.07467	7.40921	4.22101

H	12.45199	7.03674	5.92175
H	10.79270	6.95256	5.33886
H	13.92527	1.02965	5.32474
H	15.31402	1.49898	6.31756
H	15.32961	-0.04018	5.43668
H	15.65029	1.47059	1.99516
H	14.23932	0.73884	2.78317
H	15.79673	-0.04651	2.88920
H	17.45595	0.50985	4.39407
H	17.54525	2.04066	5.26444
H	17.74031	2.00280	3.49790
H	13.97025	-2.39505	-2.98764
H	11.77130	-3.15705	-3.75629
H	9.87325	-1.60366	-3.76151
H	16.25282	1.50182	-2.58677
H	15.25640	0.94038	-3.93835
H	14.59560	2.08516	-2.77792
H	14.07116	1.11450	-0.25175
H	14.56703	-0.53757	0.06809
H	15.79496	0.69998	-0.24773
H	15.57620	-1.99547	-1.64983
H	15.87196	-1.39763	-3.29717
H	16.77966	-0.73751	-1.93595
H	10.14019	1.88747	-1.04426
H	8.51774	2.22539	-1.68622
H	8.91212	0.62570	-1.03589

H	7.68252	1.04517	-3.67249
H	8.68440	-0.03006	-4.64729
H	8.14982	-0.53099	-3.02866
H	11.00381	2.68123	-3.63452
H	10.23361	1.81976	-4.95799
H	9.27528	2.91737	-3.94937
H	16.37538	6.38915	-5.61203
H	18.35385	6.82971	-4.23718
H	18.29571	6.39342	-1.82252
H	13.26927	3.52465	-4.01346
H	12.63266	3.83535	-5.63443
H	14.31975	3.34312	-5.41577
H	13.03136	7.35553	-4.43064
H	11.86058	6.12767	-4.94446
H	12.56412	6.07384	-3.31598
H	14.44752	6.94534	-6.40950
H	14.95848	5.29985	-6.84673
H	13.25503	5.75430	-6.93202
H	15.34888	7.29130	0.23930
H	14.17003	6.05826	-0.11973
H	15.05198	6.01006	1.42338
H	15.35268	3.40137	-0.53481
H	17.05945	3.36141	-0.20368
H	15.93332	3.74800	1.11524
H	17.48960	5.68475	1.47702
H	18.44877	5.30555	0.04180

H	17.75178	6.92634	0.24968
H	12.21494	-1.68870	5.07199
H	13.51000	-3.73734	4.63664
H	13.90709	-4.49239	2.30554
H	12.99190	-3.17378	0.40264
H	11.69997	-1.13295	0.82204
H	10.03162	-0.10442	5.58917
H	11.56127	0.79303	5.61993
H	10.04600	1.62362	5.22298
H	8.56344	-0.69145	2.85193
H	8.53957	1.05430	2.56378
H	9.25393	-0.04049	1.35964
H	11.23057	7.70601	1.61712

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Monomer - CO_2 coord product

C	3.05396	0.88743	-4.23866
C	3.06259	0.51369	-2.86669
C	4.18323	0.79036	-2.03541
C	5.30621	1.37723	-2.62481
C	5.33760	1.70068	-3.97340
C	4.21646	1.46714	-4.75705
O	1.98117	-0.11533	-2.33287
La	0.51111	-1.20314	-1.23606
O	-2.05446	-0.97850	0.18870
C	-3.10452	-0.98531	0.70674
O	-4.14529	-1.01318	1.21927

C	4.17699	0.48497	-0.52791
C	3.04100	1.26149	0.16870
C	1.81404	0.72707	-5.13876
C	1.41067	-0.75171	-5.27806
O	0.85030	-1.73797	1.24037
C	0.35045	-2.36042	2.18251
O	0.73729	-2.23568	3.45071
C	1.77672	-1.30989	3.76217
C	1.41015	0.02119	4.04420
C	2.47520	0.91332	4.22779
C	3.79589	0.48875	4.20444
C	4.09154	-0.86069	4.07044
C	3.08740	-1.81622	3.86536
C	-0.03730	0.49526	4.30901
C	-0.54921	-0.24110	5.56445
C	3.43453	-3.32098	3.89673
C	2.69379	-3.97296	5.08229
O	-0.63697	-3.19202	2.00377
Si	-1.41134	-4.49390	2.93913
C	-1.65584	-4.01665	4.73203
C	-0.33877	-6.01070	2.69761
C	0.16521	-6.73558	3.78912
C	0.91406	-7.89541	3.59375
C	1.17210	-8.34773	2.30082
C	0.67908	-7.64127	1.20310
C	-0.07152	-6.48498	1.40091

C	-3.04030	-4.63809	2.02674
C	-0.99766	0.24381	3.13379
C	-0.09077	2.00513	4.60344
C	3.08096	-4.04876	2.58905
C	4.93959	-3.54492	4.12927
O	0.22139	-3.11133	-2.23529
C	0.09574	-4.34966	-2.77946
C	1.22144	-5.22525	-2.81415
C	1.03055	-6.52333	-3.30039
C	-0.19963	-6.96643	-3.76205
C	-1.27039	-6.08582	-3.77743
C	-1.16051	-4.77240	-3.31076
C	2.63208	-4.79509	-2.37120
C	3.11219	-3.59425	-3.20731
C	-2.37326	-3.83230	-3.43775
C	-2.83567	-3.35696	-2.04928
F	-0.50302	1.25902	-0.65372
C	-1.66312	1.78169	-1.18851
C	-2.22959	2.93384	-0.67291
C	-3.40056	3.31465	-1.33831
C	-3.96111	2.60333	-2.40160
C	-3.35212	1.43784	-2.85929
C	-2.18600	1.03676	-2.22944
B	-1.54638	3.68609	0.62195
C	-0.32827	4.64205	0.11187
C	-0.45909	5.58600	-0.90658

C	0.59361	6.35546	-1.39074
C	1.86321	6.18867	-0.84736
C	2.04695	5.26214	0.17027
C	0.96043	4.52027	0.62676
F	-4.06820	4.40497	-0.95917
F	-5.08478	3.02161	-2.98415
F	-3.87283	0.72998	-3.86241
F	-1.55395	-0.11901	-2.60696
F	-1.65959	5.78989	-1.47567
F	0.40344	7.24557	-2.37126
F	2.89261	6.90876	-1.30090
F	3.26964	5.07270	0.68927
F	1.23448	3.63725	1.61046
C	2.65259	-4.47273	-0.86872
C	3.67920	-5.90514	-2.58008
C	-3.59412	-4.51421	-4.08119
C	-2.00385	-2.65127	-4.35560
C	-2.67096	4.36656	1.58814
C	-2.77726	5.71152	1.93944
C	-3.73238	6.20043	2.83087
C	-4.64554	5.32904	3.40963
C	-4.58518	3.97728	3.08995
C	-3.61477	3.53902	2.19740
F	-1.93807	6.62829	1.43090
F	-3.77945	7.50296	3.13164
F	-5.56803	5.78070	4.26463

F	-5.45521	3.11956	3.64079
F	-3.61144	2.20923	1.93318
C	4.05851	-1.03261	-0.29091
C	5.47727	0.91978	0.17099
C	0.65722	1.56776	-4.56304
C	2.05935	1.24282	-6.56798
H	4.59746	1.20935	4.33756
H	2.26781	1.96165	4.39602
H	5.12530	-1.17532	4.13399
H	-0.55472	-1.32500	5.42579
H	-1.57183	0.07925	5.79341
H	0.07778	-0.01398	6.43265
H	-0.58005	0.61234	2.19436
H	-1.93179	0.78737	3.29887
H	-1.25770	-0.81279	3.03552
H	0.23770	2.60453	3.74990
H	0.50286	2.27641	5.48212
H	-1.12686	2.28367	4.81670
H	1.61084	-3.88077	4.98121
H	2.98919	-3.50873	6.02874
H	2.93756	-5.03965	5.13461
H	3.51414	-3.53837	1.72582
H	2.00736	-4.15124	2.43069
H	3.48322	-5.06681	2.61483
H	5.13115	-4.62084	4.18904
H	5.28532	-3.09949	5.06719

H	5.54871	-3.14967	3.30957
H	1.86813	-7.20979	-3.33010
H	-0.31648	-7.98182	-4.12996
H	-2.21747	-6.43251	-4.17291
H	4.12174	-3.29477	-2.90463
H	3.14497	-3.86152	-4.26838
H	2.46237	-2.72408	-3.11361
H	1.91496	-3.71648	-0.58931
H	2.42345	-5.36575	-0.27848
H	3.64254	-4.11313	-0.56924
H	3.46238	-6.80141	-1.98931
H	3.76683	-6.19528	-3.63191
H	4.65859	-5.53345	-2.26081
H	-2.01282	-2.94303	-1.46718
H	-3.62226	-2.59883	-2.14307
H	-3.24754	-4.19951	-1.48277
H	-4.41035	-3.78705	-4.15098
H	-3.38372	-4.86540	-5.09632
H	-3.95913	-5.36081	-3.48990
H	-1.09259	-2.14953	-4.03274
H	-1.83026	-3.01402	-5.37384
H	-2.81279	-1.91404	-4.39051
H	4.25015	1.75244	-5.80157
H	6.22488	2.15181	-4.40829
H	6.17770	1.59416	-2.01858
H	1.17251	-1.21447	-4.31983

H	0.53302	-0.84539	-5.92769
H	2.22427	-1.33097	-5.72690
H	0.90661	2.63305	-4.59927
H	-0.25746	1.41429	-5.14758
H	0.45130	1.31638	-3.52241
H	2.32133	2.30544	-6.58433
H	2.84787	0.68214	-7.08116
H	1.14009	1.12386	-7.15127
H	3.26970	2.33008	0.19164
H	2.08281	1.16970	-0.34765
H	2.91863	0.92892	1.20456
H	3.25006	-1.48779	-0.87026
H	4.97241	-1.54149	-0.61569
H	3.89931	-1.24924	0.77047
H	5.40059	0.68735	1.23856
H	6.35508	0.39438	-0.21998
H	5.64767	1.99696	0.08077
H	-0.02617	-6.39701	4.80430
H	1.29392	-8.44587	4.44999
H	1.75441	-9.25226	2.14781
H	0.87287	-7.98960	0.19268
H	-0.44498	-5.94967	0.53108
H	-2.24657	-4.79954	5.22093
H	-0.71727	-3.90159	5.27711
H	-2.21794	-3.08193	4.80882
H	-3.61558	-5.46959	2.44693

H	-3.64319	-3.73061	2.12302
H	-2.88236	-4.84419	0.96483
H	-1.04910	2.79628	1.27541

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Monomer - CO_2 coord adduct H transf. TS

C	9.49605	0.27896	4.21449
C	9.14406	1.43865	3.50260
C	8.27262	1.30958	2.40870
C	7.76946	0.06345	2.03905
C	8.13386	-1.07578	2.75460
C	9.00008	-0.96823	3.84261
Si	9.79689	3.11642	4.01534
C	10.12027	3.22303	5.86771
O	11.29587	3.28488	3.05448
C	12.53308	3.64285	3.17859
O	12.90904	3.91427	4.43158
C	14.24656	4.32962	4.65831
C	14.50376	5.71468	4.66177
C	15.84659	6.08040	4.82285
C	16.84399	5.13176	4.99848
C	16.51928	3.78639	5.09341
C	15.20024	3.33554	4.95428
C	13.40605	6.80255	4.60810
C	14.01486	8.21312	4.70426
C	14.85661	1.85730	5.25427
C	16.12493	1.04094	5.56331

O	13.29821	3.72087	2.21254
La	13.64338	3.22606	-0.24546
O	14.71731	1.34598	-0.07058
C	15.14922	0.06563	-0.03813
C	16.54238	-0.20454	0.08538
C	16.94422	-1.54352	0.13296
C	16.03544	-2.59024	0.06277
C	14.68270	-2.30964	-0.06759
C	14.20383	-0.99814	-0.12549
C	17.59981	0.91368	0.17545
C	19.03053	0.35373	0.26636
C	12.69774	-0.73958	-0.31201
C	12.45869	-0.01859	-1.65371
O	11.39174	3.42139	-0.98992
C	10.25082	3.16122	-1.43239
O	9.54747	2.20270	-1.56428
O	14.70907	4.70446	-1.41792
C	15.71405	5.18263	-2.18426
C	15.81307	4.77191	-3.54222
C	16.93534	5.18457	-4.26754
C	17.90773	6.00440	-3.71210
C	17.74661	6.46829	-2.41386
C	16.65666	6.08994	-1.62427
C	14.68548	4.00002	-4.25487
C	15.11436	3.52488	-5.65562
C	16.48289	6.68419	-0.21469

C	17.56774	7.72521	0.11348
C	14.21302	2.74087	-3.48672
C	13.48629	4.95296	-4.43565
C	15.12820	7.41399	-0.12086
C	16.59592	5.59354	0.86486
C	17.56281	1.81029	-1.07642
C	17.37530	1.75019	1.44879
C	12.12489	0.06331	0.87359
C	11.87450	-2.03832	-0.37586
C	8.75712	4.54616	3.40246
C	12.47044	6.63242	5.82286
C	12.58202	6.77064	3.30669
C	13.97385	1.81337	6.51860
C	14.13916	1.13448	4.09766
F	9.59596	3.75473	-4.35500
C	9.57832	5.06312	-4.64377
C	9.10123	5.97953	-3.70466
C	9.12516	7.31708	-4.10763
C	9.59266	7.72797	-5.35220
C	10.07508	6.77929	-6.24672
C	10.06776	5.43510	-5.88932
B	8.53986	5.53926	-2.28046
C	7.28908	4.56511	-2.20986
C	6.42302	4.32532	-3.28286
C	5.36140	3.42713	-3.21712
C	5.13699	2.71380	-2.04541

C	5.96973	2.91918	-0.95095
C	7.00772	3.83230	-1.05306
F	8.65453	8.27845	-3.29882
F	9.58107	9.01815	-5.69241
F	10.53688	7.15345	-7.43750
F	10.54616	4.51786	-6.73382
F	6.56311	4.98274	-4.43956
F	4.55808	3.24703	-4.26621
F	4.13103	1.84677	-1.96813
F	5.76512	2.23540	0.18148
F	7.77880	3.98853	0.03839
C	8.85888	6.51773	-1.06075
C	10.16690	6.93318	-0.79674
C	10.49562	7.80374	0.23444
C	9.48836	8.30051	1.05397
C	8.16930	7.92728	0.82342
C	7.87989	7.05276	-0.22077
F	11.18341	6.47393	-1.54219
F	6.58780	6.74937	-0.40207
F	7.19695	8.40804	1.60116
F	9.79099	9.12215	2.06057
F	11.76557	8.15840	0.45351
H	17.87849	5.44697	5.09975
H	16.12303	7.12686	4.81446
H	17.31113	3.07466	5.28649
H	11.96439	5.66516	5.81593

H	11.70411	7.41564	5.81431
H	13.02850	6.71767	6.76091
H	13.22444	6.73448	2.42373
H	11.97501	7.67809	3.23386
H	11.88593	5.93082	3.26697
H	14.66342	8.44365	3.85272
H	14.58511	8.35671	5.62736
H	13.20442	8.94808	4.70435
H	13.03199	2.34583	6.37348
H	14.49050	2.26322	7.37249
H	13.73794	0.77426	6.77431
H	14.65814	1.27192	3.14590
H	13.09987	1.44692	3.98241
H	14.11369	0.05943	4.30382
H	15.83463	0.01248	5.79865
H	16.66871	1.43040	6.42956
H	16.80805	1.00072	4.70915
H	17.99696	-1.78250	0.22576
H	16.38098	-3.61949	0.10287
H	13.98535	-3.13693	-0.13046
H	18.34308	2.57744	-1.02119
H	17.73927	1.21627	-1.97939
H	16.60612	2.31932	-1.19083
H	16.37869	2.19375	1.47675
H	17.48805	1.12070	2.33820
H	18.11149	2.55965	1.51334

H	19.17891	-0.26388	1.15855
H	19.29750	-0.24006	-0.61407
H	19.73709	1.18846	0.32526
H	12.73713	0.93191	1.12958
H	11.10310	0.39621	0.66407
H	12.09731	-0.55853	1.77410
H	10.81736	-1.78374	-0.50598
H	12.16662	-2.67065	-1.22050
H	11.96186	-2.62637	0.54375
H	13.10019	0.85799	-1.77145
H	12.70565	-0.68468	-2.48705
H	11.41389	0.29153	-1.75710
H	17.05785	4.86559	-5.29555
H	18.77280	6.30236	-4.29776
H	18.49251	7.14409	-2.01158
H	15.00908	2.28394	-2.89058
H	13.34499	2.97705	-2.85841
H	13.85193	1.97493	-4.18084
H	13.77147	5.81711	-5.04416
H	12.66216	4.43803	-4.94242
H	13.12461	5.32206	-3.47224
H	15.36429	4.35999	-6.31636
H	15.97394	2.84694	-5.61350
H	14.28392	2.98584	-6.12279
H	15.09798	8.25032	-0.82708
H	14.28811	6.75839	-0.35413

H	14.98522	7.82429	0.88600
H	15.83245	4.82153	0.75255
H	17.56937	5.09620	0.81310
H	16.48286	6.02055	1.86696
H	17.37512	8.14284	1.10775
H	18.57156	7.28767	0.13213
H	17.56639	8.55667	-0.59859
H	10.16527	0.34297	5.06984
H	9.28429	-1.85448	4.40335
H	7.74107	-2.04733	2.46721
H	7.09170	-0.00901	1.19419
H	7.97713	2.18027	1.83233
H	9.78638	2.31054	6.36873
H	11.17093	3.38602	6.10764
H	9.54694	4.05946	6.27941
H	7.76536	4.49445	3.86466
H	9.21013	5.50045	3.68807
H	8.62740	4.53421	2.31865
H	9.66027	4.38355	-1.89048

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Monomer - CO_2 coord adduct H trans. product

La	2.31281	0.52566	-0.87050
O	2.62871	2.69787	-0.97781
O	3.70909	-0.63943	-2.11907
C	4.54695	-1.41352	-2.83777
C	5.95816	-1.24154	-2.71116

C	6.79656	-2.08731	-3.44351
C	6.29936	-3.07042	-4.28662
C	4.92597	-3.21131	-4.42236
C	4.02397	-2.40292	-3.72489
O	1.49487	0.17332	3.00216
Si	0.43461	0.35140	4.40315
C	-1.02845	-0.80247	4.20419
C	-1.70604	-0.90464	2.97674
C	-2.83926	-1.70688	2.85709
C	-3.32166	-2.40703	3.96324
C	-2.66623	-2.31025	5.18962
C	-1.52558	-1.51726	5.30592
O	0.14867	0.09754	-2.00177
C	-0.51373	0.03251	-0.92624
O	-0.00068	0.21168	0.21425
O	2.78146	-0.60701	1.37489
C	2.28265	-0.72583	2.49329
O	2.52473	-1.76777	3.29915
C	3.41566	-2.77094	2.82663
C	2.86301	-3.89134	2.17494
C	3.78518	-4.80128	1.64171
C	5.15278	-4.62346	1.78421
C	5.64095	-3.56528	2.53643
C	4.78793	-2.61281	3.10834
C	1.35126	-4.19673	2.09695
C	0.59805	-3.18646	1.21448

C	5.36051	-1.56546	4.09061
C	5.03825	-0.10821	3.70734
C	6.57905	-0.15941	-1.80877
C	6.21586	-0.42448	-0.33541
C	2.51302	-2.58717	-3.95123
C	2.19407	-3.70014	-4.96525
C	2.89805	4.00248	-1.18549
C	2.50849	4.62565	-2.40918
C	2.84140	5.96953	-2.60058
C	3.51659	6.70701	-1.63852
C	3.85852	6.10004	-0.43887
C	3.56205	4.75952	-0.17487
C	1.71166	3.87939	-3.49462
C	0.35348	3.43145	-2.91809
C	3.94482	4.15244	1.18730
C	4.96322	3.01427	0.99967
C	1.39304	0.03019	5.98328
C	-0.05959	2.14692	4.21603
C	6.89447	-1.66102	4.18211
C	4.79960	-1.87347	5.49417
C	1.09062	-5.58582	1.48559
C	0.75546	-4.22210	3.51937
C	8.11695	-0.14766	-1.87648
C	6.11948	1.23991	-2.26015
C	1.91135	-1.29276	-4.53098
C	1.82261	-2.99578	-2.63566

C	1.39299	4.76795	-4.71067
C	2.51771	2.68869	-4.04660
C	2.68401	3.65064	1.91642
C	4.60874	5.17702	2.12393
F	-1.61831	-2.85493	-4.59788
C	-2.44869	-2.36233	-5.52420
C	-3.75383	-1.98807	-5.17440
C	-4.53299	-1.46264	-6.21496
C	-4.06348	-1.32456	-7.51451
C	-2.75512	-1.69981	-7.80882
C	-1.93802	-2.21754	-6.80719
B	-4.30576	-2.15527	-3.72045
C	-5.27726	-1.09011	-3.10966
C	-6.33706	-1.44639	-2.26387
C	-7.21287	-0.51767	-1.71674
C	-7.03058	0.83432	-1.99506
C	-5.98613	1.23989	-2.82169
C	-5.14177	0.28156	-3.36830
F	-5.79987	-1.09914	-5.99100
F	-4.84653	-0.83963	-8.47578
F	-2.28860	-1.56530	-9.04254
F	-0.68538	-2.56761	-7.08768
F	-6.56621	-2.73185	-1.97367
F	-8.21728	-0.90475	-0.93259
F	-7.85159	1.73547	-1.47263
F	-5.80903	2.53338	-3.07934

F	-4.14957	0.72630	-4.14350
C	-3.88382	-3.40442	-2.86812
C	-3.58715	-3.31470	-1.50325
C	-3.20189	-4.40873	-0.74107
C	-3.11607	-5.66222	-1.34038
C	-3.41447	-5.80518	-2.69216
C	-3.77876	-4.68387	-3.42827
F	-3.64003	-2.12845	-0.87821
F	-2.90827	-4.27379	0.55408
F	-2.75190	-6.71660	-0.62163
F	-3.34559	-7.00476	-3.26416
F	-4.06462	-4.87797	-4.71935
H	5.84166	-5.33446	1.33750
H	6.71009	-3.48436	2.68340
H	3.42834	-5.66986	1.10358
H	3.70926	-1.82141	5.51092
H	5.18707	-1.15218	6.22315
H	5.09601	-2.87587	5.81984
H	5.25773	0.08658	2.65484
H	5.65275	0.56924	4.31014
H	3.99968	0.16130	3.90436
H	7.37870	-1.43846	3.22560
H	7.23102	-2.64428	4.52463
H	7.25104	-0.92614	4.91061
H	0.84994	-3.26189	4.02688
H	1.25062	-4.98481	4.13009

H	-0.31094	-4.46612	3.47072
H	1.05117	-3.12836	0.22048
H	0.55919	-2.18319	1.63545
H	-0.44061	-3.50941	1.09481
H	0.01349	-5.77910	1.50077
H	1.57742	-6.38605	2.05246
H	1.41575	-5.64986	0.44186
H	7.87132	-1.97803	-3.35880
H	6.97673	-3.71418	-4.84106
H	4.54924	-3.97255	-5.09558
H	6.56899	2.01543	-1.63016
H	6.43106	1.42366	-3.29374
H	5.03610	1.35683	-2.22163
H	5.13829	-0.49914	-0.18125
H	6.64788	-1.37431	-0.00308
H	6.60862	0.37255	0.30723
H	8.55550	-1.09248	-1.53789
H	8.48364	0.06030	-2.88709
H	8.49673	0.64326	-1.22039
H	2.06794	-2.31074	-1.82269
H	0.73448	-3.01793	-2.75879
H	2.15713	-3.99295	-2.32842
H	1.10886	-3.76325	-5.09379
H	2.62627	-3.49328	-5.94983
H	2.54847	-4.68170	-4.63195
H	2.12745	-0.42451	-3.91047

H	2.33081	-1.10212	-5.52476
H	0.82493	-1.38238	-4.62670
H	2.56468	6.46032	-3.52625
H	3.76483	7.74938	-1.81809
H	4.37035	6.69239	0.31067
H	3.41931	3.04290	-4.55734
H	2.85512	2.00488	-3.26621
H	1.92124	2.11801	-4.76676
H	-0.26030	4.30864	-2.68617
H	-0.19129	2.81314	-3.64007
H	0.46632	2.85894	-1.99739
H	0.78549	5.63780	-4.44012
H	2.29921	5.12102	-5.21407
H	0.82057	4.18242	-5.43850
H	2.01846	4.49068	2.14298
H	2.95824	3.16884	2.86266
H	4.58988	2.23942	0.32925
H	5.88899	3.40070	0.56091
H	5.21139	2.55419	1.96320
H	4.84619	4.69030	3.07658
H	5.54593	5.56704	1.71337
H	3.94876	6.02311	2.34187
H	-1.02051	-1.46078	6.26750
H	-3.03852	-2.85568	6.05257
H	-4.20659	-3.03070	3.86812
H	-3.33587	-1.79775	1.89608

H	-1.33097	-0.37426	2.10323
H	0.80272	0.37452	6.83954
H	1.61284	-1.03068	6.12170
H	2.33492	0.58589	5.98784
H	-1.59146	-0.20416	-0.99072
H	2.11840	2.93704	1.31626
H	-0.78217	2.41495	4.99364
H	0.80325	2.81331	4.29783
H	-0.52949	2.31017	3.24226

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Monomer - CO_2 coord adduct SiR_3 trans. TS

C	13.51739	3.39635	3.00159
C	14.45725	4.39932	3.28512
C	14.74272	4.68263	4.62937
C	14.10826	3.98853	5.65983
C	13.18109	2.99249	5.36080
C	12.88951	2.69594	4.02946
Si	15.15532	5.51035	1.94636
C	16.59829	6.62998	2.41070
O	14.66438	4.47761	0.25162
C	15.24661	4.65596	-0.86169
O	16.30544	5.29306	-1.05290
La	18.62448	4.70553	-0.57791
O	19.69740	6.60506	-0.30716
C	20.50533	7.68538	-0.38845
C	20.30846	8.64656	-1.42511

C	21.20983	9.71198	-1.51477
C	22.26306	9.86490	-0.62513
C	22.41145	8.95276	0.40911
C	21.54864	7.86448	0.56868
C	19.14303	8.55890	-2.42897
C	17.79411	8.55074	-1.68310
C	21.72424	6.93789	1.78645
C	22.06130	5.50043	1.35317
O	18.77208	2.94057	1.17222
C	17.68672	3.15113	1.77454
O	16.94142	4.14482	1.49492
O	19.15031	3.59478	-2.39197
C	19.60306	2.91296	-3.46609
C	20.98511	2.56856	-3.55566
C	21.42027	1.87130	-4.68676
C	20.55494	1.50840	-5.70802
C	19.21232	1.83984	-5.60458
C	18.69987	2.53445	-4.50461
C	22.00547	2.94492	-2.46438
C	21.62260	2.29945	-1.11828
C	17.19272	2.84817	-4.45227
C	16.43426	2.32120	-5.68410
C	19.09494	9.76863	-3.38046
C	19.29583	7.31986	-3.32912
C	20.44381	6.97095	2.64081
C	22.87300	7.38666	2.70715

C	23.42338	2.43894	-2.78672
C	22.11710	4.47662	-2.34879
C	16.95567	4.36883	-4.41702
C	16.55992	2.15846	-3.22958
O	17.25492	2.32178	2.74340
C	18.04059	1.17767	3.01284
C	19.01127	1.26156	4.03033
C	19.83641	0.14120	4.18976
C	19.67142	-0.99940	3.41781
C	18.62019	-1.08048	2.51610
C	17.75015	-0.00434	2.30217
C	19.11844	2.44556	5.01422
C	19.43672	3.78079	4.31758
C	16.48780	-0.19253	1.43320
C	16.42017	0.77871	0.23864
C	20.22955	2.21389	6.05376
C	17.78746	2.56601	5.78357
C	16.41377	-1.61502	0.85076
C	15.24885	0.00127	2.33092
C	13.79621	6.75452	1.47722
F	11.74501	0.76153	0.72664
C	11.57156	0.29306	-0.51555
C	10.95652	1.08388	-1.49533
C	10.84174	0.49613	-2.76328
C	11.29403	-0.78625	-3.04824
C	11.91325	-1.52613	-2.04515

C	12.05467	-0.98324	-0.77090
B	10.44611	2.53736	-1.21055
C	9.76959	2.89750	0.15238
C	8.95380	1.99264	0.84768
C	8.33432	2.30442	2.05085
C	8.53789	3.56104	2.61582
C	9.34770	4.49163	1.96999
C	9.93243	4.15266	0.75715
F	10.24630	1.15751	-3.76078
F	11.14564	-1.30827	-4.26307
F	12.36376	-2.74654	-2.30008
F	12.65648	-1.69033	0.18592
F	8.71226	0.77831	0.34498
F	7.55291	1.41983	2.66635
F	7.96135	3.87016	3.76879
F	9.55034	5.68804	2.51476
F	10.70841	5.08065	0.18595
C	10.62165	3.63813	-2.31481
C	9.61657	4.56607	-2.61251
C	9.75036	5.53157	-3.60321
C	10.93836	5.60581	-4.32584
C	11.97147	4.71150	-4.05642
C	11.79109	3.74702	-3.07508
F	8.45351	4.53001	-1.95423
F	8.76087	6.38181	-3.86570
F	11.08661	6.52773	-5.26724

