Supporting Information

Mechanistic Insight into the Organocalcium-catalyzed Nucleophilic Alkylation of Benzene and further Rational Design

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Content

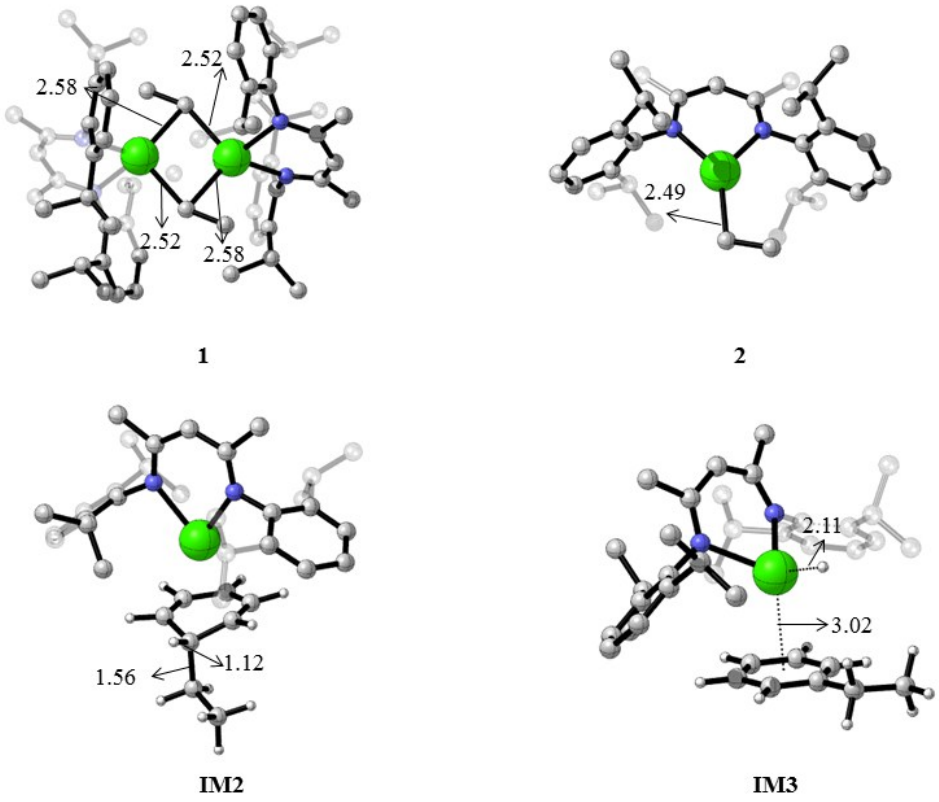


Figure S.1 Optimized geometries along with the key bond distances in Å, part of the hydrogen atoms are omitted for clarity (color code, C: grey, H: white, Ca: green, N: blue).

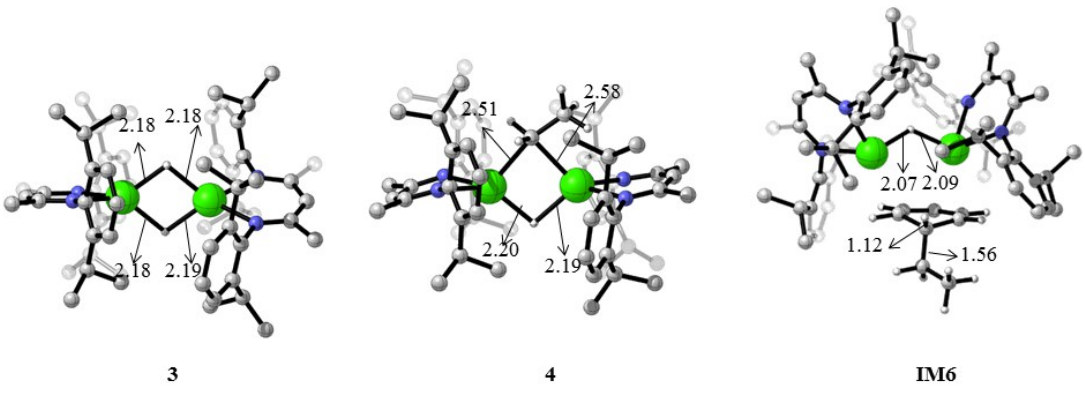


Figure S.2 Optimized geometries along with the key bond distances in Å, part of the hydrogen atoms are omitted for clarity (color code, C: grey, H: white, Ca: green, N: blue).

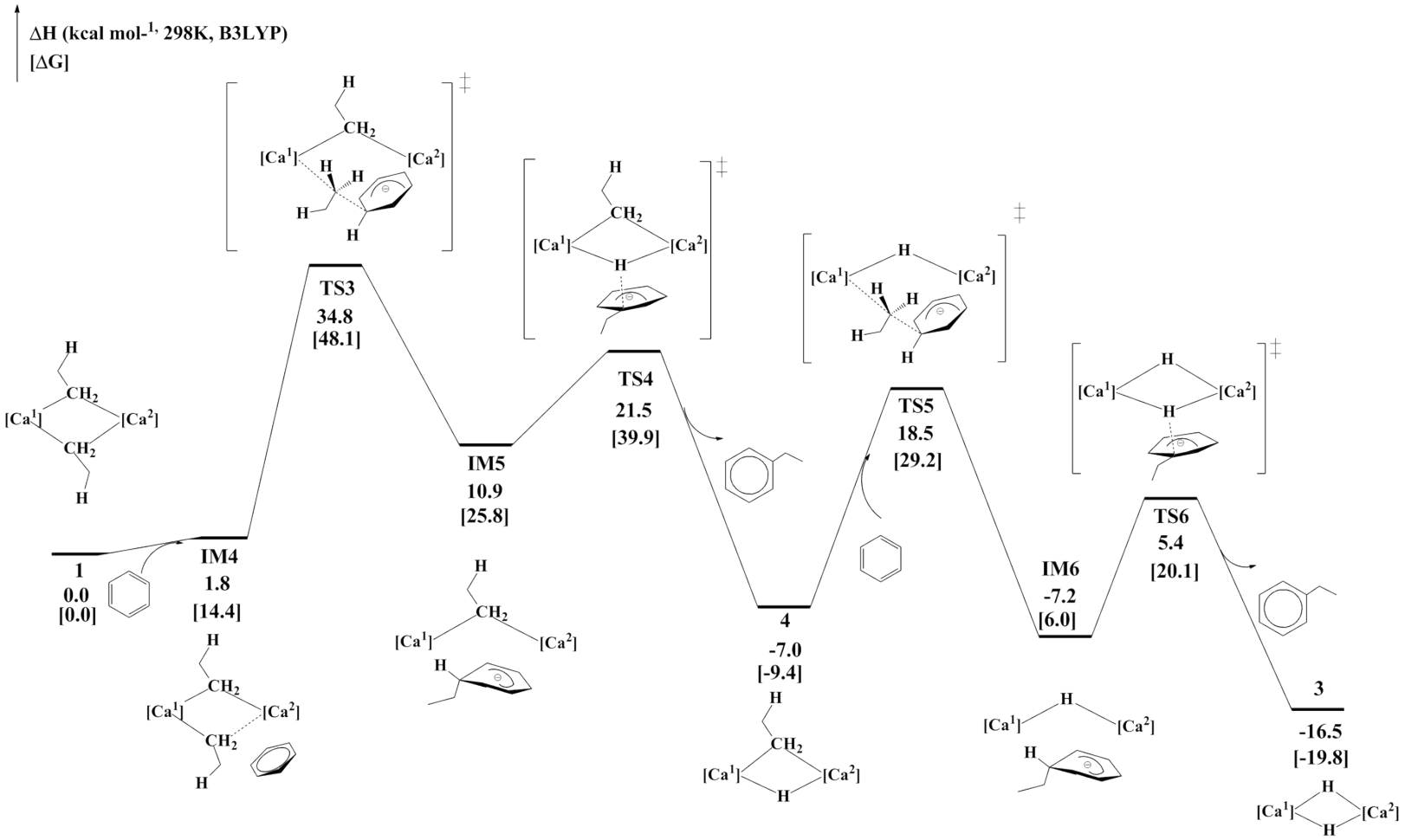


Figure S.3 Computed enthalpy (DFT, B3LYP-D3/6-311++G**/SMD//B3LYP-D3/ 6-31G**) energy profile of the dimer mechanism.

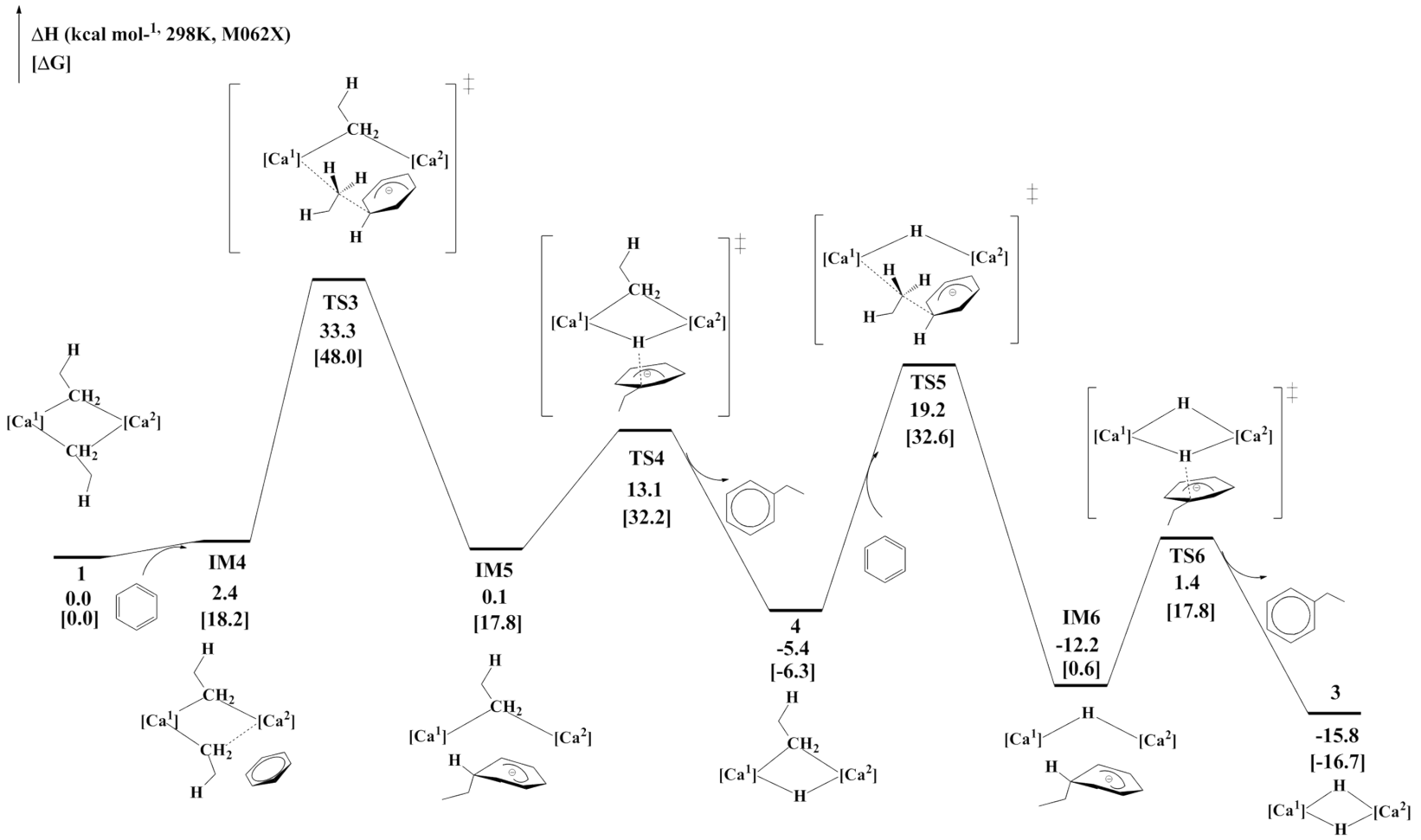


Figure S.4 Computed enthalpy (DFT, M062X/6-311++G**/SMD //M062X/6-31G**) energy profile of the dimer mechanism.

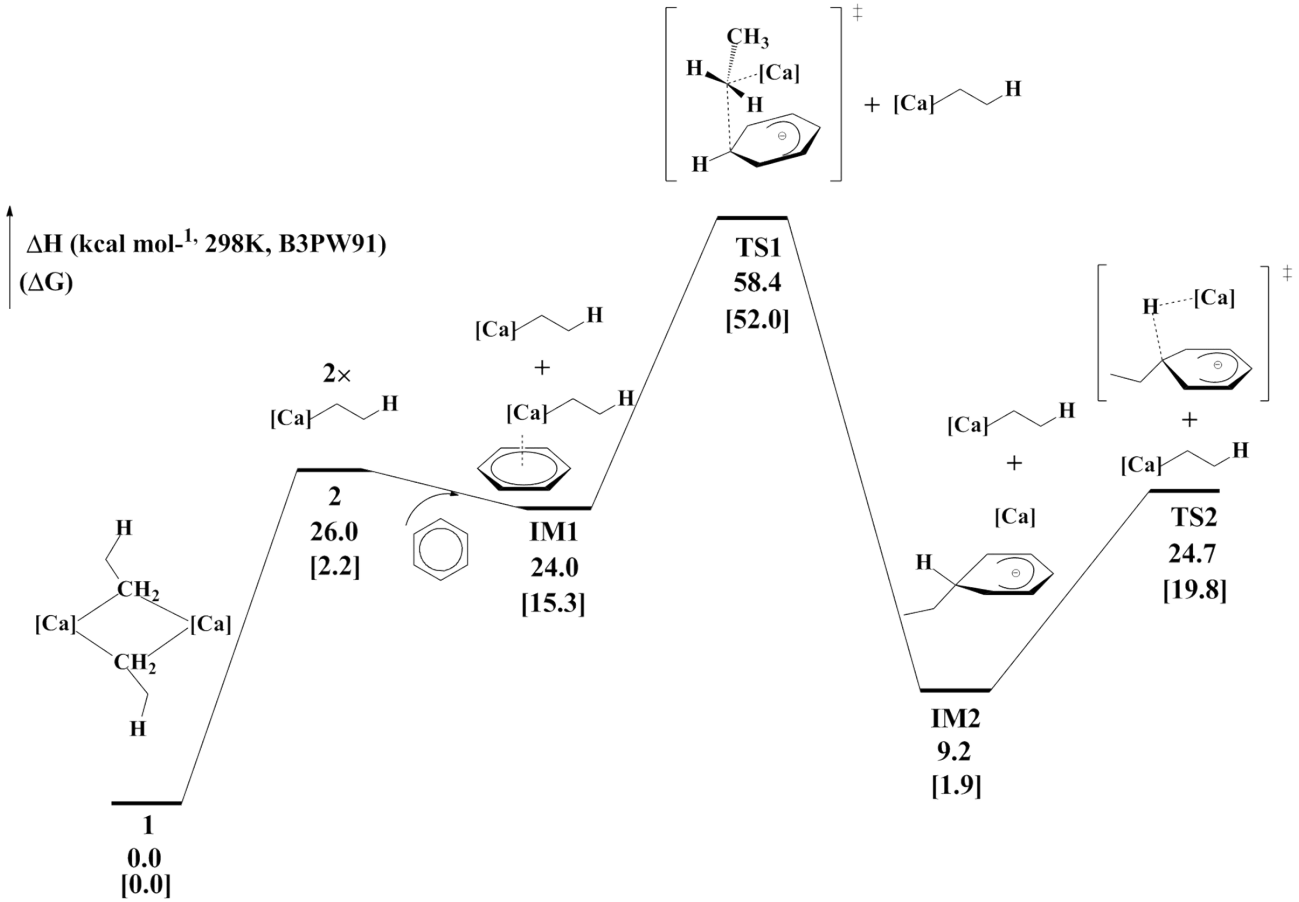


Figure S.5 Complementary enthalpy (DFT, B3PW91) energy profile of the dimer-monomer mechanism from compound **1** to **TS2**.

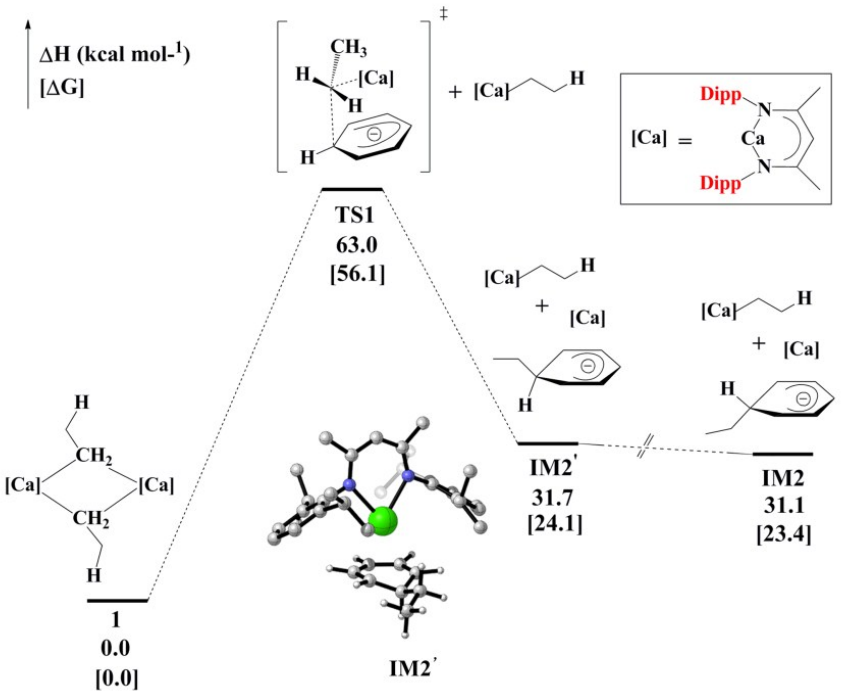
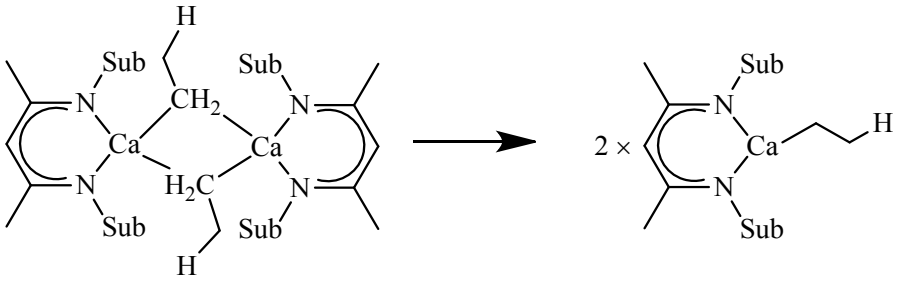


Figure S.6 Complementary enthalpy (DFT, BP86-D3BJ/def2-TZVPP/SMD//BP86-D3BJ/def2-SVP/SMD) energy profile of the monomeric mechanism from compound **1** to **IM2**.

Table S.1 The enthalpy energies of dissociation from dimeric alkylcalcium complex to monomer with different substituent.



Sub	ΔH (kcal/mol)
Dipp	50.4
Ph	44.3
$SiMe_3$	4.8

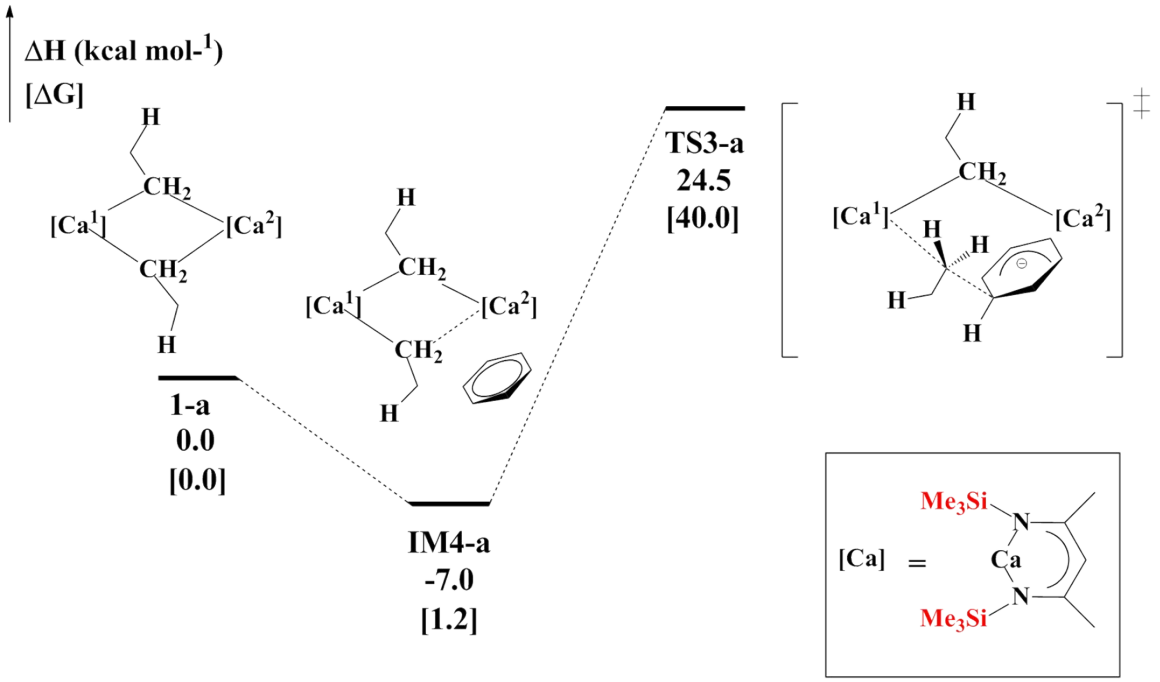


Figure S.7 Computed enthalpy (DFT, BP86-D3BJ/def2-TZVPP/SMD//BP86-D3BJ/def2-SVP/SMD) energy profile for rate determining step of the dimeric mechanism with ^{SiMe3}BDI ligand.

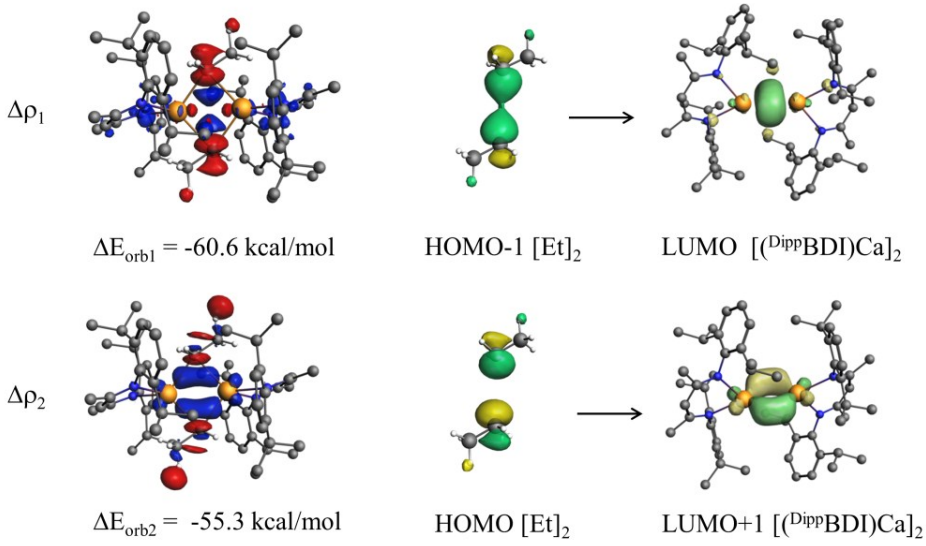


Figure S.8 Plot of deformation densities Δρ of the pairwise orbital interactions and the associated interaction energies (ΔEorb) between fragments in complex **1**, and shape of the most important interacting MOs of fragments. The direction of the charge flow is red to blue.

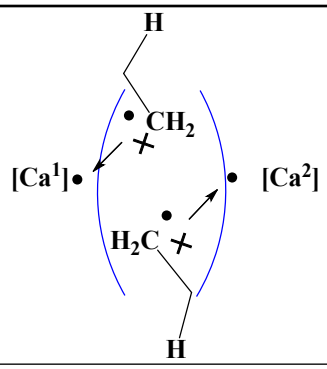
Table S.2 EDA-NOCV results of organocalcium complex **1** using the singlet (S) fragments and triplets (T) fragments at the BP86/TZ2P+ level of theory. Energy values are given in kcal/mol.