F	13.11434	4.78916	-4.73745
F	12.82337	2.92125	-2.84043
H	20.34049	-1.84536	3.54902
H	20.62326	0.15621	4.93319
H	18.47334	-2.00501	1.97208
H	16.94703	2.75591	5.11327
H	17.84451	3.39286	6.50163
H	17.57915	1.64835	6.34355
H	20.27477	3.68055	3.62281
H	19.70601	4.52929	5.07104
H	18.57984	4.17836	3.77239
H	21.22220	2.15816	5.59397
H	20.06554	1.30409	6.63963
H	20.23881	3.05503	6.75449
H	15.22089	1.00075	2.76859
H	15.24367	-0.73072	3.14562
H	14.33385	-0.14032	1.74629
H	17.36985	0.81128	-0.30253
H	16.14118	1.78930	0.54225
H	15.64845	0.44150	-0.46186
H	15.47395	-1.72204	0.30108
H	16.41874	-2.38246	1.63122
H	17.23282	-1.82154	0.15310
H	22.46570	1.60214	-4.77866
H	20.92339	0.96880	-6.57604
H	18.54656	1.54498	-6.40683

H	22.86110	4.75570	-1.59522
H	22.42989	4.90653	-3.30585
H	21.17341	4.95496	-2.08108
H	20.59691	2.51857	-0.81648
H	21.69721	1.20873	-1.18587
H	22.29795	2.63235	-0.32180
H	23.45995	1.34893	-2.88316
H	23.82361	2.88183	-3.70479
H	24.09586	2.71907	-1.96869
H	17.01824	2.48947	-2.29610
H	15.48317	2.36049	-3.18906
H	16.69476	1.07356	-3.29309
H	15.37427	2.57982	-5.58525
H	16.79437	2.77262	-6.61437
H	16.50116	1.23241	-5.77972
H	17.44628	4.83927	-3.56665
H	17.34740	4.83285	-5.32850
H	15.88336	4.58968	-4.36225
H	21.09123	10.44853	-2.30062
H	22.95231	10.69851	-0.72678
H	23.22234	9.10139	1.11246
H	20.21174	7.39133	-3.92445
H	19.36689	6.38629	-2.76776
H	18.44896	7.23495	-4.01910
H	17.65321	9.49733	-1.15019
H	16.96442	8.43216	-2.38939

H	17.73404	7.74837	-0.94758
H	18.98318	10.71367	-2.83902
H	19.98541	9.83513	-4.01411
H	18.23026	9.66521	-4.04492
H	20.25205	7.98915	2.99621
H	20.55014	6.32093	3.51594
H	21.30898	5.08434	0.68204
H	23.01778	5.47532	0.82109
H	22.14255	4.84198	2.22576
H	22.93407	6.70281	3.56085
H	23.84390	7.36431	2.20136
H	22.71316	8.39432	3.10447
H	15.46565	5.45485	4.88292
H	14.34161	4.22429	6.69471
H	12.68830	2.44832	6.16197
H	12.17260	1.91617	3.78823
H	13.27953	3.15377	1.97007
H	16.18276	7.50721	2.91866
H	17.32694	6.14056	3.05691
H	17.11545	6.99690	1.51925
H	14.74252	4.18920	-1.71929
H	19.57137	6.65054	2.07081
H	13.61152	7.41117	2.33557
H	14.10851	7.38757	0.63907
H	12.85751	6.26469	1.21176

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Monomer - CO_2 coord adduct SiR_3 trans. product

C	-3.11098	2.68206	4.06743
C	-2.90497	3.61015	3.03382
C	-3.76116	4.72083	2.96046
C	-4.78647	4.90114	3.88733
C	-4.97389	3.96974	4.90765
C	-4.13500	2.85924	4.99601
Si	-1.47511	3.43297	1.82685
C	0.06773	4.30342	2.43627
O	-1.20180	1.68091	1.91349
C	-0.22146	1.01925	1.37067
O	0.66515	1.52156	0.67624
La	3.00825	0.56343	0.07231
O	3.78628	2.62396	0.23692
C	4.37618	3.80488	0.49742
C	4.21918	4.89949	-0.40434
C	4.87631	6.09608	-0.10070
C	5.65532	6.24627	1.03862
C	5.78394	5.18031	1.91775
C	5.15807	3.95389	1.68170
C	3.35063	4.80855	-1.67424
C	1.88738	4.51583	-1.28982
C	5.30977	2.80500	2.69284
C	6.01705	1.60201	2.03504
O	3.87831	-1.35778	1.44006
C	2.71545	-1.77549	1.69547

O	1.66536	-1.16121	1.34714
O	3.44190	-0.12173	-1.94408
C	3.69457	-0.46034	-3.22370
C	5.03919	-0.67197	-3.64964
C	5.25215	-1.00254	-4.99160
C	4.20781	-1.13326	-5.89619
C	2.90450	-0.94056	-5.46137
C	2.60915	-0.60812	-4.13620
C	6.24518	-0.56106	-2.69386
C	6.12621	-1.59105	-1.55490
C	1.14114	-0.41971	-3.70617
C	0.15630	-0.65936	-4.86478
C	3.33887	6.12608	-2.46994
C	3.88407	3.72695	-2.63093
C	3.92519	2.42466	3.25696
C	6.16823	3.19238	3.90985
C	7.57907	-0.85459	-3.40443
C	6.36747	0.86486	-2.12596
C	0.89937	1.02553	-3.22923
C	0.76550	-1.43569	-2.60955
O	2.50629	-2.92989	2.36989
C	3.61362	-3.70831	2.74187
C	4.16575	-3.50473	4.02177
C	5.32003	-4.23961	4.31929
C	5.85006	-5.15346	3.41891
C	5.19297	-5.41592	2.22472

C	4.03430	-4.72080	1.85660
C	3.49575	-2.62834	5.10181
C	3.38261	-1.14720	4.69181
C	3.22501	-5.15077	0.61344
C	3.08673	-4.03282	-0.43789
C	4.28784	-2.66508	6.42046
C	2.08823	-3.19030	5.39432
C	3.88591	-6.34695	-0.09309
C	1.82142	-5.60477	1.06725
C	-1.95052	3.85085	0.06304
F	-2.95922	-0.88351	1.42665
C	-3.11442	-2.02334	0.73967
C	-4.05673	-2.09670	-0.29348
C	-4.11999	-3.31982	-0.97343
C	-3.31949	-4.40660	-0.64508
C	-2.38949	-4.28079	0.38392
C	-2.27706	-3.07828	1.07741
B	-4.98117	-0.88934	-0.66455
C	-5.62297	-0.01175	0.46175
C	-6.11319	-0.56924	1.65026
C	-6.74594	0.18456	2.63122
C	-6.88631	1.55761	2.45104
C	-6.39323	2.16148	1.29712
C	-5.78279	1.37402	0.33115
F	-5.00281	-3.49375	-1.96262
F	-3.43026	-5.55941	-1.30111

F	-1.61265	-5.30699	0.70247
F	-1.37386	-2.94857	2.04645
F	-6.02402	-1.88571	1.86503
F	-7.22053	-0.39128	3.73416
F	-7.49151	2.28875	3.37713
F	-6.51469	3.47638	1.12957
F	-5.30673	2.00606	-0.75094
C	-5.27895	-0.56760	-2.16853
C	-6.54186	-0.14881	-2.60885
C	-6.82455	0.12546	-3.94101
C	-5.81283	0.00469	-4.88994
C	-4.53834	-0.39838	-4.49983
C	-4.29846	-0.68544	-3.16243
F	-7.55259	-0.02903	-1.74180
F	-8.04491	0.50180	-4.31681
F	-6.06232	0.27382	-6.16425
F	-3.56940	-0.50197	-5.40700
F	-3.05355	-1.05476	-2.83751
H	6.75697	-5.69700	3.66916
H	5.81429	-4.10507	5.27357
H	5.59075	-6.18333	1.57224
H	1.45562	-3.17423	4.50424
H	1.60004	-2.59070	6.17176
H	2.14956	-4.22277	5.75404
H	4.32609	-0.78058	4.27895
H	3.13460	-0.54159	5.57096

H	2.59132	-0.97883	3.95952
H	5.28978	-2.23545	6.31265
H	4.38641	-3.68078	6.81620
H	3.75578	-2.07267	7.17165
H	1.26575	-4.79275	1.54000
H	1.89086	-6.43518	1.77800
H	1.24434	-5.94983	0.20197
H	4.04809	-3.55998	-0.65071
H	2.37502	-3.26475	-0.13244
H	2.70631	-4.45617	-1.37392
H	3.25755	-6.65302	-0.93549
H	3.98970	-7.21350	0.56793
H	4.87302	-6.09591	-0.49616
H	6.26247	-1.16473	-5.34791
H	4.40875	-1.38892	-6.93284
H	2.09956	-1.05462	-6.17770
H	7.22755	0.93400	-1.44980
H	6.51501	1.58913	-2.93345
H	5.47903	1.17798	-1.57553
H	5.20739	-1.47309	-0.97989
H	6.13366	-2.60837	-1.96098
H	6.97249	-1.49965	-0.86381
H	7.61297	-1.86785	-3.81836
H	7.78376	-0.14329	-4.21149
H	8.39506	-0.77014	-2.67865
H	1.41945	-1.37333	-1.73855

H	-0.26891	-1.28035	-2.28180
H	0.84560	-2.45668	-2.99698
H	-0.86833	-0.52766	-4.50413
H	0.30807	0.04576	-5.68865
H	0.23305	-1.67627	-5.26355
H	1.60140	1.32994	-2.45060
H	1.03047	1.72668	-4.05976
H	-0.12134	1.14110	-2.84562
H	4.78164	6.94193	-0.77146
H	6.15497	7.18953	1.24115
H	6.38809	5.31236	2.80830
H	4.91874	3.94485	-2.91511
H	3.86441	2.73281	-2.18575
H	3.28255	3.69927	-3.54694
H	1.47657	5.34468	-0.70211
H	1.27123	4.40384	-2.19042
H	1.79955	3.60506	-0.69574
H	2.94060	6.96210	-1.88503
H	4.33618	6.40008	-2.82996
H	2.69639	6.00496	-3.34886
H	3.52217	3.25442	3.84748
H	3.99497	1.54866	3.90987
H	5.59234	1.35164	1.06033
H	7.06968	1.84101	1.85157
H	5.97795	0.71388	2.67508
H	6.23372	2.33647	4.59069

H	7.18995	3.46206	3.62372
H	5.73449	4.02742	4.46973
H	-3.63612	5.45667	2.16853
H	-5.44093	5.76491	3.81047
H	-5.77390	4.10725	5.62967
H	-4.27970	2.12940	5.78810
H	-2.47095	1.80714	4.14163
H	-0.14219	5.37325	2.54263
H	0.35861	3.92528	3.42075
H	0.90498	4.18094	1.74603
H	-0.23725	-0.05344	1.59313
H	3.19468	2.22602	2.46859
H	-2.16840	4.92061	-0.02416
H	-1.12652	3.62267	-0.61821
H	-2.84047	3.29826	-0.24976

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$LaOAr_3$

C	17.01462	6.48321	-3.57440
C	15.93110	5.67567	-4.02229
C	15.56859	5.63770	-5.39972
C	16.30471	6.41610	-6.29723
C	17.36417	7.20791	-5.87708
C	17.70608	7.23178	-4.53135
O	15.22956	4.94142	-3.13639
La	13.82044	3.70593	-2.01660
O	14.21172	1.55968	-1.97383

C	14.23956	0.21483	-2.05679
C	15.47097	-0.48016	-1.89299
C	15.45108	-1.87362	-2.00387
C	14.28263	-2.57715	-2.26479
C	13.08929	-1.88481	-2.41566
C	13.02990	-0.49195	-2.31575
C	16.79480	0.25213	-1.60291
C	17.97710	-0.72114	-1.45439
C	11.68112	0.23584	-2.47003
C	11.71909	1.19981	-3.67458
C	14.41079	4.75962	-5.91011
C	14.19783	4.88562	-7.42894
C	17.43061	6.55121	-2.09246
C	18.62996	7.48873	-1.86746
O	13.02976	4.57557	-0.17740
C	12.35346	5.18109	0.81866
C	12.73148	4.95535	2.17237
C	11.99061	5.59567	3.17008
C	10.91743	6.42623	2.87524
C	10.56429	6.63903	1.55002
C	11.26007	6.03639	0.49826
C	13.91002	4.03933	2.55317
C	14.12637	3.97241	4.07519
C	10.84947	6.31752	-0.95929
C	9.64058	7.26439	-1.06012
C	15.22300	4.57324	1.94787

C	13.63811	2.59603	2.08651
C	12.00224	7.01273	-1.71068
C	10.42326	5.01288	-1.66517
C	17.15215	1.19789	-2.76601
C	16.69752	1.02938	-0.27553
C	11.32642	0.97989	-1.16731
C	10.51541	-0.73097	-2.74252
C	14.71421	3.27220	-5.64233
C	13.07786	5.18810	-5.26009
C	16.27579	7.10686	-1.23640
C	17.86270	5.15944	-1.59109
H	10.36097	6.90699	3.67477
H	12.25336	5.44403	4.21050
H	9.72661	7.29281	1.33576
H	15.15814	4.68599	0.86457
H	16.05351	3.89567	2.17771
H	15.46376	5.55651	2.36575
H	12.72770	2.20750	2.55515
H	14.46954	1.94013	2.36873
H	13.50818	2.52968	1.00550
H	13.25760	3.55950	4.59874
H	14.35413	4.95417	4.50352
H	14.97786	3.31685	4.28691
H	12.94230	6.45799	-1.65720
H	12.20432	7.99228	-1.26602
H	11.74462	7.17075	-2.76450

H	9.48201	4.64091	-1.24762
H	11.14706	4.20485	-1.51698
H	10.27213	5.17621	-2.73918
H	9.38882	7.41947	-2.11506
H	9.85375	8.24652	-0.62659
H	8.75388	6.85385	-0.56647
H	16.37236	-2.43191	-1.88483
H	14.30197	-3.66020	-2.34643
H	12.18506	-2.44883	-2.61333
H	18.09967	1.71029	-2.56402
H	17.26557	0.63340	-3.69764
H	16.38684	1.95747	-2.93157
H	15.86299	1.73228	-0.27317
H	16.54656	0.33903	0.56115
H	17.62249	1.58805	-0.09076
H	17.83014	-1.42677	-0.62992
H	18.15965	-1.29228	-2.37077
H	18.88603	-0.14935	-1.23904
H	12.11343	1.66426	-0.84128
H	10.39292	1.54370	-1.27944
H	11.18876	0.26465	-0.35032
H	9.58752	-0.15813	-2.84876
H	10.65901	-1.29921	-3.66715
H	10.37081	-1.43933	-1.92070
H	12.60664	1.84067	-3.66650
H	11.77343	0.63844	-4.61297

H	10.81807	1.82426	-3.70841
H	16.05096	6.40699	-7.35109
H	17.92200	7.80300	-6.59452
H	18.53668	7.85586	-4.22312
H	14.94527	3.06676	-4.59419
H	13.87459	2.63822	-5.95042
H	15.59541	2.95928	-6.21116
H	12.76631	6.16840	-5.63515
H	12.27830	4.47293	-5.48928
H	13.16353	5.30687	-4.17513
H	13.96090	5.91182	-7.72775
H	15.07552	4.55522	-7.99324
H	13.35656	4.25166	-7.73028
H	16.00026	8.11246	-1.57144
H	15.38343	6.48234	-1.29336
H	16.57761	7.17200	-0.18484
H	17.08114	4.41203	-1.73485
H	18.74935	4.81613	-2.13459
H	18.11334	5.19859	-0.52461
H	18.88460	7.49346	-0.80214
H	19.51971	7.16121	-2.41549
H	18.40699	8.52169	-2.15491

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$LaOAr_3$ - CO_2 insert. adduct

C	-1.74395	1.05261	4.09864
C	-0.61656	0.37692	3.54126

C	0.39770	-0.14518	4.39930
C	0.29004	0.08961	5.77303
C	-0.77301	0.79357	6.31921
C	-1.77916	1.25234	5.48178
O	-0.51235	0.22335	2.20483
La	-0.12212	0.05390	0.02520
O	-2.77061	0.38944	-0.61743
C	-3.90718	0.37079	-0.89882
O	-5.03269	0.36082	-1.17694
C	1.59118	-0.95750	3.86328
C	1.09436	-2.20305	3.10364
C	-2.93801	1.51148	3.24119
C	-3.58341	0.27450	2.58585
O	0.45175	1.61832	-1.43702
C	0.95898	2.54483	-2.27759
C	1.79086	3.58705	-1.76822
C	2.32943	4.50700	-2.67204
C	2.07186	4.43723	-4.03330
C	1.24244	3.43456	-4.51432
C	0.66454	2.47893	-3.67286
C	2.11116	3.72230	-0.26873
C	2.90681	2.49530	0.21212
C	-0.28124	1.42019	-4.27198
C	-1.68587	1.58479	-3.66068
O	-0.01056	-1.99018	-0.72584
C	0.30808	-3.23471	-1.12909

C	1.65825	-3.59086	-1.39441
C	1.91590	-4.90096	-1.82372
C	0.91647	-5.84418	-1.98067
C	-0.39798	-5.48331	-1.70976
C	-0.73785	-4.19773	-1.28943
C	2.90893	-2.68549	-1.27784
C	3.92737	-3.34646	-0.32216
C	-2.21757	-3.84588	-1.04165
C	-3.15168	-5.05083	-1.25341
C	3.54862	-2.53065	-2.67437
C	2.68848	-1.26313	-0.73996
C	-2.66400	-2.76685	-2.04830
C	-2.43960	-3.38495	0.41221
C	-0.44609	1.57210	-5.79470
C	0.25935	-0.00330	-4.04017
C	2.98797	4.94772	0.04515
C	0.81270	3.90477	0.54052
C	2.50403	-1.47924	4.98746
C	2.47360	-0.06682	2.97142
C	-4.04182	2.18730	4.07457
C	-2.50411	2.54765	2.18892
H	-0.82594	0.96795	7.39008
H	1.05487	-0.28789	6.44143
H	-2.61776	1.77632	5.92469
H	1.89881	0.40734	2.17263
H	3.29122	-0.64292	2.52306

H	2.91470	0.74386	3.56075
H	0.55102	-2.86781	3.78323
H	1.93978	-2.76663	2.69199
H	0.41284	-1.95642	2.28783
H	1.96744	-2.13628	5.67943
H	2.95924	-0.66704	5.56350
H	3.31904	-2.06256	4.54496
H	-1.70455	2.17254	1.54975
H	-2.12732	3.45219	2.67696
H	-3.35236	2.83802	1.55673
H	-4.42306	0.57208	1.94378
H	-3.97992	-0.39488	3.35593
H	-2.86221	-0.29480	1.99742
H	-4.86370	2.47986	3.41150
H	-3.68600	3.09497	4.57320
H	-4.45741	1.51623	4.83310
H	2.93874	-5.19215	-2.04454
H	1.15471	-6.85080	-2.31184
H	-1.17349	-6.22917	-1.83608
H	3.65659	-0.75741	-0.65892
H	2.08043	-0.65823	-1.42166
H	2.26563	-1.28883	0.27228
H	4.82842	-2.72738	-0.23879
H	3.50122	-3.46654	0.67932
H	4.23920	-4.33492	-0.66724
H	3.83191	-3.49655	-3.10078

H	2.85160	-2.05225	-3.36963
H	4.45248	-1.91255	-2.61683
H	-1.81466	-2.53185	0.67785
H	-3.49013	-3.11303	0.57188
H	-2.19652	-4.19397	1.10871
H	-4.18460	-4.74083	-1.06039
H	-3.11199	-5.43189	-2.27904
H	-2.92366	-5.87455	-0.56898
H	-2.02507	-1.88381	-2.00457
H	-2.61338	-3.15843	-3.06958
H	-3.70480	-2.47262	-1.85894
H	1.04181	3.40054	-5.57862
H	2.50796	5.16341	-4.71347
H	2.96895	5.30300	-2.30895
H	0.35818	-0.24764	-2.98228
H	-0.40716	-0.74582	-4.49392
H	1.24712	-0.11396	-4.50005
H	-2.11987	2.54418	-3.96189
H	-2.35373	0.78668	-4.00866
H	-1.64468	1.56705	-2.57138
H	-0.86341	2.54605	-6.07033
H	0.50050	1.43794	-6.32865
H	-1.13853	0.80472	-6.15747
H	0.34317	4.86182	0.29018
H	0.08084	3.12590	0.32058
H	1.01810	3.89962	1.61703

H	2.39283	1.55825	-0.01587
H	3.87665	2.44854	-0.29420
H	3.08734	2.54237	1.29153
H	3.16384	4.99400	1.12546
H	3.96625	4.89483	-0.44379
H	2.50471	5.88503	-0.24894

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$LaOAr_3$ - CO_2 insert. TS

C	13.03853	3.68536	2.82656
C	14.24820	3.17965	2.26661
C	15.26702	2.64605	3.10777
C	15.04345	2.63549	4.48792
C	13.86967	3.11946	5.04649
C	12.88589	3.63501	4.21514
O	14.43118	3.20343	0.92627
La	14.66009	3.14670	-1.24735
O	12.61353	4.44833	-1.99390
C	12.98992	5.35549	-2.71060
O	12.81321	6.36566	-3.27971
C	16.58102	2.07059	2.54860
C	16.28419	0.83721	1.67455
C	11.91886	4.29119	1.96104
C	11.36761	3.24019	0.97767
O	14.83515	4.78901	-3.00775
C	15.49769	5.59909	-3.88254
C	16.28487	6.67489	-3.38084

C	16.85517	7.55645	-4.30406
C	16.68430	7.39253	-5.66975
C	15.96709	6.30359	-6.14167
C	15.36836	5.37388	-5.28362
C	16.57715	6.87020	-1.87851
C	17.35845	5.65060	-1.35242
C	14.66799	4.13835	-5.89817
C	13.17159	4.04920	-5.54392
O	14.80115	1.13064	-1.97961
C	15.06486	-0.09412	-2.47927
C	16.39261	-0.46383	-2.81815
C	16.59199	-1.74618	-3.35057
C	15.55397	-2.63971	-3.54523
C	14.26212	-2.26304	-3.19581
C	13.98070	-1.00640	-2.66029
C	17.67624	0.38690	-2.65329
C	18.64212	-0.34740	-1.69735
C	12.53300	-0.64125	-2.27785
C	11.55001	-1.79430	-2.54964
C	18.36051	0.55295	-4.02739
C	17.50141	1.80646	-2.08551
C	12.03727	0.55298	-3.11719
C	12.43677	-0.34030	-0.76867
C	14.74313	4.14836	-7.43758
C	15.38532	2.85628	-5.43789
C	17.47234	8.09445	-1.60852

C	15.29871	7.09737	-1.05189
C	17.53413	1.59240	3.65917
C	17.35177	3.14662	1.76013
C	10.71606	4.76436	2.79639
C	12.45076	5.53742	1.22807
H	13.72276	3.09561	6.12256
H	15.80276	2.23678	5.14994
H	11.97475	4.01056	4.66583
H	16.74263	3.58537	0.96718
H	18.26040	2.72572	1.31382
H	17.65002	3.96489	2.42420
H	15.80041	0.05781	2.27212
H	17.21465	0.42000	1.27261
H	15.61648	1.05769	0.83904
H	17.10200	0.78012	4.25233
H	17.81774	2.40367	4.33767
H	18.45337	1.20938	3.20259
H	13.35240	5.31827	0.65537
H	12.70797	6.31725	1.95269
H	11.69503	5.94101	0.54522
H	10.64145	3.69193	0.29343
H	10.86790	2.43558	1.52701
H	12.15502	2.77410	0.38298
H	9.95886	5.18493	2.12585
H	10.99214	5.54774	3.50976
H	10.24574	3.94353	3.34798

H	17.59727	-2.05578	-3.62111
H	15.74611	-3.62436	-3.96155
H	13.45845	-2.97361	-3.34678
H	18.48382	2.28634	-2.01868
H	16.89384	2.43130	-2.75181
H	17.09348	1.78058	-1.06800
H	19.56969	0.22470	-1.57522
H	18.18888	-0.48154	-0.71029
H	18.91184	-1.33782	-2.07248
H	18.62786	-0.40941	-4.47068
H	17.70293	1.07102	-4.73153
H	19.28246	1.13760	-3.92553
H	13.11459	0.45587	-0.45709
H	11.41488	-0.04700	-0.50241
H	12.69400	-1.23071	-0.18544
H	10.54240	-1.48082	-2.25614
H	11.51232	-2.06448	-3.61016
H	11.79497	-2.69144	-1.97159
H	12.68951	1.42261	-3.02554
H	12.00219	0.28482	-4.17830
H	11.02697	0.84629	-2.80939
H	15.87344	6.18202	-7.21326
H	17.12431	8.10087	-6.36599
H	17.44341	8.39654	-3.95604
H	15.31424	2.71448	-4.35783
H	14.93890	1.97491	-5.91169

H	16.44481	2.88968	-5.71214
H	12.65804	4.99479	-5.73871
H	12.69531	3.27261	-6.15284
H	13.00894	3.77238	-4.50195
H	14.21081	5.00090	-7.87225
H	15.77464	4.15805	-7.80397
H	14.27004	3.23836	-7.82049
H	14.71398	7.92597	-1.46115
H	14.64400	6.22544	-1.02928
H	15.55656	7.33798	-0.01463
H	16.87640	4.70703	-1.63209
H	18.35839	5.60933	-1.79588
H	17.46898	5.68631	-0.26316
H	17.67889	8.15689	-0.53476
H	18.43569	8.02714	-2.12333
H	16.98569	9.02961	-1.90346

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2nd CO_2 inser - adduct

C	2.15067	3.23250	-2.10144
C	0.98057	2.57966	-2.58218
C	0.24897	3.12591	-3.68569
C	0.67804	4.33636	-4.23016
C	1.80007	5.00207	-3.74985
C	2.52310	4.43855	-2.71353
O	0.54143	1.44571	-2.01489
La	-0.19590	0.05536	-0.49055

O	-0.35298	-1.90858	-1.38913
C	-0.40298	-3.12947	-1.95871
C	0.80741	-3.84315	-2.19142
C	0.71733	-5.11114	-2.77286
C	-0.50234	-5.67333	-3.12320
C	-1.67157	-4.96075	-2.89577
C	-1.66345	-3.68823	-2.31677
C	2.18692	-3.25730	-1.83340
C	3.33815	-4.21971	-2.17639
C	-2.99193	-2.94099	-2.08713
C	-3.00256	-1.61123	-2.86587
C	-0.96197	2.39624	-4.30215
C	-1.52215	3.13610	-5.53076
C	3.12768	2.71581	-1.01523
C	4.46375	2.35883	-1.70316
C	-0.78971	-0.02592	2.25135
O	-1.13276	-0.10726	3.55395
C	-0.11561	-0.34135	4.49588
C	0.49084	0.77605	5.10303
C	1.55274	0.50244	5.97405
C	1.94665	-0.79892	6.25268
C	1.24111	-1.86933	5.72101
C	0.16788	-1.67747	4.84181
C	-0.02500	2.22225	4.93380
C	0.78784	3.20807	5.79155
C	-0.69398	-2.87698	4.38886

C	-0.19819	-4.18819	5.02389
O	-1.74385	0.16307	1.44278
O	0.41946	-0.13527	1.88821
C	-1.48878	2.29112	5.41850
C	0.05733	2.72598	3.47901
C	-2.14657	-2.66054	4.86449
C	-0.67876	-3.08955	2.86181
C	2.44784	-1.97200	-2.64426
C	2.28934	-2.99316	-0.31819
C	-3.22341	-2.69960	-0.58295
C	-4.20654	-3.74140	-2.58942
C	-0.54442	0.99367	-4.78779
C	-2.12306	2.30349	-3.29342
C	3.37962	3.81637	0.03897
C	2.69444	1.47265	-0.22233
H	2.78432	-0.98024	6.92049
H	2.08139	1.31798	6.45147
H	1.53152	-2.87339	6.00377
H	-2.13866	1.63912	4.83145
H	-1.86428	3.31720	5.32898
H	-1.56387	1.99613	6.47036
H	1.03572	2.51197	3.03935
H	-0.09337	3.81179	3.46283
H	-0.71788	2.29118	2.84702
H	1.83597	3.26354	5.47779
H	0.75671	2.95440	6.85585

H	0.35960	4.20963	5.68297
H	-2.58570	-1.76146	4.42786
H	-2.18970	-2.57127	5.95514
H	-2.76488	-3.51697	4.57166
H	0.33882	-3.06142	2.46290
H	-1.28674	-2.35308	2.33440
H	-1.10687	-4.06982	2.62572
H	-0.86514	-5.00190	4.72228
H	-0.20633	-4.14751	6.11784
H	0.81164	-4.45357	4.69251
H	1.62011	-5.68032	-2.96160
H	-0.54137	-6.66120	-3.57349
H	-2.61423	-5.41414	-3.17912
H	3.41647	-1.53652	-2.37060
H	2.47411	-2.19816	-3.71526
H	1.67457	-1.21390	-2.50264
H	1.48445	-2.35602	0.05382
H	2.22436	-3.93519	0.23617
H	3.24820	-2.52298	-0.07021
H	3.26317	-5.16484	-1.62874
H	3.38418	-4.44303	-3.24723
H	4.28965	-3.75383	-1.89768
H	-2.41757	-2.12947	-0.11947
H	-4.16056	-2.15428	-0.42077
H	-3.29269	-3.65416	-0.05117
H	-5.11716	-3.15860	-2.41331

H	-4.15018	-3.94668	-3.66350
H	-4.32040	-4.69340	-2.06071
H	-2.14246	-0.98411	-2.62301
H	-2.96192	-1.79823	-3.94400
H	-3.91896	-1.04760	-2.65383
H	0.13284	4.77482	-5.05733
H	2.11399	5.94250	-4.19338
H	3.41795	4.94985	-2.37142
H	-0.13514	0.38473	-3.98137
H	-1.40488	0.46815	-5.21763
H	0.22116	1.07664	-5.56645
H	-2.46720	3.30398	-3.00785
H	-2.97298	1.76816	-3.73110
H	-1.82967	1.77821	-2.38224
H	-1.89788	4.13445	-5.28193
H	-0.77499	3.23605	-6.32468
H	-2.36132	2.56379	-5.94029
H	3.81326	4.72190	-0.39106
H	2.44775	4.10148	0.53908
H	4.07558	3.45304	0.80380
H	1.80120	1.67422	0.38199
H	2.55203	0.60591	-0.87555
H	3.48024	1.21070	0.49425
H	5.20109	2.02288	-0.96404
H	4.32174	1.55700	-2.43507
H	4.88516	3.21793	-2.23214

O	-0.99066	2.86254	0.09558
C	-1.06790	3.99828	-0.18057
O	-1.16619	5.13020	-0.42433

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2nd CO_2 inser - TS

C	17.66427	5.12012	-3.00687
C	16.39705	4.66158	-3.45326
C	16.01008	4.77841	-4.82268
C	16.89055	5.42428	-5.69267
C	18.10716	5.93747	-5.26158
C	18.48183	5.77251	-3.94102
O	15.50637	4.13375	-2.56547
La	14.84586	2.37390	-1.11659
O	14.77262	0.48231	-2.14851
C	14.65910	-0.57301	-2.98419
C	15.83691	-1.20178	-3.47658
C	15.67988	-2.24509	-4.39416
C	14.42726	-2.67764	-4.80755
C	13.28998	-2.08477	-4.27646
C	13.36525	-1.03793	-3.35288
C	17.24783	-0.79154	-3.00961
C	18.34433	-1.67662	-3.62928
C	12.07659	-0.46022	-2.73476
C	11.89670	1.02634	-3.09837
C	14.69854	4.18647	-5.38610
C	14.52979	4.49285	-6.88668

C	18.23610	5.03186	-1.56997
C	19.71133	4.56982	-1.61778
C	14.45594	1.97855	1.60916
O	14.20945	1.81622	2.92034
C	15.30209	1.75010	3.80333
C	15.73554	2.95184	4.39693
C	16.87096	2.85778	5.21129
C	17.49643	1.64126	5.44731
C	16.96084	0.46905	4.93161
C	15.82659	0.47961	4.10996
C	14.97272	4.28948	4.26771
C	15.62969	5.38738	5.12301
C	15.15886	-0.84533	3.67978
C	15.91428	-2.05832	4.25118
O	13.43839	2.06874	0.86311
O	15.64373	2.04039	1.16443
C	13.53261	4.10428	4.79129
C	14.92972	4.82127	2.81987
C	13.72445	-0.88983	4.24857
C	15.11143	-1.03273	2.14954
C	17.57572	0.65255	-3.43319
C	17.36876	-0.95612	-1.48107
C	12.09712	-0.65677	-1.20557
C	10.81317	-1.17433	-3.24754
C	14.73097	2.65252	-5.25726
C	13.44386	4.75330	-4.69333

C	18.16863	6.42945	-0.92005
C	17.54117	4.04000	-0.62392
H	18.38508	1.60149	6.07126
H	17.27463	3.74807	5.67715
H	17.43461	-0.47169	5.18260
H	12.98246	3.36099	4.21130
H	12.98997	5.05438	4.72770
H	13.53893	3.78873	5.83985
H	15.91857	4.78429	2.35359
H	14.59760	5.86521	2.82515
H	14.22050	4.27663	2.19485
H	16.64107	5.63134	4.77989
H	15.67822	5.11383	6.18186
H	15.03032	6.30017	5.04878
H	13.11032	-0.07441	3.86135
H	13.73748	-0.82254	5.34151
H	13.24416	-1.83609	3.97424
H	16.07826	-0.81351	1.68844
H	14.34627	-0.41402	1.67768
H	14.85370	-2.07201	1.91827
H	15.38122	-2.97185	3.96965
H	15.96843	-2.03590	5.34434
H	16.93185	-2.13750	3.85334
H	16.55519	-2.73905	-4.79933
H	14.33771	-3.48624	-5.52745
H	12.32080	-2.45505	-4.58955

H	18.56643	0.94478	-3.06597
H	17.58123	0.74551	-4.52363
H	16.84670	1.37711	-3.06332
H	16.61669	-0.37828	-0.94124
H	17.23447	-2.00596	-1.20068
H	18.36157	-0.64107	-1.13836
H	18.21830	-2.73178	-3.36591
H	18.37603	-1.59335	-4.72063
H	19.32061	-1.35716	-3.24908
H	12.96294	-0.18975	-0.73535
H	11.19455	-0.23321	-0.75064
H	12.12842	-1.72439	-0.96469
H	9.93239	-0.73421	-2.76775
H	10.68528	-1.06695	-4.32988
H	10.82006	-2.24149	-3.00387
H	12.77810	1.62647	-2.85595
H	11.73610	1.14575	-4.17443
H	11.03389	1.45318	-2.57490
H	16.62499	5.54472	-6.73534
H	18.76143	6.45466	-5.95759
H	19.43710	6.17522	-3.62208
H	14.83264	2.32327	-4.22111
H	13.81020	2.21255	-5.65606
H	15.57251	2.23361	-5.81780
H	13.45922	5.84715	-4.68212
H	12.54630	4.43345	-5.23467

H	13.34207	4.40284	-3.66646
H	14.46487	5.56804	-7.08467
H	15.34149	4.07568	-7.49102
H	13.59824	4.03747	-7.23814
H	18.74119	7.15848	-1.50094
H	17.13728	6.78965	-0.86598
H	18.58309	6.40537	0.09505
H	16.54585	4.38021	-0.32743
H	17.51005	3.03449	-1.06892
H	18.11649	3.94207	0.30172
H	20.10385	4.47947	-0.59883
H	19.80303	3.59410	-2.10633
H	20.36049	5.26950	-2.14774
O	13.74257	4.69603	-0.96299
C	14.39240	5.44238	-1.66601
O	14.68627	6.51190	-2.05227

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2nd CO_2 inser - product

C	2.39153	2.94502	-2.12034
C	1.17141	2.51908	-2.68338
C	0.89049	2.57840	-4.06982
C	1.87286	3.15261	-4.88194
C	3.06402	3.63629	-4.35763
C	3.31719	3.52229	-3.00258
O	0.17721	1.99658	-1.84428
La	-0.68396	0.09783	-0.08536

O	-0.75842	-1.66898	-1.31951
C	-0.89240	-2.67669	-2.20927
C	0.26855	-3.36539	-2.66002
C	0.09744	-4.36278	-3.62492
C	-1.15510	-4.69757	-4.12105
C	-2.27991	-4.04607	-3.63377
C	-2.18978	-3.03621	-2.67110
C	1.67317	-3.06916	-2.09718
C	2.74758	-3.99080	-2.70142
C	-3.47045	-2.37984	-2.11837
C	-3.50476	-0.87238	-2.43490
C	-0.39374	2.01045	-4.71573
C	-0.42417	2.27651	-6.23250
C	2.79522	2.90306	-0.62711
C	4.28361	2.50783	-0.49086
C	-0.82781	-0.40162	2.64150
O	-0.98329	-0.56658	3.96438
C	0.15416	-0.43148	4.78240
C	0.43385	0.84532	5.30702
C	1.61974	0.95529	6.04400
C	2.43576	-0.14357	6.27674
C	2.05348	-1.40349	5.83681
C	0.88339	-1.59540	5.09140
C	-0.53626	2.04398	5.19896
C	0.00628	3.26572	5.96121
C	0.39762	-3.02105	4.74634

C	1.36754	-4.08421	5.29151
O	-1.88405	-0.48119	1.94447
O	0.31025	-0.17107	2.13227
C	-1.88069	1.65817	5.85186
C	-0.78460	2.50125	3.74645
C	-0.97017	-3.25829	5.42098
C	0.27232	-3.26987	3.22932
C	2.11212	-1.62898	-2.42218
C	1.69377	-3.31676	-0.57542
C	-3.57905	-2.63265	-0.60046
C	-4.74602	-2.97076	-2.74520
C	-0.42409	0.48142	-4.53268
C	-1.67996	2.63768	-4.13768
C	2.58889	4.30738	-0.02334
C	2.02905	1.88668	0.24024
H	3.35675	-0.02363	6.84058
H	1.91195	1.91443	6.45297
H	2.67825	-2.25236	6.08485
H	-2.35095	0.81448	5.34287
H	-2.57228	2.50746	5.80939
H	-1.73892	1.39091	6.90425
H	0.15284	2.59682	3.19118
H	-1.27264	3.48173	3.75036
H	-1.45472	1.82981	3.20660
H	0.93868	3.64447	5.52836
H	0.17690	3.05024	7.02079

H	-0.73084	4.07281	5.90695
H	-1.72561	-2.55729	5.06030
H	-0.89160	-3.15134	6.50795
H	-1.32028	-4.27442	5.20597
H	1.16345	-2.93241	2.69315
H	-0.60505	-2.78411	2.79922
H	0.15326	-4.34327	3.04569
H	0.96399	-5.07766	5.07224
H	1.49067	-4.01502	6.37704
H	2.35622	-4.02122	4.82397
H	0.96068	-4.89945	-4.00072
H	-1.25562	-5.47441	-4.87372
H	-3.25140	-4.33803	-4.01520
H	3.09325	-1.41873	-1.98010
H	2.19234	-1.48207	-3.50363
H	1.40238	-0.88366	-2.05616
H	0.94335	-2.72341	-0.05027
H	1.48528	-4.36940	-0.35871
H	2.68009	-3.07537	-0.16152
H	2.54463	-5.04699	-2.49685
H	2.84371	-3.86013	-3.78433
H	3.71873	-3.75064	-2.25543
H	-2.70793	-2.28031	-0.04588
H	-4.46705	-2.13784	-0.19051
H	-3.67140	-3.70572	-0.40340
H	-5.62141	-2.47450	-2.31259

H	-4.78409	-2.81738	-3.82867
H	-4.84325	-4.04216	-2.54313
H	-2.59675	-0.35373	-2.11746
H	-3.58621	-0.70641	-3.51366
H	-4.36361	-0.39224	-1.95256
H	1.70800	3.23689	-5.94819
H	3.79989	4.09480	-5.01221
H	4.25636	3.90234	-2.61820
H	-0.42712	0.19078	-3.48042
H	-1.32412	0.06178	-4.99514
H	0.44431	0.01288	-5.00659
H	-1.60124	3.72589	-4.07029
H	-2.52621	2.39663	-4.79037
H	-1.92882	2.25295	-3.14831
H	-0.43340	3.34686	-6.46465
H	0.41831	1.81261	-6.75538
H	-1.33905	1.84243	-6.64762
H	3.20839	5.04565	-0.54168
H	1.54629	4.62321	-0.11512
H	2.87033	4.31345	1.03647
H	1.01151	2.22299	0.45907
H	2.03594	0.89261	-0.22941
H	2.52358	1.77678	1.20926
H	4.54393	2.42613	0.56959
H	4.48621	1.54233	-0.96637
H	4.96171	3.24581	-0.92427

O	-1.50097	2.25449	-0.44576
C	-0.71148	2.93782	-1.19400
O	-0.60216	4.11937	-1.38849

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2nd CO_2 inser - eta 2 coord

C	18.23107	4.94068	-2.42491
C	16.83566	4.84133	-2.68455
C	16.14129	5.86581	-3.38665
C	16.87358	6.98310	-3.79875
C	18.23295	7.10424	-3.54462
C	18.89486	6.08859	-2.86807
O	16.15877	3.75426	-2.25632
La	14.97120	2.12049	-1.51357
O	14.49274	-1.13049	-4.01470
C	15.40653	-2.19987	-3.96493
C	16.52075	-2.15377	-4.82491
C	17.44653	-3.19502	-4.68243
C	17.24439	-4.22868	-3.77839
C	16.07159	-4.28991	-3.03848
C	15.09840	-3.28661	-3.12417
C	16.68873	-1.10252	-5.94421
C	17.96496	-1.36295	-6.76331
C	13.73660	-3.45298	-2.41463
C	12.62044	-3.48865	-3.48025
C	14.63568	5.77017	-3.70023
C	14.12273	6.99256	-4.48223

C	19.00931	3.83279	-1.68879
C	20.50555	4.16518	-1.55080
C	13.84366	2.39966	1.02110
O	13.25385	2.61215	2.20991
C	13.98359	2.31126	3.37492
C	14.74407	3.34324	3.95796
C	15.51505	2.98090	5.06968
C	15.48671	1.69243	5.58538
C	14.63106	0.74246	5.04482
C	13.83092	1.02683	3.93129
C	14.66856	4.81832	3.50479
C	15.55898	5.71503	4.38312
C	12.77653	0.00928	3.44306
C	12.80245	-1.27054	4.29695
O	13.15299	2.70559	0.00158
O	15.01609	1.92820	0.93870
C	13.21551	5.31296	3.66693
C	15.12255	5.03395	2.04617
C	11.37333	0.63425	3.59315
C	12.98887	-0.42913	1.97916
C	15.49099	-1.21019	-6.91180
C	16.78996	0.34177	-5.41187
C	13.43989	-2.33124	-1.39837
C	13.67228	-4.78087	-1.64009
C	14.34991	4.54155	-4.58757
C	13.81297	5.72212	-2.39723

C	18.47288	3.65465	-0.25489
C	18.93091	2.50991	-2.47690
H	16.10740	1.43798	6.44007
H	16.14661	3.71789	5.54967
H	14.58494	-0.23644	5.50562
H	12.52316	4.74110	3.04554
H	13.14511	6.36642	3.37206
H	12.89107	5.23170	4.70966
H	16.06331	4.51742	1.83728
H	15.27921	6.10331	1.86787
H	14.36866	4.70966	1.32634
H	16.62036	5.45933	4.29310
H	15.27828	5.66969	5.44021
H	15.44371	6.75433	4.05986
H	11.26698	1.53621	2.98701
H	11.17342	0.89488	4.63777
H	10.60916	-0.08300	3.27195
H	14.03529	-0.67958	1.78371
H	12.66647	0.33269	1.26698
H	12.38367	-1.31923	1.77593
H	12.01240	-1.94430	3.95052
H	12.61440	-1.06582	5.35571
H	13.75351	-1.80691	4.20907
H	18.34269	-3.20609	-5.29033
H	17.98872	-5.01392	-3.67899
H	15.91316	-5.14058	-2.38738

H	15.60249	-0.48321	-7.72446
H	15.43913	-2.20919	-7.35732
H	14.54410	-1.00983	-6.40618
H	15.82241	0.73525	-5.09511
H	17.49431	0.41279	-4.57868
H	17.14542	1.00094	-6.21133
H	18.87287	-1.25658	-6.15967
H	17.96700	-2.35626	-7.22334
H	18.02260	-0.62924	-7.57353
H	13.14275	-1.39952	-1.88311
H	12.59914	-2.63058	-0.76315
H	14.30046	-2.13929	-0.75137
H	12.67729	-4.88431	-1.19595
H	13.83073	-5.64732	-2.28997
H	14.40190	-4.81981	-0.82392
H	12.58116	-2.56130	-4.05538
H	12.77421	-4.31985	-4.17635
H	11.64693	-3.62928	-2.99638
H	16.37457	7.78281	-4.33342
H	18.77525	7.98535	-3.87588
H	19.95714	6.19807	-2.68326
H	14.71714	3.61042	-4.15136
H	13.27393	4.43615	-4.76819
H	14.84506	4.65114	-5.55796
H	13.92578	6.65837	-1.84096
H	12.74767	5.58539	-2.61552

H	14.12898	4.92259	-1.72384
H	14.24332	7.92347	-3.91851
H	14.62610	7.10487	-5.44803
H	13.05317	6.86720	-4.68253
H	18.63142	4.56871	0.32686
H	17.40197	3.44447	-0.23163
H	18.99414	2.83567	0.25417
H	17.90168	2.19889	-2.66442
H	19.41672	2.61945	-3.45215
H	19.44170	1.70656	-1.93334
H	21.00918	3.34358	-1.03017
H	20.99180	4.28427	-2.52456
H	20.67368	5.07557	-0.96601
C	14.67643	-0.10292	-3.16804
O	13.82313	0.83239	-3.24209
O	15.64722	-0.08279	-2.35402

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Monomer - CO_2

C	3.34459	10.34524	-3.18866
C	2.32740	9.50554	-3.62083
C	2.57292	8.15200	-3.80422
C	3.81295	7.58323	-3.48816
C	4.76947	8.45396	-2.93024
C	4.61249	9.85245	-2.85537
O	5.99939	7.90437	-2.52675
C	6.15569	7.53183	-1.24077

O	5.22397	7.64569	-0.39637
La	6.76043	7.07203	1.49313
O	7.22350	8.93985	2.49033
C	7.39030	10.13030	3.10396
C	6.28459	10.74520	3.75974
C	6.48993	11.99485	4.35270
C	7.72317	12.63016	4.32332
C	8.79465	12.00678	3.69968
C	8.66953	10.75770	3.08454
C	4.89597	10.08020	3.84242
C	3.88896	10.92874	4.64006
C	9.90228	10.10022	2.43348
C	10.21875	8.76455	3.13429
C	4.10999	6.11038	-3.84521
C	2.90923	5.45590	-4.55149
C	5.77233	10.82742	-2.55307
C	5.30789	12.29151	-2.64848
O	9.32528	6.21749	0.75152
C	9.87210	6.22630	-0.28892
O	10.45442	6.21529	-1.29097
O	6.64832	5.41542	2.92245
C	6.26810	4.38027	3.70048
C	7.05101	4.01193	4.83174
C	6.59508	2.95067	5.62021
C	5.42659	2.25923	5.32902
C	4.68455	2.61717	4.21231

C	5.07844	3.66591	3.37775
C	8.36524	4.72837	5.19444
C	9.02796	4.13027	6.44711
C	4.25484	4.01416	2.12808
C	3.02784	3.10349	1.94919
C	4.98826	8.72842	4.57692
C	4.28930	9.90749	2.43705
C	9.67774	9.89695	0.92310
C	11.16693	10.96737	2.56559
C	8.10416	6.21443	5.50411
C	9.38006	4.57888	4.04431
C	5.12137	3.80785	0.86798
C	3.70465	5.45486	2.22707
O	7.30260	7.07805	-0.94376
C	5.30067	6.05444	-4.82555
C	4.41978	5.24981	-2.60576
C	6.87701	10.62721	-3.61253
C	6.37225	10.64430	-1.14583
H	5.66776	12.49136	4.85435
H	7.85043	13.60234	4.79109
H	9.75341	12.51163	3.69700
H	4.00618	8.24314	4.61542
H	5.33028	8.87586	5.60640
H	5.69472	8.03846	4.11080
H	4.93940	9.35548	1.75546
H	4.11417	10.88504	1.97572

H	3.32682	9.38545	2.49001
H	3.71127	11.90471	4.17671
H	4.21379	11.08955	5.67309
H	2.92810	10.40402	4.67572
H	8.78929	9.30017	0.71285
H	10.54655	9.40493	0.46867
H	9.54398	10.86187	0.42369
H	12.00889	10.44621	2.09691
H	11.43545	11.14851	3.61133
H	11.06058	11.93464	2.06329
H	9.36818	8.08207	3.13056
H	10.48673	8.94156	4.18096
H	11.06706	8.26583	2.65027
H	7.16535	2.64860	6.49101
H	5.10074	1.44156	5.96573
H	3.78027	2.06204	3.98924
H	7.68294	6.74552	4.65042
H	9.03763	6.71411	5.78772
H	7.40276	6.31388	6.33931
H	9.63741	3.52409	3.89761
H	10.30360	5.12247	4.27635
H	8.98232	4.95978	3.10368
H	9.28194	3.07304	6.31627
H	8.39543	4.22725	7.33588
H	9.96032	4.66844	6.64926
H	5.35486	2.74510	0.74667

H	6.08534	4.32081	0.92990
H	4.59543	4.14278	-0.03116
H	4.44103	6.15579	2.63332
H	2.86441	5.49069	2.92797
H	3.34865	5.81979	1.25708
H	2.48027	3.40551	1.04938
H	2.33546	3.17575	2.79410
H	3.31206	2.05366	1.82481
H	1.34993	9.91622	-3.85819
H	1.78350	7.53057	-4.20813
H	3.14615	11.40745	-3.11994
H	6.20932	6.46718	-4.38345
H	5.50153	5.01431	-5.10748
H	5.07727	6.61419	-5.73975
H	3.67503	5.40936	-1.82067
H	4.40186	4.18950	-2.88199
H	5.41080	5.45034	-2.19604
H	2.02899	5.39394	-3.90235
H	2.62916	5.98621	-5.46724
H	3.17868	4.43351	-4.83500
H	7.28101	9.61307	-3.58753
H	6.49024	10.81987	-4.61876
H	7.70086	11.32636	-3.42806
H	5.59558	10.60194	-0.37814
H	6.99244	9.74937	-1.07491
H	7.02604	11.49185	-0.91425

H	6.16752	12.94730	-2.47873
H	4.90213	12.53434	-3.63575
H	4.55502	12.53722	-1.89176

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Monomer - CO_2 - $HSiBR_3$

O	1.32618	0.66034	3.06041
C	0.69809	0.26454	1.93901
La	-0.61277	-0.40225	-0.47820
O	-0.33965	-2.26763	-1.59956
C	-0.44982	-3.47395	-2.19760
C	-0.47879	-3.56336	-3.61997
C	-0.65644	-4.82566	-4.19465
C	-0.78153	-5.97481	-3.42696
C	-0.70438	-5.87849	-2.04500
C	-0.53193	-4.65170	-1.39800
O	-0.26690	-0.55482	1.97021
O	1.13383	0.76959	0.86140
C	-0.27588	-2.33594	-4.52879
C	-0.30841	-2.70028	-6.02343
C	-0.41602	-4.60733	0.13596
C	-1.59573	-3.82653	0.74508
O	1.09186	0.97623	-2.14058
C	1.63138	1.55084	-3.00806
O	2.15087	2.11795	-3.87509
O	-2.43882	0.71353	-0.88671
C	-3.61686	1.36649	-0.99515

C	-4.83117	0.69078	-0.67817
C	-6.02748	1.40706	-0.77926
C	-6.05879	2.73544	-1.17818
C	-4.87014	3.37521	-1.49839
C	-3.63434	2.72549	-1.42380
C	-4.86321	-0.78351	-0.23291
C	-6.29426	-1.28959	0.02272
C	-2.35417	3.48078	-1.82924
C	-1.36842	3.56958	-0.64872
C	-4.27968	-1.69141	-1.33305
C	-4.10926	-0.95217	1.09971
C	-2.63872	4.93178	-2.25662
C	-1.71136	2.78757	-3.04649
C	-1.39009	-1.29396	-4.31904
C	1.11471	-1.72902	-4.25593
C	0.93650	-3.99235	0.54520
C	-0.45707	-6.00730	0.77383
Si	3.67141	4.36260	-0.41309
C	4.66420	5.95413	-0.66645
C	3.28968	4.07587	1.41499
C	4.59742	2.87466	-1.14402
C	4.26404	1.56329	-0.76032
C	4.92481	0.46270	-1.30756
C	5.93690	0.64951	-2.24893
C	6.28528	1.94139	-2.63900
C	5.62109	3.03844	-2.09062

H	2.36634	4.51032	-1.14910
H	-0.69563	-4.92164	-5.27334
H	-0.92313	-6.94065	-3.90363
H	-0.77849	-6.78703	-1.45859
H	-1.22683	-0.42095	-4.96207
H	-2.36628	-1.71903	-4.57329
H	-1.45282	-0.94947	-3.28579
H	1.24384	-1.48025	-3.20174
H	1.89914	-2.44384	-4.52543
H	1.26609	-0.82695	-4.86269
H	0.47429	-3.41782	-6.28981
H	-1.27560	-3.11440	-6.32688
H	-0.13930	-1.79507	-6.61683
H	1.09395	-3.00494	0.10789
H	0.99995	-3.90581	1.63525
H	1.75857	-4.63085	0.20509
H	-0.36100	-5.90799	1.86050
H	-1.40034	-6.52666	0.57545
H	0.36593	-6.64026	0.42640
H	-1.75021	-2.86275	0.25494
H	-2.52864	-4.38506	0.61587
H	-1.44458	-3.64956	1.81528
H	-6.96476	0.91784	-0.54171
H	-7.00393	3.26688	-1.24474
H	-4.91102	4.41001	-1.81680
H	-4.89241	-1.62740	-2.23829

H	-3.26367	-1.41316	-1.61770
H	-4.26956	-2.73731	-1.00691
H	-4.61429	-0.39402	1.89468
H	-4.07175	-2.00575	1.39754
H	-3.08678	-0.56953	1.05685
H	-6.79435	-0.73289	0.82202
H	-6.91550	-1.23724	-0.87724
H	-6.25159	-2.33952	0.33191
H	-1.81662	4.12866	0.17909
H	-0.45116	4.08994	-0.94810
H	-1.50865	1.73313	-2.85249
H	-2.38355	2.83663	-3.90940
H	-0.77662	3.29078	-3.32424
H	-1.69607	5.41290	-2.53918
H	-3.30593	4.98427	-3.12302
H	-3.07736	5.52221	-1.44545
H	5.91086	4.03773	-2.40709
H	7.07548	2.09561	-3.36930
H	6.45394	-0.20741	-2.67274
H	4.65564	-0.54200	-0.99091
H	3.48013	1.39313	-0.02554
H	5.64278	5.89154	-0.17978
H	4.82292	6.16985	-1.72749
H	4.12608	6.80375	-0.23387
H	-1.09005	2.58920	-0.26069
H	4.21197	3.94989	1.99092

H	2.74348	4.93023	1.82808
H	2.67272	3.18300	1.55254
C	1.00679	0.03693	4.27773
C	1.94723	-0.90569	4.75481
C	1.59380	-1.60465	5.91152
C	0.39424	-1.35691	6.57026
C	-0.44016	-0.34640	6.12618
C	-0.14732	0.41569	4.98324
C	3.33723	-1.10692	4.11242
H	2.26127	-2.35686	6.31326
H	0.13058	-1.93197	7.45353
H	-1.34722	-0.13641	6.68361
C	-1.10294	1.59093	4.67054
C	4.16949	-2.13759	4.89540
C	3.25661	-1.61648	2.65975
C	4.11007	0.22841	4.15314
C	-0.65211	2.55405	3.55917
C	-2.48627	1.02864	4.29244
C	-1.23116	2.45612	5.94601
H	5.10956	0.09372	3.72365
H	3.60017	1.00843	3.58529
H	4.23052	0.57459	5.18518
H	5.15810	-2.21989	4.43280
H	4.32096	-1.84146	5.93839
H	3.71632	-3.13477	4.87876
H	4.25824	-1.90094	2.31795

H	2.61726	-2.50076	2.58543
H	2.88971	-0.85681	1.96889
H	-1.92010	3.28711	5.75891
H	-1.61814	1.89913	6.80273
H	-0.26152	2.87756	6.23127
H	-1.32041	3.42202	3.56550
H	0.36791	2.91561	3.70861
H	-0.72334	2.11999	2.56060
H	-3.18026	1.84698	4.06915
H	-2.40969	0.38889	3.40968
H	-2.91925	0.43390	5.10281

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Monomer - CO_2 - $HSiBR_3$ - Hydros. TS

O	0.57024	4.65994	-4.33413
C	-0.07641	4.34591	-5.48164
La	-1.37123	3.73669	-7.97158
O	-1.22336	1.75172	-8.90863
C	-1.35616	0.55014	-9.50547
C	-1.37252	0.46017	-10.92941
C	-1.57815	-0.79663	-11.50644
C	-1.74146	-1.94268	-10.74113
C	-1.67323	-1.84849	-9.35857
C	-1.47380	-0.62741	-8.70802
O	-1.00646	3.49407	-5.50009
O	0.32431	4.96308	-6.51041
C	-1.12857	1.68210	-11.83584

C	-1.14911	1.31629	-13.33069
C	-1.36690	-0.59279	-7.17243
C	-2.52431	0.22083	-6.56623
O	0.20827	4.98287	-9.44690
C	1.14186	5.79114	-9.43578
O	1.96042	6.18823	-10.25797
O	-3.24201	4.86159	-8.23788
C	-4.41517	5.51597	-8.34163
C	-5.63519	4.84925	-8.01918
C	-6.82807	5.57146	-8.11655
C	-6.85646	6.89956	-8.51676
C	-5.66575	7.53259	-8.84191
C	-4.43303	6.87660	-8.77166
C	-5.67640	3.37598	-7.57213
C	-7.10910	2.88273	-7.30133
C	-3.15273	7.62856	-9.18317
C	-2.16783	7.71278	-8.00150
C	-5.11183	2.46330	-8.67765
C	-4.90815	3.20238	-6.24876
C	-3.43522	9.08125	-9.60635
C	-2.51019	6.93692	-10.40065
C	-2.22698	2.74476	-11.64651
C	0.27041	2.26269	-11.54861
C	-0.00210	-0.01234	-6.75351
C	-1.44925	-1.99436	-6.54253
Si	2.59666	7.48592	-8.23082

C	2.31928	8.91482	-9.40039
C	1.97816	7.87524	-6.50023
C	4.20632	6.55734	-8.24733
C	4.79887	6.19882	-7.02382
C	6.05087	5.58832	-6.99467
C	6.72491	5.32927	-8.18669
C	6.14661	5.67507	-9.40930
C	4.89531	6.28129	-9.44158
H	1.23446	6.28559	-8.32876
H	-1.60920	-0.89064	-12.58570
H	-1.90494	-2.90439	-11.21958
H	-1.77661	-2.75537	-8.77393
H	-2.02355	3.62500	-12.26678
H	-3.20387	2.34330	-11.93527
H	-2.31762	3.07533	-10.61074
H	0.40177	2.51041	-10.49556
H	1.04075	1.53209	-11.81849
H	0.44211	3.17167	-12.13626
H	-0.37812	0.58150	-13.58464
H	-2.12046	0.92249	-13.64859
H	-0.95096	2.21730	-13.92148
H	0.17293	0.97189	-7.18977
H	0.05469	0.07434	-5.66233
H	0.80723	-0.67019	-7.08817
H	-1.34784	-1.90294	-5.45557
H	-2.40884	-2.48315	-6.74133