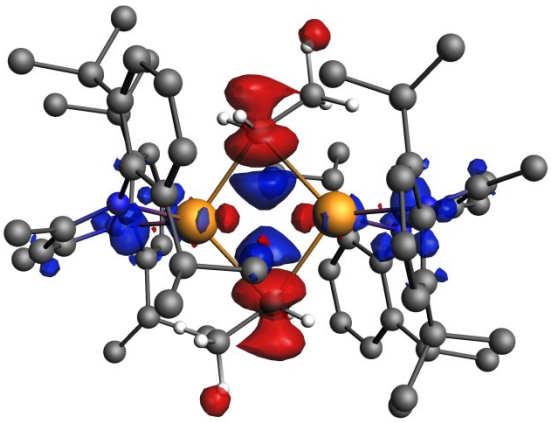
Fragments Bonding	Frag1 (S) + Frag2 (S) dative bonding	Frag1 (S) + Frag2 (T) dative bonding	Frag1(S) + Frag2 (S) electron-sharing bond
ΔE_{int}	-541.0	-487.6	-189.1
ΔE_{Pauli}	193.8	316.4	458.5
ΔE_{elstat}[a]	-479.6 (65.3%)	-488.1(60.7%)	-239.2 (36.9%)
ΔE_{orb}[a]	-221.2 (30.1%)	-281.9(35.1%)	-374.4 (57.8%)
ΔE_{disp}	-34.0 (4.6%)	-34.0(4.2%)	-34.0 (5.2%)
ΔE_{orb1}[b]	-60.6 (27.4%)		
ΔE_{orb2}[b]	-55.3 (25.0%)		
ΔE_{orb3}[b]	-10.2 (4.6%)		
ΔE_{orb4}[b]	-9.7 (4.4%)		
ΔE_{orb5}[b]	-7.8 (3.5%)		
ΔE_{orb6}[b]	-7.2 (3.2%)		
ΔE_{orb7}[b]	-5.8 (2.6%)		
$\Delta E_{orb(rest)}$	- 64.7 (29.2%)		

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

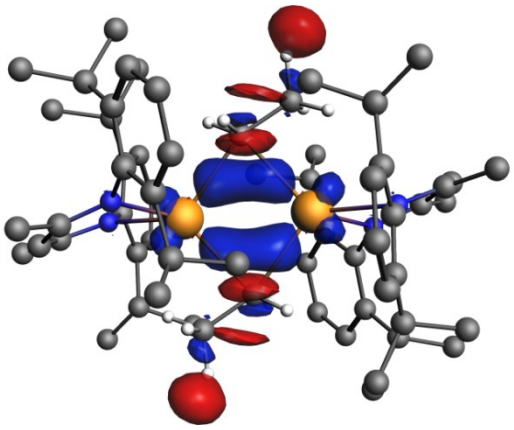
[b]The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}.

Figure S.9 Plot of deformation densities Δρ of the pairwise orbital interactions between the two fragments in complex **1** in associated interaction energies ΔE_{orb} (in kcal/mol) and eigenvalues ν. The eigenvalues ν indicate the size of the charge flow, and the direction of charge flow is red→blue.

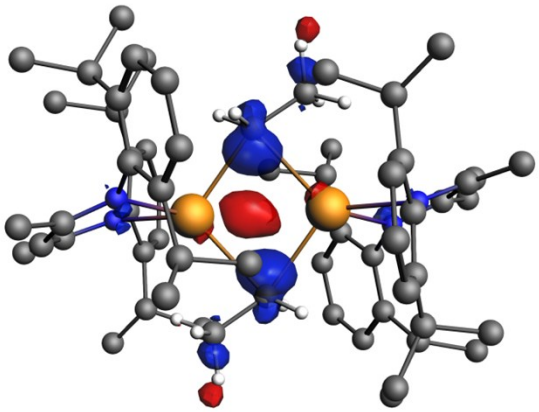




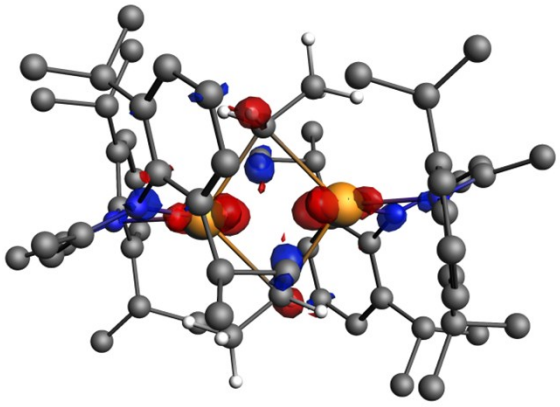
$\nu_1 = \pm 0.823$
$\Delta E_{orb(1)} = -60.6$ kcal/mol



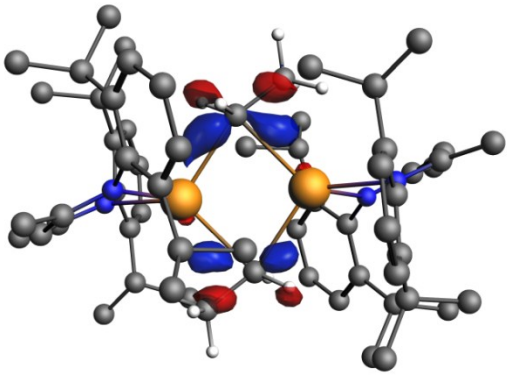
$\nu_2 = \pm 0.808$
$\Delta E_{orb(2)} = -55.3$ kcal/mol



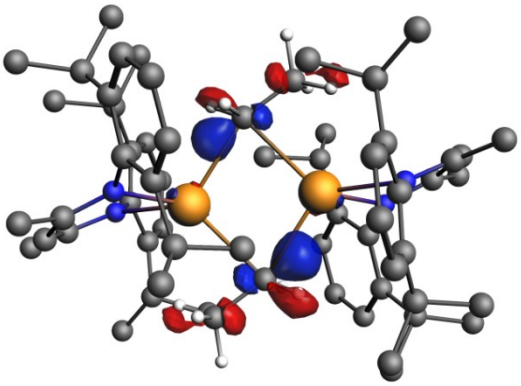
$\nu_3 = \pm 0.323$
$\Delta E_{orb(3)} = -10.2$ kcal/mol



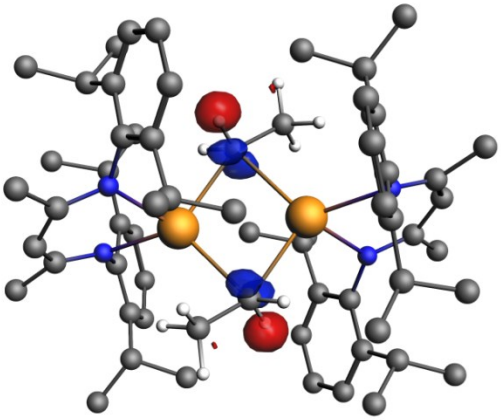
$\nu_4 = \pm 0.322$
$\Delta E_{orb(4)} = -9.7$ kcal/mol



$\nu_5 = \pm 0.227$
$\Delta E_{orb(5)} = -7.8$ kcal/mol

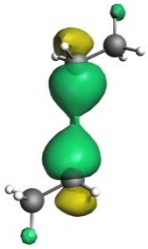
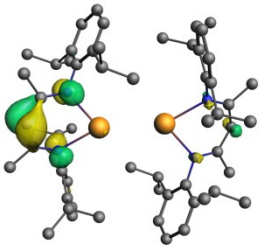
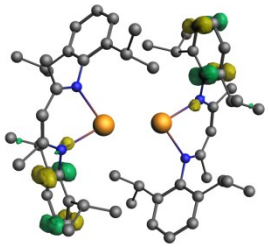
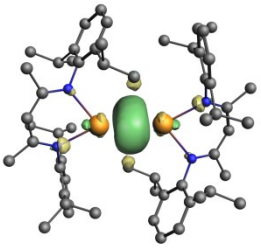


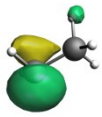
$\nu_6 = \pm 0.222$
$\Delta E_{orb(6)} = -7.2$ kcal/mol

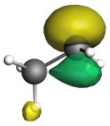


$\nu_7 = \pm 0.195$
$\Delta E_{orb(7)} = -5.8$ kcal/mol

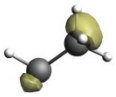
Figure S.10 Shape of the most important interacting MOs of fragments, plot of deformation densities Δρ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) between fragments in complex **1**. The direction of the charge flow is red to blue.

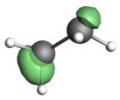
deformation densities Δρ	interacting MOs
$\nu_1 = \pm 0.823$ $\Delta E_{orb(1)} = -60.6$ kcal/mol	 frag1-17A(HOMO-1) ν =-0.435 +  frag2-247A(HOMO-1) ν = -0.093 +  frag2-239A ν = -0.089 ↓  frag2-249A(LUMO) ν = 0.662



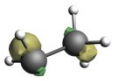


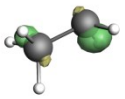
frag1-18A(HOMO)
ν = -0.530



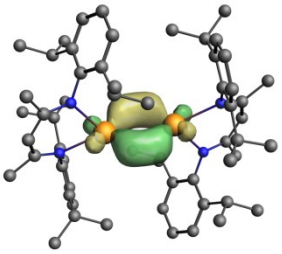


frag1-19A (LUMO)
ν = 0.076





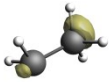
frag1-26A
ν = 0.045

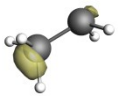


frag2-250A (LUMO+1)
ν = 0.662

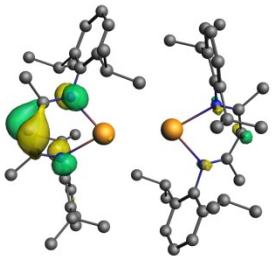
$\nu_2 = \pm 0.808$
$\Delta E_{orb(2)} = -55.3$ kcal/mol

$\nu_3 = \pm 0.323$
$\Delta E_{orb(3)} = -10.2$ kcal/mol



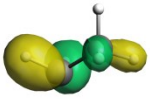


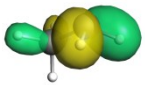
frag1-20A(LUMO+1)
$\nu = 0.021$



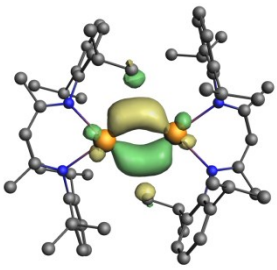
frag2-247A (HOMO-1)
$\nu = -0.015$

$\nu_4 = \pm 0.322$
$\Delta E_{orb(4)} = -9.7$ kcal/mol



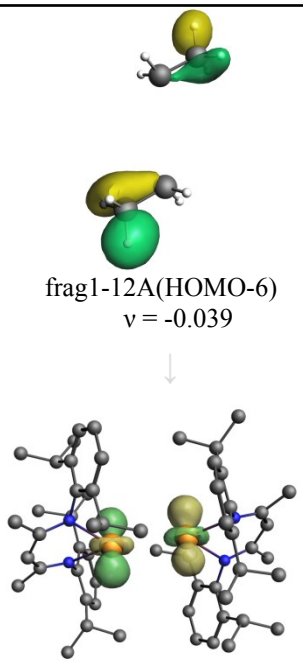


frag1-15A(HOMO-3)
$\nu = -0.030$



frag2-251A(LUMO+2)
$\nu = 0.074$

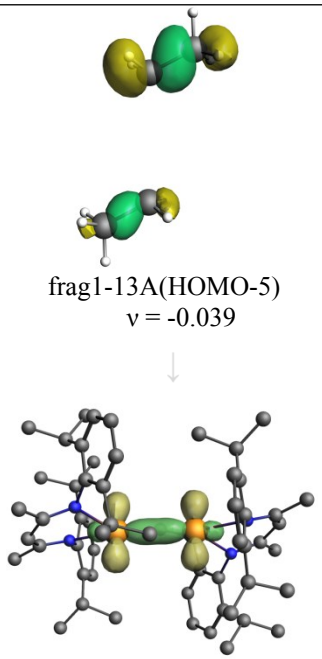
$\nu_5 = \pm 0.227$
$\Delta E_{orb(5)} = -7.8$ kcal/mol



frag1-12A(HOMO-6)
ν = -0.039

frag2-255A (LUMO+6)
ν = 0.068

$\nu_6 = \pm 0.222$
$\Delta E_{orb(6)} = -7.2$ kcal/mol

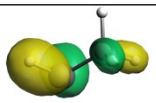


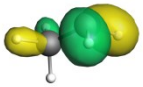
frag1-13A(HOMO-5)
ν = -0.039

f rag2-252A(LUMO+3)
ν = 0.032

$\nu_7 = \pm 0.195$

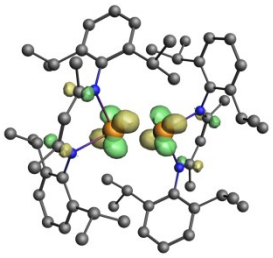
$\Delta E_{orb(7)} = -5.8$ kcal/mol





frag1-16A(HOMO-2)

$\nu = -0.029$



f rag2-253A(LUMO+4)

$\nu = 0.024$

Table S.3 EDA-NOCV results of transition state **TS3** using the doublet (D) fragments at the BP86/TZ2P+ level of theory. Energy values are given in kcal/mol.

Fragments Bonding	Frag1 (D) + Frag2 (D) electron-sharing bonding
ΔE_{int}	-63.2
ΔE_{Pauli}	102.0
ΔE_{elstat}[a]	-54.3(32.9%)
ΔE_{orb}[a]	-92.2(55.8%)
ΔE_{disp}[a]	-18.7(11.3%)
$\Delta E_{orb(\alpha 1)}$[b]	-58.3(63.2%)
$\Delta E_{orb(\beta 1)}$[b]	-14.9(16.2%)
$\Delta E_{orb(\alpha 2)}$[b]	-4.2(4.6%)
$\Delta E_{orb(\beta 2)}$[b]	-2.5(2.7%)
$\Delta E_{orb(\alpha 3)}$[b]	-1.8(2.0%)
$\Delta E_{orb(\beta 3)}$[b]	-1.7(1.8%)
$\Delta E_{orb(rest)}$ [b]	-8.8(9.5 %)

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

[b]The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}.

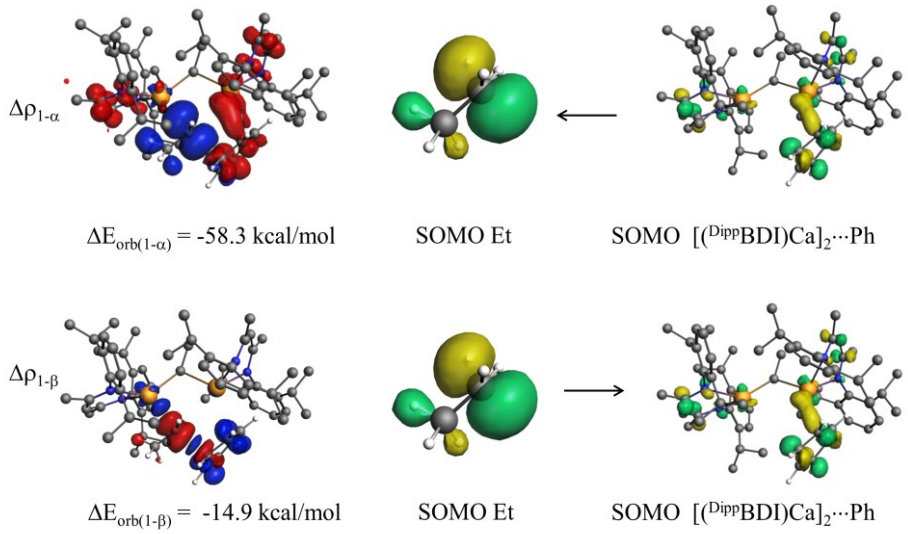
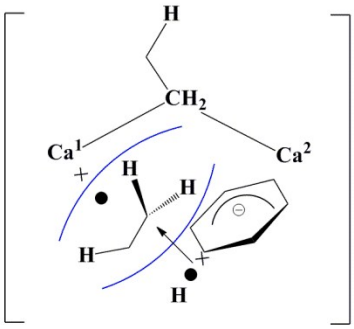
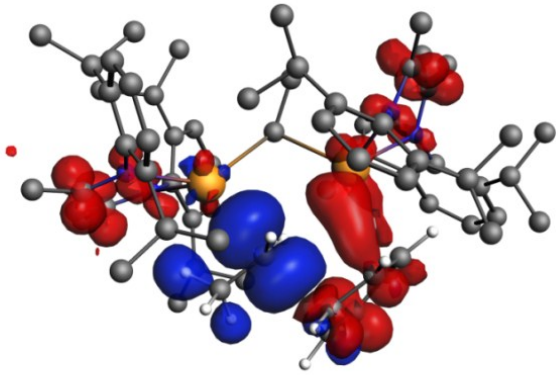


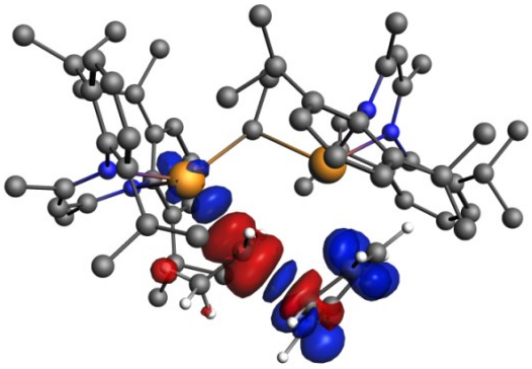
Figure S.11 Plot of deformation densities Δρ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) between fragments in transition state **TS3**, and shape of the most important interacting MOs of fragments. The direction of the charge flow is red to blue.

Figure S.12 Plot of deformation densities Δρ of the pairwise orbital interactions between the two fragments in transition state **TS3**, associated interaction energies ΔE_{orb} (in kcal/mol) and eigenvalues ν. The eigenvalues ν indicate the size of the charge flow, and the direction of charge flow is red→blue.

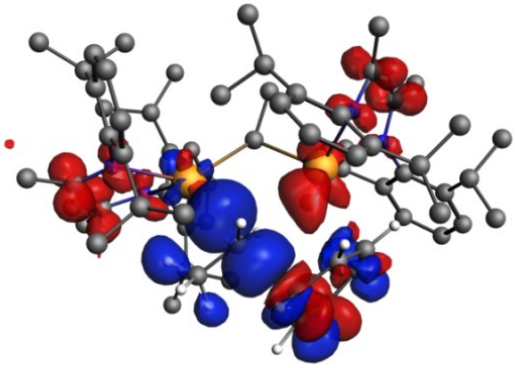




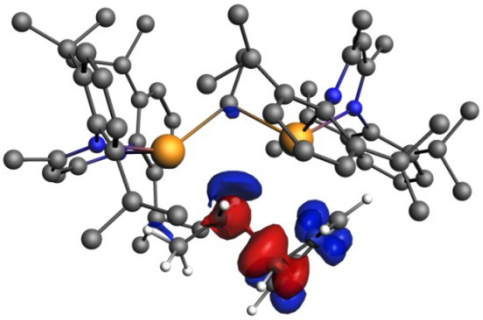
$\nu_{\alpha 1} = \pm 0.930$
$\Delta E_{orb(\alpha 1)} = -58.3$ kcal/mol



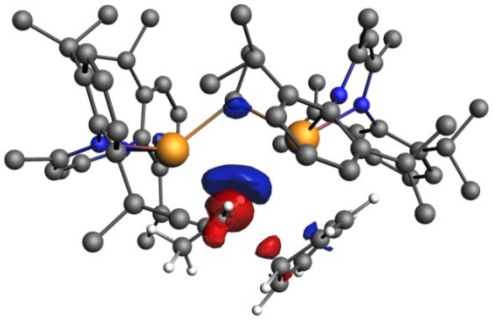
$\nu_{\beta 1} = \pm 0.454$
$\Delta E_{orb(\beta 1)} = -14.9$ kcal/mol



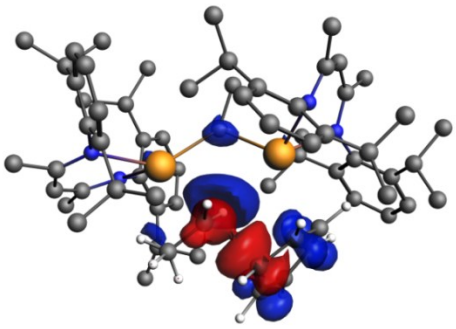
$\nu_{\alpha 1+\beta 1} = \pm 1.384$
$\Delta E_{orb(\alpha 1+\beta 1)} = -73.2$ kcal/mol



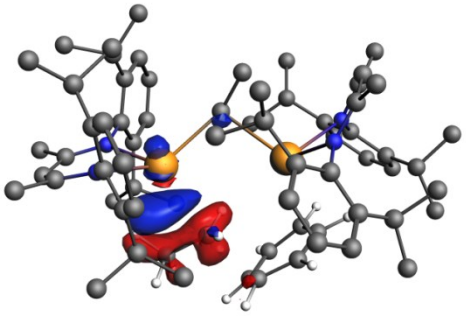
$\nu_{\alpha 2} = \pm 0.149$
$\Delta E_{orb(\alpha 2)} = -4.2$ kcal/mol



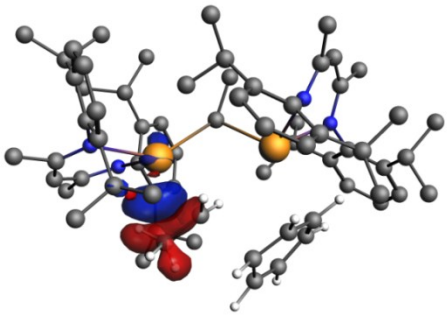
$\nu_{\beta 2} = \pm 0.119$
$\Delta E_{orb(\beta 2)} = -2.5$ kcal/mol



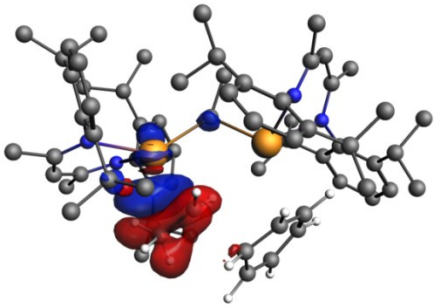
$\nu_{\alpha 2+\beta 2} = \pm 0.268$
$\Delta E_{orb(\alpha 2+\beta 2)} = -6.7$ kcal/mol



$\nu_{\alpha 3} = \pm 0.080$
$\Delta E_{orb(\alpha 1)} = -1.8$ kcal/mol

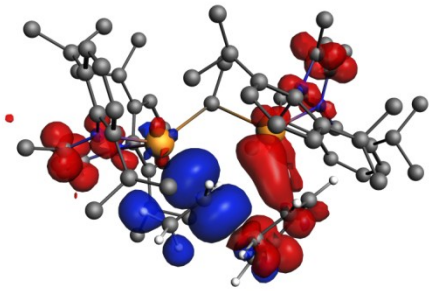
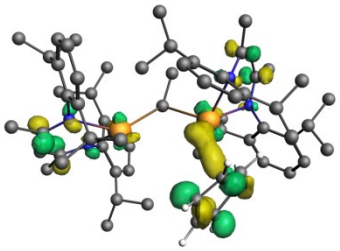
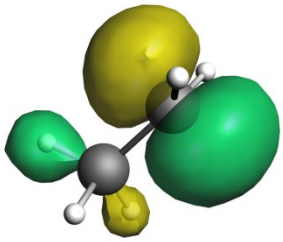
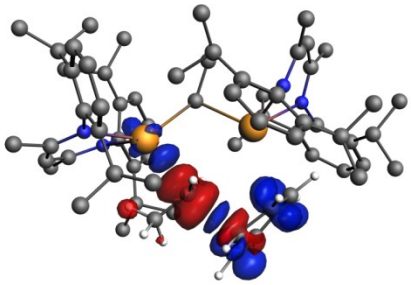
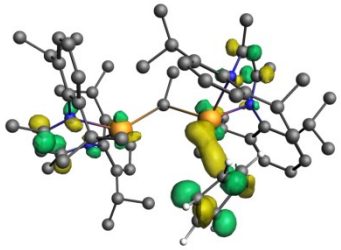
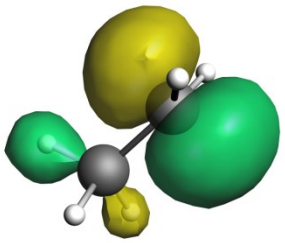


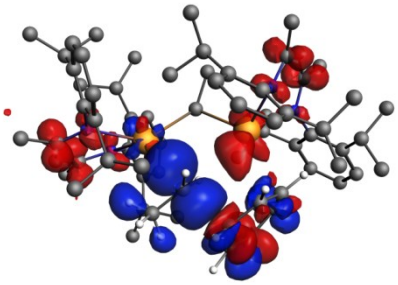
$\nu_{\beta 3} = \pm 0.078$
$\Delta E_{orb(\alpha 1)} = -1.7$ kcal/mol