H	-0.64716	-2.65139	-6.89475
H	-2.58798	1.22158	-6.99443
H	-3.48115	-0.27372	-6.76452
H	-2.40620	0.32166	-5.48165
H	-7.76657	5.08649	-7.87472
H	-7.79961	7.43504	-8.58060
H	-5.70358	8.56719	-9.16181
H	-5.73191	2.53302	-9.57757
H	-4.09573	2.73270	-8.96818
H	-5.10623	1.41749	-8.35153
H	-5.39332	3.77585	-5.45196
H	-4.88835	2.15008	-5.94480
H	-3.87916	3.56114	-6.31398
H	-7.59647	3.44493	-6.49776
H	-7.73979	2.93806	-8.19472
H	-7.07134	1.83302	-6.99068
H	-2.61325	8.27295	-7.17250
H	-1.25260	8.23705	-8.30660
H	-2.29545	5.88581	-10.21025
H	-3.18594	6.98649	-11.26082
H	-1.57349	7.43413	-10.68094
H	-2.49234	9.56024	-9.89376
H	-4.10441	9.13613	-10.47089
H	-3.87035	9.67305	-8.79395
H	4.43537	6.51799	-10.39569
H	6.66891	5.46348	-10.33783

H	7.70041	4.85115	-8.16480
H	6.49702	5.31337	-6.04338
H	4.28254	6.39090	-6.08769
H	2.68683	9.82595	-8.91332
H	2.83620	8.76661	-10.34854
H	1.25244	9.04733	-9.59996
H	-1.89073	6.73032	-7.61930
H	2.71610	8.50687	-5.98971
H	1.03691	8.42881	-6.55852
H	1.80180	6.96788	-5.91821
C	0.29600	3.90822	-3.18183
C	1.25642	2.92975	-2.83306
C	0.94586	2.11225	-1.74378
C	-0.23408	2.27797	-1.02649
C	-1.09142	3.31736	-1.34104
C	-0.84104	4.19447	-2.40916
C	2.62759	2.81130	-3.53428
H	1.63085	1.32924	-1.44379
H	-0.46534	1.61229	-0.19960
H	-1.98487	3.45720	-0.74152
C	-1.82752	5.37305	-2.58082
C	3.47981	1.69305	-2.90842
C	2.51203	2.49320	-5.03890
C	3.39852	4.13429	-3.34180
C	-1.42427	6.45429	-3.59838
C	-3.20567	4.81854	-2.98799

C	-1.94895	6.10278	-1.22249
H	4.38317	4.06531	-3.81976
H	2.86047	4.97659	-3.78175
H	3.55418	4.34338	-2.27810
H	4.45441	1.66779	-3.40646
H	3.66273	1.85781	-1.84167
H	3.02225	0.70603	-3.03459
H	3.49926	2.22486	-5.43198
H	1.84366	1.64598	-5.21477
H	2.16063	3.34562	-5.62146
H	-2.65775	6.93301	-1.31485
H	-2.30993	5.45454	-0.42042
H	-0.98310	6.51443	-0.91082
H	-2.11189	7.30010	-3.48878
H	-0.40918	6.82315	-3.43138
H	-1.50693	6.12030	-4.63378
H	-3.92340	5.63828	-3.10720
H	-3.13489	4.27887	-3.93539
H	-3.60490	4.13023	-2.23660

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Monomer - CO_2 - $HSiBR_3$ - Hydros. prod

O	1.10364	0.64612	3.23840
C	0.48372	0.36709	2.07224
La	-0.73855	-0.13259	-0.46285
O	-0.41873	-2.03838	-1.52311
C	-0.42786	-3.22454	-2.16288

C	-0.36131	-3.26560	-3.58746
C	-0.42195	-4.51429	-4.21347
C	-0.52593	-5.69629	-3.49365
C	-0.55253	-5.64473	-2.10719
C	-0.49900	-4.43463	-1.41006
O	-0.39939	-0.53128	1.98862
O	0.85368	1.06846	1.08589
C	-0.18995	-1.99357	-4.43906
C	-0.12181	-2.29926	-5.94598
C	-0.50559	-4.44006	0.12939
C	-1.76672	-3.73515	0.66262
O	0.88188	1.27026	-1.82768
C	1.86147	1.93877	-1.51544
O	2.50154	2.66197	-2.39570
O	-2.64207	0.92403	-0.74290
C	-3.82645	1.55858	-0.84513
C	-5.03719	0.84909	-0.58962
C	-6.24361	1.54905	-0.68201
C	-6.29134	2.89506	-1.01553
C	-5.10749	3.57002	-1.27644
C	-3.86230	2.93844	-1.20574
C	-5.05177	-0.64623	-0.22146
C	-6.47793	-1.18616	-0.01099
C	-2.58618	3.73487	-1.53808
C	-1.64548	3.78571	-0.31882
C	-4.44052	-1.48438	-1.36093

C	-4.30888	-0.87308	1.10888
C	-2.88656	5.19887	-1.90612
C	-1.88969	3.11376	-2.76435
C	-1.38348	-1.03729	-4.25506
C	1.14087	-1.30694	-4.07198
C	0.77738	-3.77465	0.66491
C	-0.52826	-5.86204	0.71723
Si	3.94276	3.62897	-2.05380
C	4.37211	4.26644	-3.75905
C	3.44058	4.97815	-0.85116
C	5.22326	2.45657	-1.34235
C	5.85822	2.71724	-0.11770
C	6.82537	1.84940	0.38782
C	7.16953	0.70119	-0.32310
C	6.54718	0.42206	-1.54021
C	5.58624	1.29393	-2.04525
H	2.22423	1.94898	-0.47767
H	-0.38532	-4.57255	-5.29517
H	-0.57533	-6.65122	-4.00959
H	-0.61574	-6.57616	-1.55632
H	-1.23364	-0.11746	-4.83156
H	-2.30887	-1.50869	-4.60180
H	-1.54115	-0.76157	-3.21160
H	1.20956	-1.10210	-3.00365
H	1.98214	-1.95408	-4.34372
H	1.24924	-0.35911	-4.61202

H	0.72296	-2.94897	-6.19762
H	-1.04019	-2.76792	-6.31531
H	0.01106	-1.36065	-6.49522
H	0.92223	-2.77576	0.25196
H	0.74045	-3.69572	1.75713
H	1.65308	-4.37360	0.39184
H	-0.51752	-5.79531	1.81062
H	-1.42947	-6.41489	0.43184
H	0.34652	-6.44680	0.41377
H	-1.89886	-2.74492	0.22451
H	-2.66038	-4.31464	0.40747
H	-1.72533	-3.62609	1.75184
H	-7.17669	1.03270	-0.48947
H	-7.24457	3.41269	-1.07739
H	-5.16043	4.61874	-1.54453
H	-5.03875	-1.37518	-2.27169
H	-3.42288	-1.17914	-1.60858
H	-4.42266	-2.54692	-1.09415
H	-4.83031	-0.36251	1.92529
H	-4.26281	-1.94038	1.35196
H	-3.29088	-0.47911	1.09014
H	-6.99801	-0.67563	0.80641
H	-7.08811	-1.10134	-0.91622
H	-6.42232	-2.24884	0.24899
H	-2.12821	4.31154	0.51176
H	-0.72286	4.32501	-0.56624

H	-1.67516	2.05470	-2.62320
H	-2.53287	3.20365	-3.64626
H	-0.94612	3.62888	-2.98011
H	-1.94542	5.70861	-2.14103
H	-3.52984	5.27839	-2.78848
H	-3.35927	5.74523	-1.08296
H	5.10948	1.05938	-2.99473
H	6.81091	-0.47432	-2.09444
H	7.92109	0.02251	0.07079
H	7.30658	2.06812	1.33698
H	5.59752	3.60463	0.45410
H	5.25088	4.91702	-3.71008
H	4.59926	3.44011	-4.43836
H	3.54017	4.83841	-4.18020
H	-1.37530	2.79327	0.04260
H	4.27772	5.66179	-0.67533
H	2.61329	5.56265	-1.26458
H	3.12471	4.57324	0.11499
C	0.91793	-0.20759	4.33419
C	1.98887	-1.08894	4.61526
C	1.78475	-2.00851	5.64671
C	0.59982	-2.02885	6.37483
C	-0.37457	-1.07688	6.13255
C	-0.23759	-0.10656	5.12605
C	3.35447	-1.00697	3.89719
H	2.55809	-2.72515	5.89405

H	0.45457	-2.77014	7.15576
H	-1.27155	-1.08123	6.74333
C	-1.35075	0.96400	5.04154
C	4.35083	-2.02618	4.47724
C	3.25252	-1.29832	2.38665
C	3.96093	0.39576	4.11500
C	-1.09282	2.13936	4.08295
C	-2.66964	0.28508	4.62616
C	-1.51618	1.59384	6.44420
H	4.94375	0.45364	3.63270
H	3.32815	1.17790	3.69211
H	4.09662	0.59854	5.18278
H	5.31545	-1.90527	3.97376
H	4.51968	-1.87705	5.54866
H	4.02617	-3.05980	4.31643
H	4.25983	-1.39336	1.96501
H	2.72253	-2.23641	2.19944
H	2.75518	-0.49684	1.83976
H	-2.31413	2.34404	6.41849
H	-1.78165	0.86216	7.21136
H	-0.59334	2.09119	6.76106
H	-1.86703	2.89567	4.25266
H	-0.12119	2.61010	4.25084
H	-1.16574	1.85470	3.03224
H	-3.47489	1.02646	4.56802
H	-2.56219	-0.18781	3.64686

H	-2.97520	-0.48462	5.34194

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10 + CO_2 - $ArOCOOSiR_3$

La	2.31251	0.42006	-1.31646
O	2.49540	2.57950	-1.30464
O	3.97522	-0.67277	-2.21474
C	4.76023	-1.47034	-2.96934
C	6.17635	-1.38880	-2.84893
C	6.94683	-2.23153	-3.65630
C	6.37389	-3.12616	-4.55060
C	4.99157	-3.19541	-4.65391
C	4.15724	-2.38433	-3.88058
O	-0.06299	-0.11162	-1.81150
C	-0.28021	-0.52725	-0.63588
O	0.61653	-0.55659	0.25842
O	3.21365	-0.25346	1.25899
C	2.64344	-0.68165	2.19316
O	2.12418	-1.10293	3.13999
C	6.86400	-0.42195	-1.86613
C	6.45815	-0.76373	-0.41918
C	2.62898	-2.48813	-4.02043
C	2.19327	-3.53422	-5.06169
C	2.56899	3.92487	-1.38101
C	2.36157	4.57088	-2.63298
C	2.44125	5.96602	-2.66926
C	2.71205	6.71690	-1.53379

C	2.91088	6.07095	-0.32160
C	2.84713	4.67921	-0.20600
C	2.05383	3.78523	-3.92200
C	0.72529	3.01661	-3.77697
C	3.08277	4.00961	1.16110
C	4.32293	3.09615	1.09486
C	8.39786	-0.52091	-1.92980
C	6.50421	1.03837	-2.20189
C	2.04465	-1.14442	-4.50842
C	2.00469	-2.93890	-2.68175
C	1.88435	4.70682	-5.14298
C	3.21768	2.83487	-4.26543
C	1.82882	3.22806	1.60180
C	3.36092	5.03501	2.27441
F	-1.53530	-2.53040	-4.39614
C	-2.40302	-2.02506	-5.28247
C	-3.70687	-1.70098	-4.88649
C	-4.52734	-1.15931	-5.88476
C	-4.09685	-0.95825	-7.19010
C	-2.78682	-1.28363	-7.53155
C	-1.93060	-1.81525	-6.57094
B	-4.21618	-1.92821	-3.42279
C	-5.15297	-0.87383	-2.74452
C	-6.19846	-1.24609	-1.88766
C	-7.04609	-0.32560	-1.28522
C	-6.84821	1.03314	-1.51669

C	-5.81718	1.45390	-2.35243
C	-5.00194	0.50431	-2.95543
F	-5.79641	-0.83927	-5.61216
F	-4.91794	-0.45878	-8.11112
F	-2.35492	-1.08747	-8.77021
F	-0.67402	-2.11648	-6.89562
F	-6.44083	-2.53780	-1.64126
F	-8.03844	-0.72632	-0.49322
F	-7.64179	1.92627	-0.94101
F	-5.62505	2.75364	-2.56545
F	-4.02163	0.96336	-3.73806
C	-3.78758	-3.21825	-2.64164
C	-3.48438	-3.19862	-1.27452
C	-3.08649	-4.32582	-0.56851
C	-3.00842	-5.54818	-1.23128
C	-3.31316	-5.62332	-2.58754
C	-3.68307	-4.46829	-3.26597
F	-3.53209	-2.04646	-0.58986
F	-2.78376	-4.25031	0.72569
F	-2.64208	-6.63889	-0.57155
F	-3.24651	-6.79350	-3.21825
F	-3.97495	-4.59991	-4.56380
H	8.02783	-2.19203	-3.58971
H	7.00255	-3.76624	-5.16319
H	4.55644	-3.89889	-5.35439
H	6.99629	1.72298	-1.50120

H	6.83920	1.29307	-3.21288
H	5.42968	1.21703	-2.15370
H	5.37674	-0.72981	-0.28577
H	6.79750	-1.77128	-0.15523
H	6.91632	-0.05760	0.28365
H	8.75975	-1.52088	-1.66816
H	8.78745	-0.26059	-2.91969
H	8.83131	0.18308	-1.21133
H	2.37663	-2.36551	-1.82758
H	0.91260	-2.86629	-2.71500
H	2.27169	-3.98099	-2.47784
H	1.10076	-3.54046	-5.12878
H	2.57982	-3.30323	-6.05947
H	2.51853	-4.54395	-4.79084
H	2.46132	-0.28443	-3.97494
H	2.30548	-0.98302	-5.55932
H	0.95388	-1.13278	-4.42314
H	2.28837	6.48683	-3.60722
H	2.76767	7.80015	-1.59339
H	3.12118	6.67245	0.55505
H	4.12956	3.40634	-4.46699
H	3.45739	2.14573	-3.45273
H	2.98498	2.24621	-5.16020
H	-0.10870	3.71795	-3.66901
H	0.53440	2.40210	-4.66455
H	0.70119	2.36803	-2.89907

H	1.05181	5.40720	-5.01978
H	2.79202	5.28142	-5.35462
H	1.67039	4.09558	-6.02646
H	0.98202	3.91036	1.72959
H	2.00394	2.73079	2.56369
H	4.25379	2.36001	0.29256
H	5.22105	3.69341	0.90662
H	4.46531	2.56564	2.04386
H	3.52311	4.50451	3.21906
H	4.25914	5.62783	2.07362
H	2.52020	5.72061	2.42343
H	-1.29241	-0.88244	-0.38030
H	1.52615	2.47562	0.87135

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10 + CO_2 - $ArOCOOSiR_3$ + $HSiR_3$

La	2.61134	1.53894	0.14201
O	3.22466	3.52195	-0.48955
O	4.11616	-0.03616	-0.00633
C	4.77534	-1.20026	-0.18720
C	6.17138	-1.27344	0.08262
C	6.80780	-2.50311	-0.11326
C	6.12426	-3.62756	-0.55702
C	4.76497	-3.53786	-0.82298
C	4.06224	-2.34260	-0.65168
H	0.21986	-0.40894	6.41256
Si	-1.01329	-0.95403	5.75146

C	-0.47272	-2.49008	4.78288
C	-1.34874	-3.13931	3.89704
C	-0.96410	-4.28702	3.20676
C	0.31602	-4.81128	3.38890
C	1.20491	-4.18186	4.25905
C	0.81090	-3.03390	4.94699
O	0.22435	1.23327	-0.50529
C	-0.18537	1.39214	0.68218
O	0.59765	1.59417	1.65680
O	3.13307	1.77889	2.87096
C	2.46209	2.04803	3.79698
O	1.83725	2.31716	4.73541
C	6.97831	-0.05855	0.57873
C	6.44830	0.40355	1.94975
C	2.56095	-2.27222	-0.97705
C	1.99641	-3.61154	-1.48154
C	3.64424	4.68437	-1.03318
C	3.59104	4.85975	-2.44572
C	4.04869	6.07085	-2.97261
C	4.53375	7.08795	-2.16239
C	4.56172	6.90749	-0.78655
C	4.12418	5.72332	-0.18602
C	3.03060	3.77607	-3.38581
C	1.54844	3.50942	-3.05571
C	4.17690	5.57445	1.34627
C	5.14764	4.44187	1.73269

C	-2.27164	-1.42030	7.08860
C	-1.73932	0.35600	4.59412
C	8.46875	-0.38794	0.77098
C	6.91209	1.08958	-0.44747
C	2.32162	-1.25932	-2.11716
C	1.75077	-1.92293	0.29036
C	3.06967	4.20238	-4.86431
C	3.87236	2.48776	-3.29609
C	2.76458	5.32086	1.91134
C	4.69413	6.84617	2.04124
F	-1.49193	-1.39526	-2.06478
C	-2.23058	-0.34442	-2.44144
C	-3.54058	-0.19680	-1.96444
C	-4.21926	0.95066	-2.39967
C	-3.65220	1.88475	-3.25623
C	-2.34431	1.69658	-3.69575
C	-1.62784	0.57638	-3.28669
B	-4.20765	-1.24828	-1.01679
C	-5.16488	-0.78135	0.13304
C	-6.30563	-1.51030	0.49749
C	-7.16837	-1.10929	1.50998
C	-6.89039	0.05624	2.21875
C	-5.76405	0.81094	1.90090
C	-4.93744	0.39048	0.86739
F	-5.48269	1.17015	-2.02005
F	-4.34102	2.95056	-3.65865

F	-1.78156	2.58380	-4.50515
F	-0.37658	0.40347	-3.70890
F	-6.62720	-2.63097	-0.15625
F	-8.25021	-1.82501	1.80824
F	-7.69739	0.44786	3.19548
F	-5.49443	1.92140	2.58346
F	-3.86767	1.15386	0.60849
C	-3.91842	-2.77610	-1.21910
C	-3.75098	-3.65582	-0.14191
C	-3.48634	-5.00866	-0.30645
C	-3.39726	-5.53512	-1.59219
C	-3.56947	-4.70326	-2.69510
C	-3.81343	-3.35040	-2.49307
F	-3.81261	-3.20185	1.11589
F	-3.31131	-5.80499	0.74921
F	-3.15171	-6.82683	-1.76531
F	-3.49626	-5.20826	-3.92443
F	-3.98178	-2.59940	-3.58591
H	7.86989	-2.59209	0.08332
H	6.65011	-4.56773	-0.69785
H	4.24383	-4.42164	-1.17371
H	7.49452	1.94892	-0.09536
H	7.33119	0.76934	-1.40728
H	5.88913	1.42235	-0.62512
H	5.38718	0.64946	1.90992
H	6.58048	-0.38658	2.69698

H	6.99666	1.28885	2.29271
H	8.62731	-1.17164	1.51936
H	8.94705	-0.70004	-0.16346
H	8.98995	0.50913	1.12217
H	2.19222	-1.09965	0.86002
H	0.71497	-1.67306	0.03761
H	1.73408	-2.77313	0.97911
H	0.92908	-3.49181	-1.69734
H	2.48468	-3.94053	-2.40435
H	2.09586	-4.40578	-0.73469
H	2.82961	-0.30517	-1.94556
H	2.74098	-1.64484	-3.05235
H	1.25548	-1.07511	-2.27235
H	4.02592	6.23111	-4.04420
H	4.88349	8.01843	-2.60057
H	4.93536	7.71517	-0.16810
H	4.88420	2.66520	-3.67481
H	3.99545	2.12944	-2.27070
H	3.42404	1.68716	-3.89535
H	0.95345	4.40649	-3.25695
H	1.14831	2.69609	-3.66993
H	1.38674	3.25650	-2.00616
H	2.46626	5.09674	-5.05013
H	4.08991	4.39381	-5.21272
H	2.65790	3.39568	-5.48049
H	2.11332	6.17661	1.70491

H	2.80618	5.19156	3.00012
H	4.88997	3.49566	1.25539
H	6.16627	4.69440	1.42077
H	5.15623	4.29191	2.81902
H	4.70027	6.68586	3.12500
H	5.71821	7.09309	1.74289
H	4.05658	7.71369	1.84144
H	1.51477	-2.55415	5.62399
H	2.20406	-4.58494	4.40287
H	0.61878	-5.70841	2.85515
H	-1.66205	-4.77048	2.52979
H	-2.35113	-2.74669	3.73713
H	-3.17198	-1.85686	6.64384
H	-1.84902	-2.15531	7.78005
H	-2.57211	-0.54022	7.66659
H	-1.27002	1.35063	0.87639
H	2.29269	4.44183	1.46974
H	-2.61413	-0.03317	4.06246
H	-2.05948	1.23563	5.16196
H	-1.00395	0.67897	3.85150

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10 + CO_2 - $ArOCOOSiR_3$ + $HSiR_3$ hydros. TS same CO_2

La	2.23987	0.80673	-1.20670
O	2.61849	2.89843	-1.72464
O	3.75569	-0.66063	-1.80984
C	4.56184	-1.68743	-2.14051

C	5.96110	-1.60484	-1.88105
C	6.75731	-2.69891	-2.23360
C	6.22777	-3.84145	-2.81809
C	4.86448	-3.90588	-3.06990
C	4.00583	-2.85119	-2.74912
H	0.78975	0.58731	2.17942
Si	-0.26000	-0.01293	3.53725
C	-0.50843	-1.83190	3.26782
C	-1.53617	-2.27414	2.41670
C	-1.77575	-3.63497	2.24034
C	-0.99430	-4.56844	2.91969
C	0.03044	-4.14518	3.76788
C	0.27789	-2.78695	3.93582
O	0.04286	0.42829	-2.36074
C	-0.62892	0.48731	-1.29343
O	-0.10533	0.58220	-0.14576
O	2.55847	0.48188	1.25406
C	1.93189	0.18135	2.27560
O	2.18822	-0.40863	3.31869
C	6.60491	-0.36937	-1.22392
C	6.05937	-0.18682	0.20552
C	2.50580	-2.95352	-3.07511
C	2.13082	-4.29466	-3.72955
C	2.92979	4.17090	-2.03630
C	2.88309	4.60119	-3.39481
C	3.22831	5.92682	-3.67419

C	3.59987	6.81870	-2.67753
C	3.62442	6.39020	-1.35778
C	3.29522	5.07971	-0.99997
C	2.44455	3.66831	-4.54027
C	0.98568	3.22189	-4.32108
C	3.33730	4.65546	0.48005
C	4.39889	3.55721	0.68606
C	0.29005	0.63864	5.19791
C	-1.61411	1.05434	2.78856
C	8.13239	-0.50734	-1.09243
C	6.35854	0.89032	-2.07683
C	2.11756	-1.85839	-4.08845
C	1.66506	-2.86649	-1.78398
C	2.48420	4.36739	-5.91113
C	3.38733	2.45524	-4.65424
C	1.94165	4.18882	0.94195
C	3.73022	5.81412	1.41326
F	-1.71775	-1.80949	-3.91141
C	-2.42144	-0.78114	-4.39208
C	-3.74862	-0.57629	-3.97700
C	-4.39101	0.54159	-4.53573
C	-3.77434	1.39586	-5.43855
C	-2.45196	1.15660	-5.80459
C	-1.76863	0.06402	-5.27917
B	-4.45714	-1.51491	-2.95229
C	-5.53921	-0.95096	-1.96329

C	-6.71066	-1.65858	-1.66755
C	-7.68006	-1.18327	-0.79215
C	-7.48076	0.03866	-0.15607
C	-6.32529	0.77365	-0.40956
C	-5.39076	0.27701	-1.30845
F	-5.66522	0.81028	-4.23370
F	-4.42905	2.43352	-5.95465
F	-1.84280	1.96880	-6.65583
F	-0.50794	-0.15303	-5.63689
F	-6.95431	-2.83295	-2.25943
F	-8.78821	-1.88204	-0.55566
F	-8.38924	0.50235	0.69277
F	-6.12934	1.93695	0.20872
F	-4.29332	1.01952	-1.50933
C	-4.09613	-3.03993	-2.86996
C	-3.96628	-3.70450	-1.64540
C	-3.65758	-5.05417	-1.54679
C	-3.48523	-5.80029	-2.70926
C	-3.61432	-5.18561	-3.95220
C	-3.90315	-3.82754	-4.01147
F	-4.10398	-3.03097	-0.49274
F	-3.52230	-5.63826	-0.35418
F	-3.19894	-7.09306	-2.63214
F	-3.45839	-5.89985	-5.06384
F	-4.02500	-3.28579	-5.22658
H	7.82471	-2.66382	-2.04899

H	6.87473	-4.67462	-3.07855
H	4.46462	-4.80167	-3.53170
H	6.80720	1.76901	-1.59909
H	6.81343	0.77577	-3.06661
H	5.29694	1.08831	-2.22577
H	4.97216	-0.10917	0.23192
H	6.33813	-1.04236	0.83038
H	6.47989	0.71608	0.66409
H	8.41976	-1.35335	-0.45909
H	8.62247	-0.62079	-2.06537
H	8.53295	0.39963	-0.62659
H	1.95340	-2.02013	-1.15658
H	0.59822	-2.78436	-2.01918
H	1.81478	-3.76331	-1.17341
H	1.05471	-4.30363	-3.93615
H	2.64740	-4.44549	-4.68296
H	2.34991	-5.14827	-3.07923
H	2.43776	-0.86542	-3.76914
H	2.60583	-2.05316	-5.04926
H	1.03654	-1.83568	-4.25061
H	3.20636	6.27947	-4.69864
H	3.86421	7.84243	-2.92755
H	3.90906	7.10021	-0.58965
H	4.40250	2.78039	-4.90474
H	3.45838	1.89024	-3.72339
H	3.04547	1.77517	-5.44288

H	0.31911	4.09090	-4.35210
H	0.67188	2.52596	-5.10725
H	0.84201	2.73073	-3.35863
H	1.80884	5.22820	-5.95607
H	3.49239	4.70434	-6.17462
H	2.16297	3.65878	-6.68222
H	1.23412	5.02422	0.90480
H	1.98283	3.82601	1.97643
H	4.26442	2.71755	0.00315
H	5.39889	3.96171	0.49787
H	4.37442	3.17481	1.71275
H	3.74080	5.45423	2.44821
H	4.73049	6.20030	1.19179
H	3.01957	6.64570	1.36010
H	1.10139	-2.46481	4.56593
H	0.64416	-4.87518	4.28759
H	-1.17862	-5.63026	2.78127
H	-2.55996	-3.96433	1.56687
H	-2.14861	-1.55635	1.87847
H	-0.60613	0.83165	5.79982
H	0.94125	-0.06580	5.71521
H	0.82584	1.58434	5.07822
H	-1.73132	0.46528	-1.36760
H	1.53792	3.39660	0.30986
H	-2.57997	0.77392	3.22672
H	-1.42896	2.10858	3.01366

H	-1.65039	0.93380	1.70307

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10 + CO_2 - $ArOCOOSiR_3$ + $HSiR_3$ hydros. prod same CO_2

La	2.39574	1.24003	0.26458
O	2.84063	3.28076	-0.37034
O	3.91600	-0.29291	-0.13570
C	4.73324	-1.33939	-0.35829
C	6.10978	-1.25560	0.00309
C	6.91870	-2.37065	-0.23645
C	6.42261	-3.53471	-0.80773
C	5.08186	-3.59995	-1.16042
C	4.21213	-2.52579	-0.95407
H	0.91034	-0.14467	3.15891
Si	0.81733	-0.34526	6.00772
C	0.11876	-1.89094	5.20432
C	-1.06484	-1.84656	4.44655
C	-1.55603	-2.98553	3.81136
C	-0.87541	-4.19628	3.93267
C	0.29350	-4.26591	4.68963
C	0.78618	-3.12303	5.31590
O	0.25260	0.86143	-0.97647
C	-0.44105	0.85073	0.08046
O	0.06129	0.89367	1.23946
O	2.55530	0.98235	2.80460
C	1.77504	0.40447	3.55497
O	1.92662	0.41707	4.85179

C	6.71514	0.00503	0.64938
C	6.05617	0.26495	2.01775
C	2.73959	-2.63438	-1.38731
C	2.40303	-4.00298	-2.00489
C	3.18208	4.53478	-0.72256
C	3.24076	4.89193	-2.10106
C	3.62229	6.19814	-2.42198
C	3.92728	7.13824	-1.44701
C	3.84433	6.78105	-0.10836
C	3.47408	5.49376	0.29083
C	2.87295	3.90236	-3.22385
C	1.39573	3.48280	-3.08620
C	3.39294	5.14553	1.78874
C	4.42769	4.05741	2.13726
C	1.94542	-0.69024	7.45931
C	-0.49212	0.94780	6.36650
C	8.22432	-0.14076	0.91354
C	6.55510	1.22332	-0.28065
C	2.43599	-1.58435	-2.47421
C	1.80518	-2.48064	-0.16945
C	3.01940	4.52641	-4.62301
C	3.80444	2.67512	-3.20413
C	1.96196	4.70515	2.16073
C	3.71426	6.34995	2.69097
F	-1.42258	-1.48344	-2.35101
C	-2.11638	-0.50719	-2.94373

C	-3.46154	-0.28776	-2.60164
C	-4.09133	0.77177	-3.27638
C	-3.44543	1.55820	-4.21965
C	-2.10615	1.30888	-4.50934
C	-1.43490	0.27166	-3.86884
B	-4.20455	-1.14794	-1.53248
C	-5.32479	-0.51359	-0.63427
C	-6.50410	-1.20299	-0.32735
C	-7.50722	-0.66567	0.47027
C	-7.33552	0.60418	1.01406
C	-6.17359	1.32403	0.74685
C	-5.20379	0.76331	-0.07387
F	-5.38031	1.04553	-3.05161
F	-4.08859	2.54090	-4.84626
F	-1.46970	2.05767	-5.39811
F	-0.15838	0.04248	-4.15638
F	-6.72042	-2.42266	-0.83262
F	-8.62178	-1.34994	0.72005
F	-8.27755	1.12830	1.78783
F	-6.00611	2.53406	1.27638
F	-4.10138	1.49222	-0.29183
C	-3.83609	-2.65833	-1.31530
C	-3.74925	-3.22308	-0.03764
C	-3.41676	-4.55340	0.17956
C	-3.18165	-5.38350	-0.91261
C	-3.27108	-4.87129	-2.20454

C	-3.58224	-3.52870	-2.38230
F	-3.95379	-2.46620	1.05058
F	-3.32072	-5.03988	1.41950
F	-2.87291	-6.65970	-0.72258
F	-3.05563	-5.66731	-3.24887
F	-3.66176	-3.08602	-3.64032
H	7.96903	-2.33478	0.02859
H	7.07814	-4.38384	-0.98031
H	4.70842	-4.51271	-1.61086
H	6.97302	2.12077	0.19007
H	7.08876	1.05656	-1.22237
H	5.51187	1.42242	-0.52740
H	4.97291	0.36371	1.94367
H	6.26303	-0.56463	2.70293
H	6.45426	1.18175	2.46831
H	8.44691	-0.95817	1.60777
H	8.79134	-0.30615	-0.00876
H	8.59769	0.78388	1.36697
H	2.03861	-1.59230	0.42142
H	0.75837	-2.42360	-0.48717
H	1.91371	-3.33766	0.50400
H	1.34544	-4.01603	-2.29101
H	2.98820	-4.20171	-2.90861
H	2.56548	-4.82618	-1.30084
H	2.73827	-0.57952	-2.17477
H	2.99288	-1.82193	-3.38678

H	1.37019	-1.56470	-2.71744
H	3.68256	6.49703	-3.46200
H	4.22191	8.14527	-1.72907
H	4.07474	7.52968	0.64108
H	4.83994	2.97683	-3.39322
H	3.79496	2.15899	-2.24282
H	3.51268	1.95920	-3.98110
H	0.74528	4.35470	-3.21720
H	1.12947	2.74472	-3.85156
H	1.17429	3.05073	-2.11012
H	2.36253	5.39188	-4.75885
H	4.04864	4.83643	-4.83322
H	2.73995	3.78219	-5.37665
H	1.26682	5.54307	2.04159
H	1.91979	4.37454	3.20512
H	4.35102	3.18812	1.48226
H	5.44266	4.45126	2.01925
H	4.30988	3.72014	3.17314
H	3.63443	6.04407	3.74010
H	4.73217	6.72235	2.53582
H	3.01575	7.17886	2.53524
H	1.70288	-3.19620	5.89615
H	0.82425	-5.20875	4.78799
H	-1.25787	-5.08160	3.43320
H	-2.46042	-2.93004	3.21403
H	-1.61139	-0.91218	4.34163

H	1.39112	-1.16694	8.27369
H	2.77394	-1.34539	7.17648
H	2.37032	0.24553	7.83405
H	-1.54130	0.81755	-0.01444
H	1.59627	3.89665	1.52549
H	-1.20038	0.57306	7.11248
H	-0.02848	1.85711	6.76026
H	-1.05644	1.21886	5.46931

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10 + CO_2 - $ArOCOOSiR_3$ + $HSiR_3$ hydros. TS betw 2 CO_2

C	20.42464	8.81533	-2.40501
C	20.62413	8.08129	-1.20072
C	21.50607	8.56307	-0.19072
C	22.18080	9.76449	-0.42610
C	22.00607	10.48570	-1.59915
C	21.13308	10.00944	-2.56796
O	19.96777	6.92132	-1.00892
La	18.92605	5.01870	-0.73435
O	18.78522	4.14408	1.53990
C	18.11157	3.82225	2.53417
O	18.11855	2.99739	3.40152
C	21.71771	7.80674	1.13415
C	22.70583	8.52530	2.06966
C	19.46203	8.33471	-3.50760
C	19.92765	6.98062	-4.07687
O	16.70800	5.51126	-0.36588

C	15.51741	5.32625	0.07045
O	15.18029	5.16783	1.24993
Si	16.09059	5.64183	3.56375
C	15.78776	7.36430	2.88236
C	14.66022	4.58336	4.13618
C	13.38099	4.66669	3.55871
C	12.31293	3.94841	4.08887
C	12.50864	3.12133	5.19538
C	13.77329	3.01280	5.77078
C	14.83944	3.74086	5.24736
C	17.38718	5.79536	4.93429
O	19.17849	3.38111	-2.15599
C	19.46190	2.32146	-2.93911
C	20.75207	1.72050	-2.86763
C	21.00993	0.61737	-3.68621
C	20.05276	0.10732	-4.55220
C	18.80114	0.70466	-4.61144
C	18.46835	1.81030	-3.82301
C	21.84930	2.25214	-1.92627
C	22.21620	3.70214	-2.29850
C	17.06047	2.42832	-3.92315
C	16.32890	2.30535	-2.57198
C	21.39817	2.14299	-0.45571
C	23.15570	1.44504	-2.02983
C	16.18207	1.71217	-4.96398
C	17.14720	3.90091	-4.36924

C	22.31331	6.40978	0.86996
C	20.38587	7.70831	1.90609
C	18.02247	8.24564	-2.96200
C	19.40999	9.30505	-4.70106
F	12.97285	6.79028	-2.46542
C	11.78901	6.23497	-2.20816
C	11.68241	4.87303	-1.96333
C	10.47042	4.24527	-1.65437
C	9.34629	5.07990	-1.62294
C	9.40944	6.44277	-1.88818
C	10.64180	7.02360	-2.17530
B	10.37944	2.71248	-1.33414
C	11.21428	1.68127	-2.15958
C	11.74896	0.51794	-1.58417
C	12.53123	-0.38569	-2.29214
C	12.79194	-0.14995	-3.63918
C	12.27150	0.98224	-4.26050
C	11.50730	1.87256	-3.51882
F	11.55222	0.25045	-0.29044
F	13.03417	-1.46458	-1.69783
F	13.53914	-1.00016	-4.32926
F	12.52207	1.20639	-5.54878
F	11.02682	2.93610	-4.17031
F	12.81927	4.16417	-1.99269
F	10.72356	8.32537	-2.41651
F	8.31093	7.19440	-1.86542

F	8.13871	4.57059	-1.35765
C	9.46010	2.23666	-0.15722
C	9.38516	2.93939	1.05110
C	8.60313	2.52285	2.11997
C	7.82748	1.37459	1.98893
C	7.85398	0.65176	0.79854
C	8.67102	1.08274	-0.23906
F	10.11837	4.04497	1.23701
F	8.66094	0.35690	-1.36141
F	7.10513	-0.44115	0.67043
F	7.06529	0.96869	2.99601
F	8.59592	3.20672	3.26502
H	17.13180	4.64751	2.61570
H	21.98207	0.13945	-3.65153
H	20.28042	-0.75159	-5.17720
H	18.06568	0.29181	-5.29215
H	22.96350	4.10476	-1.60535
H	22.63976	3.73804	-3.30744
H	21.35224	4.37012	-2.30315
H	20.41707	2.58979	-0.27746
H	21.30839	1.09199	-0.16243
H	22.12649	2.61652	0.21306
H	23.01463	0.39389	-1.75776
H	23.58658	1.48746	-3.03547
H	23.89372	1.86625	-1.33847
H	16.87839	2.79051	-1.76417

H	15.33376	2.76186	-2.63095
H	16.20625	1.25150	-2.29993
H	15.20507	2.20473	-5.01211
H	16.61622	1.75531	-5.96821
H	16.00678	0.66151	-4.71002
H	17.78438	4.49032	-3.70903
H	17.56890	3.96875	-5.37764
H	16.14972	4.35592	-4.38730
H	21.00441	10.58861	-3.47497
H	22.54479	11.41590	-1.75629
H	22.86153	10.15321	0.32261
H	20.92029	7.07781	-4.52871
H	20.00156	6.20597	-3.31126
H	19.23689	6.62942	-4.85173
H	17.66122	9.24090	-2.68184
H	17.34514	7.84473	-3.72515
H	17.94841	7.61879	-2.07149
H	19.06093	10.30077	-4.40845
H	20.38373	9.40990	-5.19089
H	18.70810	8.91765	-5.44743
H	20.04606	8.70694	2.20054
H	20.51238	7.10919	2.81572
H	21.71363	5.83392	0.16223
H	23.31426	6.50073	0.43549
H	22.39881	5.83995	1.80263
H	22.81273	7.94639	2.99363

H	23.70147	8.61861	1.62394
H	22.35682	9.52535	2.34699
H	15.81839	3.64404	5.70673
H	13.93098	2.36227	6.62646
H	11.67482	2.55800	5.60601
H	11.33047	4.02472	3.63370
H	13.23240	5.27952	2.67663
H	16.93103	6.30640	5.79053
H	17.77767	4.83141	5.26605
H	18.22616	6.40693	4.58738
H	14.73272	5.31421	-0.70593
H	19.59443	7.26235	1.30066
H	15.84610	8.07797	3.71157
H	16.56156	7.62397	2.15454
H	14.81707	7.44102	2.39289

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10 + CO_2 - $ArOCOOSiR_3$ + $HSiR_3$ hydros. prod betw 2 CO_2

C	5.47203	4.27408	0.38468
C	5.39886	2.99960	1.02043
C	6.00274	2.79426	2.29704
C	6.64957	3.87157	2.90739
C	6.71941	5.11947	2.30376
C	6.13675	5.30444	1.05707
O	4.75739	1.98228	0.41657
La	3.67707	0.14409	-0.14651
O	2.20237	-1.61125	0.98409

C	3.22608	-2.27982	1.30506
O	4.40730	-1.89096	1.07282
C	5.96741	1.42175	2.99051
C	6.68866	1.42209	4.34987
C	4.85043	4.53917	-0.99995
C	5.48191	3.61715	-2.06013
O	1.42443	1.25088	0.46618
C	0.41159	0.73667	0.94432
O	-0.58635	1.40140	1.44942
Si	-0.68496	3.17406	1.58748
C	-0.72676	3.89891	-0.13931
C	-2.32354	3.35466	2.48953
C	-2.96406	2.27228	3.11266
C	-4.15877	2.44918	3.80953
C	-4.73334	3.71603	3.89709
C	-4.11330	4.80441	3.28388
C	-2.92083	4.62278	2.58680
C	0.76717	3.75714	2.61881
O	3.92676	-0.44962	-2.22866
C	4.03419	-0.75737	-3.53497
C	5.27858	-1.21753	-4.05457
C	5.35260	-1.49045	-5.42387
C	4.25984	-1.34025	-6.26697
C	3.04624	-0.92190	-5.73928
C	2.89461	-0.62865	-4.38133
C	6.51248	-1.44394	-3.15885

C	6.96202	-0.12791	-2.49683
C	1.52218	-0.19304	-3.83565
C	1.03450	-1.19331	-2.76733
C	6.20319	-2.51695	-2.09578
C	7.72339	-1.95885	-3.95678
C	0.43413	-0.17023	-4.92363
C	1.59887	1.24166	-3.27680
C	6.69986	0.37820	2.12090
C	4.50783	1.01428	3.28912
C	3.32369	4.33733	-0.94379
C	5.08438	5.98247	-1.47883
F	-1.84412	0.77467	-1.36527
C	-2.98154	0.29862	-0.84964
C	-3.02001	-0.94750	-0.24159
C	-4.18062	-1.47089	0.33820
C	-5.31944	-0.65983	0.25913
C	-5.32049	0.58674	-0.35569
C	-4.13657	1.07135	-0.90383
B	-4.19655	-2.86170	1.06540
C	-3.45208	-4.08397	0.44013
C	-2.81146	-5.05363	1.22633
C	-2.12855	-6.13452	0.68485
C	-2.08655	-6.28861	-0.69869
C	-2.71602	-5.35903	-1.52258
C	-3.37133	-4.27808	-0.94732
F	-2.80812	-4.94743	2.55844

F	-1.51835	-7.01971	1.46925
F	-1.44826	-7.32083	-1.23082
F	-2.68328	-5.51377	-2.84363
F	-3.96838	-3.42385	-1.78376
F	-1.87020	-1.63329	-0.18960
F	-4.10240	2.27130	-1.47130
F	-6.43033	1.31773	-0.41768
F	-6.48108	-1.08509	0.76726
C	-4.95960	-2.99304	2.42794
C	-4.95239	-1.96586	3.37980
C	-5.63252	-2.04504	4.58719
C	-6.37431	-3.18769	4.87432
C	-6.41680	-4.23581	3.95801
C	-5.70890	-4.12724	2.76726
F	-4.24190	-0.85132	3.16244
F	-5.79456	-5.15471	1.91750
F	-7.13174	-5.32471	4.23033
F	-7.03864	-3.27841	6.01838
F	-5.58375	-1.04207	5.46419
H	3.08611	-3.25239	1.81142
H	6.28786	-1.83310	-5.85083
H	4.35147	-1.55773	-7.32748
H	2.19807	-0.82542	-6.40729
H	7.83037	-0.30031	-1.85040
H	7.24713	0.60736	-3.25650
H	6.17364	0.32501	-1.89371

H	5.34905	-2.25447	-1.47070
H	5.97709	-3.47395	-2.57837
H	7.06890	-2.66659	-1.43996
H	7.52013	-2.92004	-4.44029
H	8.04717	-1.24698	-4.72357
H	8.56515	-2.10822	-3.27201
H	1.75926	-1.33833	-1.96445
H	0.08766	-0.86207	-2.32754
H	0.86814	-2.17544	-3.22274
H	-0.51659	0.13515	-4.47238
H	0.66174	0.54333	-5.72237
H	0.28296	-1.15638	-5.37488
H	2.40943	1.36379	-2.55578
H	1.79212	1.95249	-4.08704
H	0.65539	1.52328	-2.79590
H	6.20724	6.28336	0.59721
H	7.22918	5.94152	2.79851
H	7.11496	3.73779	3.87755
H	6.55730	3.80862	-2.13898
H	5.34941	2.56379	-1.81550
H	5.03318	3.80090	-3.04344
H	2.87047	5.06301	-0.25888
H	2.88044	4.48638	-1.93583
H	3.06152	3.33805	-0.59343
H	4.63212	6.72134	-0.80844
H	6.14974	6.21447	-1.58003

H	4.62596	6.11108	-2.46544
H	4.10840	1.62340	4.10711
H	4.44408	-0.03780	3.58777
H	6.36456	0.38928	1.08206
H	7.77157	0.60185	2.10148
H	6.56551	-0.63367	2.51646
H	6.62563	0.42067	4.79018
H	7.75034	1.66995	4.25087
H	6.23516	2.12282	5.05883
H	-2.45584	5.48531	2.11241
H	-4.55941	5.79320	3.34687
H	-5.66398	3.85565	4.44042
H	-4.63767	1.59509	4.27902
H	-2.52966	1.27937	3.04929
H	0.62869	4.81401	2.87142
H	0.82616	3.19835	3.55737
H	1.71233	3.65250	2.08101
H	0.28666	-0.35059	0.98679
H	3.84317	1.18845	2.43853
H	-0.91443	4.97658	-0.08401
H	0.23027	3.74673	-0.64430
H	-1.52190	3.44648	-0.73641

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10 + CO_2 - $ArOCOOSiR_3$ + $HSiR_3$ h act TS

C	5.78929	1.98353	-1.66942
C	6.72790	2.84175	-2.25714

C	6.20629	3.81400	-3.12064
C	4.84779	3.94253	-3.38032
C	3.95476	3.05842	-2.78068
C	4.42633	2.06779	-1.92324
B	8.26400	2.71839	-1.97374
C	8.76788	2.38916	-0.52827
C	8.12713	2.88735	0.61564
C	8.54675	2.59456	1.90701
C	9.63953	1.75203	2.09277
C	10.30157	1.22308	0.98866
C	9.87244	1.56009	-0.28795
F	7.07954	3.70858	0.49757
F	7.91747	3.10683	2.96197
F	10.04710	1.45227	3.31812
F	11.34296	0.40941	1.16483
F	10.55198	1.02346	-1.30853
F	7.02041	4.69460	-3.71273
F	4.39427	4.89497	-4.19250
F	2.65515	3.15999	-3.02596
F	3.57190	1.21778	-1.35776
F	6.19176	1.00775	-0.84828
C	9.28331	2.91640	-3.14787
C	10.50285	3.58460	-2.97878
C	11.40350	3.78266	-4.01651
C	11.10993	3.28308	-5.28220
C	9.91461	2.60288	-5.49751

C	9.02618	2.44155	-4.44133
F	10.83447	4.09318	-1.78712
F	7.90044	1.76956	-4.70099
F	9.63578	2.11721	-6.70488
F	11.96683	3.45547	-6.27970
F	12.54820	4.43861	-3.81302
C	13.81897	2.47936	0.14904
C	14.34523	2.23037	1.41501
C	15.23703	3.13993	1.98524
C	15.60649	4.28556	1.28462
C	15.07878	4.55818	0.01414
C	14.17191	3.64126	-0.53756
Si	15.42985	6.17942	-0.87554
C	13.73783	6.95475	-1.23394
O	15.79330	5.85770	-2.61516
C	16.80097	5.90753	-3.40942
O	17.97900	6.16399	-3.13675
La	19.63744	5.35262	-1.51727
O	19.83569	3.60306	0.65037
C	19.29481	2.79897	1.30843
O	18.78403	2.00126	1.97925
O	20.25513	3.50480	-2.58391
C	20.75890	2.36547	-3.09427
C	19.88119	1.29287	-3.43840
C	20.44502	0.10565	-3.91512
C	21.81470	-0.04962	-4.07631

C	22.65543	1.01234	-3.77575
C	22.16641	2.22929	-3.29308
C	18.34905	1.41122	-3.32312
C	17.84740	2.56110	-4.21867
C	23.14436	3.38387	-3.01186
C	24.60242	3.02452	-3.34714
O	20.64189	7.13764	-0.66505
C	21.29042	8.22698	-0.21172
C	21.52646	9.33169	-1.08571
C	22.20942	10.44180	-0.58075
C	22.64948	10.50136	0.73362
C	22.40175	9.42879	1.57822
C	21.72911	8.28216	1.14598
C	21.03418	9.34593	-2.54529
C	21.42328	10.63540	-3.28993
C	21.49349	7.12451	2.13523
C	19.98533	6.85244	2.29894
C	21.66246	8.18774	-3.34177
C	19.49525	9.27366	-2.57661
C	22.02865	7.43425	3.54451
C	22.24191	5.86766	1.65419
C	22.78614	4.59541	-3.89421
C	23.12792	3.74817	-1.51530
C	17.92188	1.63185	-1.86006
C	17.62383	0.13959	-3.79793
C	16.45241	7.52165	-0.04245

H	17.65202	5.16334	-0.63433
H	23.72146	0.88552	-3.92554
H	22.22206	-0.98665	-4.44557
H	19.80031	-0.72631	-4.17299
H	23.42201	5.45482	-3.65350
H	22.93607	4.34878	-4.95053
H	21.74062	4.88950	-3.78221
H	22.11332	3.90640	-1.14406
H	23.55051	2.93186	-0.91997
H	23.71858	4.65057	-1.32154
H	24.97157	2.18807	-2.74456
H	24.73087	2.77173	-4.40464
H	25.24226	3.88823	-3.13506
H	18.32184	2.56274	-1.45731
H	16.83051	1.67916	-1.77721
H	18.27264	0.80456	-1.23296
H	16.54237	0.29455	-3.71651
H	17.84413	-0.09520	-4.84455
H	17.87495	-0.73435	-3.18746
H	18.35464	3.49782	-3.98511
H	18.03774	2.33257	-5.27292
H	16.76634	2.69925	-4.09228
H	22.40341	11.28934	-1.22772
H	23.17761	11.37798	1.09805
H	22.74480	9.49253	2.60424
H	22.74608	8.32371	-3.42213

H	21.50292	7.22352	-2.85666
H	21.25055	8.14288	-4.35678
H	19.06690	10.16705	-2.10986
H	19.12958	9.21904	-3.60871
H	19.11862	8.40698	-2.03229
H	20.98332	11.52687	-2.83125
H	22.50867	10.77178	-3.33957
H	21.05175	10.57968	-4.31912
H	19.48863	7.72779	2.73099
H	19.81960	6.00493	2.97548
H	21.96676	5.59529	0.63491
H	23.32250	6.04506	1.66136
H	22.03639	5.01484	2.31214
H	21.82802	6.57938	4.19995
H	23.11068	7.60093	3.54795
H	21.54246	8.30942	3.98817
H	16.32274	4.97399	1.72619
H	15.64907	2.95109	2.97299
H	14.05773	1.33300	1.95555
H	13.12450	1.77481	-0.29862
H	13.73183	3.83080	-1.51246
H	15.78448	8.30256	0.33769
H	17.05742	7.12596	0.77419
H	17.13373	7.98416	-0.76189
H	16.52431	5.70457	-4.45387
H	19.49958	6.63874	1.34582

H	13.25196	7.21719	-0.28729
H	13.83963	7.87211	-1.82387
H	13.07558	6.27296	-1.77367

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10 + CO_2 - $ArOCOOSiR_3$ + $HSiR_3$ hydros. h act prod

C	2.68215	-1.09747	-2.58050
C	2.62048	-1.35111	-1.17818
C	2.48760	-2.68377	-0.68750
C	2.44317	-3.72639	-1.61758
C	2.51843	-3.49545	-2.98505
C	2.63104	-2.19166	-3.44891
O	2.68246	-0.32610	-0.31038
La	2.82838	1.34894	1.10458
O	4.39753	2.86414	0.94752
C	5.48446	3.64038	0.78313
C	6.76621	3.15239	1.17172
C	7.87372	3.97890	0.96337
C	7.75274	5.24413	0.40499
C	6.49512	5.71492	0.05362
C	5.34057	4.94716	0.23248
C	6.95142	1.76752	1.82077
C	6.53324	0.64999	0.84509
C	3.96508	5.52914	-0.14568
C	3.06037	5.59801	1.10102
C	2.39545	-2.99353	0.81845
C	2.24865	-4.49964	1.09930

C	2.81037	0.32727	-3.15297
C	4.13845	0.96548	-2.70345
O	0.62828	2.48690	0.90848
C	-0.43144	3.01449	0.56764
O	-1.33149	3.48096	1.36769
Si	-1.34560	3.37332	3.17017
C	-2.68746	4.63263	3.52799
C	-1.84266	1.62183	3.59959
C	-3.18455	1.21527	3.49568
C	-3.57149	-0.07630	3.84338
C	-2.61902	-0.98113	4.31318
C	-1.28456	-0.59560	4.42437
C	-0.89524	0.69423	4.06557
C	0.32564	3.87867	3.83973
C	6.16062	1.68584	3.14175
C	8.41991	1.48166	2.18374
C	4.06612	6.96439	-0.69112
C	3.30784	4.68887	-1.25702
C	1.14887	-2.31960	1.42607
C	3.68266	-2.54380	1.53678
C	2.82279	0.34096	-4.69208
C	1.60789	1.19196	-2.72609
F	-0.50044	-5.64553	-1.26426
C	-1.15501	-4.74668	-1.99795
C	-2.10572	-3.91520	-1.42429
C	-2.81361	-2.94961	-2.15328

C	-2.49299	-2.86054	-3.51482
C	-1.56200	-3.69005	-4.12633
C	-0.89073	-4.63893	-3.36070
F	-2.31222	-4.04630	-0.10855
B	-3.91392	-2.04952	-1.50471
C	-4.89985	-2.64529	-0.44219
C	-5.37337	-1.89437	0.64286
C	-6.24135	-2.40923	1.59634
C	-6.68850	-3.72181	1.47560
C	-6.25911	-4.50384	0.40706
C	-5.37426	-3.96302	-0.51788
F	-3.12617	-1.98113	-4.29975
F	-1.31226	-3.59117	-5.43019
F	-0.00749	-5.44602	-3.93108
F	-4.97073	-0.63171	0.81867
F	-6.64782	-1.66278	2.62555
F	-7.52329	-4.22439	2.37524
F	-6.69573	-5.75505	0.28354
F	-5.00917	-4.75603	-1.52896
C	-4.04299	-0.54478	-1.93192
C	-2.91877	0.26716	-2.12417
C	-3.01241	1.60703	-2.47798
C	-4.26606	2.17657	-2.67943
C	-5.41208	1.40319	-2.51484
C	-5.28278	0.07260	-2.13574
F	-1.69124	-0.22456	-1.93018

F	-1.91329	2.35612	-2.61957
F	-4.36851	3.45371	-3.02525
F	-6.61184	1.94434	-2.71500
F	-6.41263	-0.62809	-1.99414
O	4.10554	-0.86258	4.99143
C	3.10674	-0.47086	5.45334
O	2.12112	-0.11975	5.97414
H	2.43501	0.95196	3.21520
H	2.68381	-2.02904	-4.51920
H	2.48571	-4.32562	-3.68399
H	2.34711	-4.74881	-1.27139
H	1.72036	2.21589	-3.10129
H	0.67590	0.78352	-3.12870
H	1.49657	1.22936	-1.64064
H	4.22740	1.02027	-1.61732
H	4.98587	0.37586	-3.06823
H	4.23587	1.98088	-3.10395
H	3.67679	-0.20712	-5.10321
H	1.90503	-0.07980	-5.11636
H	2.90164	1.37673	-5.03980
H	3.90960	-1.49182	1.35622
H	3.60055	-2.69467	2.61844
H	4.53938	-3.12271	1.17580
H	2.17876	-4.65576	2.18136
H	1.34404	-4.91697	0.64643
H	3.11085	-5.07212	0.74146

H	1.12533	-1.24547	1.23702
H	0.23629	-2.74839	0.99824
H	1.11769	-2.47551	2.51020
H	6.41719	6.70998	-0.36915
H	8.63254	5.86285	0.25202
H	8.86097	3.63158	1.24497
H	3.91581	4.71959	-2.16718
H	3.20540	3.64112	-0.97142
H	2.31393	5.08338	-1.50215
H	3.48961	6.27906	1.84346
H	2.06601	5.97620	0.83147
H	2.94868	4.62206	1.57537
H	4.49840	7.65404	0.04121
H	4.66214	7.01678	-1.60823
H	3.06150	7.32901	-0.93266
H	6.55921	2.40791	3.86247
H	6.24353	0.68704	3.58384
H	5.52535	0.78917	0.44576
H	7.20002	0.62878	-0.02319
H	6.58099	-0.33074	1.33170
H	8.48754	0.49080	2.64577
H	9.07213	1.47897	1.30408
H	8.81283	2.20666	2.90396
H	0.15643	0.96121	4.14246
H	-0.54015	-1.29403	4.79444
H	-2.91878	-1.98743	4.59411

H	-4.60941	-0.37744	3.74296
H	-3.94060	1.91188	3.14056
H	0.21964	4.10150	4.90729
H	1.07055	3.08413	3.73196
H	0.69334	4.78140	3.34331
H	-0.69146	3.12253	-0.49317
H	5.09987	1.91555	3.01998
H	-2.87135	4.68651	4.60560
H	-2.38341	5.62562	3.18353
H	-3.62886	4.37614	3.03439

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10 + CO_2 - $ArOCOOSiR_3$ + $HSiR_3$ hydros. CO_2 ins TS

C	13.40083	0.29635	-2.84695
C	12.72073	1.36005	-3.45921
C	13.02221	1.57087	-4.81317
C	13.91063	0.77317	-5.52239
C	14.55458	-0.27437	-4.86997
C	14.30226	-0.51354	-3.52185
B	11.67278	2.23220	-2.69872
C	11.53037	3.76061	-3.02951
C	12.64205	4.58937	-3.21633
C	12.53006	5.94493	-3.49443
C	11.26781	6.51868	-3.61467
C	10.13254	5.73007	-3.44994
C	10.28146	4.38087	-3.15063
F	13.87988	4.09702	-3.09019

F	13.62174	6.70524	-3.63218
F	11.14761	7.81215	-3.88480
F	8.92362	6.27366	-3.57304
F	9.16045	3.66599	-3.00798
F	12.41447	2.54665	-5.49701
F	14.14568	0.99552	-6.81376
F	15.39961	-1.04861	-5.53513
F	14.92079	-1.51347	-2.89722
F	13.21701	0.03974	-1.54703
C	10.73579	1.59334	-1.61631
C	10.36789	2.28000	-0.45150
C	9.53599	1.73240	0.51593
C	9.02026	0.45326	0.32897
C	9.34488	-0.26336	-0.81958
C	10.19609	0.30747	-1.75770
F	9.23115	2.41461	1.62211
F	10.84154	3.50832	-0.21329
F	10.46210	-0.41925	-2.84693
F	8.84202	-1.48157	-1.00547
F	8.21937	-0.07981	1.24196
C	12.62292	4.70477	2.54696
C	13.90440	5.27657	2.63425
C	14.92576	4.53828	3.25625
C	14.66647	3.27459	3.78582
C	13.38869	2.72577	3.69339
C	12.36620	3.43877	3.06658

Si	14.22255	7.01176	2.01008
C	15.81169	7.76156	2.64792
O	14.27103	6.94266	0.20812
C	15.25069	6.56052	-0.54332
O	16.36336	6.20908	-0.15057
La	18.62331	5.24530	0.16053
O	20.14349	3.38867	2.92148
C	19.32349	3.54236	3.74535
O	18.56817	3.61911	4.63179
O	20.04990	6.90033	-0.06043
C	21.06600	7.73325	-0.35728
C	22.39875	7.38127	0.00830
C	23.43460	8.23920	-0.37155
C	23.19544	9.41823	-1.06384
C	21.88845	9.77470	-1.36576
C	20.80085	8.96655	-1.02133
C	22.71001	6.12387	0.84097
C	21.98192	6.21055	2.19793
C	19.36873	9.43229	-1.34471
C	19.33797	10.82446	-1.99980
O	18.36588	3.50908	-1.18314
C	18.23135	2.50291	-2.06694
C	17.86767	1.20096	-1.60937
C	17.79074	0.16788	-2.54782
C	18.03548	0.37840	-3.89817
C	18.34348	1.65828	-4.33780