$\nu_{\alpha 3+\beta 3} = \pm 0.158$
$\Delta E_{orb(\alpha 3+\beta 3)} = -3.5$ kcal/mol

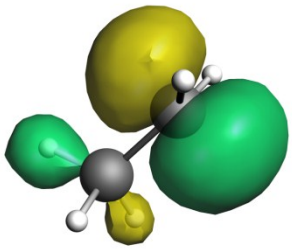
Figure S.13 Shape of the most important interacting MOs of fragments, plot of deformation densities Δρ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) between fragments in **TS3**. The direction of the charge flow is red to blue.

deformation densities Δρ	interacting MOs
	
$\nu_{\alpha 1} = \pm 0.930$ $\Delta E_{orb(\alpha 1)} = -58.3$ kcal/mol	frag1-280A(SOMO) ν = -0.902
	
	frag2-9A(SOMO) ν = 0.727
	
$\nu_{\beta 1} = \pm 0.454$ $\Delta E_{orb(\beta 1)} = -14.9$ kcal/mol	frag1-280A(SOMO) ν = 0.094
	
	frag2-9A(SOMO) ν = -0.254

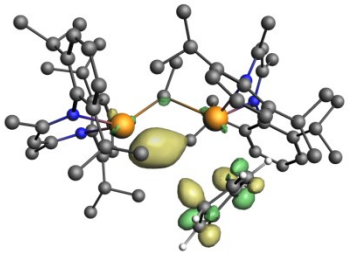


$\nu_{\alpha1+\beta1} = \pm 1.384$
$\Delta E_{orb(\alpha1+\beta1)} = -73.2$ kcal/mol

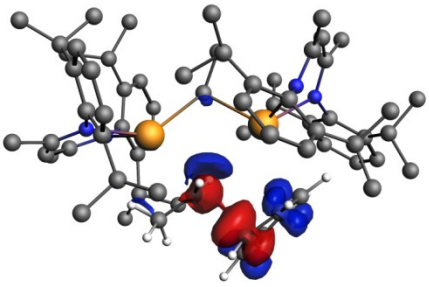
frag1-280A(SOMO)



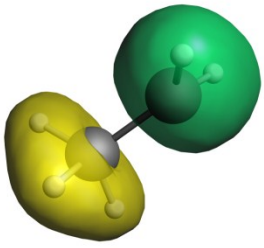
frag2-9A(SOMO)



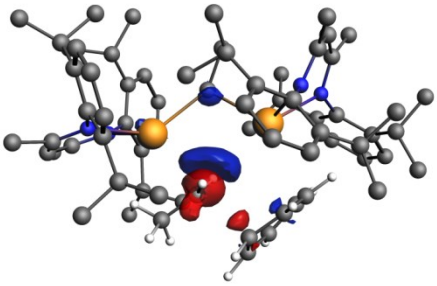
frag1-279A(LUMO)
$\nu = 0.029$



$\nu_{\alpha2} = \pm 0.149$
$\Delta E_{orb(\alpha2)} = -4.2$ kcal/mol



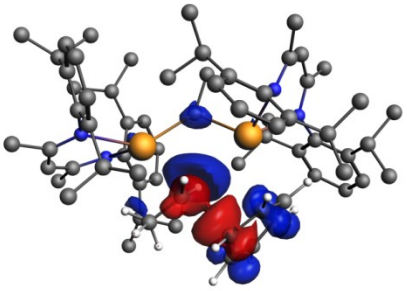
frag2-4A(SOMO-5)
$\nu = -0.009$



$\nu_{\beta 2} = \pm 0.119$
$\Delta E_{orb(\beta 2)} = -2.5$ kcal/mol

frag1-279A(LUMO)
ν = 0.021

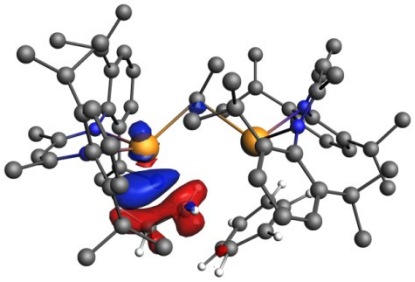
frag2-4A(SOMO-5)
ν = -0.008



$\nu_{(\alpha 2+\beta 2)} = \pm 0.268$
$\Delta E_{orb(\alpha 2+\beta 2)} = -6.7$ kcal/mol

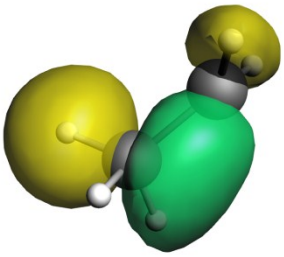
frag1-279A(LUMO)

frag2-4A(SOMO-5)

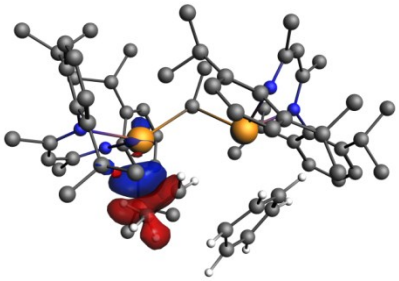


$\nu_{\alpha 3} = \pm 0.080$
$\Delta E_{orb(\alpha 3)} = -1.8$ kcal/mol

frag1-279A(LUMO)
ν = 0.008

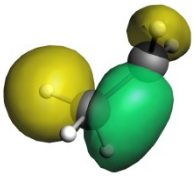


frag2-6A(SOMO-3)
ν = -0.018

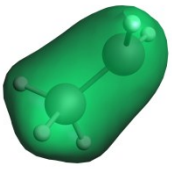


$\nu_{\beta 3} = \pm 0.078$
$\Delta E_{orb(\beta 3)} = -1.7$ kcal/mol

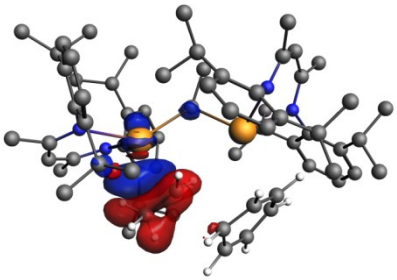
frag1-279A(LUMO)
ν = 0.009



frag2-6A(SOMO-3)
ν = -0.017



frag2-3A(SOMO-6)
ν = -0.009



$\nu_{\alpha 3+\beta 3} = \pm 0.158$

$\Delta E_{orb(\alpha 3+\beta 3)} = -3.5$ kcal/mol

frag1-279A(LUMO)

frag2-6A(SOMO-3)

frag2-3A(SOMO-6)

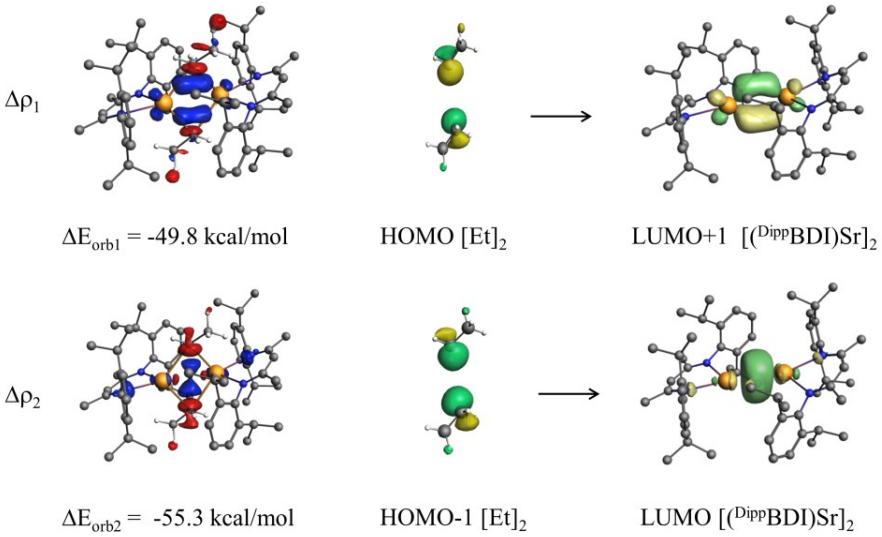


Figure S.14 Plot of deformation densities Δρ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) between fragments in strontium complex **6**, and shape of the most important interacting MOs of fragments. The direction of the charge flow is red to blue

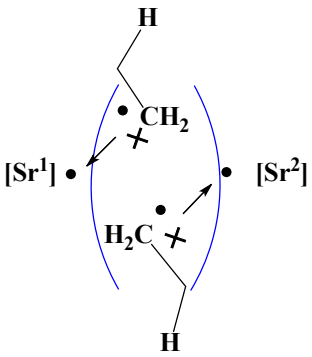
Table S.4 EDA-NOCV results of organostrontium complex **6** using the singlet (S) fragments and triplets (T) fragments at the BP86/TZ2P+ level of theory. Energy values are given in kcal/mol.

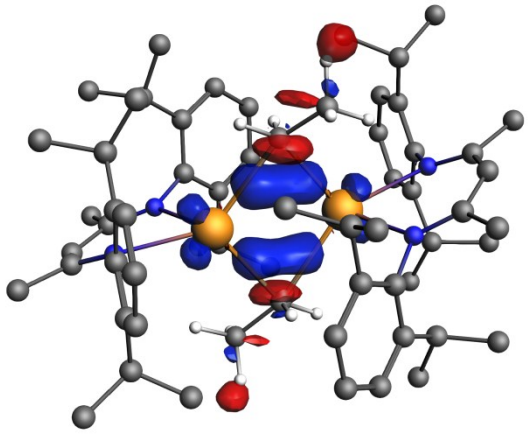
Fragments Bonding	Frag1 (S) + Frag2(S) dative bonding	Frag1 (S) + Frag2(T) dative bonding	Frag1(T) + Frag2(S) electron-sharing bond
ΔE_{int}	-505.0	-460.9	-114.8
ΔE_{Pauli}	182.7	299.6	335.6
ΔE_{elstat}[a]	-462.8 (67.3%)	-467.0(61.4%)	-199.1 (44.2%)
ΔE_{orb}[a]	-190.2 (27.7%)	-258.8(34.0%)	-216.6 (48.1%)
ΔE_{disp}	-34.7 (5.0%)	-34.7(4.6%)	-34.7 (7.7%)
ΔE_{orb1}[b]	-49.8 (26.2%)		
ΔE_{orb2}[b]	-40.0 (21.0%)		
ΔE_{orb3}[b]	-8.0 (4.2%)		
ΔE_{orb4}[b]	-7.8 (4.1%)		
ΔE_{orb5}[b]	-6.8 (3.6%)		
ΔE_{orb6}[b]	-7.4 (3.9%)		
ΔE_{orb7}[b]	-5.2 (2.7%)		
$\Delta E_{orb(rest)}$	- 65.2(34.3%)		

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

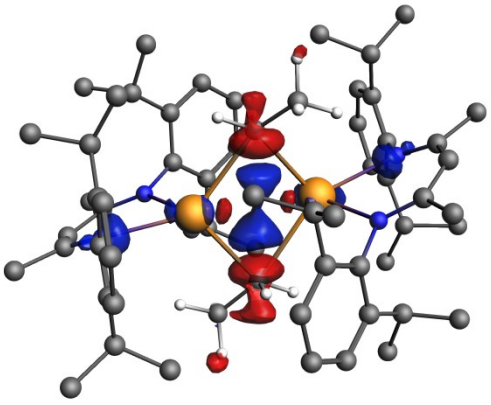
[b]The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}.

Figure S.15 Plot of deformation densities Δρ of the pairwise orbital interactions between the two fragments in complex **6** in associated interaction energies ΔE_{orb} (in kcal/mol) and eigenvalues ν. The eigenvalues ν indicate the size of the charge flow, and the direction of charge flow is red→blue.

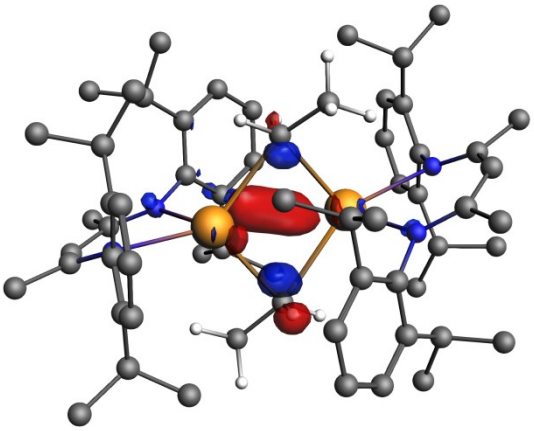




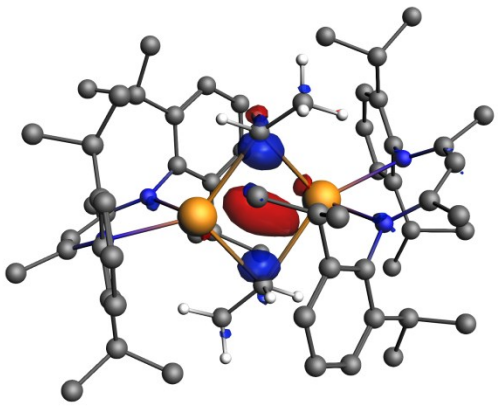
$\nu_1 = \pm 0.759$
$\Delta E_{orb(1)} = -49.8$ kcal/mol



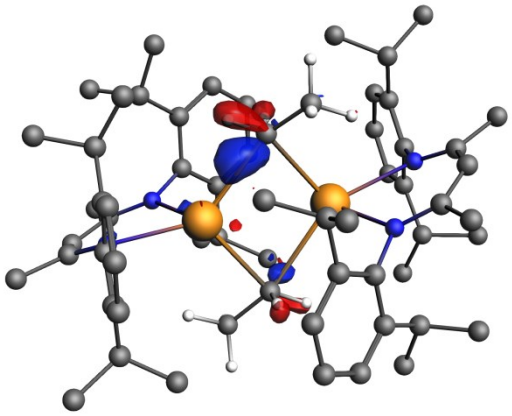
$\nu_2 = \pm 0.660$
$\Delta E_{orb(2)} = -40.0$ kcal/mol

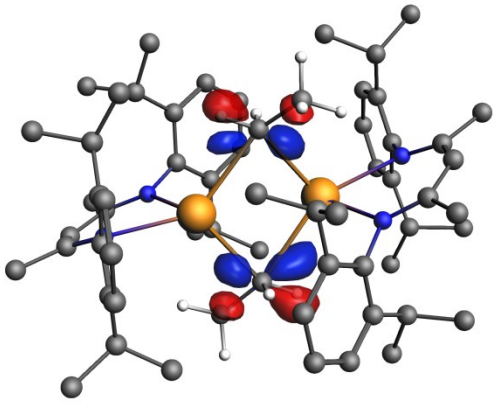


$\nu_3 = \pm 0.283$
$\Delta E_{orb(3)} = -8.0$ kcal/mol



$\nu_4 = \pm 0.275$
$\Delta E_{orb(4)} = -7.8$ kcal/mol



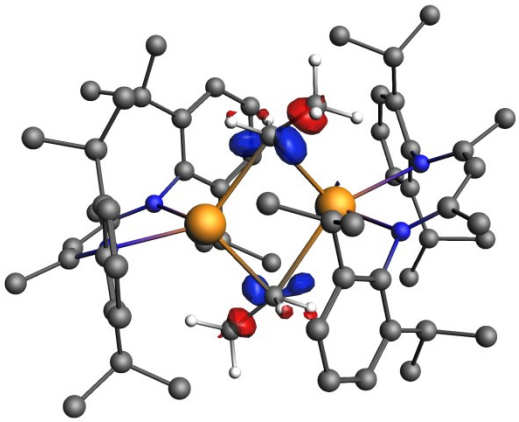


$\nu_5 = \pm 0.226$

$\nu_6 = \pm 0.217$

$\Delta E_{orb(5)}$ = -6.8 kcal/mol

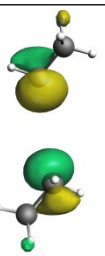
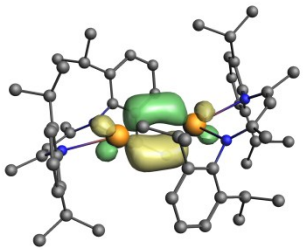
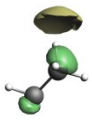
$\Delta E_{orb(6)}$ = -7.4 kcal/mol



$\nu_7 = \pm 0.186$

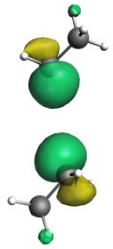
$\Delta E_{orb(7)}$ = -5.2 kcal/mol

Figure S.16 Shape of the most important interacting MOs of fragments, plot of deformation densities Δρ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) between fragments in complex **6**. The direction of the charge flow is red to blue.

deformation densities Δρ	interacting MOs
$\nu_1 = \pm 0.759$ $\Delta E_{orb(1)}$ = -49.8 kcal/mol	 frag1-18A(HOMO) ν =-0.483 ↓  frag2-268A(LUMO+1) ν = 0.312 +   frag1- 20A(LUMO+1) ν = 0.048

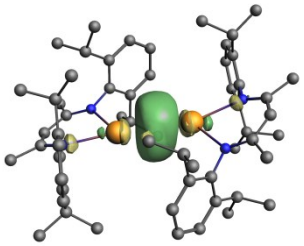
$\nu_2 = \pm 0.660$

$\Delta E_{orb(2)} = -40.0$ kcal/mol



frag1-17A(HOMO-1)

$\nu = -0.380$

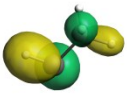


frag2-267A (LUMO)

$\nu = 0.436$

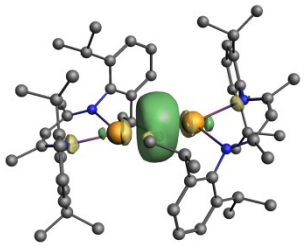
$\nu_3 = \pm 0.283$

$\Delta E_{orb(3)} = -8.0$ kcal/mol



frag1-15A(HOMO-3)

$\nu = -0.010$



frag2-269A (LUMO+2)

$\nu = 0.050$

frag1-15A(HOMO-3)

ν = -0.010

+

frag2-267A(LUMO)

ν = -0.011

↓

$\nu_4 = \pm 0.275$

$\Delta E_{orb(4)} = -7.8$ kcal/mol

frag1-17A(HOMO-1)

ν = 0.019

+

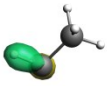
frag2-269A (LUMO+2)

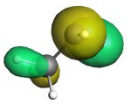
ν = 0.019

frag1-15A(HOMO-3)

ν = -0.011

+





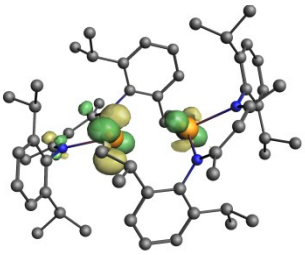
frag1-16A(HOMO-2)

ν = -0.038

↓

$\nu_5 = \pm 0.226$

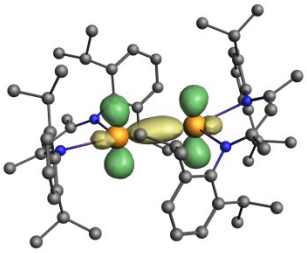
$\Delta E_{orb(5)} = -6.8$ kcal/mol



frag2-271A(LUMO+4)

ν = 0.018

+



frag2-270A (LUMO+3)

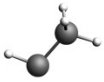
ν = 0.013

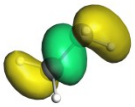
interacting MOs

frag1-15A(HOMO-3)

ν = -0.026

+





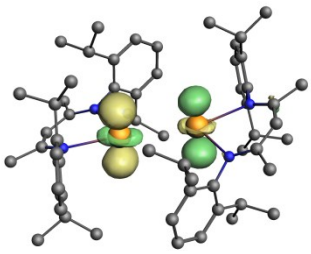
frag1-14A(HOMO-4)

ν = -0.017

↓

$\nu_6 = \pm 0.217$

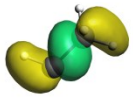
$\Delta E_{orb(6)} = -7.4$ kcal/mol

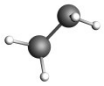


frag2-272A(LUMO+5)

ν = 0.070

interacting MOs





frag1-13A(HOMO-5)

ν = -0.017

+

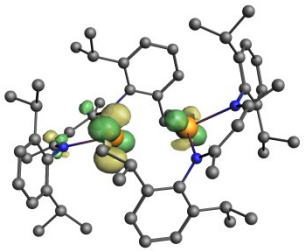
frag1-14A(HOMO-4)

ν = -0.013

↓

$\nu_7 = \pm 0.186$

$\Delta E_{orb(7)} = -5.2$ kcal/mol



frag2-271A(LUMO+4)

ν = 0.013

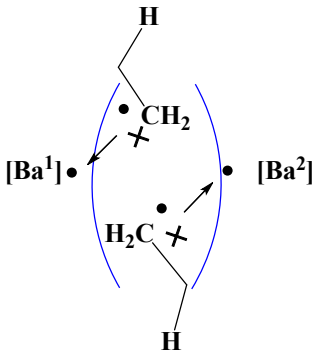
Table S.5 EDA-NOCV results of organobarium complex **7** using singlet (S) fragments and triplets (T) fragments at the BP86/TZ2P+ level of theory. Energy values are given in kcal/mol.

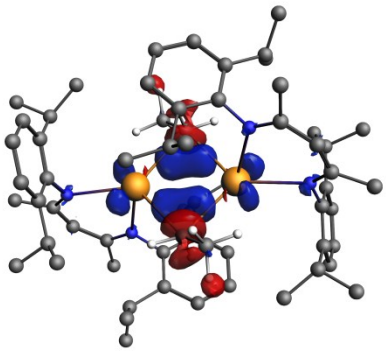
Fragments Bonding	Frag1 (S) + Frag2 (S) dative bonding	Frag1 (S) + Frag2 (T) dative bonding	Frag1 (S) + Frag2 (S) electron-sharing bonding
ΔE_{int}	-475.6	-401.3	-202.0
ΔE_{Pauli}	171.9	256.9	227.8
ΔE_{elstat}[a]	- 433.7(67.0%)	-436.4(66.3%)	-167.7 (39.0%)
ΔE_{orb}[a]	-179.7 (27.7%)	-187.7(28.5%)	-228.0 (53.0%)
ΔE_{disp}	-34.1 (5.3%)	-34.1 (5.2%)	-34.1 (8.0%)
ΔE_{orb1}[b]	-55.3(30.8%)		
ΔE_{orb2}[b]	-25.1 (14.0%)		
ΔE_{orb3}[b]	-8.3 (4.6%)		
ΔE_{orb4}[b]	-6.3(3.5%)		
ΔE_{orb5}[b]	-6.0(3.3%)		
ΔE_{orb6}[b]	-6.1(3.4%)		
ΔE_{orb7}[b]	-4.7(2.6%)		
$\Delta E_{orb(rest)}$	-67.9(37.8%)		

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$

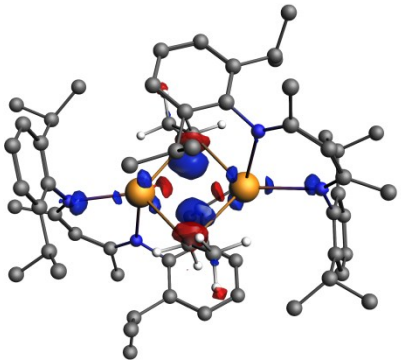
[b]The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}

Figure S.17 Plot of deformation densities $\Delta\rho_{1\text{-}7}$ of the pairwise orbital interactions between the two fragments in their singlet (S) states of complex **7**, associated interaction energies ΔE_{orb} (in kcal/mol) and eigenvalues ν. The eigenvalues ν indicate the size of the charge flow, and the direction of charge flow is red→blue.