C	18.44101	2.74092	-3.45904
C	17.55649	0.90823	-0.13022
C	16.38269	1.78399	0.35093
C	18.73888	4.14498	-4.01659
C	18.87531	4.15470	-5.54947
C	18.81250	1.13417	0.73002
C	17.12458	-0.55086	0.10107
C	17.56857	5.09198	-3.68514
C	20.07241	4.68002	-3.46226
C	18.70178	8.46763	-2.34141
C	18.54217	9.54107	-0.04782
C	24.20849	5.98809	1.16495
C	22.32855	4.84240	0.07466
C	12.74276	8.14527	2.21482
H	18.06119	5.08051	2.26642
H	18.51276	1.81234	-5.39716
H	17.97252	-0.44524	-4.60298
H	17.52851	-0.83132	-2.22238
H	17.77213	6.10308	-4.05477
H	16.64668	4.73632	-4.15729
H	17.37567	5.14535	-2.61131
H	20.10035	4.67195	-2.37172
H	20.90323	4.05491	-3.80585
H	20.25610	5.70496	-3.80304
H	19.70655	3.53099	-5.89403
H	17.96018	3.81786	-6.04777

H	19.07446	5.17838	-5.88465
H	19.20612	2.14547	0.62587
H	18.59182	0.95794	1.78913
H	19.60733	0.44224	0.43192
H	16.89278	-0.69005	1.16276
H	16.22719	-0.81115	-0.46915
H	17.91616	-1.26287	-0.15528
H	16.56448	2.84613	0.18168
H	15.46537	1.51553	-0.18410
H	16.20090	1.63394	1.42080
H	21.71717	10.71190	-1.88248
H	24.02074	10.06367	-1.35104
H	24.45816	7.98797	-0.11808
H	19.25120	8.45709	-3.28861
H	18.68351	7.44414	-1.96542
H	17.67109	8.77860	-2.55215
H	18.96874	10.30513	0.61053
H	17.50997	9.83331	-0.27840
H	18.52641	8.60041	0.50386
H	19.77810	11.59218	-1.35502
H	19.85937	10.84173	-2.96260
H	18.29685	11.11009	-2.18757
H	22.35402	7.07023	2.76518
H	22.16271	5.30726	2.79002
H	21.30935	4.87966	-0.31838
H	22.97825	4.70737	-0.79606

H	22.42463	3.95812	0.71401
H	24.36459	5.08574	1.76619
H	24.82133	5.89098	0.26258
H	24.58036	6.83811	1.74596
H	15.93810	4.93186	3.31397
H	15.46800	2.72393	4.26968
H	13.18830	1.74101	4.10754
H	11.37129	3.01286	2.98115
H	11.81159	5.24726	2.06782
H	15.66486	8.05411	3.69363
H	16.64286	7.05016	2.60427
H	16.08073	8.65846	2.08249
H	15.00795	6.57408	-1.61301
H	20.90335	6.33968	2.08730
H	12.52114	8.28232	3.27785
H	12.94851	9.12769	1.77928
H	11.85009	7.73969	1.73088

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Y monomer

C	14.58291	2.37566	1.11407
O	13.72635	2.59046	0.19667
O	15.80670	2.17105	0.83925
C	15.04287	2.22655	3.42391
O	14.12082	2.36775	2.36441
C	15.54021	3.40904	4.00508
C	16.92507	1.97506	5.40105

H	17.69655	1.87378	6.15929
C	16.51797	3.23776	4.99312
H	16.96771	4.10434	5.46105
C	15.32656	0.92896	3.89131
C	16.31113	0.84280	4.88403
H	16.60191	-0.12635	5.26920
C	14.98888	4.81697	3.68506
C	13.47991	4.85122	4.00876
H	12.91696	4.14310	3.39746
H	13.08254	5.85438	3.81675
H	13.30237	4.61401	5.06291
C	15.21158	5.23527	2.21784
H	16.24342	5.05842	1.90357
H	15.00705	6.30635	2.11011
H	14.53671	4.72384	1.52927
C	15.66670	5.88834	4.55752
H	16.73921	5.97258	4.35134
H	15.53099	5.69882	5.62706
H	15.21459	6.86068	4.33865
C	13.04949	-0.13018	3.75055
H	12.63373	0.71376	3.19662
H	12.88622	0.04575	4.81897
H	12.49018	-1.02916	3.46739
C	14.55039	-0.33275	3.45210
C	14.73925	-0.66966	1.96013
H	15.79461	-0.65031	1.67429

H	14.18580	0.00736	1.30820
H	14.35119	-1.67461	1.76158
C	15.00709	-1.57027	4.24521
H	14.39479	-2.42666	3.94617
H	14.88180	-1.43997	5.32487
H	16.05197	-1.82973	4.04359
Y	15.32691	2.29983	-1.40842
O	16.17508	3.96346	-2.26586
O	14.98470	0.51944	-2.37137
C	16.10497	-2.60924	-3.88577
H	17.01807	-3.11499	-4.17692
C	16.17120	-1.33190	-3.32172
C	14.95031	-0.70047	-2.94682
C	14.89527	-3.25585	-4.09350
H	14.87233	-4.24866	-4.53387
C	13.71404	-2.61899	-3.74012
H	12.77860	-3.13599	-3.91798
C	13.69795	-1.34366	-3.16613
C	17.53685	-0.63924	-3.15833
C	17.58133	0.63233	-4.02853
H	18.54466	1.14282	-3.92342
H	17.45114	0.36905	-5.08334
H	16.78864	1.34255	-3.78237
C	17.82801	-0.32377	-1.67707
H	17.00587	0.20211	-1.18215
H	17.96686	-1.24966	-1.10913

H	18.74035	0.27471	-1.57540
C	18.70537	-1.52251	-3.63247
H	18.76946	-2.45921	-3.06927
H	18.63179	-1.76322	-4.69773
H	19.64706	-0.98318	-3.48293
C	12.35098	-0.69411	-2.79266
C	12.26487	-0.47110	-1.27136
H	13.05360	0.18629	-0.90677
H	11.30247	-0.01821	-1.00549
H	12.34863	-1.42540	-0.74083
C	11.15097	-1.57960	-3.17322
H	10.22556	-1.06202	-2.89868
H	11.10893	-1.77958	-4.24907
H	11.15825	-2.53734	-2.64243
C	12.16430	0.63656	-3.54628
H	12.97780	1.33395	-3.34394
H	12.13828	0.46543	-4.62791
H	11.21983	1.11034	-3.25352
C	16.49943	5.11397	-2.89119
C	15.55898	5.72088	-3.77273
C	15.91896	6.91983	-4.39472
H	15.22308	7.40388	-5.06983
C	17.15303	7.51528	-4.17685
H	17.40790	8.44705	-4.67378
C	18.06020	6.90800	-3.31979
H	19.02004	7.38646	-3.16467

C	17.77248	5.70964	-2.65876
C	14.18779	5.08588	-4.06919
C	14.37875	3.71521	-4.74831
H	14.98589	3.02485	-4.15707
H	13.41163	3.24051	-4.94662
H	14.89711	3.83842	-5.70483
C	13.34541	4.96998	-2.78192
H	13.04965	5.96359	-2.42915
H	12.43144	4.39157	-2.95924
H	13.89155	4.51768	-1.94898
C	13.34615	5.92791	-5.04506
H	13.14257	6.93004	-4.65426
H	13.82801	6.02875	-6.02279
H	12.38105	5.43476	-5.20454
C	18.82084	5.08531	-1.71751
C	18.27332	5.00761	-0.28003
H	18.04386	6.01054	0.09543
H	17.36137	4.41306	-0.22138
H	19.01663	4.55675	0.38826
C	19.22307	3.68511	-2.21698
H	18.35973	3.02439	-2.30035
H	19.68647	3.74857	-3.20748
H	19.94710	3.22833	-1.53155
C	20.11423	5.91576	-1.65047
H	20.82045	5.42284	-0.97367
H	20.60187	6.00199	-2.62712

H	19.93766	6.92396	-1.26154

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Y Monomer - $PhMe_2Si$-H-B_R_3 coordination

C	6.30126	1.71548	-0.34559
C	5.49925	2.25482	0.70443
C	6.06564	3.14938	1.66140
C	7.42828	3.44662	1.55064
C	8.22558	2.90994	0.55127
C	7.65563	2.06022	-0.38442
O	4.19382	1.91030	0.79125
Y	2.22721	1.39300	1.03015
O	2.26925	0.45206	3.16628
C	1.97798	-0.69054	2.70475
O	1.63091	-0.84500	1.49230
Si	-2.92422	-2.55587	0.46788
C	-3.34901	-1.18255	1.67395
C	5.25274	3.79208	2.80344
C	6.09635	4.76743	3.64554
C	5.72730	0.80476	-1.44744
C	4.65580	1.57404	-2.24229
F	1.72482	0.13168	-1.17386
C	0.90623	-0.55400	-2.01783
C	-0.45535	-0.63559	-1.77628
C	-1.34460	-1.29131	-2.63183
C	-0.75869	-1.86294	-3.76384
C	0.60866	-1.81198	-4.02769

C	1.45352	-1.15270	-3.14517
B	-2.93066	-1.28904	-2.35355
C	-3.82719	-2.40458	-3.06889
C	-3.47769	-3.75520	-2.99910
C	-4.22046	-4.78061	-3.56444
C	-5.37856	-4.46252	-4.26740
C	-5.76369	-3.13267	-4.38513
C	-4.99337	-2.13538	-3.79080
F	-2.35707	-4.11196	-2.34272
F	-3.83703	-6.05232	-3.44605
F	-6.10827	-5.42440	-4.82497
F	-6.86589	-2.81948	-5.06698
F	-5.42379	-0.88004	-3.96845
F	-0.91037	-0.03105	-0.66415
F	2.75857	-1.09195	-3.38849
F	1.11032	-2.38066	-5.12129
F	-1.50247	-2.47850	-4.68677
C	-3.58581	0.15212	-2.10156
C	-3.07435	1.33372	-2.64278
C	-3.64315	2.58459	-2.41974
C	-4.78017	2.68905	-1.62722
C	-5.33895	1.53724	-1.08055
C	-4.74500	0.31029	-1.34155
F	-1.99280	1.31280	-3.43707
F	-5.34033	-0.77480	-0.80881
F	-6.43460	1.61908	-0.32369

F	-5.33413	3.87476	-1.39767
F	-3.10389	3.67663	-2.95999
O	0.98492	2.99869	0.66027
C	0.23008	4.11819	0.56901
C	-0.64749	4.46345	1.63951
C	-1.39290	5.64126	1.53589
C	-1.31100	6.46535	0.42419
C	-0.47385	6.10635	-0.62120
C	0.30726	4.94627	-0.59058
C	-0.81468	3.57587	2.88444
C	-1.85776	4.12834	3.87280
C	1.20946	4.62251	-1.79591
C	1.05169	5.64040	-2.93999
C	-1.32926	2.18729	2.46049
C	0.50875	3.48862	3.66761
C	2.69008	4.66489	-1.37871
C	0.83464	3.25181	-2.38837
O	2.03786	-1.80166	3.45547
C	2.51316	-1.70241	4.78135
C	1.56545	-1.57145	5.81473
C	2.07968	-1.37700	7.10262
C	3.44579	-1.36750	7.34483
C	4.33484	-1.64060	6.31501
C	3.89750	-1.85037	5.00105
C	0.04680	-1.74033	5.60283
C	-0.72074	-1.63974	6.93295

C	4.88899	-2.34335	3.92451
C	6.30787	-2.49538	4.50060
C	-0.22499	-3.14481	5.02484
C	-0.54080	-0.66809	4.66898
C	4.43750	-3.73923	3.44371
C	4.99975	-1.39732	2.71573
C	-1.17712	-3.21287	0.65842
C	-4.21924	-3.91299	0.41007
C	-3.83913	-5.24983	0.19950
C	-4.78372	-6.27382	0.20963
C	-6.12818	-5.97847	0.43058
C	-6.52495	-4.65837	0.64253
C	-5.57925	-3.63600	0.63242
C	4.08465	4.62474	2.24256
C	4.74868	2.70997	3.77501
C	5.15927	-0.49404	-0.84672
C	6.79185	0.36913	-2.47025
H	-2.94154	-1.83866	-0.96419
H	3.81759	-1.19354	8.35066
H	1.40321	-1.23516	7.93593
H	5.39128	-1.70067	6.54355
H	0.25968	-3.28415	4.05627
H	-1.30372	-3.29225	4.89400
H	0.13874	-3.92191	5.70506
H	-0.20744	0.33119	4.96077
H	-1.63517	-0.69071	4.72615

H	-0.27363	-0.83094	3.62381
H	-0.62776	-0.64937	7.39148
H	-0.39324	-2.39122	7.65824
H	-1.78488	-1.81260	6.74246
H	3.44456	-3.70845	2.98964
H	4.41431	-4.44985	4.27669
H	5.14089	-4.11999	2.69428
H	5.14151	-0.35776	3.02161
H	4.12871	-1.46281	2.06160
H	5.86268	-1.68545	2.10665
H	6.96460	-2.89402	3.72122
H	6.34131	-3.19280	5.34365
H	6.72789	-1.53650	4.82267
H	7.88618	4.11986	2.26497
H	9.28144	3.15991	0.49668
H	8.28630	1.65859	-1.16840
H	3.52591	5.09475	3.05994
H	4.46165	5.42036	1.59152
H	3.38255	4.03519	1.65250
H	4.15545	1.93941	3.28369
H	5.59615	2.20953	4.25625
H	4.13237	3.15689	4.56422
H	6.93445	4.26962	4.14432
H	6.48985	5.59694	3.04865
H	5.46175	5.19749	4.42773
H	4.43465	-0.29919	-0.05566

H	4.67579	-1.09836	-1.62095
H	5.96443	-1.08965	-0.40455
H	6.31940	-0.26835	-3.22564
H	7.23669	1.22175	-2.99335
H	7.59675	-0.21204	-2.00789
H	3.87150	1.96942	-1.59655
H	5.11034	2.42908	-2.75355
H	4.19726	0.92947	-2.99843
H	-0.43056	6.75402	-1.48830
H	-1.90111	7.37571	0.36843
H	-2.05995	5.92495	2.34113
H	2.93200	3.93242	-0.60818
H	3.33562	4.47144	-2.24280
H	2.94463	5.65393	-0.98352
H	-0.18659	3.26940	-2.78017
H	1.51060	2.99264	-3.21210
H	0.88514	2.46441	-1.63700
H	0.02439	5.68390	-3.31634
H	1.35730	6.64918	-2.64345
H	1.69493	5.33825	-3.77354
H	-2.30293	2.28910	1.96900
H	-0.66227	1.69443	1.75045
H	-1.45376	1.53927	3.33299
H	1.35259	3.20894	3.03571
H	0.75333	4.46521	4.09850
H	0.43954	2.76291	4.48484

H	-1.93142	3.45004	4.73007
H	-1.57860	5.11352	4.25987
H	-2.85406	4.20239	3.42451
H	-5.90818	-2.61419	0.79469
H	-7.57191	-4.42478	0.81475
H	-6.86618	-6.77596	0.43748
H	-4.47054	-7.30064	0.04344
H	-2.79656	-5.49734	0.02211
H	-2.63412	-0.36141	1.58697
H	-4.35493	-0.79201	1.51167
H	-3.29150	-1.58176	2.69216
H	-0.87109	-3.80097	-0.20965
H	-0.45878	-2.40239	0.80697
H	-1.13901	-3.86011	1.54161

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Y Monomer - $PhMe_2Si$-H-B_R_3 coord TS

C	24.56602	8.24807	-1.18510
C	23.56368	8.79722	-0.33153
C	23.92732	9.61397	0.77777
C	25.28952	9.81582	1.02417
C	26.27585	9.26376	0.22173
C	25.90561	8.49885	-0.87338
O	22.25419	8.53898	-0.57935
Y	20.27643	8.07975	-0.76060
O	19.68052	6.34655	0.46427
C	19.01597	5.37065	0.98036

O	17.89543	4.97820	0.64258
Si	16.40934	4.52736	-1.17120
C	15.69832	6.16292	-0.59758
C	22.89381	10.30416	1.68706
C	23.55619	11.11947	2.81378
C	24.23269	7.41790	-2.43677
C	23.41139	8.27073	-3.42117
F	20.43910	6.94961	-2.97307
C	19.64321	6.32165	-3.90462
C	18.28189	6.25392	-3.68828
C	17.39078	5.56051	-4.50239
C	17.99745	4.99323	-5.62761
C	19.36822	5.06474	-5.89583
C	20.21685	5.72492	-5.01623
B	15.81212	5.39721	-4.10225
C	14.99235	4.28988	-4.95913
C	15.14137	2.92132	-4.74573
C	14.43619	1.94203	-5.43488
C	13.53523	2.32743	-6.42065
C	13.36692	3.67919	-6.69527
C	14.09357	4.62389	-5.97470
F	16.02470	2.47941	-3.82679
F	14.62454	0.64673	-5.16898
F	12.84871	1.41053	-7.10111
F	12.51919	4.06091	-7.65311
F	13.90004	5.90450	-6.32627

F	17.86084	6.88105	-2.56117
F	21.52780	5.77702	-5.23414
F	19.87211	4.49034	-6.98531
F	17.27984	4.33032	-6.53634
C	15.00679	6.79199	-3.93581
C	15.40760	8.01852	-4.46387
C	14.67698	9.19455	-4.31943
C	13.46820	9.16905	-3.63462
C	13.01072	7.96505	-3.10897
C	13.77567	6.81740	-3.27968
F	16.54690	8.12218	-5.17377
F	13.28200	5.68190	-2.74788
F	11.85132	7.92296	-2.44767
F	12.75514	10.28335	-3.48229
F	15.12702	10.33932	-4.83783
O	19.14414	9.76779	-0.98627
C	18.44770	10.91620	-1.19927
C	17.50320	11.36573	-0.22940
C	16.79973	12.54572	-0.49346
C	16.99532	13.27892	-1.65262
C	17.91843	12.83239	-2.58425
C	18.66071	11.66221	-2.39690
C	17.23957	10.63042	1.09780
C	16.15616	11.31567	1.95036
C	19.66102	11.24084	-3.48961
C	19.68778	12.21945	-4.67863

C	16.74008	9.20048	0.83775
C	18.51998	10.61967	1.94803
C	21.09412	11.21738	-2.93018
C	19.25516	9.87671	-4.07366
O	19.56773	4.66679	2.00436
C	20.78333	5.00537	2.60973
C	20.73694	5.82450	3.75784
C	21.97237	6.17152	4.31986
C	23.16761	5.69089	3.80250
C	23.15350	4.77123	2.76294
C	21.95709	4.36336	2.15918
C	19.42209	6.21023	4.47198
C	19.69675	7.04527	5.73507
C	21.95134	3.15993	1.19108
C	23.36839	2.59744	0.98277
C	18.70584	4.91907	4.92235
C	18.47338	7.03938	3.58737
C	21.09922	2.03377	1.81604
C	21.40060	3.50143	-0.20250
C	18.02843	3.81046	-1.81278
C	15.30224	3.13159	-0.58072
C	15.63587	1.78390	-0.80189
C	14.82014	0.75595	-0.33781
C	13.65170	1.05522	0.36191
C	13.30210	2.38447	0.59399
C	14.11910	3.41033	0.12558

C	22.05875	11.30454	0.86614
C	22.00329	9.26819	2.39323
C	23.48664	6.13209	-2.03766
C	25.48683	6.96388	-3.20505
H	15.84299	4.87334	-2.88120
H	24.11230	5.99232	4.24616
H	22.00538	6.82094	5.18566
H	24.09369	4.34703	2.43389
H	18.44091	4.28750	4.07212
H	17.78346	5.17295	5.45733
H	19.34001	4.33903	5.60086
H	18.99934	7.87555	3.11945
H	17.66937	7.45501	4.20548
H	17.99291	6.44272	2.81173
H	20.17303	8.00427	5.50341
H	20.32278	6.51153	6.45704
H	18.74511	7.26275	6.23020
H	20.05981	2.33984	1.95163
H	21.50082	1.73921	2.79110
H	21.11373	1.15176	1.16530
H	21.93094	4.35006	-0.64076
H	20.33605	3.72499	-0.17967
H	21.53316	2.64213	-0.86995
H	23.31008	1.72738	0.32114
H	23.82437	2.26374	1.92021
H	24.03799	3.32401	0.51006

H	25.59434	10.42556	1.86559
H	27.32523	9.43840	0.44162
H	26.68503	8.08789	-1.50351
H	21.35770	11.84063	1.51467
H	22.71458	12.04434	0.39530
H	21.48240	10.82516	0.07448
H	21.47003	8.61659	1.69561
H	22.60445	8.60487	3.02072
H	21.26205	9.76538	3.02826
H	24.16740	10.49574	3.47457
H	24.18064	11.93021	2.42503
H	22.77307	11.57790	3.42684
H	22.63435	6.34331	-1.38973
H	23.13338	5.59488	-2.92449
H	24.15325	5.46692	-1.47898
H	25.17633	6.38378	-4.08081
H	26.07787	7.81117	-3.56769
H	26.13580	6.32169	-2.60048
H	22.51768	8.68482	-2.95629
H	24.01212	9.11565	-3.77387
H	23.11306	7.67770	-4.29182
H	18.06155	13.41475	-3.48566
H	16.43151	14.19030	-1.82924
H	16.07549	12.90734	0.22580
H	21.22897	10.50529	-2.11438
H	21.80792	10.96182	-3.72104

H	21.36447	12.20374	-2.53932
H	18.30593	9.95532	-4.61012
H	20.01503	9.51300	-4.77581
H	19.10803	9.12988	-3.29240
H	18.71456	12.29761	-5.17325
H	20.01070	13.22282	-4.38259
H	20.40359	11.85248	-5.42207
H	15.80688	9.22055	0.26579
H	17.46111	8.61120	0.26991
H	16.54714	8.68077	1.78285
H	19.34574	10.12976	1.43024
H	18.83765	11.64360	2.17063
H	18.34866	10.10343	2.89873
H	16.01606	10.74201	2.87289
H	16.43739	12.33340	2.23930
H	15.18920	11.35464	1.43841
H	13.82789	4.43878	0.31598
H	12.39235	2.62275	1.13792
H	13.01407	0.25342	0.72441
H	15.09464	-0.27859	-0.52398
H	16.53568	1.52858	-1.35245
H	16.21880	7.02272	-1.00892
H	14.65348	6.20609	-0.90842
H	15.75871	6.19281	0.49149
H	17.89934	3.37314	-2.80280
H	18.84194	4.53216	-1.82912

H	18.30101	3.02316	-1.10556

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Y Monomer - $PhMe_2Si$-H-B_R_3 coord product - 8-Y

C	5.93228	1.94150	0.97575
C	4.75981	2.33086	1.69018
C	4.86209	3.15275	2.85068
C	6.13742	3.57292	3.24433
C	7.28315	3.21528	2.55069
C	7.16948	2.40508	1.43182
O	3.54349	1.90926	1.26166
Y	1.71667	1.31716	0.56356
O	1.14584	-0.44932	1.89000
C	0.42908	-1.41717	2.21748
O	-0.78330	-1.53401	1.81203
Si	-2.09385	-2.77880	1.85438
C	-3.55238	-1.75696	1.31463
C	3.64312	3.60598	3.67641
C	4.04716	4.42877	4.91424
C	5.88603	1.02710	-0.26055
C	5.08847	1.70389	-1.39209
F	2.55420	-0.09442	-1.27363
C	1.75278	-0.62643	-2.26351
C	0.38605	-0.48811	-2.14402
C	-0.54436	-0.96302	-3.05265
C	0.05148	-1.62095	-4.13536
C	1.43038	-1.79072	-4.29385

C	2.31168	-1.28138	-3.34522
B	-2.14569	-0.74148	-2.75408
C	-3.14933	-1.68241	-3.62918
C	-3.74619	-2.81819	-3.08588
C	-4.66968	-3.60905	-3.76528
C	-5.03171	-3.26880	-5.06216
C	-4.45991	-2.14854	-5.65567
C	-3.54066	-1.39141	-4.93660
F	-3.44756	-3.22104	-1.83160
F	-5.20806	-4.68911	-3.18348
F	-5.91431	-4.01253	-5.73419
F	-4.79442	-1.81810	-6.90777
F	-3.01089	-0.33551	-5.57542
F	0.00387	0.19248	-1.00341
F	3.63185	-1.42226	-3.46413
F	1.91684	-2.43374	-5.35439
F	-0.69657	-2.13944	-5.11087
C	-2.56305	0.83640	-2.85821
C	-1.97606	1.78275	-3.69541
C	-2.36400	3.11831	-3.74802
C	-3.40133	3.56352	-2.93895
C	-4.02043	2.66058	-2.08346
C	-3.59822	1.33508	-2.06721
F	-0.95219	1.43946	-4.50450
F	-4.24672	0.52390	-1.20738
F	-5.00138	3.07458	-1.27065

F	-3.79174	4.83862	-2.97746
F	-1.73299	3.97877	-4.55993
O	0.51465	2.93098	0.42144
C	-0.26236	3.98652	0.07243
C	-1.45082	4.25131	0.80980
C	-2.21664	5.35787	0.42902
C	-1.85553	6.17247	-0.63362
C	-0.70414	5.88628	-1.35112
C	0.11953	4.80237	-1.03042
C	-1.91780	3.37603	1.98908
C	-3.23796	3.87870	2.59973
C	1.39689	4.55760	-1.86019
C	1.52397	5.54240	-3.03713
C	-2.18276	1.93291	1.52328
C	-0.87485	3.39491	3.12120
C	2.64986	4.75753	-0.98766
C	1.38973	3.15702	-2.50052
O	0.87126	-2.39076	3.00754
C	2.19945	-2.29557	3.51194
C	2.38546	-1.63543	4.74159
C	3.71890	-1.46873	5.13820
C	4.77301	-1.97192	4.38923
C	4.52213	-2.73080	3.25500
C	3.21918	-2.93977	2.78520
C	1.23930	-1.25413	5.70607
C	1.77526	-0.53605	6.95720

C	2.96159	-3.92810	1.62614
C	4.27280	-4.55898	1.12372
C	0.57226	-2.56385	6.17547
C	0.17285	-0.32732	5.08908
C	2.07943	-5.08048	2.15091
C	2.30303	-3.26860	0.40014
C	-1.56909	-4.08966	0.63042
C	-2.31202	-3.45177	3.59471
C	-1.89849	-4.75285	3.92689
C	-2.16009	-5.29236	5.18531
C	-2.84461	-4.53812	6.13717
C	-3.26734	-3.24577	5.82712
C	-3.00568	-2.71142	4.56742
C	2.73090	4.51426	2.83331
C	2.87206	2.38682	4.21386
C	5.30324	-0.34409	0.13509
C	7.28101	0.73916	-0.84549
H	-2.26994	-1.06101	-1.59154
H	5.79564	-1.80847	4.71626
H	3.94122	-0.94098	6.05648
H	5.35874	-3.17366	2.73025
H	0.13478	-3.12067	5.34397
H	-0.23103	-2.34094	6.88554
H	1.29965	-3.21028	6.67754
H	0.62219	0.54038	4.59963
H	-0.48215	0.04407	5.88426

H	-0.47521	-0.84532	4.38123
H	2.26683	0.41117	6.71271
H	2.47364	-1.15660	7.52699
H	0.93474	-0.30879	7.62000
H	1.12191	-4.72267	2.53503
H	2.58603	-5.61489	2.96105
H	1.88204	-5.79862	1.34678
H	2.87938	-2.40073	0.06902
H	1.27136	-2.96220	0.57561
H	2.27503	-3.98491	-0.42807
H	4.03725	-5.28976	0.34382
H	4.80685	-5.09033	1.91729
H	4.94739	-3.81721	0.68363
H	6.24367	4.20347	4.11839
H	8.25736	3.56385	2.88153
H	8.07204	2.12685	0.90128
H	1.90901	4.90122	3.44568
H	3.29725	5.36958	2.45084
H	2.29207	3.99749	1.98024
H	2.56224	1.70413	3.42031
H	3.50348	1.80890	4.89674
H	1.98090	2.71207	4.76272
H	4.70170	3.86877	5.59045
H	4.54571	5.36525	4.64418
H	3.14319	4.69232	5.47342
H	4.35289	-0.25659	0.66391

H	5.16572	-0.97662	-0.74916
H	5.99316	-0.85466	0.81483
H	7.17213	0.08225	-1.71541
H	7.78365	1.65038	-1.18525
H	7.93383	0.22953	-0.12934
H	4.11547	2.06388	-1.05549
H	5.63503	2.57865	-1.75929
H	4.94225	1.01692	-2.23262
H	-0.44729	6.52717	-2.18536
H	-2.47673	7.01876	-0.91056
H	-3.12694	5.59124	0.96741
H	2.72375	4.04176	-0.16664
H	3.55619	4.66152	-1.59655
H	2.64692	5.75787	-0.54325
H	0.62838	3.08175	-3.28024
H	2.36202	2.93208	-2.95326
H	1.14553	2.37171	-1.77797
H	0.66873	5.47983	-3.71654
H	1.62937	6.57790	-2.69814
H	2.42284	5.29605	-3.61280
H	-3.00744	1.89613	0.80647
H	-1.31366	1.48542	1.04099
H	-2.45385	1.30725	2.38195
H	0.10029	3.04168	2.78449
H	-0.74141	4.41253	3.50332
H	-1.20649	2.76251	3.95360

H	-3.52373	3.21707	3.42504
H	-3.14649	4.89008	3.00924
H	-4.05626	3.86825	1.87288
H	-3.35775	-1.70832	4.33933
H	-3.80898	-2.65818	6.56325
H	-3.05491	-4.95913	7.11651
H	-1.83591	-6.30241	5.42002
H	-1.37615	-5.36212	3.19350
H	-3.37512	-1.30813	0.33434
H	-4.43198	-2.40481	1.23941
H	-3.77724	-0.95897	2.02713
H	-2.35754	-4.84688	0.56565
H	-1.46403	-3.64625	-0.36251
H	-0.63740	-4.58679	0.90917

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Y Monomer - CO_2 coord adduct

C	0.78742	-7.03214	1.18141
C	0.37984	-6.37833	2.35788
C	0.97991	-6.75492	3.57058
C	1.96144	-7.74401	3.60957
C	2.35849	-8.37557	2.43226
C	1.76973	-8.01944	1.21883
Si	-1.01121	-5.12305	2.31288
C	-1.62509	-4.65796	4.01840
O	-0.41963	-3.67723	1.43537
C	0.26432	-2.61678	1.71790

O	0.56103	-2.46277	3.00214
C	1.30267	-1.30372	3.38709
C	0.58157	-0.13272	3.68530
C	1.36115	1.01359	3.89415
C	2.74833	0.95885	3.89206
C	3.40110	-0.26051	3.76331
C	2.69651	-1.44784	3.52231
C	-0.94036	-0.09430	3.95671
C	-1.80966	-0.51232	2.75608
C	3.42077	-2.81171	3.58454
C	3.27657	-3.65670	2.30661
O	0.60194	-1.80382	0.83742
Y	0.50599	-1.18519	-1.40050
O	0.15811	-3.02147	-2.22839
C	-0.17434	-4.30451	-2.49244
C	0.84676	-5.29467	-2.59407
C	0.44958	-6.62522	-2.77224
C	-0.88503	-6.99429	-2.86676
C	-1.86288	-6.00984	-2.83387
C	-1.54647	-4.65754	-2.66809
C	2.34956	-4.95783	-2.53491
C	2.72612	-4.43729	-1.13778
C	-2.66217	-3.60164	-2.77565
C	-4.04960	-4.22367	-3.01765
F	-0.58263	0.80161	-0.40717
C	-1.40871	1.64562	-1.15129

C	-1.74358	2.90920	-0.71499
C	-2.56401	3.59377	-1.62094
C	-3.02108	3.06062	-2.82591
C	-2.64511	1.77286	-3.20447
C	-1.82211	1.07744	-2.33953
B	-1.26684	3.49153	0.74307
C	0.09961	4.37784	0.68255
C	0.72132	4.88596	-0.45542
C	1.93269	5.57590	-0.43302
C	2.57447	5.79211	0.77941
C	1.99226	5.31215	1.94778
C	0.78263	4.63276	1.87255
F	0.17379	4.71529	-1.67606
F	2.48243	6.02658	-1.56615
F	3.73889	6.44572	0.82360
F	2.60228	5.50450	3.12456
F	0.26694	4.20405	3.04413
F	-1.37119	-0.18666	-2.64906
F	-3.04508	1.24164	-4.35774
F	-3.80252	3.77262	-3.63502
F	-2.94625	4.84271	-1.35379
C	-2.53030	4.21407	1.48522
C	-3.58598	3.43246	1.95153
C	-4.69122	3.93440	2.62776
C	-4.77873	5.30153	2.86087
C	-3.75850	6.12966	2.40886

C	-2.67166	5.57923	1.73134
F	-3.57133	2.09366	1.74748
F	-1.74198	6.45033	1.31020
F	-3.83470	7.44758	2.62053
F	-5.82996	5.81103	3.50767
F	-5.67012	3.11882	3.05179
O	1.87958	-0.17880	-2.50919
C	2.97175	0.34812	-3.12094
C	2.95710	0.57886	-4.52616
C	4.14339	1.01990	-5.12156
C	5.29178	1.27137	-4.38464
C	5.26012	1.12335	-3.00607
C	4.11496	0.67696	-2.34003
C	1.68386	0.44558	-5.38312
C	0.62997	1.43385	-4.84612
C	4.11099	0.58578	-0.80513
C	3.95885	-0.87742	-0.35480
C	1.92505	0.81807	-6.85674
C	1.14274	-0.99438	-5.38859
C	5.42362	1.08843	-0.17819
C	2.99417	1.47344	-0.22020
C	-2.40519	-5.65691	1.18801
C	3.23664	-6.18925	-2.79202
C	2.71715	-3.92670	-3.61797
C	-2.36670	-2.71450	-4.00249
C	-2.80334	-2.77977	-1.47853

C	-1.39555	1.31620	4.36893
C	-1.22135	-1.02590	5.15446
C	4.93026	-2.63293	3.82476
C	2.85640	-3.59327	4.78967
O	-5.81818	-0.11746	2.49060
C	-6.08297	0.52083	1.54827
O	-6.36486	1.12649	0.59146
H	3.32163	1.86870	4.04439
H	0.87819	1.96810	4.05533
H	4.47931	-0.28686	3.85812
H	-0.92845	-2.05718	4.94902
H	-2.29150	-1.01580	5.39048
H	-0.67773	-0.68913	6.04309
H	-1.55565	0.06807	1.86697
H	-2.86009	-0.31152	2.98500
H	-1.73911	-1.57883	2.53006
H	-1.23924	2.05179	3.57650
H	-0.88549	1.65927	5.27459
H	-2.46701	1.28832	4.58825
H	1.78719	-3.78763	4.67864
H	3.00654	-3.03577	5.71973
H	3.36624	-4.55848	4.88313
H	3.59960	-3.10226	1.42249
H	2.26123	-4.01780	2.14343
H	3.90710	-4.54833	2.38842
H	5.39663	-3.62034	3.89849

H	5.14254	-2.10260	4.75809
H	5.41963	-2.10053	3.00232
H	1.20330	-7.39949	-2.85068
H	-1.15899	-8.03710	-2.99901
H	-2.89828	-6.30478	-2.95636
H	3.79238	-3.71618	-3.58944
H	2.47695	-4.31633	-4.61288
H	2.18598	-2.98482	-3.49280
H	2.11304	-3.58485	-0.83814
H	2.58493	-5.21671	-0.38252
H	3.77657	-4.12653	-1.11383
H	3.10740	-6.96615	-2.03101
H	3.05132	-6.63187	-3.77617
H	4.28698	-5.88084	-2.76368
H	-1.84328	-2.42887	-1.09292
H	-3.45904	-1.91617	-1.63354
H	-3.23870	-3.39346	-0.68460
H	-4.79160	-3.42118	-3.09017
H	-4.08933	-4.78905	-3.95373
H	-4.35919	-4.88343	-2.19998
H	-1.36328	-2.29100	-3.97448
H	-2.44012	-3.31608	-4.91439
H	-3.09123	-1.89632	-4.07939
H	4.17246	1.18372	-6.19195
H	6.19742	1.61004	-4.87962
H	6.14899	1.36943	-2.43739

H	0.90746	-1.35930	-4.38920
H	0.23139	-1.05339	-5.99511
H	1.87894	-1.67953	-5.82153
H	0.96284	2.46547	-4.99965
H	-0.32579	1.30306	-5.36666
H	0.46858	1.30154	-3.77612
H	2.27845	1.84758	-6.97127
H	2.64268	0.14776	-7.34192
H	0.97878	0.73464	-7.40193
H	3.19685	2.52690	-0.43548
H	2.01331	1.25670	-0.64576
H	2.93391	1.35576	0.86687
H	3.13639	-1.39162	-0.86243
H	4.85880	-1.45096	-0.60170
H	3.79318	-0.93418	0.72561
H	5.34723	1.01879	0.91219
H	6.28825	0.49162	-0.48692
H	5.61907	2.13614	-0.42678
H	0.67894	-6.27761	4.49939
H	2.41172	-8.02385	4.55791
H	3.12104	-9.14917	2.46045
H	2.06966	-8.51709	0.30096
H	0.33752	-6.77642	0.22499
H	-2.11854	-5.53542	4.45163
H	-0.82746	-4.34482	4.69470
H	-2.36415	-3.85439	3.96124

H	-2.79031	-6.62445	1.52653
H	-3.22598	-4.93447	1.21987
H	-2.07433	-5.76218	0.15091
H	-0.99261	2.51142	1.40483

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Y Monomer - CO_2 coord TS

C	8.85325	8.51219	2.52198
C	9.89115	9.26916	1.98154
C	9.81043	10.63496	2.24989
C	8.79650	11.20774	3.01621
C	7.79251	10.40285	3.54040
C	7.81892	9.03593	3.28887
B	11.07558	8.51415	1.14730
C	12.44843	9.37028	0.96573
C	12.94323	9.91383	-0.21717
C	14.16208	10.58351	-0.31067
C	14.94256	10.74464	0.82697
C	14.48959	10.23003	2.03684
C	13.26794	9.56879	2.07808
F	12.25244	9.80034	-1.36940
F	14.58529	11.07151	-1.48190
F	16.11492	11.38185	0.76024
F	15.23344	10.37122	3.14174
F	12.88855	9.10030	3.28680
F	10.73041	11.48412	1.76615
F	8.77532	12.52496	3.24608

F	6.81138	10.93503	4.27438
F	6.85652	8.24517	3.78270
F	8.81578	7.17680	2.30646
C	10.46651	7.92218	-0.26034
C	10.75931	6.64764	-0.70174
C	10.19935	6.04672	-1.81618
C	9.28884	6.73011	-2.60124
C	8.96702	8.03132	-2.22120
C	9.55525	8.59083	-1.08676
F	11.66597	5.84546	-0.02792
Y	12.42024	3.66520	-0.92208
F	10.56553	4.75516	-2.14318
F	9.20130	9.84472	-0.80654
F	8.10244	8.72735	-2.95659
F	8.75340	6.16812	-3.68271
O	13.85955	4.66779	-1.95437
C	14.94776	5.16200	-2.60649
C	14.90244	5.38331	-4.01466
C	16.08857	5.76058	-4.65303
C	17.27040	5.96616	-3.95800
C	17.26937	5.84779	-2.57689
C	16.12600	5.46804	-1.86733
C	13.60563	5.30387	-4.84178
C	13.81472	5.70774	-6.31256
C	16.17217	5.43127	-0.33095
C	17.51343	5.93285	0.23409

O	12.73796	3.19571	1.35944
C	12.40186	2.41189	2.26299
O	11.64761	1.38404	2.01798
Si	11.04237	-0.02591	2.93248
C	9.60690	-0.54864	1.85055
O	12.13545	1.83877	-1.82482
C	12.04658	0.58201	-2.33005
C	13.20416	-0.25629	-2.37247
C	13.04354	-1.58150	-2.79336
C	11.81867	-2.08967	-3.19453
C	10.72115	-1.24499	-3.22229
C	10.79543	0.09173	-2.81732
C	14.62141	0.22671	-2.00743
C	15.69359	-0.85445	-2.24251
C	9.54486	0.97369	-2.99281
C	9.86904	2.11479	-3.97336
C	15.08943	6.36008	0.24985
C	16.00881	3.98982	0.17526
C	13.03606	3.87709	-4.87059
C	12.58931	6.30420	-4.25846
O	12.76089	2.54993	3.53487
C	13.60988	3.64277	3.89754
C	13.00671	4.87031	4.23305
C	13.88978	5.94669	4.39723
C	15.26545	5.77556	4.33406
C	15.80390	4.50277	4.19862

C	14.99027	3.37991	3.99615
C	11.51894	5.03579	4.61889
C	11.19906	6.48763	5.01454
C	15.59473	1.95943	4.05694
C	17.11365	2.00662	4.29914
C	11.27367	4.15341	5.86149
C	10.52578	4.65744	3.51100
C	14.96791	1.22127	5.25829
C	15.37860	1.14699	2.77100
C	10.48868	0.50474	4.63972
C	12.39200	-1.32621	2.95462
C	12.95104	-1.77053	4.16379
C	13.90048	-2.79110	4.18407
C	14.30569	-3.38715	2.99122
C	13.75751	-2.96382	1.78024
C	12.80746	-1.94532	1.76202
C	15.02937	1.42287	-2.88505
C	14.70316	0.58466	-0.51782
C	9.06322	1.52046	-1.63977
C	8.35273	0.20973	-3.59743
O	9.80890	3.86699	0.40532
C	8.70403	4.25925	0.44623
O	7.60341	4.62472	0.47979
H	15.92070	6.63394	4.44954
H	13.49624	6.93902	4.57115
H	16.87830	4.38232	4.25568

H	11.46003	3.09678	5.65517
H	10.23447	4.25735	6.19391
H	11.92330	4.45737	6.68849
H	10.70799	5.25079	2.61407
H	9.50845	4.87931	3.85124
H	10.54898	3.59535	3.26105
H	11.35589	7.18603	4.18755
H	11.78952	6.81868	5.87456
H	10.14500	6.54754	5.30262
H	13.88563	1.12085	5.15154
H	15.17073	1.75555	6.19206
H	15.39189	0.21451	5.34096
H	15.74021	1.69347	1.89770
H	14.33603	0.87505	2.60710
H	15.93403	0.20497	2.83166
H	17.48979	0.98228	4.38287
H	17.36998	2.52479	5.22836
H	17.65052	2.48489	3.47314
H	13.90405	-2.23854	-2.82071
H	11.72704	-3.12492	-3.51061
H	9.77843	-1.63891	-3.58100
H	16.04899	1.74256	-2.64354
H	15.00650	1.14202	-3.94292
H	14.37575	2.28375	-2.75853
H	13.96584	1.33591	-0.22656
H	14.52049	-0.29527	0.10670

H	15.69788	0.97015	-0.27462
H	15.54578	-1.73794	-1.61233
H	15.73193	-1.17550	-3.28831
H	16.67462	-0.43724	-1.99203
H	9.88160	1.96936	-1.07997
H	8.27791	2.27121	-1.79485
H	8.64130	0.71730	-1.02630
H	7.50367	0.89622	-3.68567
H	8.56844	-0.17223	-4.60039
H	8.03010	-0.62731	-2.96903
H	10.69809	2.73423	-3.63296
H	10.15361	1.69864	-4.94530
H	8.99470	2.75916	-4.12387
H	16.09004	5.90965	-5.72580
H	18.17598	6.25185	-4.48550
H	18.18320	6.06653	-2.03780
H	12.84055	3.47750	-3.87564
H	12.09841	3.85534	-5.43746
H	13.73910	3.19439	-5.35884
H	12.93429	7.33134	-4.41538
H	11.61331	6.19464	-4.74595
H	12.46579	6.16723	-3.18463
H	14.20419	6.72579	-6.41153
H	14.48897	5.02426	-6.83949
H	12.84853	5.67407	-6.82763
H	15.30312	7.40007	-0.01610

H	14.09537	6.13284	-0.13329
H	15.06332	6.28903	1.34214
H	15.12339	3.50153	-0.23751
H	16.86696	3.38033	-0.12920
H	15.93313	3.97043	1.26685
H	17.46266	5.91700	1.32793
H	18.35743	5.30187	-0.06452
H	17.72488	6.96263	-0.07046
H	12.64481	-1.31983	5.10416
H	14.31997	-3.12239	5.12992
H	15.04351	-4.18466	3.00461
H	14.06378	-3.43232	0.84922
H	12.39153	-1.63479	0.80657
H	9.89832	-0.30378	5.08481
H	11.32282	0.73063	5.30671
H	9.84982	1.39008	4.57986
H	9.19740	-1.49136	2.22770
H	8.81015	0.19904	1.86070
H	9.92195	-0.70449	0.81531
H	11.38015	7.53506	1.79931

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Y Monomer - CO_2 coord product - 9-Y

O	-2.89405	-1.15530	0.31817
Y	-0.45933	-1.21983	-0.95974
O	0.97079	-0.19653	-1.98489
C	2.05154	0.32057	-2.63188

C	2.00632	0.53927	-4.04049
C	3.18375	0.95054	-4.67390
C	4.35667	1.18852	-3.97423
C	4.35655	1.06068	-2.59405
C	3.22304	0.64489	-1.88873
O	-0.10505	-1.66549	1.33782
C	-0.48934	-2.38085	2.27633
O	-0.11018	-2.22345	3.54003
C	0.76868	-1.14836	3.87928
C	0.19279	0.09851	4.19157
C	1.09882	1.15589	4.35128
C	2.47063	0.95005	4.30546
C	2.97933	-0.33644	4.18556
C	2.14141	-1.44229	3.98718
C	-1.29786	0.30571	4.54384
C	-1.59812	-0.55365	5.79004
C	2.71572	-2.87498	4.05531
C	2.07835	-3.59490	5.26193
O	-0.72670	-3.05218	-1.87019
C	-0.76086	-4.26988	-2.47561
C	0.42725	-5.06094	-2.56493
C	0.33418	-6.33003	-3.14768
C	-0.85544	-6.83402	-3.64740
C	-1.99313	-6.04654	-3.58653
C	-1.98708	-4.76811	-3.02010
F	-1.23773	1.00712	-0.08175

C	-2.16246	1.78894	-0.75585
C	-2.48305	3.06003	-0.32431
C	-3.40933	3.70193	-1.15487
C	-3.98364	3.12146	-2.28593
C	-3.62764	1.82715	-2.65911
C	-2.70214	1.17205	-1.86828
F	-2.28584	-0.10208	-2.19006
C	1.80920	-4.58544	-2.07756
C	2.25211	-3.33573	-2.85739
C	-3.29596	-3.95793	-3.04169
C	-3.74419	-3.65272	-1.60230
B	-1.87599	3.68128	1.06884
C	-3.06375	4.43511	1.89922
C	-4.10461	3.67664	2.43401
C	-5.14314	4.19995	3.19559
C	-5.17168	5.56662	3.44834
C	-4.16535	6.37218	2.92990
C	-3.14719	5.80049	2.16824
F	-3.79004	4.95117	-0.88448
F	-4.86398	3.79262	-3.02684
F	-4.14310	1.24815	-3.74222
F	-4.14415	2.34079	2.21533
F	-6.10880	3.40833	3.68237
F	-6.15714	6.09778	4.17749
F	-4.18830	7.68934	3.16044
F	-2.22627	6.65127	1.68881

C	0.71488	0.42501	-4.87271
C	0.16566	-1.01074	-4.88511
C	3.27648	0.58337	-0.35286
C	2.18419	1.48509	0.25290
C	-3.96252	-1.29024	0.77876
O	-5.01885	-1.43007	1.23778
O	-1.33063	-3.35325	2.08523
Si	-1.95405	-4.73176	3.03692
C	-3.54838	-5.07349	2.11877
C	-0.72240	-6.12865	2.84495
C	-0.48401	-6.69440	1.57988
C	0.37150	-7.78386	1.43417
C	1.00074	-8.33054	2.55301
C	0.77474	-7.78491	3.81560
C	-0.08003	-6.69294	3.95885
C	-2.27076	-4.25703	4.81918
C	-2.26877	-0.06433	3.41056
C	-1.58982	1.76867	4.91793
C	2.47819	-3.69065	2.77507
C	4.23656	-2.85825	4.29026
C	1.78928	-4.32051	-0.56517
C	2.91241	-5.63733	-2.30186
C	-4.46576	-4.71149	-3.70063
C	-3.09472	-2.67565	-3.86698
C	-0.50806	4.54222	0.86012
C	-0.00854	5.03573	-0.34281

C	1.21260	5.69794	-0.46073
C	1.99097	5.90429	0.67071
C	1.53347	5.44106	1.89960
C	0.31029	4.78514	1.96400
F	-0.69558	4.87702	-1.49195
F	1.63980	6.13526	-1.65043
F	3.16507	6.53557	0.58085
F	2.27424	5.62646	3.00008
F	-0.07481	4.36852	3.18908
C	-0.31657	1.42020	-4.30745
C	0.92507	0.80989	-6.34840
C	3.13899	-0.87043	0.12732
C	4.61278	1.09521	0.21512
H	3.14609	1.79281	4.41939
H	0.72608	2.15930	4.50881
H	4.05009	-0.48126	4.25078
H	-1.41566	-1.61502	5.60832
H	-2.64710	-0.43168	6.08324
H	-0.97519	-0.24288	6.63485
H	-1.99430	0.44330	2.48364
H	-3.27684	0.26740	3.67632
H	-2.31881	-1.14356	3.24544
H	-1.41387	2.45381	4.08530
H	-0.99828	2.09731	5.77812
H	-2.64393	1.85437	5.19888
H	0.99478	-3.67944	5.15402

H	2.28768	-3.05744	6.19237
H	2.48777	-4.60708	5.35263
H	2.84971	-3.15804	1.89753
H	1.42938	-3.94093	2.61396
H	3.01425	-4.64348	2.84122
H	4.59164	-3.89001	4.37433
H	4.50855	-2.34343	5.21687
H	4.77807	-2.39283	3.46013
H	1.22183	-6.94565	-3.22320
H	-0.89168	-7.82358	-4.09408
H	-2.91371	-6.43981	-3.99943
H	3.24589	-3.01120	-2.52953
H	2.30775	-3.55856	-3.92768
H	1.57322	-2.49350	-2.73420
H	1.00799	-3.61723	-0.26950
H	1.60524	-5.24701	-0.01210
H	2.75383	-3.91869	-0.24058
H	2.71674	-6.57139	-1.76464
H	3.05494	-5.86861	-3.36225
H	3.86036	-5.23730	-1.92685
H	-2.92798	-3.23791	-1.01237
H	-4.58992	-2.95330	-1.60292
H	-4.07794	-4.57387	-1.11264
H	-5.35518	-4.07227	-3.67489
H	-4.26754	-4.94987	-4.75041
H	-4.71547	-5.63912	-3.17477

H	-2.23713	-2.10009	-3.52711
H	-2.91514	-2.93350	-4.91579
H	-3.98556	-2.03837	-3.82463
H	3.18521	1.10109	-5.74642
H	5.25493	1.50311	-4.49780
H	5.26407	1.29833	-2.05244
H	-0.03490	-1.40010	-3.88728
H	-0.76600	-1.05439	-5.46053
H	0.88308	-1.69026	-5.35664
H	0.01584	2.44898	-4.47947
H	-1.29025	1.29076	-4.79466
H	-0.43996	1.29816	-3.23189
H	1.29222	1.83472	-6.46114
H	1.61777	0.13316	-6.86000
H	-0.03671	0.74731	-6.86897
H	2.37136	2.53201	-0.00589
H	1.18821	1.24385	-0.11470
H	2.17737	1.40255	1.34466
H	2.26714	-1.37038	-0.30052
H	4.01203	-1.45666	-0.18045
H	3.05704	-0.90955	1.21796
H	4.57023	1.05218	1.30859
H	5.46498	0.48609	-0.10469
H	4.80503	2.13551	-0.06550
H	-0.24718	-6.28225	4.95131
H	1.26067	-8.21103	4.68890

H	1.66447	-9.18342	2.44047
H	0.54148	-8.20671	0.44819
H	-0.96433	-6.28405	0.69496
H	-2.79638	-5.08787	5.30355
H	-1.35764	-4.05416	5.38173
H	-2.91613	-3.37669	4.87822
H	-4.03103	-5.95523	2.55294
H	-4.24634	-4.23483	2.19599
H	-3.36242	-5.27735	1.06150
H	-1.55796	2.71725	1.73666

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Y Monomer - CO_2 coord adduct H transf. TS

C	16.47893	-0.49329	-0.23667
C	15.08314	-0.20536	-0.21911
C	14.12426	-1.24559	-0.39980
C	14.59464	-2.54580	-0.60631
C	15.94952	-2.84041	-0.63524
C	16.86986	-1.81931	-0.44981
O	14.66069	1.06546	-0.02470
Y	13.79531	2.91330	0.14533
O	13.46245	3.18120	2.42705
C	12.69179	2.98442	3.38117
O	12.98884	3.32724	4.63273
C	14.22742	3.97052	4.90532
C	14.22245	5.37880	4.95519
C	15.46531	5.98122	5.18898

C	16.61403	5.22840	5.38449
C	16.54326	3.84346	5.42061
C	15.33854	3.15899	5.21174
C	12.94731	6.24948	4.87400
C	13.27390	7.74134	5.07007
C	15.27073	1.63910	5.49370
C	14.48912	1.45296	6.81138
C	12.60728	-0.98459	-0.38643
C	12.17347	-0.38228	0.96358
C	17.55630	0.58564	-0.01967
C	17.48149	1.66161	-1.11867
O	11.54447	3.12306	-0.19079
C	10.36341	3.05754	-0.51581
O	9.50291	2.24882	-0.47869
O	14.99502	4.38995	-0.58110
C	15.76838	5.13962	-1.39944
C	15.67563	5.00808	-2.81032
C	16.52856	5.79868	-3.59514
C	17.43282	6.68953	-3.04735
C	17.49450	6.82137	-1.66569
C	16.68025	6.07238	-0.81619
C	14.70960	4.10727	-3.61601
C	13.77003	3.20183	-2.80586
C	16.78498	6.27446	0.70593
C	15.42734	6.72332	1.27663
C	13.79752	5.00604	-4.47902

C	15.51957	3.16696	-4.53478
C	17.26339	4.97772	1.38326
C	17.79951	7.36752	1.08551
O	11.53833	2.42167	3.23530
Si	10.11478	2.10972	4.29557
C	10.69636	1.65629	6.01830
C	9.28916	0.65336	3.46119
C	8.34691	0.84459	2.43747
C	7.71939	-0.24267	1.83256
C	8.01786	-1.53985	2.24684
C	8.94442	-1.74934	3.26798
C	9.57365	-0.66144	3.86808
C	9.10177	3.69130	4.25384
C	11.98866	5.85003	6.01497
C	12.23159	6.13910	3.51408
C	14.60776	0.80460	4.38060
C	16.67493	1.04318	5.70478
C	11.78111	-2.27166	-0.55898
C	12.21911	-0.07128	-1.56464
C	17.39564	1.21070	1.37844
C	18.98253	0.00870	-0.07493
F	12.85596	8.41537	-0.35540
C	11.53565	8.21136	-0.31453
C	10.96721	7.07565	-0.87801
C	9.59756	6.81016	-0.87446
C	8.80991	7.77566	-0.24606

C	9.33783	8.92405	0.33954
C	10.70992	9.14372	0.30481
B	9.02405	5.49192	-1.61655
C	9.28363	5.51603	-3.21230
C	9.89130	4.48567	-3.92414
C	10.14405	4.54273	-5.29140
C	9.77347	5.67313	-6.00795
C	9.15035	6.72537	-5.34446
C	8.92501	6.62843	-3.97569
F	10.28406	3.35471	-3.30072
F	10.76215	3.53057	-5.91321
F	10.00909	5.74766	-7.31778
F	8.77779	7.81170	-6.02519
F	8.30755	7.66626	-3.39064
F	11.81690	6.19382	-1.44640
F	11.23194	10.23661	0.86298
F	8.53929	9.81725	0.93007
F	7.47729	7.64358	-0.19364
C	7.60563	4.93397	-1.10183
C	6.46470	4.76857	-1.88984
C	5.26269	4.26309	-1.39704
C	5.16898	3.88851	-0.06251
C	6.27994	4.03301	0.76043
C	7.45388	4.54762	0.23047
F	6.46564	5.10634	-3.18546
F	4.20148	4.13401	-2.19598

F	4.03046	3.39601	0.42462
F	6.21020	3.65626	2.04743
F	8.50129	4.64842	1.07752
H	9.87483	4.59335	-1.18095
H	17.56603	5.72544	5.54696
H	15.53950	7.06034	5.22276
H	17.44641	3.28569	5.62977
H	11.66705	4.81015	5.93584
H	11.09498	6.48323	5.98981
H	12.46916	5.98441	6.98958
H	12.91741	6.34023	2.68738
H	11.42399	6.87741	3.46636
H	11.76938	5.16528	3.35027
H	13.91283	8.13486	4.27304
H	13.75325	7.93711	6.03438
H	12.34038	8.31178	5.04854
H	13.47541	1.85227	6.73792
H	14.99331	1.96270	7.63865
H	14.41993	0.38797	7.06179
H	15.03495	1.01883	3.39828
H	13.52620	0.93975	4.33522
H	14.77334	-0.25880	4.58255
H	16.57725	-0.02886	5.90091
H	17.18972	1.47898	6.56617
H	17.30927	1.16126	4.82040
H	17.92410	-2.06727	-0.47342

H	16.28670	-3.85975	-0.80099
H	13.88659	-3.35315	-0.75069
H	18.26704	2.41187	-0.97527
H	17.62786	1.20569	-2.10372
H	16.52551	2.18401	-1.12645
H	16.41141	1.66364	1.50929
H	17.51716	0.44357	2.15114
H	18.15239	1.98528	1.54343
H	19.15664	-0.74767	0.69784
H	19.21233	-0.43324	-1.05010
H	19.69943	0.81951	0.09265
H	12.77145	0.48555	1.24827
H	11.11971	-0.08745	0.93945
H	12.29763	-1.12127	1.76221
H	10.71660	-2.01824	-0.51665
H	11.96518	-2.75666	-1.52315
H	11.97851	-2.99712	0.23701
H	12.78713	0.86054	-1.57271
H	12.42954	-0.56989	-2.51664
H	11.15200	0.17245	-1.53450
H	16.47582	5.71572	-4.67641
H	18.07793	7.28422	-3.68765
H	18.19622	7.53124	-1.24517
H	14.33965	2.44489	-2.24600
H	13.09485	3.79480	-2.17714
H	13.12564	2.64269	-3.49094

H	14.37409	5.63481	-5.16228
H	13.11962	4.39257	-5.08193
H	13.19617	5.66653	-3.84695
H	16.14930	3.71770	-5.23773
H	16.17120	2.51213	-3.94745
H	14.84144	2.53728	-5.12263
H	15.13857	7.69469	0.86490
H	14.63721	6.01257	1.03333
H	15.49150	6.81362	2.36671
H	16.60792	4.13736	1.15647
H	18.26940	4.71683	1.03690
H	17.29765	5.10172	2.47137
H	17.81624	7.47275	2.17586
H	18.81725	7.11903	0.76628
H	17.53275	8.34296	0.66548
H	10.29141	-0.84498	4.66380
H	9.17472	-2.75881	3.59718
H	7.52456	-2.38712	1.77837
H	6.99586	-0.07479	1.04028
H	8.09142	1.84658	2.10839
H	11.41851	0.83641	6.01795
H	11.14261	2.51108	6.53042
H	9.82002	1.33310	6.59169
H	8.98231	4.08224	5.26856
H	9.57383	4.46431	3.64448
H	8.10908	3.51118	3.83541

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Y Monomer - CO_2 coord adduct H trans. product - 10-Y