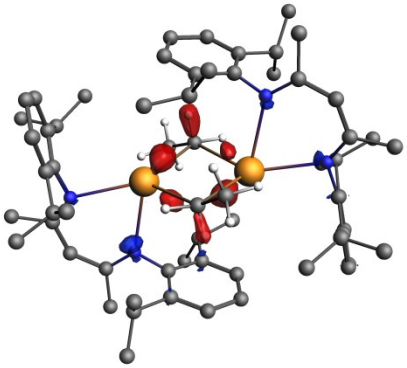




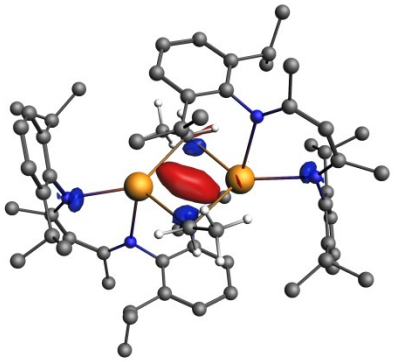
$\nu_1 = \pm 0.844$
$\Delta E_{orb(1)} = -55.3$ kcal/mol



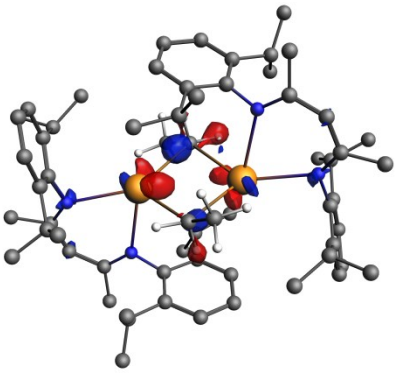
$\nu_2 = \pm 0.567$
$\Delta E_{orb(2)} = -25.1$ kcal/mol



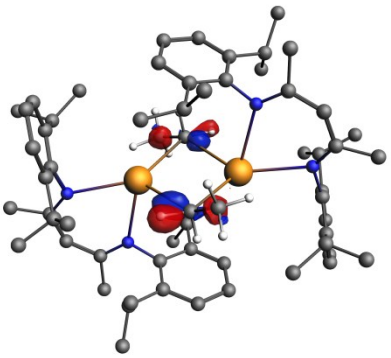
$\nu_3 = \pm 0.304$
$\Delta E_{orb(3)} = -8.3$ kcal/mol



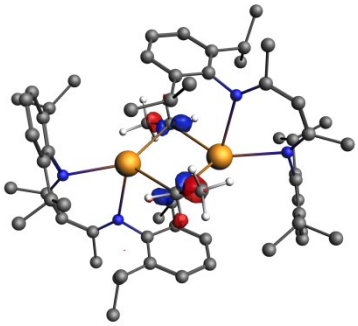
$\nu_4 = \pm 0.236$
$\Delta E_{orb(4)} = -6.3$ kcal/mol



$\nu_5 = \pm 0.225$
$\Delta E_{orb(5)} = -6.0$ kcal/mol

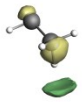
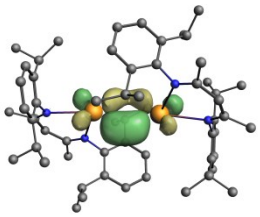
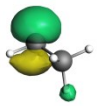
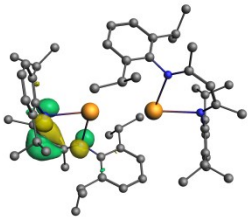


$\nu_6 = \pm 0.216$
$\Delta E_{orb(6)} = -6.1$ kcal/mol



$\nu_7 = \pm 0.188$
$\Delta E_{orb(7)} = -4.7$ kcal/mol

Figure S.18 Shape of the most important interacting MOs of fragments, plot of deformation densities Δρ of the pairwise orbital interactions and the associated interaction energies (ΔE_{orb}) between fragments in complex **7**. The direction of the charge flow is red to blue.

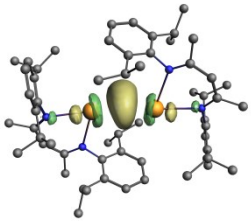
deformation densities Δρ	interacting MOs
$\nu_1 = \pm 0.844$ $\Delta E_{orb(1)} = -55.3$ kcal/mol	  frag1-20A(LUMO+1) ν = 0.037  frag2-285A（LUMO） ν = 0.493   frag1-18A(HOMO) ν = -0.547  frag2-283A(HOMO-1) ν = -0.025

Interacting MOs

frag1-19A(LUMO)

ν = 0.018

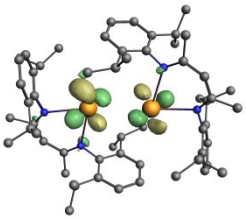
+



frag2-286A（LUMO+1）

ν = 0.164

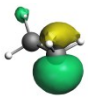
+

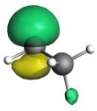


frag2-293A

ν = 0.015

↑





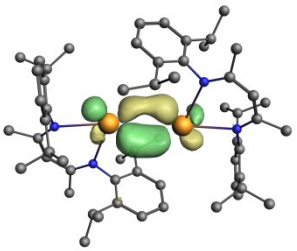
frag1-17A(HOMO-1)

ν = -0.234

$\nu_2 = \pm 0.567$

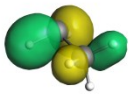
$\Delta E_{orb(2)} = -25.1$ kcal/mol

Interacting MOs



frag2-287A（LUMO+2）
ν = 0.064

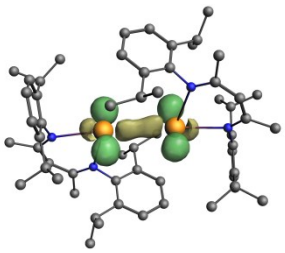
frag1-16A(HOMO-2)
ν = -0.009



frag1-15A(HOMO-3)
ν = -0.007

$\nu_3 = \pm 0.304$
$\Delta E_{orb(3)} = -8.3$ kcal/mol

Interacting MOs

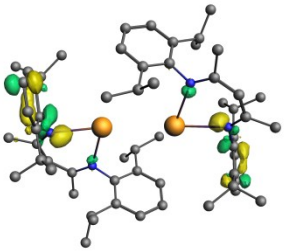


frag2-
288A（LUMO+3）
ν = 0.020

↑

frag1-16A(HOMO-2)
ν = -0.017

+



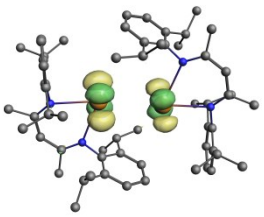
frag2-281A(HOMO-3)
ν = -0.011

$\nu_4 = \pm 0.236$
$\Delta E_{orb(4)} = -6.3$ kcal/mol

Interacting MOs

frag1-17A(HOMO-1)
ν = 0.010

+



frag2-289A(LUMO+4)
ν = 0.009

↑

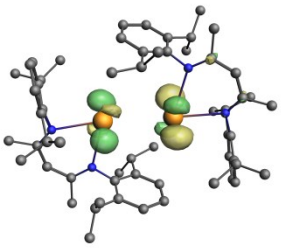
$\nu_5 = \pm 0.225$
$\Delta E_{orb(5)} = -6.0$ kcal/mol

frag1-16A(HOMO-2)
ν = -0.018

+

frag1-15A(HOMO-3)
ν = -0.010

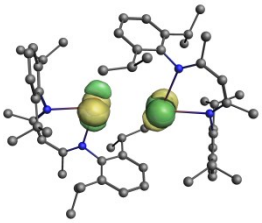
Interacting MOs



frag2-290A

ν = 0.025

+



frag2-291A

ν = 0.015

↑

frag1-12A(HOMO-6)

ν = -0.011

+

frag1-15A(HOMO-3)

ν = -0.014

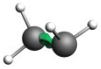
$\nu_6 = \pm 0.216$

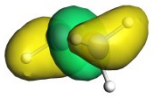
$\Delta E_{orb(6)} = -6.1$ kcal/mol

Interacting MOs

frag2-289A(LUMO+4)

ν = 0.017





$\nu_7 = \pm 0.188$

$\Delta E_{orb(7)} = -4.7$ kal/mol

frag1-13A(HOMO-5)

ν = -0.023

Table S.6 HOMO-LUMO gap of organocalcium complex **1**, organostrontium complex **6** and organobarium complex **7**.

Complex	HOMO-LUMO gap (eV)
organocalcim complex **1**	2．74
organostrontium complex **6**	2．60
organobarium complex **7**	2．18

Table S.7 Coordinates and energies (hatree) of the calculated structures at the BP86-D3BJ/def2-TZVPP/SMD//BP86-D3BJ/def2-SVP/SMD level.

1

Enthalpy: -3992.430097

Free energy: -3992.625726

C	4.050361	-1.692557	0.150800
C	4.432641	-1.661305	-1.228205
C	4.675747	-2.875973	-1.896601
C	4.516210	-4.109356	-1.246189
C	4.090905	-4.135190	0.088077
N	3.751880	-0.459202	0.792051
C	4.607780	0.118434	1.644389
C	5.877365	-0.612206	2.052937
C	4.574166	-0.322987	-1.948327
C	5.924452	0.350018	-1.631576
C	3.333591	-3.032827	2.239077
C	4.280621	-3.828244	3.156893
C	4.426564	1.412244	2.215792
C	3.546059	2.470649	1.862590
C	3.824912	3.826261	2.489607
N	2.519333	2.355847	1.003441
C	1.903595	3.524953	0.470468
C	0.745705	4.093404	1.078541
C	0.127931	5.205861	0.473529
C	0.636787	5.765059	-0.706861
C	1.763998	5.191100	-1.312127
C	2.404649	4.068729	-0.752242
C	0.129068	3.464052	2.321668
C	-0.260626	4.484764	3.402609
C	3.617156	3.453032	-1.445812
C	4.892892	4.280431	-1.198332
C	-1.082932	2.609867	1.909229
C	3.379787	3.242202	-2.950421
C	4.350990	-0.419762	-3.463898
C	1.916271	-3.636909	2.265742
Ca	1.509602	0.282418	0.463692
C	-0.456513	-0.817086	1.728321
C	0.443183	-0.503506	2.935837
Ca	-1.511303	-0.270570	-0.491195
N	-2.512279	-2.352773	-1.012719
C	-1.887304	-3.520556	-0.487369
C	-0.734278	-4.086051	-1.107120
C	-0.112204	-5.201895	-0.512701
C	-0.611552	-5.766152	0.669226
C	-1.731231	-5.192282	1.288548
C	-2.375833	-4.066919	0.739384
C	-0.127416	-3.449478	-2.351295
C	0.260524	-4.463845	-3.438756
C	-3.580041	-3.450242	1.446352
C	-4.866433	-4.256197	1.183709
C	-3.548549	-2.470944	-1.860263
C	-3.824225	-3.825352	-2.491764
C	-4.441101	-1.417480	-2.198004
C	-4.625497	-0.127131	-1.619356
C	-5.905851	0.595031	-2.009325
N	-3.763570	0.454803	-0.775966
C	-4.063440	1.684769	-0.128686
C	-4.429185	1.648111	1.254515
C	-4.673576	2.859484	1.928284
C	-4.531361	4.095203	1.278402
C	-4.121675	4.126751	-0.060707
C	-3.878959	2.940013	-0.783212
C	-4.550987	0.307329	1.973070
C	-5.904024	-0.370897	1.680798
C	-3.380539	3.033599	-2.222419
C	-4.342523	3.826452	-3.126848
C	-1.966450	3.644483	-2.265065
C	-4.297130	0.400367	3.483971
C	1.083041	-2.591696	-1.941235
C	-3.340884	-3.270551	2.954514
C	0.449972	0.836512	-1.755451
C	-0.450112	0.522166	-2.962649
H	-0.214385	1.083089	-3.897341
H	-2.944598	-4.169206	-3.075794
H	-3.993463	-4.599212	-1.715169
H	-4.704885	-3.800707	-3.160623
H	-5.219504	-1.700606	-2.921191
H	-6.694705	-0.115931	-2.320654
H	-6.290695	1.217780	-1.178235
H	-5.717114	1.280545	-2.8630

H	-0.896310	-2.771512	-2.778822
H	-0.591224	-5.122639	-3.707795
H	0.590044	-3.939184	-4.360054
H	1.101726	-5.114202	-3.118141
H	1.868486	-3.208385	-1.460720
H	1.534893	-2.069255	-2.809162
H	0.775937	-1.811575	-1.211720
H	0.785541	-5.633370	-0.983178
H	-0.120627	-6.645050	1.116240
H	-2.110752	-5.626969	2.226931
H	-3.728011	-2.444107	1.000962
H	-5.735812	-3.793330	1.697324
H	-5.105763	-4.303621	0.102608
H	-4.770016	-5.299479	1.554789
H	-2.433725	-2.662372	3.147632
H	-4.206457	-2.761984	3.427666
H	-3.216528	-4.242291	3.477718
H	-3.768606	-0.355963	1.538228
H	-6.747833	0.279003	1.996925
H	-6.027527	-0.593441	0.602723
H	-5.990010	-1.330665	2.231982
H	-4.236607	-0.613736	3.927102
H	-3.344603	0.922856	3.710716
H	-5.112764	0.936707	4.014021
H	-4.966458	2.839861	2.988587
H	-4.723155	5.032888	1.823600
H	-3.981334	5.097205	-0.563262
H	-3.316847	1.998705	-2.618757
H	-4.384767	4.897388	-2.834158
H	-4.009412	3.787890	-4.185554
H	-5.377284	3.429556	-3.078686
H	-1.255748	3.096450	-1.615997
H	-1.554987	3.636372	-3.296023
H	-1.974911	4.696693	-1.913527
H	4.020054	4.591338	1.710363
H	4.691018	3.796145	3.176992
H	2.937767	4.186045	3.052001
H	5.198438	1.692531	2.947035
H	6.667112	0.093776	2.373174
H	6.268902	-1.239366	1.228298
H	5.672197	-1.294126	2.905630
H	0.892513	2.784596	2.756552
H	0.592306	5.141101	3.673894
H	-0.597655	3.965302	4.324130
H	-1.097192	5.137283	3.074395
H	-1.863774	3.228056	1.423005
H	-1.540925	2.092738	2.777007
H	-0.776197	1.825486	1.184242
H	-0.774134	5.638949	0.934263
H	0.148424	6.640980	-1.162440
H	2.152476	5.622710	-2.248359
H	3.777508	2.457200	-0.981947
H	5.769908	3.815523	-1.696970
H	5.126874	4.357955	-0.117617
H	4.786156	5.313063	-1.595502
H	2.481446	2.617292	-3.131323
H	4.252479	2.738262	-3.415391
H	3.239768	4.202573	-3.490459
H	3.786159	0.345899	-1.531989
H	6.771045	-0.304051	-1.931204
H	6.028715	0.573267	-0.551759
H	6.025170	1.308914	-2.181815
H	4.307102	0.593048	-3.911854
H	3.400032	-0.936665	-3.709286
H	5.173868	-0.963555	-3.974689
H	4.981259	-2.861003	-2.953361
H	4.707093	-5.049485	-1.787482
H	3.937257	-5.103530	0.590818
H	3.269905	-1.996752	2.632298
H	4.321379	-4.899959	2.866902
H	3.934534	-3.785885	4.211281
H	5.317757	-3.436379	3.120899
H	1.218472	-3.090919	1.601258
H	1.489221	-3.618700	3.290202
H	1.925185	-4.691905	1.922832
H	0.517269	1.945850	-1.634127
H	1.493634	0.536166	-2.038371
H	-1.531415	0.751669	-2.782921
H	-1.499119	-0.511026	2.008537
H	-0.529351	-1.926288	1.609633
H	0.417530	0.576483	3.207464
H	1.522526	-0.743086	2.759353
C	3.849245	-2.945232	0.805580
H	-0.416052	-0.555985	-3.240549
H	0.200184	-1.056550	3.873349

2

Enthalpy: -1996.174913

Free energy: -1996.291461

Ca	2.776278	0.509412	0.221228
N	4.882920	-0.495454	0.524499
C	4.659049	-1.897544	0.497966
C	4.302797	-2.578603	1.702119
C	3.950733	-3.940361	1.634273
C	3.946578	-4.628833	0.412102
C	4.288160	-3.951518	-0.767655
C	4.644515	-2.589136	-0.750510
C	4.252825	-1.826519	3.030100
C	4.944054	-2.583086	4.176699
C	4.935327	-1.845828	-2.051633
C	5.956399	-2.572702	-2.943077
C	6.113793	0.004369	0.705802
C	7.274314	-0.958853	0.871053
C	6.404893	1.392626	0.764237
C	5.526387	2.499968	0.627487
C	6.120059	3.886641	0.795072
N	4.216522	2.380920	0.377779
C	3.376332	3.512472	0.224776
C	3.250485	4.143941	-1.052059
C	2.303398	5.173316	-1.205334
C	1.479609	5.572566	-0.139978
C	1.591192	4.933128	1.101982
C	2.529824	3.902135	1.307145
C	4.077585	3.645804	-2.235144
C	4.504185	4.762634	-3.200663
C	2.622223	3.197072	2.659022
C	2.943301	4.175411	3.803548
C	1.344810	2.388641	2.968099
C	3.319283	2.532952	-2.987616
C	2.796812	-1.480628	3.404266
C	3.623522	-1.572808	-2.816470
C	0.594287	-0.215063	-0.723029
C	0.315799	-1.696956	-0.394435
H	0.333020	-1.897842	0.704210
H	7.110940	-1.626712	1.742873
H	7.356726	-1.626049	-0.012583
H	8.236742	-0.430652	1.005947
H	7.458180	1.645928	0.949339
H	7.205444	3.850157	1.005092
H	5.956781	4.504054	-0.112426
H	5.617025	4.425097	1.625961
H	4.794298	-0.869334	2.882797
H	5.988511	-2.850852	3.915238
H	4.973728	-1.960884	5.096015
H	4.412506	-3.523093	4.436295
H	2.190202	-2.398590	3.553298
H	2.747509	-0.881266	4.337707
H	2.282589	-0.898763	2.608033
H	3.671898	-4.473715	2.557261
H	3.667761	-5.693798	0.377990
H	4.271265	-4.492859	-1.726927
H	5.370157	-0.862716	-1.775660
H	6.200640	-1.961224	-3.837280
H	6.903775	-2.771523	-2.400224
H	5.569433	-3.547153	-3.309910
H	2.870778	-1.044034	-2.190249
H	3.805687	-0.954708	-3.720712
H	3.145663	-2.520716	-3.143257
H	4.999894	3.186260	-1.824034
H	3.640558	5.197919	-3.746676
H	5.018003	5.590165	-2.668801
H	5.203210	4.366123	-3.966558
H	3.931202	2.122908	-3.818294
H	3.055733	1.682735	-2.323277
H	2.367370	2.913569	-3.413960
H	2.198670	5.671107	-2.181956
H	0.743210	6.378847	-0.283673
H	0.935838	5.240890	1.933011
H	3.470366	2.483000	2.590558
H	2.126927	4.913770	3.953823
H	3.079452	3.632562	4.762839
H	3.873962	4.743781	3.599360
H	1.081485	1.674081	2.156322
H	1.454830	1.808118	3.907935
H	0.462603	3.053063	3.084159
H	0.491960	-0.068008	-1.828562
H	-0.241753	0.405615	-0.305141
H	1.087562	-2.376878	-0.826947
H	-0.668341	-2.101683	-0.750241

Benzene

Enthalpy: -232.2483381

Free energy: -232.2813161

C	-0.229766	-0.898639	0.000063
C	1.176685	-0.898780	0.000511
C	1.879920	0.319217	-0.000044
C	1.176773	1.537238	-0.001048
C	-0.229677	1.537379	-0.001497
C	-0.932913	0.319381	-0.000941
H	-0.780970	-1.852655	0.000498
H	1.727586	-1.853003	0.001298
H	2.981725	0.319446	0.000306
H	1.727978	2.491253	-0.001484
H	-0.780579	2.491601	-0.002283
H	-2.034717	0.319152	-0.001292

IM1

Enthalpy: -2228.441835

Free energy: -2228.566393

Ca	0.044206	1.232664	0.131138
N	1.525168	-0.291531	-0.939593
C	2.785022	-0.550402	-0.334037
C	3.857708	0.387674	-0.412401
C	5.058953	0.111961	0.273751
C	5.216244	-1.056671	1.028193
C	4.149205	-1.963597	1.125359
C	2.926905	-1.729862	0.465910
C	3.730829	1.693682	-1.190603
C	4.780230	1.808917	-2.312304
C	1.762291	-2.707661	0.604853
C	1.659418	-3.660319	-0.603944
C	1.283114	-0.636040	-2.214654
C	2.436601	-1.079059	-3.100189
C	-0.003401	-0.621035	-2.821975
C	-1.304885	-0.539270	-2.248715
C	-2.435968	-0.989903	-3.162265
N	-1.563137	-0.129780	-0.998039
C	-2.813255	-0.375134	-0.374411
C	-3.165156	-1.695121	0.049541
C	-4.367481	-1.890366	0.758168
C	-5.212659	-0.819215	1.073453
C	-4.858894	0.476037	0.667303
C	-3.675619	0.723482	-0.055690
C	-2.258613	-2.896778	-0.203408
C	-2.937786	-3.959911	-1.087683
C	-3.371831	2.129993	-0.566817
C	-3.884917	2.298919	-2.010813
C	-3.912279	3.248694	0.335437
C	-1.796267	-3.520423	1.125574
C	3.814743	2.906178	-0.244033
C	1.805245	-3.511045	1.914004
C	0.367177	3.567699	-0.620669
C	-0.731252	4.602850	-0.912744
H	-1.455413	4.242653	-1.679138
H	3.154387	-1.713923	-2.543872
H	2.083547	-1.631735	-3.991241
H	3.004406	-0.192244	-3.453968
H	-0.000998	-0.890057	-3.889009
H	-2.367810	-2.078859	-3.365944
H	-3.433648	-0.781265	-2.733150
H	-2.356925	-0.479338	-4.144022
H	2.726053	1.703025	-1.662346
H	4.761556	0.928819	-2.987271
H	4.598352	2.715201	-2.927529
H	5.809400	1.887850	-1.901094
H	4.814616	2.976129	0.235372
H	3.631471	3.853244	-0.791473
H	3.060154	2.841924	0.565957
H	5.890635	0.832453	0.210323
H	6.164867	-1.259217	1.550358
H	4.273391	-2.872992	1.732179
H	0.837093	-2.088548	0.598357
H	0.821301	-4.376652	-0.470846
H	1.477578	-3.112441	-1.548194
H	2.592625	-4.251218	-0.723458
H	1.932448	-2.859454	2.803585
H	0.868894	-4.088527	2.046806
H	2.636998	-4.247063	1.921077
H	-1.355237	-2.533638	-0.733746
H	-3.804661	-4.424820	-0.570345
H	-3.313316	-3.528553	-2.036954
H	-2.227049	-4.774999	-1.340783
H	-1.097304	-4.363047	0.944817
H	-1.279752	-2.775031	1.762956
H	-2.651932	-3.921214	1.709428
H	-4.640043	-2.909169	1.078311
H	-6.145969	-0.990857	1.632743
H	-5.527941	1.315648	0.908660
H	-2.266648	2.253756	-0.619093
H	-4.986434	2.159786	-2.053948
H	-3.649629	3.312309	-2.398364

H	-3.424171	1.560258	-2.695088
H	-3.565426	3.139289	1.384382
H	-3.568673	4.235517	-0.033159
H	-5.022372	3.276252	0.346764
H	0.977554	3.434069	-1.553674
H	1.093073	4.032309	0.096235
H	-0.370353	5.596884	-1.287925
H	-1.336843	4.829811	-0.005262
C	-1.069386	0.482600	3.208261
C	0.087984	-0.304091	3.029890
C	1.362532	0.300646	3.015678
C	1.477483	1.696860	3.173545
C	0.321011	2.486097	3.340773
C	-0.951022	1.878722	3.365021
H	-2.062755	0.007145	3.215209
H	-0.002610	-1.393695	2.903090
H	2.263829	-0.313889	2.865078
H	2.471103	2.170604	3.156635
H	0.411471	3.577781	3.449382
H	-1.853350	2.494976	3.499697

TS1

Enthalpy: -2228.403202

Free energy: -2228.526156

Ca	-0.038662	-0.922741	0.223413
N	-1.568915	0.314303	-1.055561
C	-2.855928	0.322057	-0.450457
C	-3.674733	-0.850407	-0.518432
C	-4.901327	-0.858004	0.174017
C	-5.324873	0.249973	0.923639
C	-4.513387	1.389616	0.992927
C	-3.275638	1.447924	0.321716
C	-3.244569	-2.049938	-1.361806
C	-3.539131	-1.829963	-2.858590
C	-2.411784	2.700326	0.453880
C	-3.130744	3.954206	-0.078845
C	-1.335219	0.989290	-2.190756
C	-2.484218	1.628098	-2.956242
C	-0.043790	1.224503	-2.726952
C	1.237168	1.097969	-2.126907
C	2.362857	1.780766	-2.892826
N	1.480551	0.466010	-0.967803
C	2.751211	0.588727	-0.330701
C	2.900676	1.581184	0.690720
C	4.133615	1.686220	1.362634
C	5.201605	0.826269	1.064304
C	5.035503	-0.166905	0.091964
C	3.821695	-0.312857	-0.611914
C	1.735088	2.501069	1.053199
C	1.590626	3.681369	0.071822
C	3.698277	-1.420051	-1.656626
C	4.499826	-1.098415	-2.934115
C	4.141807	-2.787588	-1.101075
C	1.799256	3.019616	2.497813
C	-3.840977	-3.381424	-0.884996
C	-1.961446	2.911112	1.911107
C	-0.428155	-3.728006	0.322681
C	0.757233	-3.273573	-0.465703
H	0.618867	-2.546161	-1.347778
H	-3.468277	1.206767	-2.677726
H	-2.516666	2.719648	-2.753202
H	-2.337755	1.511869	-4.048824
H	-0.041136	1.747806	-3.695264
H	2.067609	2.802208	-3.206427
H	3.296162	1.847758	-2.304605
H	2.577900	1.214828	-3.823708
H	-2.138494	-2.140074	-1.262122
H	-3.000288	-0.951208	-3.260338
H	-3.224255	-2.714477	-3.451833
H	-4.625353	-1.672171	-3.031394
H	-4.934752	-3.437940	-1.071925
H	-3.374546	-4.225227	-1.433390
H	-3.668699	-3.548797	0.197626
H	-5.542297	-1.750935	0.126943
H	-6.288870	0.221260	1.455839
H	-4.845057	2.256733	1.586959
H	-1.500499	2.546530	-0.159194
H	-2.447041	4.829302	-0.083328
H	-3.499753	3.804898	-1.113622
H	-4.006446	4.220479	0.550811
H	-1.401252	2.034977	2.295398
H	-1.306523	3.802893	2.000300
H	-2.829106	3.068196	2.586295
H	0.808886	1.891076	0.946536
H	2.520006	4.289143	0.043268
H	1.373595	3.340425	-0.957619
H	0.759250	4.348009	0.384378
H	0.853753	3.534067	2.763392

H	1.961617	2.204656	3.232779
H	2.615672	3.759894	2.635217
H	4.262870	2.452125	2.141434
H	6.159160	0.925740	1.599440
H	5.868892	-0.852111	-0.130535
H	2.625533	-1.486862	-1.937046
H	5.587657	-1.040441	-2.715051
H	4.353882	-1.890566	-3.699074
H	4.199704	-0.133488	-3.384536
H	3.653830	-3.023480	-0.134674
H	3.894681	-3.600334	-1.815573
H	5.239793	-2.822844	-0.936939
H	-1.043816	-4.492820	-0.189858
H	-1.094445	-2.975193	0.796674
H	1.270885	-4.128401	-0.950142
H	1.557247	-2.789885	0.170267
C	1.407742	-0.966178	2.724882
C	0.177095	-0.300681	2.963312
C	-0.984680	-1.074078	3.253333
C	-0.916263	-2.471095	3.253846
C	0.295137	-3.146630	2.925060
C	1.470482	-2.372050	2.712384
H	2.323857	-0.377525	2.555402
H	0.143966	0.797110	3.019502
H	-1.935634	-0.567050	3.483816
H	-1.820308	-3.061619	3.471100
H	0.351588	-4.239425	2.980657
H	2.435979	-2.871433	2.537207

IM2’

Enthalpy: -2228.453144

Free energy: -2228.577202

Ca	-0.013976	0.351515	-0.447696
N	-1.559374	-0.685359	1.026921
C	-2.823977	-0.331970	0.498982
C	-3.315659	0.992668	0.719903
C	-4.502613	1.389313	0.074232
C	-5.193830	0.512306	-0.775208
C	-4.697346	-0.780870	-0.997497
C	-3.513806	-1.225469	-0.377545
C	-2.564858	1.935245	1.660697
C	-2.842608	1.591498	3.138514
C	-2.931167	-2.601585	-0.695480
C	-4.000040	-3.695778	-0.846170
C	-1.426118	-1.536828	2.050427
C	-2.659230	-2.082565	2.753812
C	-0.172637	-2.005941	2.521398
C	1.120502	-1.790029	1.980191
C	2.282532	-2.452364	2.701547
N	1.355239	-1.037474	0.896603
C	2.665911	-0.871931	0.381531
C	3.025439	-1.566768	-0.815333
C	4.285537	-1.313660	-1.390589
C	5.173185	-0.390130	-0.816966
C	4.799637	0.310352	0.339578
C	3.549649	0.093784	0.950078
C	2.044387	-2.555688	-1.442764
C	2.076883	-3.921310	-0.728212
C	3.100562	0.938860	2.139932
C	4.201066	1.150928	3.190767
C	2.533247	2.285790	1.647305
C	2.223647	-2.730261	-2.957410
C	-2.832911	3.422516	1.394226
C	-2.034058	-2.536314	-1.947599
C	0.216064	4.284799	-0.897158
C	1.447660	5.192330	-0.852005
H	1.360109	5.956907	-0.051735
H	-3.528659	-1.404094	2.655925
H	-2.956583	-3.059183	2.313136
H	-2.458377	-2.260819	3.828633
H	-0.213576	-2.665326	3.400593
H	1.942467	-3.303887	3.321440
H	3.055021	-2.807832	1.991406
H	2.785150	-1.726178	3.377262
H	-1.474132	1.754900	1.502378
H	-2.532834	0.558650	3.387592
H	-2.291497	2.279737	3.813980
H	-3.925987	1.686823	3.364242
H	-3.869243	3.709961	1.671691
H	-2.150155	4.052415	2.001275
H	-2.679708	3.685950	0.328698
H	-4.896650	2.403779	0.235383
H	-6.120241	0.841295	-1.271829
H	-5.241103	-1.458667	-1.674152
H	-2.274703	-2.891442	0.148266
H	-3.522263	-4.692526	-0.949681
H	-4.676518	-3.732216	0.032890
H	-4.629048	-3.543990	-1.748921

H	-1.204799	-1.807860	-1.826181
H	-1.571132	-3.523122	-2.159124
H	-2.610854	-2.226713	-2.844472
H	1.022393	-2.144888	-1.269851
H	3.089548	-4.373964	-0.788712
H	1.805656	-3.831700	0.341317
H	1.358564	-4.628071	-1.195658
H	1.379678	-3.313736	-3.379989
H	2.260855	-1.756983	-3.487593
H	3.154097	-3.284736	-3.203876
H	4.577343	-1.842066	-2.310703
H	6.154611	-0.206088	-1.281898
H	5.491407	1.050716	0.771940
H	2.265685	0.401202	2.632312
H	5.037092	1.770235	2.801779
H	3.794709	1.676603	4.080204
H	4.630149	0.185608	3.530838
H	1.745384	2.142334	0.875239
H	2.090516	2.872778	2.479706
H	3.324169	2.903806	1.172731
H	-0.699066	4.910895	-0.994032
H	0.109073	3.750224	0.076518
H	1.583604	5.730982	-1.814697
H	2.379966	4.621286	-0.659254
C	1.309011	1.055168	-2.677593
C	0.064122	0.504755	-3.121056
C	-1.123619	1.209973	-2.740083
C	-1.063210	2.419987	-2.056635
C	0.215920	3.252925	-2.045014
C	1.372813	2.258590	-1.979371
H	2.228876	0.450729	-2.769455
H	0.018683	-0.433089	-3.692833
H	-2.107510	0.727672	-2.881965
H	-1.998890	2.888521	-1.706299
H	0.288078	3.865371	-2.992537
H	2.348593	2.595364	-1.593245

IM2

Enthalpy: -2228.454087

Free energy: -2228.578356

Ca	0.029104	0.233925	-0.495359
N	-1.255572	-1.360915	0.693888
C	-2.601158	-0.980484	0.465418
C	-3.132302	0.124606	1.200546
C	-4.429072	0.578027	0.892907
C	-5.184180	-0.021631	-0.126935
C	-4.641133	-1.083053	-0.865990
C	-3.351761	-1.578177	-0.590933
C	-2.284884	0.792014	2.283537
C	-2.258102	-0.029536	3.587994
C	-2.729706	-2.672622	-1.456310
C	-3.719027	-3.786001	-1.836113
C	-0.950665	-2.459008	1.396249
C	-2.065553	-3.339520	1.936252
C	0.380890	-2.870351	1.670843
C	1.594742	-2.235672	1.307113
C	2.885284	-2.833088	1.834692
N	1.656938	-1.133705	0.546535
C	2.889044	-0.477812	0.293795
C	3.616100	-0.769158	-0.899903
C	4.712942	0.046658	-1.239209
C	5.104698	1.115890	-0.418692
C	4.409338	1.369991	0.773052
C	3.305141	0.583575	1.154026
C	3.190508	-1.932054	-1.793948
C	4.383578	-2.781322	-2.265701
C	2.544545	0.878216	2.445467
C	3.477091	0.998521	3.662833
C	1.659594	2.131778	2.302411
C	2.352575	-1.450483	-2.994131
C	-2.677455	2.247447	2.572444
C	-2.079488	-2.063127	-2.714582
C	-0.677888	4.831388	-1.503151
C	-1.958473	5.551298	-1.072838
H	-2.074146	6.529081	-1.586373
H	-2.934695	-2.738238	2.269483
H	-2.438901	-4.022612	1.142388
H	-1.716062	-3.967944	2.777618
H	0.481874	-3.782010	2.276580
H	2.710872	-3.774878	2.388208
H	3.598284	-3.031881	1.007504
H	3.396165	-2.118136	2.514261
H	-1.234447	0.795250	1.906992
H	-1.832201	-1.038801	3.430871
H	-1.636295	0.477546	4.356252
H	-3.282050	-0.147255	4.001831
H	-3.664222	2.316932	3.077349
H	-1.935492	2.716020	3.251322

H	-2.724688	2.858712	1.648756
H	-4.856433	1.423144	1.452957
H	-6.195503	0.349857	-0.355689
H	-5.231692	-1.533009	-1.679678
H	-1.912209	-3.136831	-0.868792
H	-3.192842	-4.612530	-2.358175
H	-4.219348	-4.212229	-0.941831
H	-4.512788	-3.423728	-2.523474
H	-1.333162	-1.279725	-2.461504
H	-1.554342	-2.838021	-3.312221
H	-2.838061	-1.581058	-3.366710
H	2.533025	-2.583753	-1.181975
H	5.042372	-2.223760	-2.964720
H	5.008715	-3.115650	-1.411845
H	4.030379	-3.685921	-2.803953
H	2.028876	-2.305927	-3.624014
H	1.431086	-0.913028	-2.681216
H	2.928851	-0.751737	-3.636842
H	5.275104	-0.158499	-2.164074
H	5.960976	1.746825	-0.704872
H	4.730667	2.200511	1.422081
H	1.864430	0.020832	2.626002
H	4.142413	1.885212	3.590309
H	2.887763	1.106169	4.597899
H	4.123661	0.102911	3.769236
H	0.978071	2.059585	1.428103
H	1.037558	2.291865	3.207862
H	2.271115	3.044753	2.141087
H	0.209204	5.476262	-1.303304
H	-0.690802	4.649258	-2.600937
H	-1.965936	5.748645	0.022191
H	-2.861596	4.948544	-1.306889
C	-1.495611	1.648903	-2.218497
C	-0.259989	1.414118	-2.903480
C	0.917593	2.000399	-2.335460
C	0.860813	2.810113	-1.203577
C	-0.455500	3.465336	-0.792438
C	-1.562186	2.453130	-1.083362
H	-2.392834	1.077163	-2.515231
H	-0.214428	0.803322	-3.816430
H	1.907270	1.702741	-2.725579
H	1.799728	3.167302	-0.748331
H	-0.435414	3.683545	0.303127
H	-2.511576	2.509160	-0.527386

TS2

Enthalpy: -2228.438030

Free energy: -2228.562784

Ca	-0.004878	0.669096	-0.226120
N	-1.531208	-0.589377	1.064129
C	-2.807886	-0.449281	0.467874
C	-3.491288	0.804913	0.572908
C	-4.706971	0.974031	-0.117884
C	-5.244704	-0.052916	-0.909091
C	-4.556660	-1.268156	-1.028688
C	-3.337293	-1.488246	-0.358332
C	-2.907558	1.923379	1.435546
C	-3.092433	1.642292	2.939599
C	-2.570524	-2.789847	-0.585699
C	-3.439434	-4.038404	-0.355413
C	-1.333497	-1.389977	2.119582
C	-2.523821	-2.024564	2.820019
C	-0.051593	-1.736538	2.621436
C	1.228067	-1.523732	2.043834
C	2.411575	-2.163269	2.751046
N	1.434123	-0.809886	0.929003
C	2.709924	-0.746223	0.313447
C	2.933617	-1.537654	-0.858548
C	4.156186	-1.405980	-1.543395
C	5.139106	-0.502905	-1.106855
C	4.901126	0.286816	0.025966
C	3.697787	0.183978	0.752956
C	1.842692	-2.489425	-1.346115
C	1.814257	-3.803099	-0.539793
C	3.457248	1.089389	1.958755
C	4.616634	1.030728	2.970518
C	3.174277	2.539070	1.517855
C	1.910698	-2.786319	-2.850676
C	-3.437708	3.319814	1.083466
C	-1.944172	-2.804781	-1.993920
C	0.649574	4.495997	-1.236205
C	-0.474226	5.217642	-0.496778
H	-0.181008	6.258990	-0.250621
H	-3.429763	-1.390180	2.757796
H	-2.776459	-2.997553	2.346511
H	-2.297906	-2.229386	3.884844
H	-0.057383	-2.346682	3.536204
H	2.092780	-2.969721	3.438567

H	3.142305	-2.576103	2.027184
H	2.958140	-1.404234	3.351099
H	-1.804162	1.941953	1.255850
H	-2.606778	0.695769	3.243606
H	-2.645440	2.456879	3.547761
H	-4.171167	1.574826	3.196395
H	-4.506773	3.439257	1.361313
H	-2.871154	4.094831	1.638571
H	-3.341411	3.542132	0.001158
H	-5.246844	1.928928	-0.037623
H	-6.197638	0.099959	-1.440049
H	-4.971648	-2.064636	-1.667417
H	-1.732942	-2.822605	0.139630
H	-2.825562	-4.961418	-0.420838
H	-3.923427	-4.021615	0.642888
H	-4.246817	-4.128128	-1.113105
H	-1.272020	-1.935384	-2.146285
H	-1.348976	-3.728139	-2.155288
H	-2.724562	-2.762619	-2.783649
H	0.873946	-1.979843	-1.137786
H	2.782868	-4.340559	-0.624273
H	1.611298	-3.624303	0.533407
H	1.017020	-4.477358	-0.919117
H	0.997443	-3.323314	-3.179719
H	1.997359	-1.861935	-3.457532
H	2.775053	-3.435443	-3.106820
H	4.345159	-2.014438	-2.440738
H	6.088888	-0.410261	-1.657060
H	5.669662	1.003575	0.357313
H	2.543630	0.723411	2.470112
H	5.545978	1.482586	2.562527
H	4.359261	1.592054	3.893427
H	4.854985	-0.013685	3.261001
H	2.235010	2.607607	0.922782
H	3.041444	3.199465	2.401461
H	4.008591	2.949925	0.910155
H	1.593193	4.568867	-0.655244
H	0.845548	5.005179	-2.209388
H	-0.704993	4.688152	0.451695
H	-1.406598	5.275053	-1.096695
C	-1.024113	1.367629	-2.753870
C	0.088353	0.519875	-3.005966
C	1.378172	1.018764	-2.674787
C	1.535869	2.237698	-2.011557
C	0.404686	3.022945	-1.547847
C	-0.872638	2.588181	-2.085736
H	-2.031610	1.053286	-3.071396
H	-0.031787	-0.427319	-3.549850
H	2.275700	0.433139	-2.927044
H	2.551176	2.584315	-1.761799
H	0.291925	2.689012	0.209369
H	-1.766353	3.199687	-1.888740

IM3

Enthalpy: -2228.457419

Free energy: -2228.585105

Ca	0.030999	0.902027	0.525200
N	-1.522102	-0.819184	1.024996
C	-2.773683	-0.640669	0.384259
C	-3.566386	0.508470	0.700736
C	-4.737506	0.755895	-0.041662
C	-5.139334	-0.101500	-1.076983
C	-4.360299	-1.227231	-1.380750
C	-3.176764	-1.515243	-0.672422
C	-3.188579	1.414918	1.869248
C	-3.922998	0.977273	3.151914
C	-2.341348	-2.729085	-1.070038
C	-3.121225	-4.045347	-0.892967
C	-1.293307	-1.804421	1.901543
C	-2.448733	-2.620291	2.459601
C	0.002609	-2.178671	2.353181
C	1.279489	-1.849526	1.825094
C	2.464321	-2.610716	2.395792
N	1.485488	-0.917332	0.881052
C	2.738532	-0.769546	0.229065
C	2.917382	-1.390161	-1.049845
C	4.118633	-1.168953	-1.750578
C	5.122565	-0.334591	-1.232689
C	4.925470	0.297247	0.001114
C	3.745314	0.098973	0.747909
C	1.805562	-2.254333	-1.642601
C	1.776795	-3.672158	-1.035134
C	3.579132	0.820514	2.082836
C	4.655077	0.389520	3.098576
C	3.583571	2.349751	1.901340
C	1.856031	-2.338609	-3.175531
C	-3.400828	2.908212	1.581387
C	-1.820016	-2.595017	-2.512062

C	0.423341	4.968705	-0.834884
C	-0.876873	5.752024	-0.661155
H	-0.678107	6.726394	-0.170418
H	-3.431635	-2.201649	2.172128
H	-2.400815	-3.669860	2.100967
H	-2.388481	-2.659301	3.566923
H	0.012317	-2.948062	3.139837
H	2.159959	-3.582457	2.829623
H	3.246175	-2.785098	1.630764
H	2.934639	-2.014381	3.207183
H	-2.104330	1.273763	2.074468
H	-3.703448	-0.080594	3.401270
H	-3.614476	1.601279	4.017148
H	-5.023825	1.073169	3.033486
H	-4.476298	3.173469	1.495312
H	-2.967329	3.522521	2.396582
H	-2.899672	3.213150	0.639398
H	-5.353523	1.635202	0.203708
H	-6.060209	0.106306	-1.644582
H	-4.675077	-1.901078	-2.194405
H	-1.457475	-2.762088	-0.401170
H	-2.466533	-4.920264	-1.091274
H	-3.525625	-4.146889	0.134104
H	-3.980213	-4.106609	-1.595290
H	-1.215502	-1.674366	-2.638408
H	-1.183964	-3.462859	-2.785079
H	-2.653083	-2.550958	-3.245520
H	0.847780	-1.768240	-1.347937
H	2.745288	-4.192512	-1.194984
H	1.571808	-3.652895	0.051992
H	0.981195	-4.284926	-1.509929
H	0.941173	-2.828176	-3.565899
H	1.934887	-1.338600	-3.650308
H	2.719034	-2.941977	-3.528953
H	4.273815	-1.649525	-2.728157
H	6.054239	-0.173031	-1.797876
H	5.707031	0.963280	0.401282
H	2.587769	0.536248	2.495362
H	5.666850	0.727232	2.786930
H	4.451485	0.829198	4.097781
H	4.695520	-0.712947	3.211536
H	2.761810	2.684883	1.235282
H	3.432982	2.862011	2.874366
H	4.545276	2.704500	1.472614
H	0.875096	4.787948	0.166505
H	1.167018	5.578690	-1.394845
H	-1.598141	5.205447	-0.018724
H	-1.371596	5.962870	-1.633051
C	-1.016042	1.767896	-2.457536
C	0.160421	1.041435	-2.727608
C	1.413845	1.603530	-2.400206
C	1.479438	2.875576	-1.803521
C	0.305180	3.620570	-1.519932
C	-0.941045	3.045602	-1.864027
H	-2.000024	1.338210	-2.703462
H	0.104574	0.046177	-3.194095
H	2.340280	1.040759	-2.593929
H	2.461894	3.299603	-1.539925
H	0.151361	2.537733	1.856322
H	-1.872033	3.594110	-1.659786

3

Enthalpy: -3835.231749

Free energy: -3835.421999

C	-3.105224	-2.533343	0.787636
C	-2.855181	-2.837532	2.161522
C	-2.259708	-4.072135	2.484939
C	-1.893966	-4.989067	1.488143
C	-2.126591	-4.677071	0.140955
N	-3.589046	-1.250459	0.419858
C	-4.900638	-0.984587	0.366844
C	-5.883682	-2.096860	0.680270
C	-3.194233	-1.838059	3.264870
C	-4.137161	-2.436120	4.324992
C	-2.989275	-3.148260	-1.704578
C	-3.729954	-4.287132	-2.427467
C	-5.437801	0.285508	0.028284
C	-4.763264	1.482771	-0.330826
C	-5.618654	2.693181	-0.655240
N	-3.430817	1.598314	-0.400653
C	-2.809892	2.804098	-0.824828
C	-2.482369	2.985756	-2.204179
C	-1.757359	4.132093	-2.584575
C	-1.341691	5.078712	-1.637685
C	-1.648615	4.884775	-0.282676
C	-2.384417	3.763390	0.145918
C	-2.886562	1.956567	-3.257821
C	-3.809706	2.563468	-4.330904

C	-2.691480	3.555743	1.627285	H	5.714234	2.527143	1.726939
C	-3.163418	4.841800	2.327196	H	6.924678	1.817728	0.600103
C	-1.649920	1.295971	-3.897730	H	3.375362	-2.641974	1.758668
C	-1.475193	2.955895	2.359275	H	4.171231	-5.037380	1.910777
C	-1.912800	-1.277561	3.913579	H	3.498287	-4.435176	3.461668
C	-1.675953	-2.792004	-2.429448	H	2.535694	-5.542794	2.441542
Ca	-1.689963	0.070397	0.021274	H	0.562103	-3.788795	2.351180
Ca	1.698941	-0.081472	0.098618	H	1.527341	-2.740915	3.448781
N	3.453953	-1.582658	-0.369029	H	0.902335	-2.105525	1.897981
C	2.843907	-2.798996	-0.779144	H	1.309403	-5.576261	0.555572
C	2.389362	-3.726684	0.207935	H	0.846148	-6.003622	-1.864748
C	1.668889	-4.864307	-0.203588	H	1.619421	-4.366744	-3.587284
C	1.403702	-5.104084	-1.559564	H	3.550408	-1.220769	-2.721939
C	1.843320	-4.184801	-2.523575	H	4.235143	-1.884024	-5.020271
C	2.554165	-3.024391	-2.160273	H	4.783511	-3.120450	-3.843072
C	2.639270	-3.469925	1.691463	H	3.356980	-3.436478	-4.877647
C	3.243957	-4.687723	2.410575	H	1.089612	-0.872184	-3.117337
C	2.971155	-2.018987	-3.231310	H	2.045996	-0.581043	-4.611215
C	3.885861	-2.650844	-4.296687	H	1.116413	-2.101824	-4.418691
C	4.785347	-1.458517	-0.294259	H	3.669742	2.239226	-1.698743
C	5.649362	-2.666220	-0.605377	H	3.090220	5.172948	-2.505781
C	5.450747	-0.255196	0.062666	H	4.656520	4.562185	-1.886181
C	4.901258	1.009672	0.400157	H	4.006380	3.960171	-3.446171
C	5.870419	2.137593	0.699077	H	1.904434	2.451377	-3.476919
N	3.586867	1.255853	0.466519	H	1.184507	1.872834	-1.946016
C	3.080827	2.535657	0.812520	H	0.972155	3.572210	-2.423792
C	2.719692	3.452121	-0.223146	H	1.787731	5.360874	-0.667954
C	2.078496	4.655963	0.126522	H	1.313252	5.923643	1.720583
C	1.808424	4.973497	1.465619	H	1.944792	4.318601	3.528372
C	2.166505	4.070638	2.477715	H	3.662188	1.008458	2.826426
C	2.792008	2.845007	2.177374	H	3.572764	3.311322	4.896163
C	2.999346	3.123503	-1.687723	H	4.352981	1.714866	5.107519
C	3.727019	4.266980	-2.416101	H	4.990768	2.872531	3.894459
C	3.125262	1.859934	3.294818	H	1.169571	0.836786	3.187186
C	4.060818	2.474667	4.351958	H	2.084705	0.530748	4.703450
C	1.841721	1.301246	3.940900	H	1.261660	2.102698	4.446497
C	1.700810	2.735392	-2.422759	H	-5.386088	3.531956	0.034399
C	1.344564	-3.002867	2.385128	H	-6.699971	2.470391	-0.586850
C	1.738597	-1.356979	-3.877917	H	-5.396842	3.067424	-1.676142
H	5.404874	-3.506034	0.079075	H	-6.534990	0.348509	0.034054
H	5.448171	-3.040301	-1.630626	H	-6.933653	-1.769585	0.562165
H	6.728720	-2.440974	-0.516652	H	-5.744093	-2.463345	1.718874
H	6.548439	-0.308370	0.067493	H	-5.706652	-2.972681	0.021076
H	5.693950	2.995644	0.016560	H	-3.459644	1.162156	-2.735364