C	4.21983	-4.42671	-0.99000
C	2.86117	-4.04923	-0.76708
C	1.80181	-4.93919	-1.11997
C	2.13401	-6.15380	-1.72798
C	3.44856	-6.51653	-1.98090
C	4.47053	-5.65835	-1.60294
O	2.57811	-2.85258	-0.21459
Y	2.06033	-0.96630	0.46917
O	2.11677	-1.08176	2.80194
C	1.32069	-1.32268	3.72141
O	1.62444	-1.11935	5.00585
C	2.91539	-0.62020	5.32571
C	3.05319	0.77151	5.49554
C	4.35431	1.22655	5.74611
C	5.42528	0.35095	5.85144
C	5.21514	-1.01875	5.78151
C	3.94428	-1.55856	5.54407
C	1.86914	1.76446	5.52787
C	2.34439	3.19343	5.84755
C	3.72268	-3.08410	5.67375
C	2.81870	-3.33097	6.89948
C	0.32144	-4.61327	-0.85031
C	0.09107	-4.37368	0.65380
C	5.40772	-3.54290	-0.56602

C	5.39027	-2.20211	-1.32215
O	0.03052	-0.36869	0.32362
C	-1.19971	-0.00129	0.14276
O	-2.01470	0.24702	1.02038
O	3.18619	0.62850	-0.22430
C	4.07264	1.31413	-0.97146
C	3.81967	1.51273	-2.35897
C	4.82353	2.10753	-3.13005
C	6.01803	2.54327	-2.57347
C	6.20544	2.43526	-1.20271
C	5.25051	1.84483	-0.36951
C	2.45691	1.18550	-3.00002
C	2.02518	-0.28727	-2.79941
C	5.46992	1.82594	1.15325
C	4.29093	2.53557	1.84770
C	1.39390	2.12234	-2.38808
C	2.46565	1.43338	-4.51969
C	5.62314	0.38688	1.67474
C	6.74428	2.57952	1.57179
O	0.14447	-1.81059	3.51428
Si	-1.38597	-1.95051	4.43798
C	-1.01315	-2.63378	6.14610
C	-2.40347	-3.15510	3.43050
C	-3.17040	-2.69196	2.34748
C	-3.98350	-3.56406	1.62550
C	-4.04148	-4.91355	1.97272

C	-3.28765	-5.39024	3.04487
C	-2.47880	-4.51627	3.76835
C	-2.12192	-0.23404	4.43263
C	0.90564	1.35234	6.66015
C	1.11593	1.84668	4.18656
C	3.09791	-3.73969	4.42654
C	5.04980	-3.82093	5.93171
C	-0.61804	-5.76731	-1.24411
C	-0.11782	-3.39800	-1.68801
C	5.37305	-3.32163	0.95823
C	6.76686	-4.19508	-0.87680
F	-3.71881	7.29921	-5.48388
C	-4.46614	6.42245	-4.81595
C	-4.05466	5.10419	-4.66410
C	-4.79631	4.15158	-3.95263
C	-6.00283	4.60691	-3.40459
C	-6.45592	5.91129	-3.55430
C	-5.67790	6.82438	-4.26106
B	-4.31028	2.67038	-3.78947
C	-3.59700	1.95704	-4.99162
C	-2.48634	1.12362	-4.81337
C	-1.83080	0.50151	-5.86707
C	-2.29912	0.68718	-7.16495
C	-3.40857	1.49683	-7.39213
C	-4.02522	2.12133	-6.31483
F	-1.98575	0.92114	-3.58705

F	-0.76062	-0.26461	-5.65171
F	-1.68989	0.09311	-8.18280
F	-3.86274	1.66708	-8.63224
F	-5.09161	2.88124	-6.58724
F	-2.87809	4.77463	-5.20724
F	-6.09125	8.07712	-4.40550
F	-7.61922	6.29526	-3.03164
F	-6.79457	3.76836	-2.72802
C	-4.53338	1.90532	-2.44569
C	-4.81311	0.53136	-2.40666
C	-5.02704	-0.15980	-1.22206
C	-4.94429	0.51845	-0.01051
C	-4.65492	1.87916	0.00578
C	-4.46564	2.54393	-1.19741
F	-4.92050	-0.17094	-3.54020
F	-5.30525	-1.46608	-1.23485
F	-5.14869	-0.13301	1.12519
F	-4.56114	2.52429	1.16400
F	-4.17249	3.84639	-1.12358
H	-1.48464	0.07988	-0.92448
H	6.42506	0.73682	6.02887
H	4.53718	2.28659	5.86607
H	6.05928	-1.68058	5.92504
H	0.49877	0.35128	6.50716
H	0.06766	2.05665	6.71403
H	1.41719	1.36499	7.62825

H	1.80141	2.05516	3.36146
H	0.38496	2.66156	4.22713
H	0.55389	0.94405	3.94846
H	2.99822	3.59753	5.06792
H	2.86553	3.25234	6.80836
H	1.47028	3.84886	5.91061
H	1.84735	-2.84499	6.78940
H	3.28797	-2.95010	7.81249
H	2.64855	-4.40593	7.03017
H	3.62241	-3.45166	3.51248
H	2.03731	-3.51302	4.30970
H	3.16753	-4.82874	4.51935
H	4.84253	-4.88863	6.05145
H	5.54255	-3.48289	6.84844
H	5.74993	-3.71376	5.09654
H	5.49306	-5.96233	-1.79266
H	3.67546	-7.46515	-2.45959
H	1.34629	-6.84130	-2.01306
H	6.25046	-1.58554	-1.03906
H	5.44170	-2.37437	-2.40258
H	4.48944	-1.62249	-1.12324
H	4.43475	-2.86462	1.27834
H	5.46966	-4.27960	1.48112
H	6.19892	-2.67492	1.27461
H	6.89571	-5.15315	-0.36210
H	6.91176	-4.35644	-1.95007

H	7.56692	-3.52857	-0.53687
H	0.74148	-3.59599	1.05517
H	-0.94752	-4.08636	0.84602
H	0.29775	-5.29144	1.21540
H	-1.64781	-5.48568	-0.99934
H	-0.58345	-5.98427	-2.31700
H	-0.38989	-6.68820	-0.69715
H	0.50410	-2.52254	-1.50393
H	-0.04567	-3.62906	-2.75632
H	-1.15761	-3.13127	-1.46531
H	4.67406	2.24147	-4.19472
H	6.78393	2.99228	-3.19965
H	7.12123	2.82612	-0.77433
H	2.87529	-0.97174	-2.73945
H	1.38952	-0.39848	-1.91320
H	1.39331	-0.61984	-3.62950
H	1.62592	3.16721	-2.62020
H	0.40099	1.89426	-2.79232
H	1.35625	2.01608	-1.30097
H	2.68866	2.47571	-4.76722
H	3.18977	0.79256	-5.03506
H	1.47564	1.20417	-4.92532
H	4.25565	3.59006	1.55249
H	3.33753	2.07916	1.57739
H	4.40899	2.48752	2.93645
H	4.76328	-0.23220	1.41748

H	6.50951	-0.08511	1.23842
H	5.72978	0.37775	2.76518
H	6.82321	2.56830	2.66445
H	7.65229	2.11330	1.17466
H	6.72608	3.62680	1.25240
H	-1.90393	-4.90494	4.60560
H	-3.33223	-6.44083	3.31871
H	-4.67688	-5.59323	1.41104
H	-4.57106	-3.18301	0.79562
H	-3.12947	-1.64629	2.05661
H	-0.43970	-3.56364	6.10260
H	-0.46047	-1.91655	6.75695
H	-1.96360	-2.84767	6.64737
H	-3.15855	-0.29001	4.78203
H	-1.57715	0.44784	5.08985
H	-2.11881	0.16667	3.41319

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Y Monomer - CO_2 coord adduct H trans. product with BR_3 coord - 10'-Y

C	2.23163	-3.75397	2.27353
C	2.88514	-2.73328	2.99087
C	4.26376	-2.71293	3.27700
C	5.03076	-3.69275	2.63425
C	4.45164	-4.64339	1.80621
C	3.07266	-4.69392	1.66309
O	2.08331	-1.68153	3.52911
C	1.88545	-0.60981	2.76682

O	1.14263	0.31386	3.27577
Y	2.35869	0.51787	-0.42831
O	2.38662	-0.49267	1.63507
C	4.91645	-1.79006	4.32934
C	6.43208	-2.03716	4.43327
C	0.70049	-3.95711	2.24827
C	0.31625	-5.21596	1.45074
O	0.22215	0.12232	-0.74380
C	-0.99922	-0.01736	-0.99925
O	-1.82539	0.92691	-0.87646
Si	0.26720	0.62729	4.81145
C	1.53144	0.68890	6.19410
O	3.53915	-0.63529	-1.64412
C	4.29065	-1.39476	-2.47169
C	5.71226	-1.30794	-2.41523
C	6.45402	-2.11317	-3.28589
C	5.84969	-2.97801	-4.18605
C	4.46547	-3.05382	-4.22754
C	3.65491	-2.28277	-3.38922
C	6.44951	-0.36348	-1.44747
C	7.97989	-0.48096	-1.56728
C	2.12421	-2.42065	-3.48360
C	1.49300	-1.07787	-3.89686
O	2.74990	2.52989	-0.50219
C	3.04731	3.83565	-0.69321
C	2.70461	4.47206	-1.92234

C	3.05747	5.81514	-2.08575
C	3.71089	6.53344	-1.09554
C	4.01399	5.90871	0.10460
C	3.69407	4.56880	0.34405
C	1.95329	3.74775	-3.05470
C	1.67474	4.66576	-4.25922
C	4.03582	3.94574	1.70962
C	2.74848	3.47083	2.40898
C	6.10408	1.10357	-1.76567
C	6.10785	-0.71626	0.01293
C	1.56114	-2.92817	-2.14238
C	1.68401	-3.44368	-4.54630
C	-0.45071	2.30974	4.44549
C	-1.03374	-0.69547	5.05248
C	-2.06911	-0.84843	4.11433
C	-3.06894	-1.79915	4.30530
C	-3.06494	-2.59407	5.45163
C	-2.05519	-2.44463	6.40136
C	-1.04353	-1.50758	6.19805
C	2.79391	2.57995	-3.60307
C	0.57710	3.27101	-2.55178
C	4.70287	4.94985	2.66657
C	5.03397	2.78750	1.53784
C	4.30409	-2.12900	5.70421
C	4.74025	-0.29073	4.02399
C	0.21807	-4.17136	3.69780

C	-0.06688	-2.78603	1.61002
F	-2.19550	-0.22666	-3.61635
C	-2.71657	1.01174	-3.77862
C	-3.33918	1.63876	-2.69822
C	-3.80182	2.92632	-2.96863
C	-3.68780	3.53184	-4.22029
C	-3.07107	2.85367	-5.26280
C	-2.57279	1.57452	-5.03900
B	-3.34325	0.89082	-1.24441
C	-3.91029	-0.65606	-1.24235
C	-3.66918	-1.48315	-0.14459
C	-4.18246	-2.76488	0.00321
C	-5.01726	-3.27501	-0.98364
C	-5.31026	-2.48765	-2.09075
C	-4.76355	-1.20918	-2.19995
F	-4.37620	3.67729	-2.01847
F	-4.15398	4.76702	-4.41811
F	-2.94663	3.42412	-6.46036
F	-1.95891	0.91184	-6.02360
F	-2.87239	-1.04615	0.85913
F	-3.88151	-3.50132	1.08213
F	-5.52759	-4.50003	-0.86923
F	-6.11523	-2.96238	-3.04236
F	-5.11382	-0.52347	-3.29310
C	-4.14021	1.66009	-0.04381
C	-5.51641	1.85619	-0.17920

C	-6.32089	2.42741	0.79852
C	-5.74560	2.82528	2.00125
C	-4.38393	2.63809	2.19181
C	-3.61517	2.06191	1.18195
F	-6.12254	1.48382	-1.31840
F	-7.63030	2.59396	0.59942
F	-6.49338	3.37341	2.95935
F	-3.81605	3.00270	3.34877
F	-2.30753	1.90095	1.47913
H	5.07543	-5.37702	1.30402
H	6.10205	-3.71913	2.78552
H	2.64166	-5.48917	1.06871
H	3.21908	-2.00379	5.70462
H	4.72680	-1.47820	6.47813
H	4.52060	-3.16635	5.97912
H	5.02395	-0.06157	2.99391
H	5.38668	0.29418	4.68737
H	3.72293	0.06283	4.19585
H	6.95432	-1.79752	3.50117
H	6.66621	-3.06947	4.71035
H	6.84258	-1.39134	5.21577
H	0.41616	-3.30282	4.32854
H	0.70916	-5.04260	4.14402
H	-0.86251	-4.34669	3.70856
H	0.33541	-2.53946	0.62369
H	-0.06845	-1.88865	2.22913

H	-1.11778	-3.06272	1.48822
H	-0.76967	-5.34140	1.49576
H	0.76658	-6.12344	1.86507
H	0.59354	-5.13865	0.39408
H	7.53625	-2.06561	-3.26620
H	6.45371	-3.58843	-4.85144
H	4.00687	-3.73390	-4.93519
H	6.65534	1.77953	-1.10240
H	6.38377	1.34262	-2.79696
H	5.04108	1.32111	-1.65807
H	5.03232	-0.72164	0.19894
H	6.47433	-1.71862	0.25796
H	6.57991	-0.00305	0.69906
H	8.33603	-1.49219	-1.34429
H	8.33942	-0.19902	-2.56215
H	8.44682	0.19915	-0.84658
H	1.87878	-2.31056	-1.30149
H	0.46506	-2.95334	-2.16925
H	1.91761	-3.94527	-1.94750
H	0.58963	-3.49157	-4.56257
H	2.01251	-3.16265	-5.55200
H	2.05391	-4.45139	-4.32981
H	1.78830	-0.26155	-3.23736
H	1.81953	-0.80541	-4.90592
H	0.39971	-1.14211	-3.90360
H	2.81399	6.32038	-3.01232

H	3.97361	7.57534	-1.25491
H	4.51219	6.48547	0.87464
H	3.73157	2.95301	-4.02844
H	3.06945	1.84935	-2.84001
H	2.25089	2.05341	-4.39579
H	-0.05314	4.13097	-2.30219
H	0.06202	2.69352	-3.32764
H	0.64323	2.65836	-1.65205
H	1.05580	5.52733	-3.98890
H	2.59658	5.03178	-4.72307
H	1.12935	4.09755	-5.02041
H	2.09616	4.32604	2.61638
H	2.98980	2.98650	3.36323
H	4.65394	2.01329	0.86978
H	5.97033	3.15400	1.10463
H	5.26519	2.33149	2.50711
H	4.91242	4.45071	3.61925
H	5.65529	5.32352	2.27672
H	4.05649	5.80720	2.88003
H	-0.25887	-1.40943	6.94433
H	-2.05271	-3.05995	7.29680
H	-3.85015	-3.32945	5.60470
H	-3.84195	-1.92423	3.55390
H	-2.10096	-0.22351	3.22620
H	1.03493	1.04411	7.10400
H	1.98692	-0.27926	6.41042

H	2.32523	1.40151	5.95240
H	-1.35729	-0.99299	-1.34446
H	2.18088	2.76840	1.79788
H	-0.96250	2.67988	5.34034
H	0.33917	3.01869	4.18249
H	-1.17881	2.28075	3.63249

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Y Monomer - CO_2 coord adduct SiR_3 trans. TS

C	18.58590	-0.15712	3.00853
C	19.07832	1.06939	3.49665
C	20.32793	1.22135	4.12992
C	21.18056	0.11177	4.07659
C	20.79055	-1.07828	3.48026
C	19.49966	-1.21875	2.99305
O	18.22834	2.20771	3.41369
C	18.32898	2.96839	2.31941
O	17.53462	3.97084	2.22016
Y	18.44253	4.21874	-0.28463
O	19.15340	2.73271	1.40435
C	20.73147	2.46315	4.95244
C	22.11958	2.28946	5.59417
C	17.11037	-0.40796	2.63002
C	16.88652	-1.86118	2.17546
O	16.24890	4.04621	-0.37252
C	15.19847	3.69888	0.24860
O	14.99858	3.70635	1.48020

Si	15.83132	4.71061	3.31413
C	17.06356	5.39374	4.58077
O	19.14846	3.18894	-1.93252
C	19.67666	2.49921	-2.96529
C	21.07950	2.56764	-3.22356
C	21.58877	1.84761	-4.30872
C	20.77961	1.07614	-5.12859
C	19.42057	1.00944	-4.86291
C	18.83456	1.69866	-3.79661
C	22.04537	3.40346	-2.36322
C	23.50386	3.29854	-2.84622
C	17.31720	1.56498	-3.56804
C	16.63013	2.93201	-3.73166
O	18.90369	6.24229	-0.34388
C	19.30574	7.50675	-0.59466
C	18.72981	8.24172	-1.67555
C	19.22604	9.52182	-1.94190
C	20.23259	10.09858	-1.18270
C	20.74435	9.39831	-0.10115
C	20.30011	8.11479	0.23063
C	17.57895	7.69416	-2.54046
C	17.07300	8.72589	-3.56612
C	20.86972	7.42999	1.48611
C	19.72477	7.12136	2.46794
C	21.67672	4.89670	-2.44565
C	22.04392	2.89427	-0.90870

C	17.04631	0.97011	-2.17509
C	16.64673	0.61772	-4.57935
C	15.14091	6.24383	2.47361
C	14.69956	3.53244	4.25953
C	13.43323	3.13294	3.79648
C	12.58368	2.37269	4.59589
C	12.98241	1.98301	5.87431
C	14.23284	2.36646	6.35307
C	15.07660	3.13765	5.55521
C	18.04237	6.47625	-3.35893
C	16.36938	7.34910	-1.65001
C	21.86457	8.32372	2.24895
C	21.63854	6.15132	1.11479
C	19.71957	2.63155	6.10489
C	20.79808	3.74888	4.10920
C	16.24413	-0.18046	3.88519
C	16.61656	0.49350	1.48504
F	12.90374	3.50182	-4.34446
C	12.60816	4.79978	-4.21061
C	11.54636	5.19617	-3.38661
C	11.33576	6.57784	-3.28453
C	12.10802	7.51037	-3.96567
C	13.15495	7.06649	-4.76886
C	13.41791	5.70374	-4.88497
B	10.64727	4.16277	-2.63105
C	10.22216	2.82600	-3.32391

C	10.10992	1.62122	-2.61575
C	9.73681	0.42474	-3.21408
C	9.43735	0.40953	-4.57385
C	9.52485	1.58245	-5.31914
C	9.92215	2.75646	-4.69198
F	10.33367	7.05261	-2.53698
F	11.85825	8.81318	-3.85947
F	13.90937	7.94343	-5.41903
F	14.43592	5.28739	-5.63367
F	10.40123	1.57623	-1.31106
F	9.66268	-0.70004	-2.50566
F	9.06936	-0.72213	-5.15882
F	9.22956	1.56695	-6.61679
F	9.97624	3.85499	-5.45094
C	10.17053	4.47350	-1.16966
C	8.86588	4.20380	-0.73910
C	8.42273	4.48500	0.54743
C	9.31154	5.03511	1.46714
C	10.62280	5.30891	1.08732
C	11.02338	5.03824	-0.21435
F	7.97391	3.68209	-1.58743
F	7.16712	4.23082	0.90906
F	8.91067	5.29595	2.70462
F	11.47645	5.81926	1.97587
F	12.29881	5.30623	-0.52548
H	21.48173	-1.91510	3.43552

H	22.16962	0.17383	4.51228
H	19.19646	-2.17907	2.59638
H	18.69890	2.74432	5.73346
H	19.96862	3.51723	6.70073
H	19.74109	1.76079	6.76852
H	21.38994	3.59552	3.20305
H	21.27304	4.54422	4.69447
H	19.81448	4.12068	3.82161
H	22.91440	2.20815	4.84510
H	22.16775	1.41565	6.25146
H	22.33672	3.16984	6.20725
H	16.32911	0.84160	4.25843
H	16.53644	-0.86611	4.68760
H	15.18924	-0.36123	3.65129
H	17.31454	0.48269	0.64431
H	16.44768	1.52188	1.80539
H	15.65079	0.12485	1.12216
H	15.82359	-2.00031	1.95509
H	17.15389	-2.58587	2.95096
H	17.44494	-2.10123	1.26421
H	22.64934	1.88915	-4.52558
H	21.20477	0.52980	-5.96598
H	18.80032	0.39974	-5.50888
H	22.39124	5.50128	-1.87659
H	21.70680	5.23370	-3.48723
H	20.67801	5.11089	-2.06497

H	21.04595	2.87167	-0.46896
H	22.42638	1.86858	-0.86640
H	22.68718	3.52063	-0.27986
H	23.87924	2.27044	-2.81267
H	23.63144	3.68123	-3.86423
H	24.13948	3.90149	-2.18857
H	17.52235	1.55789	-1.39076
H	15.96915	0.92902	-1.97361
H	17.44320	-0.04910	-2.11254
H	15.57727	0.55391	-4.34980
H	16.73795	0.97891	-5.60907
H	17.05407	-0.39774	-4.53115
H	17.01605	3.66892	-3.02987
H	16.79106	3.31543	-4.74459
H	15.54939	2.84003	-3.57453
H	18.81486	10.09113	-2.76656
H	20.60191	11.09213	-1.42084
H	21.50985	9.87100	0.50244
H	18.84679	6.76421	-4.04387
H	18.43226	5.66387	-2.74365
H	17.21598	6.07878	-3.95845
H	15.98075	8.25711	-1.17565
H	15.56519	6.90876	-2.25124
H	16.62538	6.64379	-0.86011
H	16.71335	9.64254	-3.08680
H	17.84199	8.99581	-4.29736

H	16.23459	8.29579	-4.12278
H	19.22904	8.05016	2.77165
H	20.11482	6.63539	3.36941
H	21.01941	5.44764	0.55743
H	22.49851	6.39360	0.48225
H	22.01053	5.64816	2.01408
H	22.21345	7.78839	3.13892
H	22.74725	8.56907	1.64927
H	21.40493	9.25839	2.58646
H	16.04178	3.43198	5.95520
H	14.55283	2.06864	7.34781
H	12.31961	1.38570	6.49480
H	11.60689	2.08104	4.21910
H	13.11816	3.41886	2.80058
H	16.49783	5.90700	5.36807
H	17.69644	4.63872	5.05007
H	17.71306	6.12895	4.09952
H	14.36716	3.34741	-0.38521
H	18.97195	6.47212	2.01917
H	15.09622	7.05183	3.21147
H	15.81514	6.56285	1.67265
H	14.15097	6.07778	2.04966

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Y Monomer - CO_2 coord adduct SiR_3 trans. product

O	0.91962	1.12596	-0.27770
Y	3.16982	0.64679	-0.01790

O	2.25722	0.29544	2.17987
C	2.74590	-0.86968	2.19898
O	3.49865	-1.29634	1.27370
Si	-1.38179	2.57267	1.47443
C	0.27049	3.22215	2.04973
O	3.95096	2.57088	0.02414
C	4.55128	3.77783	0.04598
C	4.32680	4.70970	-1.01461
C	4.98686	5.94187	-0.96136
C	5.83566	6.28413	0.07993
C	6.02894	5.38153	1.11419
C	5.40467	4.13090	1.13643
O	3.75518	-0.24982	-1.80091
C	4.22570	-0.90090	-2.88203
C	5.62655	-1.14981	-3.02020
C	6.06807	-1.81412	-4.16865
C	5.19868	-2.23924	-5.16188
C	3.84096	-2.00321	-5.01264
C	3.32065	-1.34397	-3.89492
C	3.39221	4.42099	-2.20553
C	3.91796	3.23528	-3.03487
C	5.64572	3.19917	2.33819
C	6.59874	3.81214	3.38075
O	2.40496	-1.64536	3.24819
C	2.86329	-2.97514	3.27855
C	2.04256	-3.96783	2.70628

C	2.57552	-5.26229	2.66995
C	3.81686	-5.55274	3.21856
C	4.52669	-4.56842	3.89156
C	4.06069	-3.24997	3.96793
C	0.58914	-3.71197	2.25118
C	-0.22651	-3.20872	3.46052
C	4.78741	-2.21758	4.85561
C	3.81678	-1.72159	5.94844
C	-0.25820	1.05577	-0.62960
O	-1.25836	1.62883	-0.04721
C	6.66267	-0.72505	-1.96135
C	6.67331	0.80581	-1.79448
C	1.79972	-1.12385	-3.80133
C	1.24054	-1.84115	-2.55903
C	-2.13953	1.34868	2.67864
C	-3.12723	0.43305	2.28046
C	-3.70861	-0.43776	3.19909
C	-3.31902	-0.40077	4.53806
C	-2.33997	0.50024	4.95231
C	-1.75239	1.36297	4.02836
C	-2.56779	3.92304	0.94202
C	1.95955	4.15480	-1.70512
C	3.29118	5.61172	-3.17679
C	6.30851	1.88748	1.88136
C	4.31717	2.93620	3.07161
C	0.48484	-2.69108	1.10124

C	-0.07712	-5.00722	1.75510
C	5.32034	-1.01619	4.05424
C	5.99457	-2.84759	5.57199
C	6.37891	-1.43526	-0.62426
C	8.09975	-1.11523	-2.35490
C	1.03844	-1.69741	-5.01030
C	1.47925	0.38158	-3.76817
F	-4.58944	-1.95480	0.22160
C	-4.37891	-2.64715	-0.90506
C	-4.60184	-2.05047	-2.15499
C	-4.32421	-2.85934	-3.26778
C	-3.86875	-4.16727	-3.15783
C	-3.65155	-4.70840	-1.89320
C	-3.90389	-3.94294	-0.75743
B	-5.12434	-0.58387	-2.29678
C	-4.66208	0.31830	-3.49131
C	-3.34181	0.33865	-3.95546
C	-2.92070	1.14436	-5.00374
C	-3.84710	1.96296	-5.64631
C	-5.17418	1.97270	-5.22630
C	-5.55388	1.16781	-4.15873
F	-3.68542	-4.45667	0.45223
F	-3.20565	-5.94945	-1.76977
F	-3.63757	-4.90234	-4.24167
F	-4.52562	-2.39732	-4.50441
F	-2.40742	-0.41673	-3.35564

F	-1.64876	1.14791	-5.39694
F	-3.46363	2.73270	-6.65489
F	-6.06043	2.74890	-5.84439
F	-6.84158	1.20512	-3.80126
C	-6.11326	0.01150	-1.23624
C	-5.96761	1.31241	-0.74185
C	-6.82112	1.86219	0.20538
C	-7.89450	1.10666	0.67001
C	-8.08916	-0.18911	0.19685
C	-7.19722	-0.71495	-0.72950
F	-4.93904	2.07252	-1.14491
F	-7.42648	-1.96051	-1.15792
F	-9.11873	-0.90763	0.63805
F	-8.72805	1.61774	1.56578
F	-6.61960	3.09365	0.67061
H	4.21273	-6.56282	3.15998
H	5.45987	-4.83743	4.37060
H	2.01070	-6.06428	2.21149
H	2.94347	-1.22638	5.51923
H	4.32762	-1.00439	6.60136
H	3.47139	-2.55542	6.56889
H	5.87839	-1.34135	3.17194
H	5.99414	-0.42725	4.68741
H	4.52279	-0.34495	3.73392
H	6.76923	-3.17377	4.86969
H	5.70698	-3.70078	6.19484

H	6.44548	-2.09896	6.23122
H	0.16591	-2.26563	3.84615
H	-0.21328	-3.94600	4.27026
H	-1.26970	-3.04535	3.16733
H	1.20075	-2.91353	0.30574
H	0.63825	-1.66711	1.44650
H	-0.52358	-2.73065	0.67328
H	-1.11529	-4.79271	1.48399
H	-0.09533	-5.78433	2.52583
H	0.41869	-5.41245	0.86612
H	7.12599	-2.00878	-4.29635
H	5.57602	-2.75200	-6.04224
H	3.17043	-2.34414	-5.79230
H	7.43196	1.10283	-1.06149
H	6.91977	1.28796	-2.74647
H	5.71488	1.20979	-1.46778
H	5.35640	-1.29586	-0.27476
H	6.52607	-2.51566	-0.73081
H	7.06468	-1.07804	0.15361
H	8.21845	-2.19701	-2.47647
H	8.42512	-0.62382	-3.27801
H	8.78203	-0.79908	-1.55828
H	1.72672	-1.50332	-1.64332
H	0.15865	-1.67790	-2.47123
H	1.40828	-2.92070	-2.63618
H	-0.03137	-1.49941	-4.88253

H	1.34561	-1.22883	-5.95097
H	1.16670	-2.78071	-5.10594
H	1.95369	0.88256	-2.92489
H	1.84175	0.86301	-4.68224
H	0.39553	0.54118	-3.72245
H	4.83755	6.66109	-1.75735
H	6.33692	7.24800	0.08802
H	6.68536	5.66522	1.92794
H	4.92829	3.44822	-3.39941
H	3.96375	2.30497	-2.46894
H	3.27530	3.06754	-3.90684
H	1.55257	5.05492	-1.22968
H	1.30404	3.89046	-2.54453
H	1.93175	3.34736	-0.97398
H	2.90965	6.51520	-2.68928
H	4.25332	5.84934	-3.64218
H	2.59502	5.35371	-3.98238
H	3.90833	3.87908	3.45143
H	4.47414	2.26814	3.92648
H	5.73333	1.37931	1.10549
H	7.29734	2.08955	1.45638
H	6.43451	1.20152	2.72480
H	6.73065	3.09974	4.20247
H	7.59038	4.02062	2.96554
H	6.20172	4.73744	3.81110
H	-0.97742	2.04639	4.36639

H	-2.02650	0.52601	5.99218
H	-3.77327	-1.07864	5.25555
H	-4.45977	-1.14908	2.86862
H	-3.43761	0.38576	1.24019
H	0.10566	3.90411	2.89209
H	0.92155	2.40841	2.37768
H	0.77602	3.78631	1.26186
H	-0.54768	0.47937	-1.51588
H	3.56553	2.48508	2.42500
H	-2.79866	4.56189	1.80098
H	-2.12056	4.54997	0.16432
H	-3.50628	3.51218	0.56263