H	-4.713338	3.026138	-3.882341
H	-4.148495	1.783759	-5.045694
H	-3.290116	3.349499	-4.919490
H	-1.035422	2.036863	-4.452296
H	-1.953074	0.506763	-4.618373
H	-0.993738	0.826757	-3.133428
H	-1.505507	4.280782	-3.647216
H	-0.772279	5.966637	-1.954751
H	-1.311216	5.624321	0.459355
H	-3.516552	2.815683	1.688060
H	-3.487442	4.621277	3.365980
H	-4.017667	5.310526	1.795701
H	-2.353395	5.598942	2.394458
H	-1.699170	2.772100	3.431518
H	-0.597315	3.631983	2.298885
H	-1.145237	1.985374	1.929234
H	-3.723273	-0.989044	2.783641
H	-3.651200	-3.261314	4.888126
H	-5.063136	-2.844542	3.868851
H	-4.436033	-1.663577	5.064830
H	-2.157899	-0.496768	4.664949
H	-1.233900	-0.824597	3.159368
H	-1.341778	-2.076624	4.432987
H	-2.068122	-4.316441	3.542388
H	-1.424486	-5.947102	1.761902
H	-1.833386	-5.394602	-0.641264
H	-3.643762	-2.252335	-1.734291
H	-3.110126	-5.206644	-2.496265
H	-3.989847	-3.989398	-3.465281
H	-4.671801	-4.556753	-1.905763
H	-1.149235	-1.933980	-1.956201
H	-1.863639	-2.515869	-3.488665
H	-0.960899	-3.640617	-2.415082
C	-2.736890	-3.464063	-0.232235
H	-0.029134	0.003267	1.433490
H	0.035182	-0.035208	-1.307339

Ethyl benzene

Enthalpy: -310.8568259

Free energy: -310.8971979

C	4.592114	-0.441220	-6.372074
C	4.879919	-1.944529	-6.532965
H	5.969496	-2.139689	-6.620677
H	5.009924	0.109552	-7.242587
H	5.122298	-0.058309	-5.473191
H	4.386563	-2.351793	-7.440518
H	4.499437	-2.520395	-5.663179
C	0.937657	0.308602	-7.291002
C	0.316902	0.306062	-6.029658
C	1.090917	0.079808	-4.878122
C	2.473599	-0.143587	-4.989906
C	3.111318	-0.143193	-6.249752
C	2.320685	0.084687	-7.397305
H	0.340706	0.489314	-8.199442
H	-0.766883	0.483583	-5.943984
H	0.614792	0.080145	-3.884354
H	3.073889	-0.317954	-4.081190
H	2.800166	0.090670	-8.390572

IM4

Enthalpy: -4224.682620

Free energy: -4224.889661

C	1.481129	3.717165	-0.101555
C	2.128687	3.939539	1.149492
C	1.610317	4.920714	2.018196
C	0.478416	5.671752	1.669309
C	-0.174377	5.420613	0.453233
N	1.988043	2.704485	-0.961249
C	2.706029	3.038320	-2.040535
C	2.872487	4.500993	-2.419259
C	3.385658	3.150862	1.504501
C	4.644205	3.825688	0.922771
C	-0.493779	4.078972	-1.690945
C	-1.207320	5.269030	-2.348537
C	3.361974	2.085811	-2.874228
C	3.772449	0.755534	-2.599122
C	4.616220	0.079327	-3.670151
N	3.469273	0.066453	-1.476941
C	4.259565	-1.080288	-1.189210
C	3.801407	-2.386776	-1.527032
C	4.635926	-3.493352	-1.274828
C	5.898391	-3.326660	-0.686072
C	6.315350	-2.045470	-0.293033
C	5.509428	-0.911383	-0.517296
C	2.385268	-2.583485	-2.050666
C	2.251254	-3.630518	-3.164857
C	5.941683	0.467860	-0.020917
C	6.781138	1.241125	-1.058416

C	1.467449	-2.933270	-0.863549	H	-6.910642	-0.231864	2.457593
C	6.687706	0.403467	1.322811	H	-5.766514	-2.064995	2.326653
C	3.547731	2.901836	3.010545	H	-5.717916	-4.188685	1.431526
C	-1.503606	2.973275	-1.339310	H	-4.218277	-4.870505	0.702384
Ca	1.233595	0.455401	-0.640896	H	-4.278195	-4.471270	2.443209
C	-0.742318	-0.303085	-2.110389	H	-3.382191	1.502960	2.865446
C	0.034239	0.341373	-3.271877	H	-5.177563	3.024790	3.832764
Ca	-1.868537	-0.432301	0.158509	H	-3.665263	3.028199	4.798882
N	-4.020417	0.388134	0.802093	H	-4.043656	4.405664	3.724737
C	-4.282896	1.737074	0.433405	H	-1.777284	4.119293	2.473274
C	-3.989942	2.825556	1.307212	H	-1.362907	2.797134	3.607513
C	-4.241649	4.139888	0.863987	H	-1.301893	2.526287	1.838871
C	-4.760955	4.391494	-0.414109	H	-4.017997	4.984550	1.535216
C	-5.009853	3.318754	-1.284115	H	-4.956232	5.425419	-0.739832
C	-4.769418	1.989552	-0.887596	H	-5.391658	3.521188	-2.296600
C	-3.349531	2.595750	2.672947	H	-4.364738	-0.004200	-1.505185
C	-4.102646	3.299948	3.814962	H	-6.656882	-0.552787	-2.383569
C	-5.033001	0.822178	-1.834886	H	-6.673408	-0.071097	-0.661790
C	-6.473345	0.293672	-1.688637	H	-7.213020	1.090309	-1.919131
C	-4.942672	-0.293604	1.502708	H	-3.678790	1.541891	-3.417938
C	-6.126462	0.457815	2.093241	H	-4.780002	0.221758	-3.921382
C	-4.925650	-1.695381	1.721642	H	-5.410032	1.879013	-3.739559
C	-4.121449	-2.726688	1.160181	H	-3.374352	-1.875067	-1.886173
C	-4.611438	-4.141671	1.435909	H	-4.920251	-4.416044	-2.688650
N	-3.020017	-2.522625	0.426684	H	-5.187421	-3.412663	-1.225745
C	-2.323467	-3.603229	-0.179862	H	-5.532702	-2.735840	-2.845489
C	-2.431403	-3.760959	-1.598282	H	-3.631128	-1.896756	-4.322707
C	-1.684459	-4.771917	-2.231992	H	-1.936258	-2.332439	-3.945312
C	-0.849030	-5.627528	-1.495989	H	-3.109674	-3.597815	-4.449499
C	-0.740024	-5.461854	-0.109715	H	-1.762696	-4.899336	-3.322204
C	-1.453602	-4.452622	0.568411	H	-0.274333	-6.414923	-2.008462
C	-3.389421	-2.870484	-2.384544	H	-0.071656	-6.122936	0.465353
C	-4.837342	-3.387934	-2.275959	H	-1.962773	-3.492214	2.409374
C	-1.255849	-4.277359	2.071159	H	-0.836690	-6.369210	2.625802
C	-1.570006	-5.566365	2.853459	H	-1.525479	-5.382410	3.947765
C	0.168843	-3.787280	2.390542	H	-2.577856	-5.960827	2.612894
C	-2.988628	-2.669292	-3.851713	H	0.420902	-2.853757	1.851534
C	-1.870205	3.028555	2.647480	H	0.287224	-3.584936	3.474531
C	-4.706566	1.139320	-3.301518	H	0.928466	-4.545272	2.107882
C	0.186740	0.055459	1.604959	H	5.570249	-0.309615	-3.262439
C	-0.740398	-0.356441	2.760323	H	4.841256	0.763753	-4.509581
H	-1.231292	-1.345196	2.589018	H	4.073955	-0.802957	-4.074071
H	-5.801356	1.089550	2.946996	H	3.750852	2.494615	-3.817957
H	-6.576131	1.148584	1.351535	H	3.596890	4.628816	-3.245240

H	3.223070	5.091146	-1.547703
H	1.907041	4.953383	-2.727757
H	2.057629	-1.610529	-2.475331
H	2.935670	-3.416271	-4.011579
H	1.212359	-3.644840	-3.554600
H	2.472228	-4.655758	-2.799848
H	1.756377	-3.908460	-0.423772
H	0.404494	-3.002567	-1.167460
H	1.554070	-2.198658	-0.034166
H	4.289767	-4.503729	-1.544522
H	6.546092	-4.199080	-0.505640
H	7.284895	-1.926627	0.214588
H	5.002958	1.044402	0.128489
H	7.136698	2.203105	-0.632397
H	6.199782	1.482226	-1.968887
H	7.675558	0.655807	-1.362607
H	6.837611	1.425887	1.729082
H	7.697240	-0.047540	1.216527
H	6.132491	-0.188437	2.078669
H	3.293911	2.164404	0.996042
H	4.737668	4.869153	1.292805
H	4.619234	3.856308	-0.183935
H	5.560654	3.276436	1.223307
H	4.377303	2.189309	3.197755
H	2.623265	2.480406	3.456305
H	3.792923	3.833540	3.563812
H	2.107392	5.104461	2.982970
H	0.092128	6.441838	2.355634
H	-1.082560	5.986803	0.196636
H	0.214251	3.655724	-2.432496
H	-2.031129	5.659000	-1.714441
H	-1.663948	4.958939	-3.311524
H	-0.509450	6.107211	-2.554878
H	-0.994260	2.075501	-0.926045
H	-2.071904	2.643443	-2.232118
H	-2.226664	3.330506	-0.582972
H	0.623025	1.059482	1.851701
H	1.068168	-0.636870	1.642863
H	-1.571374	0.367284	2.914735
H	-0.731428	-1.413190	-2.254114
H	-1.820485	-0.030862	-2.268156
H	1.134821	0.145427	-3.231972
H	-0.067502	1.449497	-3.276618
C	0.299124	4.440438	-0.439439
H	-0.242405	-0.461300	3.753448
H	-0.263659	0.001965	-4.292958
C	3.567639	-3.370342	3.113439
C	3.763764	-2.328218	2.190001
C	3.458836	-1.004988	2.554529
C	2.949861	-0.724643	3.835779
C	2.752729	-1.768114	4.756416
C	3.065375	-3.092123	4.396587
H	3.810708	-4.405830	2.826851
H	4.159460	-2.545380	1.188951
H	3.628143	-0.186908	1.836053
H	2.703792	0.310524	4.114634
H	2.354641	-1.547668	5.759708
H	2.911362	-3.910194	5.118343

TS3

Enthalpy: -4224.638799

Free energy: -4224.847617

C	-2.143074	-3.283255	-0.446129
C	-2.960938	-3.833788	0.590133
C	-2.484160	-4.946224	1.310739
C	-1.236084	-5.521561	1.024253
C	-0.446460	-4.986820	-0.002145
N	-2.559833	-2.084095	-1.092437
C	-3.062148	-2.108303	-2.335922
C	-3.096261	-3.407015	-3.126718
C	-4.343821	-3.248602	0.860309
C	-5.357491	-3.708170	-0.208145
C	0.032379	-3.275369	-1.812525
C	0.561841	-4.314085	-2.814412
C	-3.577026	-0.964763	-3.009201
C	-3.966624	0.298988	-2.495620
C	-4.701797	1.223512	-3.452588
N	-3.714703	0.714417	-1.241710
C	-4.483748	1.776194	-0.680569
C	-4.009324	3.118494	-0.671890
C	-4.767955	4.109979	-0.016771
C	-5.972978	3.797459	0.625059
C	-6.433174	2.471469	0.620683
C	-5.710913	1.447373	-0.020814
C	-2.682608	3.495617	-1.317344
C	-2.840034	4.546089	-2.430667
C	-6.228331	0.010706	-0.018393
C	-7.141949	-0.267679	-1.229160

C	-1.674452	3.964981	-0.252878	H	7.281204	-0.654385	1.938781
C	-6.942407	-0.374672	1.286596	H	6.508080	1.393385	1.687043
C	-4.884955	-3.541201	2.266319	H	6.464378	3.524844	1.325687
C	1.195642	-2.546977	-1.125597	H	5.329502	4.194872	0.099957
Ca	-1.816200	-0.066921	-0.034488	H	4.887243	4.227574	1.816942
C	0.190935	0.986344	-1.174772	H	2.813289	-1.765578	2.297930
C	-0.180489	0.397263	-2.551881	H	5.038345	-2.135984	3.286625
Ca	2.052140	0.289074	0.518295	H	3.771870	-2.566941	4.476979
N	4.208192	-0.817835	0.581399	H	4.656515	-3.859571	3.600478
C	4.245791	-2.179298	0.169701	H	2.187342	-4.709105	3.022200
C	3.721885	-3.194249	1.026670	H	1.435133	-3.235256	3.684958
C	3.727015	-4.530960	0.582509	H	1.158965	-3.688768	1.972306
C	4.201716	-4.868626	-0.694205	H	3.335017	-5.320607	1.241811
C	4.679754	-3.860698	-1.544999	H	4.190188	-5.917603	-1.029864
C	4.721625	-2.514102	-1.132577	H	5.033558	-4.128455	-2.553616
C	3.145442	-2.821337	2.387630	H	5.362360	-0.504908	-1.500746
C	4.214076	-2.845588	3.496676	H	6.976798	-0.928008	-3.301181
C	5.223601	-1.434056	-2.089444	H	7.331554	-2.058916	-1.954060
C	6.579362	-1.789436	-2.724140	H	6.500200	-2.645503	-3.427677
C	5.342185	-0.251768	1.023909	H	3.234969	-0.729831	-2.736043
C	6.588979	-1.105631	1.201872	H	4.552672	-0.367072	-3.889422
C	5.521170	1.135946	1.276761	H	3.911668	-2.036174	-3.755471
C	4.735687	2.256627	0.899129	H	3.403316	1.523706	-1.939614
C	5.398821	3.617001	1.044160	H	5.262692	3.741782	-2.989264
N	3.488276	2.182512	0.405901	H	5.562132	2.632700	-1.609219
C	2.882631	3.360564	-0.119884	H	5.492371	1.985158	-3.274352
C	2.872839	3.544384	-1.537358	H	3.255880	1.540040	-4.388730
C	2.254123	4.692405	-2.068702	H	1.759611	2.287019	-3.743633
C	1.644152	5.641361	-1.233727	H	3.053701	3.309732	-4.449256
C	1.621128	5.431865	0.151575	H	2.245174	4.848584	-3.158040
C	2.222391	4.295632	0.729232	H	1.168857	6.535291	-1.667494
C	3.525416	2.506490	-2.448128	H	1.112303	6.161611	0.801476
C	5.044685	2.730809	-2.583298	H	2.782117	3.213519	2.485326
C	2.100901	4.051549	2.230599	H	1.819535	6.123066	2.937515
C	2.513525	5.267447	3.078168	H	2.503241	5.012421	4.158760
C	0.668668	3.605552	2.581742	H	3.533909	5.621357	2.822786
C	2.858560	2.410395	-3.827560	H	0.358575	2.711440	2.003760
C	1.918817	-3.658740	2.780115	H	0.577411	3.352696	3.657369
C	4.173660	-1.126530	-3.174207	H	-0.066617	4.405909	2.356716
C	0.478571	-0.267413	2.511313	H	-5.516139	1.778582	-2.947757
C	1.586460	0.243714	3.384310	H	-5.119594	0.679376	-4.320783
H	2.504660	0.701537	2.902096	H	-3.992460	1.987147	-3.840780
H	6.350254	-2.140511	1.513226	H	-3.857575	-1.140923	-4.057895
H	7.137386	-1.182020	0.237840	H	-3.947101	-3.424272	-3.834699

H	-3.159490	-4.292970	-2.466436
H	-2.167078	-3.513750	-3.727177
H	-2.279184	2.574713	-1.789483
H	-3.567287	4.217278	-3.201423
H	-1.866716	4.732252	-2.932177
H	-3.197308	5.518035	-2.027960
H	-1.999240	4.919263	0.213841
H	-0.669474	4.130188	-0.689674
H	-1.576168	3.225963	0.569023
H	-4.400538	5.148973	-0.008672
H	-6.551861	4.583343	1.135563
H	-7.373852	2.226310	1.137173
H	-5.336046	-0.641848	-0.133203
H	-7.504577	-1.317282	-1.214071
H	-6.615678	-0.114159	-2.190439
H	-8.030150	0.400391	-1.217531
H	-7.186271	-1.457195	1.284208
H	-7.904365	0.166288	1.411037
H	-6.319699	-0.163533	2.179862
H	-4.248215	-2.146396	0.746936
H	-5.436820	-4.816048	-0.226835
H	-5.075252	-3.367083	-1.222523
H	-6.366514	-3.300689	0.011751
H	-5.818365	-2.969446	2.441548
H	-4.167673	-3.256014	3.062200
H	-5.133148	-4.615822	2.399548
H	-3.103423	-5.375375	2.112367
H	-0.880604	-6.387535	1.604541
H	0.534181	-5.435380	-0.227101
H	-0.550724	-2.520792	-2.374227
H	1.241476	-5.044615	-2.327727
H	1.142967	-3.816918	-3.619399
H	-0.264355	-4.883073	-3.288216
H	0.798407	-1.818078	-0.384429
H	1.825385	-2.001685	-1.855528
H	1.842734	-3.258775	-0.582371
H	0.410889	-1.325298	2.217792
H	-0.085407	0.470784	1.914156
H	1.990625	-0.557742	4.037431
H	-0.508283	1.836313	-0.967848
H	1.129270	1.574928	-1.328621
H	-1.130593	-0.189183	-2.558461
H	0.594928	-0.310378	-2.916609
C	-0.880894	-3.873218	-0.749636
H	1.216468	1.052966	4.058601
H	-0.320173	1.154195	-3.360827
C	-2.275283	1.924864	3.606066
C	-3.125598	1.482046	2.558374
C	-3.228680	0.080646	2.340014
C	-2.380905	-0.824022	2.994598
C	-1.321116	-0.329093	3.842771
C	-1.461499	1.031858	4.303217
H	-2.301052	2.986779	3.902800
H	-3.807311	2.176459	2.046551
H	-4.026685	-0.300721	1.678151
H	-2.484637	-1.908133	2.824483
H	-0.814461	-1.048209	4.504350
H	-0.863012	1.383453	5.158697

IM5

Enthalpy: -4224.680163

Free energy: -4224.887887

C	3.916622	2.408512	-0.352210
C	4.960736	2.390121	0.625264
C	5.246238	3.569555	1.339311
C	4.515939	4.748451	1.120554
C	3.469579	4.748466	0.189399
N	3.591383	1.196854	-1.022654
C	4.156566	0.905104	-2.205330
C	4.904314	1.994365	-2.957019
C	5.724491	1.097431	0.898818
C	6.892189	0.890669	-0.086583
C	1.961174	3.613586	-1.507020
C	2.017443	4.769031	-2.520113
C	4.088459	-0.368770	-2.833687
C	3.667602	-1.628759	-2.319882
C	3.952273	-2.837754	-3.198169
N	3.030678	-1.790431	-1.152557
C	2.838047	-3.073052	-0.570414
C	1.674343	-3.843080	-0.858412
C	1.438232	-5.034133	-0.141894
C	2.334991	-5.478348	0.837389
C	3.489172	-4.725941	1.109222
C	3.762312	-3.526544	0.423748
C	0.653764	-3.370688	-1.883112
C	0.384001	-4.411745	-2.982741
C	5.018143	-2.713161	0.719551
C	6.135024	-2.997985	-0.304809

C	-0.654355	-2.973993	-1.182293	H	-6.675782	2.580143	0.836686
C	5.548798	-2.901347	2.147865	H	-6.158017	0.625035	1.987247
C	6.217897	0.980740	2.348729	H	-6.676810	-1.899011	0.800548
C	0.644206	3.651391	-0.710747	H	-5.560852	-2.872875	1.790732
Ca	1.696291	-0.023849	-0.232712	H	-6.486292	-1.513974	2.531530
C	-0.411522	0.440552	-1.729441	H	-3.038331	3.281440	2.286064
C	0.532055	0.363752	-2.940273	H	-4.597810	5.310259	2.150349
Ca	-1.803288	0.139132	0.287393	H	-3.563352	5.307035	3.617033
N	-3.495246	1.842094	0.318258	H	-3.166112	6.376567	2.240537
C	-3.152719	3.062230	-0.337464	H	-0.792287	5.395891	2.055658
C	-2.738307	4.221989	0.384723	H	-1.148478	4.390666	3.492952
C	-2.373379	5.378402	-0.335659	H	-0.562018	3.627997	1.980638
C	-2.391908	5.405353	-1.734346	H	-2.060983	6.277663	0.219162
C	-2.783106	4.257787	-2.440554	H	-2.096705	6.316734	-2.277589
C	-3.173508	3.083716	-1.768306	H	-2.797236	4.281179	-3.540171
C	-2.668006	4.257547	1.909897	H	-3.371384	0.968464	-1.979492
C	-3.551130	5.369576	2.508364	H	-5.590795	0.970416	-3.152833
C	-3.681686	1.873397	-2.547851	H	-5.660830	1.808251	-1.572937
C	-5.222713	1.853601	-2.589110	H	-5.615871	2.763840	-3.089993
C	-4.680930	1.710889	0.932106	H	-1.984365	1.804786	-3.944027
C	-5.634239	2.893965	1.046000	H	-3.390043	0.807176	-4.430453
C	-5.188640	0.500788	1.480952	H	-3.455586	2.576327	-4.626360
C	-4.835602	-0.858384	1.270613	H	-4.707017	-1.008359	-1.413603
C	-5.937594	-1.847161	1.628660	H	-6.230026	-3.243432	-2.918610
N	-3.693159	-1.297208	0.710379	H	-6.787198	-2.454960	-1.412055
C	-3.638175	-2.667004	0.302745	H	-6.610060	-1.493473	-2.915411
C	-4.109688	-3.021887	-0.997143	H	-4.311143	-1.104535	-3.919890
C	-4.025809	-4.365045	-1.413768	H	-2.826859	-1.433927	-2.975603
C	-3.503248	-5.357163	-0.572864	H	-3.714828	-2.782240	-3.747811
C	-3.038479	-5.002657	0.701357	H	-4.384338	-4.639806	-2.419016
C	-3.087400	-3.669453	1.156719	H	-3.453930	-6.404258	-0.910919
C	-4.702135	-1.981417	-1.945909	H	-2.620724	-5.779476	1.360947
C	-6.160111	-2.312755	-2.315700	H	-2.499453	-2.225815	2.605188
C	-2.550678	-3.333811	2.544986	H	-3.636762	-4.901696	3.642231
C	-3.495739	-3.799846	3.669292	H	-3.077852	-3.537866	4.664503
C	-1.134877	-3.900849	2.758621	H	-4.496429	-3.330672	3.590430
C	-3.841344	-1.817864	-3.211869	H	-0.463447	-3.668015	1.908229
C	-1.214158	4.423594	2.386379	H	-0.676375	-3.486115	3.679865
C	-3.092281	1.765414	-3.960134	H	-1.150465	-5.005886	2.867416
C	-0.547741	0.474626	4.224739	H	4.118676	-3.753267	-2.598135
C	-0.903901	1.757796	4.976177	H	4.825680	-2.673080	-3.857965
H	-1.132533	1.551602	6.042711	H	3.073977	-3.035226	-3.851571
H	-5.623230	3.296808	2.080728	H	4.554435	-0.412963	-3.828773
H	-5.368128	3.718501	0.359636	H	5.482024	1.587465	-3.808366

H	5.593300	2.548642	-2.288992
H	4.185724	2.744263	-3.353789
H	1.073801	-2.466384	-2.367485
H	1.320935	-4.730460	-3.484104
H	-0.296868	-3.997359	-3.756288
H	-0.103084	-5.321151	-2.571310
H	-1.153163	-3.853088	-0.731594
H	-1.367352	-2.514978	-1.893385
H	-0.458140	-2.252788	-0.359438
H	0.527865	-5.618082	-0.353802
H	2.136368	-6.408400	1.393134
H	4.189663	-5.081150	1.880145
H	4.727331	-1.647393	0.588339
H	7.048152	-2.415367	-0.060143
H	5.834470	-2.720671	-1.332899
H	6.409196	-4.074996	-0.305760
H	6.377850	-2.191765	2.347258
H	5.958690	-3.921169	2.308759
H	4.764322	-2.729923	2.913922
H	4.999887	0.274183	0.712966
H	7.597527	1.748975	-0.056763
H	6.538685	0.772177	-1.128853
H	7.465756	-0.024731	0.171465
H	6.624555	-0.034065	2.535606
H	5.403143	1.157185	3.080966
H	7.034194	1.700097	2.573453
H	6.050736	3.565115	2.090610
H	4.754099	5.661507	1.689093
H	2.880769	5.666969	0.034005
H	1.984460	2.665382	-2.080928
H	1.923710	5.757549	-2.022068
H	1.183807	4.691110	-3.249429
H	2.971813	4.769958	-3.086672
H	0.583079	2.813761	0.016746
H	-0.239371	3.595529	-1.377437
H	0.562965	4.588894	-0.124486
H	-1.400360	-0.241483	4.274258
H	0.313938	-0.035065	4.709327
H	-1.799115	2.248377	4.536490
H	-1.305753	-0.181605	-2.010574
H	-0.816149	1.484094	-1.674715
H	0.755702	-0.688445	-3.218851
H	1.525345	0.838995	-2.765195
C	3.152269	3.593851	-0.555099
H	-0.070414	2.490807	4.954212
H	0.146299	0.850383	-3.867986
C	2.313675	0.877538	2.444277
C	2.450007	-0.553547	2.331326
C	1.277130	-1.294650	2.111440
C	0.011717	-0.663740	2.004476
C	-0.188159	0.671571	2.725183
C	1.080122	1.492678	2.501998
H	3.216841	1.508373	2.413478
H	3.435820	-1.033535	2.357205
H	1.357810	-2.375689	1.902899
H	-0.855112	-1.354816	2.012560
H	-1.054280	1.259837	2.303208
H	1.033283	2.591238	2.550088

TS4

Enthalpy: -4224.661172

Free energy: -4224.863550

C	-2.423402	3.243878	-0.309682
C	-2.989421	3.379610	-1.614254
C	-2.501331	4.391791	-2.464237
C	-1.479202	5.258696	-2.049489
C	-0.928102	5.117917	-0.768073
N	-2.851025	2.172865	0.521843
C	-3.661177	2.411330	1.562647
C	-4.070112	3.838783	1.898576
C	-4.130926	2.464612	-2.047637
C	-5.475293	2.929908	-1.451825
C	-0.706450	3.927200	1.470614
C	-0.407180	5.245557	2.201256
C	-4.206778	1.399179	2.399448
C	-4.331951	0.001328	2.185206
C	-5.218631	-0.737465	3.177457
N	-3.729517	-0.675218	1.193819
C	-4.209746	-1.965061	0.830077
C	-3.664000	-3.161253	1.378604
C	-4.120165	-4.406507	0.898291
C	-5.090564	-4.489823	-0.107520
C	-5.627683	-3.309262	-0.645186
C	-5.209508	-2.043886	-0.193334
C	-2.602932	-3.133121	2.473168
C	-3.122614	-3.741664	3.789913
C	-5.821590	-0.767261	-0.765925
C	-7.007225	-0.278815	0.091380

C	-1.312595	-3.845454	2.031772	H	7.258231	1.228479	-0.762812
C	-6.257771	-0.894180	-2.233914	H	6.529038	-0.653903	-1.354129
C	-4.251807	2.301018	-3.569443	H	6.663853	-2.894574	-0.770277
C	0.574931	3.099572	1.298880	H	5.224012	-3.958263	-0.941181
Ca	-1.643529	0.124973	0.177247	H	5.891831	-3.092493	-2.361373
C	0.251827	-0.479666	1.757742	H	4.000546	2.579612	-1.985359
C	-0.601677	0.150164	2.877194	H	5.685822	4.506094	-1.924077
Ca	1.852219	-0.144430	-0.204656	H	4.627954	4.518812	-3.373337
N	3.938806	1.080005	-0.053709	H	4.322853	5.661167	-2.035445
C	3.855213	2.333888	0.621973	H	1.874058	4.799173	-1.702194
C	3.786657	3.563180	-0.098095	H	2.154915	3.807503	-3.166213
C	3.721490	4.771137	0.624268	H	1.561939	3.044005	-1.655018
C	3.708173	4.781628	2.026564	H	3.671990	5.725272	0.075786
C	3.735464	3.567889	2.728361	H	3.659803	5.736449	2.573384
C	3.801329	2.335587	2.049031	H	3.700014	3.579026	3.828489
C	3.702124	3.584468	-1.621768	H	3.394210	0.247368	2.151568
C	4.636546	4.621350	-2.267861	H	5.310238	-0.365889	3.687584
C	3.840804	1.018367	2.818850	H	5.831291	0.360944	2.138587
C	5.289817	0.565462	3.083325	H	5.852028	1.344009	3.641944
C	5.149742	0.712507	-0.517369	H	1.989841	1.423061	3.941877
C	6.310949	1.694560	-0.434114	H	2.925155	0.016139	4.530468
C	5.481364	-0.563639	-1.032611	H	3.487126	1.668970	4.900022
C	4.791887	-1.806705	-0.996039	H	3.127601	-1.762712	1.701028
C	5.683875	-3.010191	-1.274000	H	4.775714	-4.250114	2.453895
N	3.497474	-1.962027	-0.697062	H	5.270893	-2.923874	1.354341
C	2.935602	-3.259462	-0.519930	H	5.047850	-2.595821	3.096944
C	2.619924	-3.651213	0.823093	H	2.757843	-2.288777	4.067437
C	1.902638	-4.841137	1.041738	H	1.291993	-2.754738	3.154692
C	1.517159	-5.662790	-0.028821	H	2.448274	-4.010141	3.723153
C	1.881877	-5.308619	-1.333149	H	1.648533	-5.139608	2.069297
C	2.592646	-4.120745	-1.611108	H	0.945808	-6.585463	0.158002
C	3.160000	-2.835619	1.997729	H	1.603122	-5.969997	-2.168891
C	4.647523	-3.168749	2.234669	H	3.507636	-2.858390	-3.086733
C	3.008826	-3.849917	-3.060919	H	3.510708	-5.899240	-3.677076
C	4.016161	-4.919087	-3.543433	H	4.450074	-4.635638	-4.525755
C	1.829991	-3.810592	-4.054989	H	4.850061	-5.074718	-2.833037
C	2.365095	-2.986786	3.299805	H	1.101067	-3.011443	-3.822658
C	2.245303	3.817195	-2.060781	H	2.206612	-3.640349	-5.085958
C	3.016632	1.040664	4.114326	H	1.275169	-4.772695	-4.065624
C	0.609197	0.591817	-3.390095	H	-5.793291	-1.552123	2.696264
C	-0.039229	1.911099	-3.798881	H	-5.923492	-0.055795	3.690529
H	0.644403	2.515193	-4.427812	H	-4.583204	-1.208769	3.957922
H	6.133300	2.593677	-1.057471	H	-4.774441	1.780245	3.260343
H	6.442583	2.063793	0.603860	H	-4.976686	3.860236	2.532504

H	-4.262053	4.429014	0.980662
H	-3.261469	4.366608	2.447791
H	-2.360476	-2.067026	2.662928
H	-4.066651	-3.264709	4.120912
H	-2.374822	-3.621468	4.602540
H	-3.322795	-4.828918	3.678627
H	-1.486343	-4.926607	1.845803
H	-0.532938	-3.766447	2.816051
H	-0.900099	-3.414041	1.099607
H	-3.699062	-5.331912	1.323594
H	-5.430464	-5.471539	-0.473759
H	-6.390695	-3.376392	-1.435734
H	-5.031690	0.012541	-0.698138
H	-7.462069	0.634409	-0.347075
H	-6.695371	-0.027390	1.122185
H	-7.797555	-1.057689	0.151672
H	-6.553936	0.098028	-2.632524
H	-7.139330	-1.559562	-2.352004
H	-5.451635	-1.294336	-2.883478
H	-3.919865	1.464429	-1.607874
H	-5.693755	3.978481	-1.746469
H	-5.477999	2.875591	-0.346253
H	-6.308511	2.295227	-1.820134
H	-4.967098	1.488779	-3.812457
H	-3.280896	2.048478	-4.043898
H	-4.630132	3.224229	-4.057604
H	-2.927596	4.507364	-3.471990
H	-1.109550	6.043009	-2.728794
H	-0.124189	5.797709	-0.445312
H	-1.392822	3.334883	2.107209
H	0.355287	5.850968	1.667691
H	-0.001803	5.042131	3.214441
H	-1.316766	5.872087	2.315275
H	0.367366	2.146411	0.764699
H	1.031424	2.852485	2.276956
H	1.326727	3.655630	0.709158
H	1.620652	0.775363	-2.956654
H	0.780931	-0.041723	-4.290568
H	-0.318742	2.518807	-2.913715
H	0.068286	-1.582067	1.751563
H	1.311165	-0.407765	2.116390
H	-1.699553	0.167017	2.665627
H	-0.326256	1.210740	3.055610
C	-1.378996	4.118476	0.115510
H	-0.959704	1.742140	-4.394524
H	-0.527910	-0.365261	3.864373
C	-2.417753	-1.381195	-2.113948
C	-1.821451	-2.518352	-1.514287
C	-0.411595	-2.583108	-1.505278
C	0.369185	-1.528744	-2.001932
C	-0.207255	-0.249324	-2.401261
C	-1.656055	-0.299817	-2.567299
H	-3.509897	-1.349196	-2.239020
H	-2.438185	-3.347299	-1.142374
H	0.094001	-3.498467	-1.161744
H	1.454293	-1.688303	-2.137668
H	0.067253	0.798081	-1.187903
H	-2.162250	0.549870	-3.045135

4

Enthalpy: -3913.828255

Free energy: -3914.023329

C	2.907387	2.947956	-0.084493
C	3.011440	3.125992	1.333208
C	2.576214	4.338583	1.899777
C	2.021954	5.356123	1.107858
C	1.875308	5.154847	-0.269755
N	3.306961	1.696335	-0.630197
C	4.497137	1.530244	-1.219669
C	5.381678	2.736213	-1.496302
C	3.605241	2.021620	2.205506
C	5.146453	2.049526	2.181057
C	2.077547	3.777511	-2.384137
C	2.817479	4.839022	-3.219850
C	5.031968	0.270139	-1.613693
C	4.601454	-1.051989	-1.324327
C	5.580612	-2.169820	-1.637038
N	3.426383	-1.365951	-0.756743
C	3.178909	-2.687523	-0.290549
C	2.413207	-3.602390	-1.074005
C	2.106019	-4.871345	-0.542319
C	2.542344	-5.249838	0.734293
C	3.283447	-4.342616	1.506219
C	3.606937	-3.061370	1.020921
C	1.933432	-3.237418	-2.474869
C	2.553069	-4.151198	-3.548749
C	4.359118	-2.080808	1.916002
C	5.695564	-2.652123	2.422117

C	0.396647	-3.252426	-2.557694	H	-5.246795	-3.512857	1.086292
C	3.464881	-1.632195	3.087991	H	-4.641840	-3.305984	2.742668
C	3.078730	2.036401	3.646854	H	-2.773138	2.349058	2.867001
C	0.571918	3.782906	-2.712418	H	-3.900220	4.565627	3.354719
Ca	1.597625	0.072296	-0.367253	H	-2.679990	4.119000	4.594292
C	-0.556068	0.275672	-1.774058	H	-2.298991	5.366192	3.370633
C	0.438044	0.328689	-2.945884	H	-0.170666	3.993500	2.553862
Ca	-1.612590	-0.019182	0.488528	H	-0.539108	2.860968	3.898366
N	-3.522368	1.319943	0.807247	H	-0.349936	2.249867	2.227023
C	-3.224790	2.617827	0.316855	H	-1.627363	5.541397	1.176757
C	-2.558352	3.579147	1.133896	H	-2.057110	6.031190	-1.233314
C	-2.147868	4.796730	0.553787	H	-3.197189	4.334367	-2.667960
C	-2.383545	5.073181	-0.799032	H	-3.917156	0.854818	-1.490164
C	-3.027312	4.118029	-1.602194	H	-6.206776	1.227324	-2.441635
C	-3.448719	2.884913	-1.071591	H	-6.046662	1.918464	-0.798839
C	-2.261227	3.297739	2.603618	H	-6.007189	2.999688	-2.225960
C	-2.817364	4.396369	3.527689	H	-2.588353	1.719923	-3.467621
C	-4.157622	1.845763	-1.935042	H	-4.156025	0.989777	-3.942546
C	-5.688280	2.006257	-1.843203	H	-3.975149	2.763164	-3.935477
C	-4.630993	1.031332	1.496923	H	-3.656219	-1.201650	-1.500813
C	-5.562497	2.149209	1.934181	H	-5.801896	-3.336552	-2.068032
C	-5.002158	-0.289376	1.873173	H	-5.786560	-2.138679	-0.730275
C	-4.426140	-1.535472	1.506294	H	-5.969815	-1.583034	-2.418285
C	-5.181836	-2.786785	1.921688	H	-3.934796	-1.357345	-3.928769
N	-3.275620	-1.665270	0.826683	H	-2.403683	-2.185132	-3.504849
C	-2.879842	-2.928392	0.308493	H	-3.867931	-3.139866	-3.909991
C	-3.182078	-3.224341	-1.058633	H	-3.017214	-4.708737	-2.635516
C	-2.777861	-4.463530	-1.589377	H	-1.744980	-6.348617	-1.247894
C	-2.054394	-5.384106	-0.814853	H	-1.101770	-5.765670	1.094090
C	-1.701788	-5.057278	0.501031	H	-2.229734	-2.584734	2.807809
C	-2.101802	-3.837420	1.083745	H	-1.443298	-5.539080	3.310462
C	-3.924962	-2.199740	-1.912783	H	-1.795378	-4.298556	4.547760
C	-5.454476	-2.323834	-1.770447	H	-3.101510	-4.882435	3.462632
C	-1.673057	-3.498142	2.508128	H	0.089307	-2.307152	1.907374
C	-2.025521	-4.614023	3.508278	H	0.145153	-2.897539	3.590486
C	-0.167907	-3.168389	2.560023	H	0.450031	-4.027679	2.226791
C	-3.506183	-2.227511	-3.389977	H	6.456957	-1.805918	-2.205654
C	-0.751797	3.090657	2.832595	H	5.089265	-2.980906	-2.212815
C	-3.689129	1.835222	-3.395958	H	5.945902	-2.637853	-0.698569
H	-5.255047	2.527835	2.933738	H	6.009017	0.330655	-2.114527
H	-5.526927	3.010362	1.238736	H	6.454337	2.462509	-1.487648
H	-6.608918	1.798272	2.022843	H	5.211096	3.548435	-0.763370
H	-5.932738	-0.360157	2.454767	H	5.155749	3.151633	-2.502003
H	-6.204385	-2.555358	2.274951	H	2.285071	-2.203580	-2.678390

H	3.661622	-4.144223	-3.499078
H	2.257422	-3.821465	-4.567401
H	2.219311	-5.203886	-3.427949
H	-0.009692	-4.263538	-2.356005
H	0.045314	-2.944912	-3.564907
H	-0.065613	-2.569426	-1.815129
H	1.514117	-5.577621	-1.146147
H	2.297626	-6.247239	1.132571
H	3.611793	-4.633472	2.517295
H	4.588872	-1.182891	1.306763
H	6.260750	-1.883450	2.990470
H	6.338339	-2.990899	1.583122
H	5.545744	-3.518849	3.101065
H	4.001948	-0.915945	3.743869
H	3.161831	-2.497269	3.715296
H	2.534628	-1.139558	2.733607
H	3.300229	1.053947	1.747450
H	5.529770	3.023193	2.554636
H	5.544471	1.895448	1.159239
H	5.566252	1.249357	2.826734
H	3.446401	1.147886	4.198541
H	1.970443	2.016047	3.676523
H	3.424178	2.929058	4.210087
H	2.663513	4.489945	2.985947
H	1.687156	6.297985	1.570783
H	1.412724	5.941539	-0.887207
H	2.486886	2.781982	-2.656109
H	2.396310	5.852786	-3.048679
H	2.725296	4.622028	-4.305309
H	3.896879	4.883261	-2.970081
H	0.009999	3.049139	-2.101560
H	0.393768	3.545058	-3.782066
H	0.123607	4.778108	-2.512669
H	-1.388478	-0.414654	-2.068398
H	-1.053771	1.279710	-1.697721
H	0.819967	-0.681442	-3.208237
H	1.344907	0.950219	-2.731730
C	2.302467	3.961139	-0.886726
H	0.039674	0.757179	-3.895548
H	0.371960	0.038874	1.444931

TS5

Enthalpy: -4146.048447

Free energy: -4146.253215

C	3.432883	2.823256	-0.372837
C	4.688605	3.051989	0.271927
C	4.889194	4.265577	0.957098
C	3.878422	5.236978	1.033519
C	2.640833	4.992805	0.425127
N	3.195867	1.565018	-0.993526
C	3.398747	1.397492	-2.309096
C	3.655024	2.612018	-3.185033
C	5.776556	1.984897	0.225087
C	6.657805	2.107667	-1.033674
C	1.021588	3.550110	-0.888461
C	0.623044	4.652584	-1.884363
C	3.380857	0.132509	-2.960642
C	3.404854	-1.173454	-2.399637
C	3.642894	-2.328552	-3.357384
N	3.222626	-1.430336	-1.094669
C	3.489564	-2.721308	-0.562290
C	2.464457	-3.707487	-0.505478
C	2.729485	-4.937401	0.130184
C	3.981085	-5.201721	0.701299
C	4.984747	-4.220954	0.654303
C	4.762609	-2.974900	0.036810
C	1.069995	-3.419795	-1.048224
C	0.560951	-4.516816	-1.996141
C	5.843263	-1.898799	0.013998
C	6.680083	-1.950289	-1.279632
C	0.097743	-3.195695	0.121871
C	6.754525	-1.929453	1.249818
C	6.644310	1.954750	1.492157
C	-0.042765	3.389876	0.210987
Ca	1.900819	0.010750	0.243464
Ca	-2.255662	0.001457	0.321468
N	-4.101601	1.472213	-0.000734
C	-3.702472	2.802912	-0.322684
C	-3.588941	3.802365	0.689683
C	-3.200954	5.104676	0.317093
C	-2.917227	5.428963	-1.016624
C	-2.983007	4.429937	-1.998419
C	-3.354024	3.111001	-1.673392
C	-3.846595	3.481230	2.159554
C	-4.965771	4.348414	2.765121
C	-3.356643	2.034038	-2.756080
C	-4.400086	2.313152	-3.852376
C	-5.416442	1.191200	-0.010474

C	-6.411007	2.315680	-0.245090	H	-1.946383	1.038774	-4.116542
C	-5.969844	-0.105455	0.135644	H	-1.589620	2.770102	-3.850984
C	-5.355510	-1.385109	0.130289	H	-4.523417	-1.895380	-2.246208
C	-6.312314	-2.563094	0.013845	H	-3.573629	-4.121646	-4.176483
N	-4.030785	-1.605012	0.146581	H	-5.207288	-4.042476	-3.442398
C	-3.576190	-2.946342	-0.008431	H	-4.642746	-2.742067	-4.541310
C	-3.464298	-3.505882	-1.317573	H	-2.706690	-1.198148	-3.826013
C	-3.023599	-4.836230	-1.448360	H	-2.110673	-1.224022	-2.140299
C	-2.688913	-5.603469	-0.321486	H	-1.676771	-2.548717	-3.248289
C	-2.760032	-5.031864	0.955799	H	-2.944115	-5.286565	-2.449631
C	-3.187755	-3.701003	1.137249	H	-2.356108	-6.646281	-0.443306
C	-3.761503	-2.644881	-2.543469	H	-2.470136	-5.630900	1.832667
C	-4.325767	-3.434526	-3.733793	H	-3.162734	-1.976781	2.380858
C	-3.237989	-3.076344	2.528622	H	-4.768597	-4.417643	3.364075
C	-4.585670	-3.329649	3.231029	H	-4.598906	-2.856622	4.235842
C	-2.062582	-3.514392	3.416306	H	-5.433813	-2.911180	2.654368
C	-2.500549	-1.862086	-2.961461	H	-1.088344	-3.373608	2.905121
C	-2.551201	3.617663	2.983178	H	-2.040812	-2.924804	4.356154
C	-1.948682	1.844560	-3.353187	H	-2.136068	-4.582687	3.710371
C	-1.032923	0.020415	2.606476	H	4.388049	-3.042902	-2.953284
C	-2.060506	0.225611	3.686672	H	3.983845	-1.980248	-4.350522
H	-3.091999	0.527820	3.368710	H	2.703965	-2.907022	-3.496477
H	-6.290372	3.127705	0.500049	H	3.506548	0.171586	-4.052090
H	-6.239166	2.785670	-1.236277	H	4.067860	2.330388	-4.172100
H	-7.454870	1.952704	-0.206860	H	4.346270	3.326432	-2.695793
H	-7.068681	-0.132104	0.138869	H	2.705566	3.164241	-3.353720
H	-7.321983	-2.297140	0.380871	H	1.122271	-2.473165	-1.627056
H	-6.414892	-2.865380	-1.051463	H	1.273475	-4.691483	-2.828847
H	-5.950878	-3.455392	0.559668	H	-0.419435	-4.232668	-2.429239
H	-4.171873	2.420744	2.209474	H	0.412848	-5.482465	-1.469589
H	-5.906321	4.275509	2.181050	H	0.009600	-4.105958	0.747837
H	-5.189818	4.031812	3.805668	H	-0.919379	-2.943776	-0.239529
H	-4.678027	5.420911	2.799948	H	0.447869	-2.380901	0.792409
H	-2.172158	4.661540	2.966024	H	1.935763	-5.700342	0.180277
H	-2.725246	3.343626	4.044255	H	4.174613	-6.168206	1.193164
H	-1.744646	2.965896	2.592667	H	5.960864	-4.427414	1.119101
H	-3.119981	5.883946	1.091781	H	5.301530	-0.928344	0.003934
H	-2.626613	6.455562	-1.289270	H	7.470360	-1.170175	-1.265728
H	-2.738327	4.677456	-3.044175	H	6.059951	-1.773477	-2.179585
H	-3.651379	1.083204	-2.264031	H	7.177864	-2.937345	-1.394480
H	-4.419160	1.488975	-4.596580	H	7.444127	-1.060532	1.241123
H	-5.419752	2.407446	-3.425164	H	7.391578	-2.838907	1.279810
H	-4.176831	3.253498	-4.400737	H	6.174776	-1.891805	2.195177
H	-1.202305	1.572153	-2.576416	H	5.240834	1.014656	0.144747

H	7.149153	3.103347	-1.081637
H	6.072964	1.970618	-1.963882
H	7.456035	1.335533	-1.028089
H	7.315407	1.071742	1.479939
H	6.031418	1.898607	2.415249
H	7.296303	2.850429	1.573890
H	5.854077	4.451888	1.453030
H	4.055473	6.178967	1.576494
H	1.840294	5.746824	0.496218
H	1.070604	2.592423	-1.448985
H	0.481778	5.630540	-1.377623
H	-0.335460	4.400041	-2.379242
H	1.395149	4.791803	-2.669051
H	0.226048	2.583794	0.927117
H	-1.033331	3.153931	-0.226690
H	-0.156395	4.321117	0.802119
H	-0.621115	0.881537	2.055476
H	-0.835797	-0.982446	2.196375
H	-1.736445	1.008102	4.413655
C	2.395986	3.795304	-0.277619
H	-2.191326	-0.704414	4.280374
C	2.850285	-1.304843	2.688783
C	3.497392	-0.069022	2.398041
C	2.895587	1.130491	2.882358
C	1.682537	1.101304	3.574106
C	0.953377	-0.130366	3.779706
C	1.634763	-1.340192	3.379426
H	3.327921	-2.249984	2.381267
H	4.487481	-0.051574	1.922416
H	3.406315	2.094706	2.722521
H	1.260427	2.043628	3.960827
H	0.246037	-0.179416	4.621174
H	1.179241	-2.315599	3.616086
H	-0.191376	0.090548	-0.475340

IM6

Enthalpy: -4146.088376

Free energy: -4146.289595

C	3.361445	-2.543075	-0.424224
C	4.336813	-2.501666	-1.467329
C	4.392132	-3.568748	-2.384545
C	3.506433	-4.654426	-2.291140
C	2.544565	-4.680454	-1.270941
N	3.249714	-1.422604	0.444666
C	3.835840	-1.472151	1.653059
C	4.431219	-2.784223	2.141466
C	5.283064	-1.306370	-1.577087
C	6.467478	-1.416131	-0.595311
C	1.365242	-3.647392	0.739224
C	1.213884	-5.009767	1.432235
C	3.966354	-0.368425	2.531223
C	3.642004	1.002485	2.350223
C	4.189841	1.938488	3.418908
N	2.926292	1.482512	1.325307
C	2.689867	2.875603	1.205217
C	1.777652	3.565309	2.061264
C	1.600380	4.951893	1.879400
C	2.264378	5.649633	0.860097
C	3.109497	4.953884	-0.017998
C	3.334474	3.572401	0.134624
C	0.955244	2.833931	3.119565
C	1.047100	3.500238	4.504330
C	4.306531	2.826242	-0.777261
C	5.708550	2.752175	-0.141722
C	-0.515624	2.700763	2.674919
C	4.367176	3.381593	-2.206635
C	5.792461	-1.054962	-3.004064
C	0.020390	-3.172477	0.157407
Ca	1.792099	0.271430	-0.412182
Ca	-1.933569	-0.253211	-0.243982
N	-3.147863	-0.677527	1.746144
C	-2.835320	-1.970980	2.248519
C	-3.467699	-3.105821	1.649860
C	-3.105941	-4.398498	2.075171
C	-2.146112	-4.587409	3.079844
C	-1.514805	-3.472225	3.649304
C	-1.827846	-2.159289	3.245279
C	-4.491152	-2.922792	0.530600
C	-5.777419	-3.736755	0.750395
C	-1.059029	-0.987183	3.851307
C	-1.189172	-0.932193	5.385408
C	-4.011895	0.111601	2.402852
C	-4.620301	-0.383856	3.702335
C	-4.453772	1.378827	1.940544
C	-4.246369	2.022602	0.691959
C	-5.011685	3.315144	0.463884
N	-3.450060	1.545529	-0.274956
C	-3.403821	2.155874	-1.557866

C	-2.625779	3.325113	-1.802649	H	0.289698	4.122868	-0.071975
C	-2.550029	3.824770	-3.118507	H	-0.151265	2.533067	-0.763426
C	-3.198176	3.182719	-4.181594	H	0.076735	3.944480	-1.841891
C	-3.932195	2.011062	-3.941178	H	-1.950195	4.727390	-3.316035
C	-4.049088	1.480322	-2.643206	H	-3.118392	3.584022	-5.204032
C	-1.805185	3.980274	-0.697239	H	-4.419676	1.499232	-4.784277
C	-1.997652	5.505266	-0.629163	H	-4.329288	-0.333242	-1.556765
C	-4.857860	0.212116	-2.373381	H	-6.843104	1.133500	-2.544577
C	-6.256858	0.536608	-1.814072	H	-6.821682	-0.396189	-1.601611
C	-4.958502	-0.726598	-3.582910	H	-6.196929	1.111908	-0.870271
C	-0.314783	3.626596	-0.853139	H	-3.962319	-0.959882	-4.013111
C	-3.866282	-3.256512	-0.838468	H	-5.439441	-1.683350	-3.292090
C	0.426942	-1.023370	3.442875	H	-5.581111	-0.291194	-4.392342
C	-0.495573	-2.149722	-4.675249	H	4.284910	2.978847	3.054459
C	0.135863	-3.473824	-5.114594	H	5.180369	1.592236	3.773401
H	-0.150283	-3.742601	-6.153385	H	3.517549	1.957401	4.303057
H	-5.162208	-1.338759	3.535703	H	4.511944	-0.586129	3.460616
H	-3.838484	-0.605450	4.456110	H	5.074218	-2.635510	3.029448
H	-5.326942	0.349321	4.133842	H	5.024122	-3.284785	1.350122
H	-5.144178	1.900688	2.617950	H	3.623744	-3.494597	2.421210
H	-4.342057	4.191946	0.595838	H	1.358777	1.805305	3.201824
H	-5.408978	3.374609	-0.569259	H	2.098383	3.668503	4.815966
H	-5.850629	3.423531	1.176989	H	0.559014	2.867258	5.275245
H	-4.773746	-1.849539	0.523626	H	0.533102	4.484953	4.521635
H	-6.230253	-3.516886	1.738886	H	-0.972908	3.695000	2.486648
H	-6.529945	-3.495223	-0.029532	H	-1.121880	2.201238	3.459398
H	-5.593369	-4.830996	0.701049	H	-0.599955	2.092819	1.751978
H	-3.518089	-4.310095	-0.876308	H	0.908757	5.495259	2.543089
H	-4.589985	-3.106346	-1.665681	H	2.106567	6.732508	0.735829
H	-2.973855	-2.633241	-1.070959	H	3.612220	5.499391	-0.831156
H	-3.588569	-5.275229	1.614453	H	3.954578	1.770551	-0.835773
H	-1.882578	-5.604039	3.410856	H	6.410893	2.188692	-0.791847
H	-0.744664	-3.622727	4.422847	H	5.678496	2.245245	0.843049
H	-1.495258	-0.057310	3.433309	H	6.123930	3.771089	0.009912
H	-0.708804	-0.013828	5.784131	H	4.945622	2.699124	-2.863140
H	-2.248357	-0.929351	5.716785	H	4.869756	4.371052	-2.246917
H	-0.692490	-1.799678	5.870554	H	3.354986	3.499984	-2.646089
H	0.545898	-0.919318	2.346505	H	4.696236	-0.414887	-1.255539
H	0.984927	-0.187263	3.912510	H	7.052500	-2.341542	-0.783563
H	0.916379	-1.966340	3.765106	H	6.130776	-1.430020	0.459020
H	-2.139102	3.551864	0.268891	H	7.154942	-0.551180	-0.709673
H	-1.585120	6.014923	-1.525858	H	6.340176	-0.090818	-3.054309
H	-3.069523	5.783505	-0.551468	H	4.965922	-1.016938	-3.743799
H	-1.468399	5.923363	0.252429	H	6.500918	-1.843659	-3.335912

H	5.135816	-3.548312	-3.195222
H	3.561338	-5.476129	-3.022500
H	1.841983	-5.526633	-1.208802
H	1.652806	-2.904084	1.508696
H	0.815307	-5.784799	0.743733
H	0.501032	-4.932220	2.277368
H	2.184526	-5.377677	1.825322
H	0.138048	-2.170852	-0.313952
H	-0.750130	-3.107709	0.951757
H	-0.342949	-3.866388	-0.628993
H	-1.603937	-2.201253	-4.788941
H	-0.154327	-1.320239	-5.334157
H	-0.179181	-4.311134	-4.453073
C	2.453859	-3.637086	-0.328938
H	1.244672	-3.428437	-5.078190
C	1.908305	-0.333767	-3.055968
C	1.149378	0.894175	-3.039210
C	-0.259474	0.769159	-2.918065
C	-0.898803	-0.474031	-2.786939
C	-0.183290	-1.759895	-3.199923
C	1.314245	-1.578117	-2.969179
H	3.013344	-0.280006	-3.058984
H	1.627063	1.869491	-3.215005
H	-0.878808	1.681233	-2.880562
H	-2.005577	-0.479436	-2.875021
H	-0.539123	-2.622732	-2.585257
H	1.946345	-2.475371	-2.899283
H	-0.075147	0.254335	0.522884

TS6

Enthalpy: -4146.073048

Free energy: -4146.270990

C	-3.495562	2.295498	-1.015619
C	-4.246247	1.875245	-2.159738
C	-4.358680	2.744642	-3.261868
C	-3.755957	4.012221	-3.249641
C	-3.005416	4.409145	-2.135597
N	-3.363542	1.379942	0.066429
C	-4.141970	1.526102	1.152678
C	-4.983478	2.784163	1.303556
C	-4.943735	0.517416	-2.152804
C	-6.296051	0.584301	-1.413615
C	-1.938265	4.000308	0.128375
C	-2.283804	5.395258	0.678190
C	-4.273888	0.567961	2.190010
C	-3.829595	-0.781145	2.278723
C	-4.419075	-1.576394	3.435303
N	-2.979066	-1.355282	1.422354
C	-2.666834	-2.739556	1.486382
C	-1.749919	-3.272025	2.443551
C	-1.416744	-4.639914	2.372676
C	-1.948122	-5.475458	1.382344
C	-2.844202	-4.947278	0.440440
C	-3.221393	-3.591646	0.476382
C	-1.125378	-2.415662	3.542487
C	-1.475072	-2.948988	4.945703
C	-4.251437	-3.031784	-0.503155
C	-5.629804	-2.864033	0.169656
C	0.400964	-2.290397	3.375427
C	-4.391644	-3.844134	-1.797288
C	-5.122796	-0.093214	-3.550454
C	-0.458554	3.940655	-0.296278
Ca	-1.675606	-0.286287	-0.283203
Ca	1.823927	0.135688	-0.171040
N	3.004471	1.370500	1.497826
C	2.459793	2.648611	1.823908
C	3.026540	3.816964	1.223620
C	2.537856	5.081133	1.600877
C	1.499225	5.206477	2.539241
C	0.905909	4.055151	3.072344
C	1.359779	2.766428	2.719488
C	4.099326	3.665244	0.146970
C	5.063568	4.855248	0.041228
C	0.648533	1.536847	3.274469
C	0.738942	1.445389	4.807412
C	4.078714	0.969493	2.203226
C	4.551665	1.818574	3.372590
C	4.857459	-0.183615	1.927659
C	4.802380	-1.115186	0.858070
C	5.930896	-2.133314	0.808742
N	3.849423	-1.138806	-0.085751
C	3.942400	-2.082251	-1.143152
C	3.541332	-3.438591	-0.959564
C	3.603804	-4.314463	-2.062793
C	4.027836	-3.871592	-3.323383
C	4.380226	-2.524837	-3.505927
C	4.343657	-1.613719	-2.433309
C	2.988313	-3.933578	0.375576

C	3.650061	-5.242806	0.843527	H	4.016054	0.440883	-1.960195
C	4.702198	-0.138892	-2.623001	H	6.880311	-0.413331	-2.685611
C	6.126609	0.182293	-2.128295	H	6.362492	1.256984	-2.281373
C	4.497380	0.367050	-4.057934	H	6.246364	-0.032464	-1.048924
C	1.456445	-4.092888	0.317478	H	3.492078	0.109243	-4.450431
C	3.425224	3.392737	-1.213923	H	4.604195	1.471183	-4.096262
C	-0.815430	1.506318	2.802262	H	5.250375	-0.053840	-4.757122
C	0.556272	1.435693	-3.486751	H	-4.377314	-2.666991	3.253202
C	-0.451985	2.562867	-3.682788	H	-5.471075	-1.285614	3.623762
H	0.041507	3.480497	-4.063004	H	-3.853783	-1.370463	4.369136
H	4.895177	2.815830	3.025766	H	-4.947916	0.873070	3.003711
H	3.722686	2.015218	4.082533	H	-5.756281	2.667798	2.086358
H	5.383136	1.335244	3.918621	H	-5.479347	3.056661	0.350176
H	5.694876	-0.340595	2.621742	H	-4.344980	3.649212	1.581025
H	5.574603	-3.133611	1.132811	H	-1.550181	-1.396597	3.442228
H	6.316906	-2.259532	-0.222859	H	-2.566062	-3.095983	5.076399
H	6.768113	-1.841892	1.470360	H	-1.127726	-2.246629	5.733105
H	4.698523	2.765244	0.397863	H	-0.984104	-3.926789	5.138865
H	5.535457	5.088696	1.018052	H	0.901629	-3.278674	3.456061
H	5.876008	4.628799	-0.680365	H	0.830576	-1.638326	4.165001
H	4.557686	5.776043	-0.319517	H	0.645303	-1.848533	2.388272
H	2.796199	4.250944	-1.529991	H	-0.716746	-5.057731	3.114442
H	4.173638	3.198000	-2.010289	H	-1.664032	-6.538905	1.341673
H	2.752433	2.511518	-1.163446	H	-3.264865	-5.607881	-0.332382
H	2.974072	5.988058	1.155178	H	-3.912324	-2.004885	-0.776344
H	1.136707	6.204238	2.832462	H	-6.383451	-2.507835	-0.563797
H	0.064599	4.153575	3.777168	H	-5.600214	-2.130093	0.997024
H	1.153345	0.642893	2.852191	H	-5.986276	-3.832960	0.579284
H	0.229825	0.531630	5.178996	H	-5.037538	-3.304070	-2.520193
H	1.792799	1.409564	5.152912	H	-4.871607	-4.829318	-1.615625
H	0.254149	2.316227	5.298776	H	-3.415271	-4.033015	-2.286768
H	-0.878308	1.591084	1.697872	H	-4.298301	-0.165808	-1.554811
H	-1.313529	0.560515	3.094087	H	-6.957111	1.350437	-1.871981
H	-1.406305	2.343016	3.229487	H	-6.168443	0.833256	-0.342244
H	3.202977	-3.154409	1.134893	H	-6.821327	-0.392412	-1.466063
H	3.378652	-6.099303	0.190180	H	-5.472695	-1.143502	-3.470587
H	4.757814	-5.170091	0.852614	H	-4.178602	-0.093455	-4.132682
H	3.317513	-5.499213	1.871343	H	-5.884675	0.451439	-4.147840
H	1.064708	-4.476612	1.279572	H	-4.936223	2.431037	-4.144717
H	0.941617	-3.130883	0.119920	H	-3.861834	4.684206	-4.115949
H	1.152032	-4.809908	-0.474214	H	-2.511493	5.394187	-2.139191
H	3.300733	-5.365781	-1.932300	H	-2.074136	3.267376	0.948439
H	4.066910	-4.572547	-4.172036	H	-2.071676	6.194373	-0.063857
H	4.685125	-2.178628	-4.504806	H	-1.672527	5.615763	1.578054

H	-3.354421	5.479330	0.958872
H	-0.179221	2.917600	-0.629086
H	0.202544	4.224607	0.543642
H	-0.254053	4.634253	-1.139530
H	1.448831	1.812417	-2.940312
H	0.934436	1.093306	-4.477491
H	-0.958166	2.821539	-2.733836
C	-2.846272	3.565456	-1.017190
H	-1.240624	2.287684	-4.411968
C	-1.770726	-1.552034	-2.859254
C	-0.858984	-2.578091	-2.517566
C	0.515966	-2.244892	-2.488116
C	0.946405	-0.928923	-2.668513
C	0.018171	0.191047	-2.767808
C	-1.358959	-0.220099	-3.020013
H	-2.829199	-1.802187	-3.036468
H	-1.192791	-3.615652	-2.376161
H	1.273929	-3.034765	-2.379919
H	2.026738	-0.742667	-2.792029
H	0.006247	0.914976	-1.307805
H	-2.092597	0.541335	-3.326031
H	0.144072	-0.742340	0.721779

IM1-a

Enthalpy: -2110.778948

Free energy: -2110.878015

Ca	-0.020574	0.817595	-0.307843
N	1.612477	-0.934761	-0.195579
C	1.406798	-1.947336	0.653800
C	2.583101	-2.767555	1.178694
C	0.131194	-2.399897	1.107129
C	-1.186459	-2.093416	0.658180
C	-2.274822	-3.017770	1.196534
N	-1.515216	-1.072709	-0.148574
C	0.101916	2.950580	-1.772027
C	-0.945665	4.071417	-1.683662
H	-0.785797	4.933909	-2.377175
H	2.902771	-3.515130	0.422162
H	3.457172	-2.123682	1.405235
H	2.321085	-3.324638	2.099737
H	0.181392	-3.241923	1.814282
H	-1.863979	-3.870088	1.770898
H	-2.968092	-2.461232	1.862217
H	-2.884728	-3.430821	0.366550
H	1.084573	3.421793	-1.505627
H	0.230687	2.500788	-2.772706
H	-0.982253	4.499726	-0.655407
H	-1.974666	3.696530	-1.889907
C	-1.268454	1.225180	2.610494
C	-0.087941	0.508799	2.966127
C	1.182627	1.078792	2.658393
C	1.287314	2.324269	1.994836
C	0.086097	3.082231	1.620889
C	-1.202061	2.473592	1.942550
H	-2.258030	0.800847	2.833269
H	-0.141184	-0.477991	3.445166
H	2.110487	0.538602	2.904113
H	2.271257	2.771060	1.770723
H	0.159187	4.093196	1.170084
H	-2.115813	3.026031	1.668803
Si	-3.098515	-0.792358	-0.888017
C	-4.594418	-0.598916	0.258261
H	-5.434309	-0.149564	-0.315859
H	-4.955374	-1.570340	0.654365
H	-4.401313	0.067095	1.124157
C	-3.492085	-2.141723	-2.163569
H	-3.680508	-3.132938	-1.699624
H	-4.396951	-1.877676	-2.753881
H	-2.648878	-2.260691	-2.877206
C	-2.877123	0.862123	-1.801253
H	-2.650268	1.702350	-1.105889
H	-2.054580	0.820419	-2.551424
H	-3.804947	1.159080	-2.333674
Si	3.155323	-0.529361	-0.979587
C	4.126961	-1.990697	-1.707526
H	3.458751	-2.687720	-2.258444
H	4.864008	-1.596415	-2.441114
H	4.691147	-2.581969	-0.958821
C	2.711128	0.593164	-2.440211
H	3.630285	0.838188	-3.015153
H	2.010261	0.097505	-3.146563
H	2.250259	1.554498	-2.131889
C	4.273671	0.451752	0.199675
H	3.758168	1.366551	0.561017
H	4.581721	-0.146670	1.082495
H	5.203133	0.778241	-0.316431

TS1-a

Enthalpy: -2110.765820

Free energy: -2110.862239

Ca	0.098093	0.926089	-0.197050
N	-1.497385	-0.535405	0.793709
C	-1.194356	-1.839765	0.833841
C	-2.303565	-2.882534	0.953047
C	0.124443	-2.386760	0.826495
C	1.394772	-1.766516	0.987284
C	2.565581	-2.721418	1.194392
N	1.617621	-0.444562	0.961128
C	-0.155141	3.493021	-0.734816
C	0.840112	4.597008	-1.048729
H	0.641081	5.549822	-0.504075
H	-2.648386	-2.959858	2.006464
H	-3.182834	-2.613786	0.333498
H	-1.960752	-3.889728	0.644965
H	0.154884	-3.487003	0.831260
H	2.245951	-3.777726	1.281218
H	3.279207	-2.647035	0.346580
H	3.128973	-2.459639	2.115187
H	-1.198177	3.810184	-0.952536
H	-0.126469	3.277970	0.366291
H	0.834572	4.854897	-2.133092
H	1.883083	4.305589	-0.795366
C	1.407437	0.161188	-2.507564
C	0.267368	-0.683379	-2.411567
C	-1.009454	-0.069766	-2.518751
C	-1.151498	1.319390	-2.600492
C	-0.006562	2.219499	-2.498462
C	1.288066	1.551930	-2.597397
H	2.412624	-0.290350	-2.516975
H	0.370798	-1.772979	-2.327613
H	-1.913188	-0.699657	-2.526817
H	-2.158527	1.756431	-2.697568
H	-0.096706	3.203535	-2.985952
H	2.195467	2.168091	-2.701923
Si	3.096917	0.403219	1.417960
C	4.651439	-0.084952	0.445996
H	5.448170	0.677060	0.593097
H	5.069294	-1.063031	0.761020
H	4.442075	-0.138382	-0.643434
C	3.431576	0.282770	3.277939
H	3.710940	-0.746048	3.588507
H	4.262946	0.957419	3.577402
H	2.529800	0.573222	3.857834
C	2.719312	2.210854	0.985635
H	2.513851	2.338115	-0.100221
H	1.863484	2.624676	1.562375
H	3.589110	2.863865	1.209666
Si	-3.103735	0.168548	1.065713
C	-3.970729	-0.465405	2.629527
H	-3.259500	-0.549505	3.478822
H	-4.768663	0.248284	2.930133
H	-4.451911	-1.454787	2.487053
C	-2.793223	2.023684	1.299252
H	-3.748350	2.551020	1.508917
H	-2.111667	2.228304	2.153360
H	-2.368344	2.505718	0.393282
C	-4.259419	-0.021123	-0.426074
H	-3.824968	0.464581	-1.324353
H	-4.467136	-1.081126	-0.681586
H	-5.236651	0.469060	-0.222430

IM2-a

Enthalpy: -2110.799517

Free energy: -2110.899492

Ca	0.061069	0.178478	-0.871599
N	-0.880702	-1.571263	0.369873
C	-0.665520	-1.617886	1.689449
C	-1.678472	-2.311973	2.590638
C	0.479964	-1.069805	2.339167
C	1.697698	-0.595907	1.770680
C	2.835107	-0.329449	2.748148
N	1.893853	-0.389067	0.461672
C	-1.976053	4.004687	0.969020
C	-3.325784	3.909173	1.684618
H	-3.768153	4.911533	1.866065
H	-2.680204	-1.848821	2.470129
H	-1.776734	-3.381606	2.306783
H	-1.402799	-2.270094	3.662073
H	0.479224	-1.153316	3.436450
H	2.567611	-0.563430	3.796648
H	3.727572	-0.934556	2.480495
H	3.139777	0.737142	2.696708
H	-1.270468	4.627940	1.566141
H	-2.095584	4.520841	-0.009832
H	-3.227177	3.404615	2.671176
H	-4.061145	3.328576	1.087984

C	-1.983125	1.801232	-1.592853
C	-0.825410	2.384272	-2.202290
C	0.207751	2.839912	-1.319331
C	0.074929	2.778044	0.064960
C	-1.301548	2.625932	0.707312
C	-2.127037	1.723645	-0.209953
H	-2.724089	1.291170	-2.235961
H	-0.730148	2.471002	-3.294512
H	1.179768	3.145275	-1.748413
H	0.933961	3.031937	0.708680
H	-1.192530	2.132891	1.702225
H	-2.965225	1.149816	0.217537
Si	3.396303	-0.112684	-0.411737
C	2.832273	0.066198	-2.225698
H	2.346660	-0.861296	-2.604065
H	2.152526	0.931006	-2.408110
H	3.708903	0.243946	-2.884342
C	4.567942	-1.597168	-0.327228
H	5.421858	-1.467296	-1.027296
H	4.992501	-1.739101	0.688809
H	4.039126	-2.533806	-0.603972
C	4.319776	1.469675	0.069205
H	4.830670	1.372478	1.049734
H	5.098373	1.713571	-0.686198
H	3.627734	2.335733	0.132453
Si	-2.048004	-2.453428	-0.610730
C	-1.621775	-1.911146	-2.388128
H	-1.833970	-0.836791	-2.596383
H	-0.560053	-2.130277	-2.642596
H	-2.234844	-2.475809	-3.122374
C	-3.861454	-2.022271	-0.279355
H	-4.516872	-2.435838	-1.076763
H	-4.217261	-2.435081	0.687596
H	-4.011427	-0.922343	-0.253944
C	-1.802170	-4.329478	-0.519876
H	-2.146062	-4.751651	0.447581
H	-2.373238	-4.841874	-1.324505
H	-0.730452	-4.594300	-0.641204

TS2-a

Enthalpy: -2110.774986

Free energy: -2110.873225

Ca	0.299312	0.623778	-0.429046
N	-1.336379	-0.579023	0.766569
C	-1.151527	-0.599590	2.094064
C	-2.345079	-0.742406	3.033182
C	0.121448	-0.563580	2.737578
C	1.419946	-0.756932	2.184509
C	2.541263	-1.001355	3.186910
N	1.696500	-0.741886	0.872964
C	0.349889	4.677278	-0.204373
C	-0.653636	4.830746	0.937415
H	-0.437844	5.740717	1.534637
H	-3.217081	-0.162080	2.669005
H	-2.655142	-1.807194	3.102752
H	-2.105658	-0.403366	4.060385
H	0.082709	-0.543834	3.837442
H	2.179926	-1.055169	4.232019
H	3.066077	-1.953286	2.958364
H	3.297132	-0.190148	3.123027
H	1.385129	4.748025	0.189615
H	0.228389	5.523165	-0.922427
H	-0.598202	3.950822	1.614554
H	-1.698291	4.922180	0.572030
C	-1.243935	1.993659	-2.462315
C	-0.150334	1.560998	-3.251073
C	1.111731	2.175157	-3.009209
C	1.288512	3.089568	-1.970512
C	0.237305	3.388152	-1.014757
C	-1.070297	2.897792	-1.404250
H	-2.256982	1.617836	-2.680565
H	-0.292096	0.864719	-4.090345
H	1.963303	1.940967	-3.669288
H	2.279030	3.548113	-1.813558
H	0.709131	2.466965	0.473790
H	-1.946896	3.196330	-0.808934
Si	3.153454	-1.291946	0.048427
C	2.782180	-0.930692	-1.780905
H	1.870855	-1.461236	-2.135983
H	2.652957	0.158410	-1.972947
H	3.617723	-1.257019	-2.436044
C	3.431756	-3.155948	0.238345
H	4.258530	-3.501023	-0.420142
H	3.697817	-3.438640	1.278644
H	2.516557	-3.720889	-0.039091
C	4.731563	-0.347044	0.510340
H	5.125157	-0.642956	1.504844
H	5.535784	-0.538281	-0.233605

H	4.545780	0.748223	0.531224
Si	-2.776974	-1.043514	-0.144473
C	-2.098424	-1.522368	-1.851521
H	-1.427306	-0.754166	-2.293575
H	-1.512245	-2.463302	-1.770201
H	-2.913929	-1.696574	-2.585747
C	-4.002566	0.395106	-0.304931
H	-4.786410	0.178346	-1.062926
H	-4.518818	0.592407	0.658708
H	-3.491687	1.334645	-0.600954
C	-3.692968	-2.567838	0.514207
H	-4.303878	-2.356733	1.415528
H	-4.383211	-2.951886	-0.269120
H	-2.984288	-3.387098	0.760963

IM3-a

Enthalpy: -2110.792402

Free energy: -2110.896676

Ca	-0.108773	0.499306	0.383880
N	0.213162	-1.850851	0.231572
C	0.980988	-2.287594	1.241820
C	0.781001	-3.688432	1.811774
C	2.052353	-1.547011	1.824200
C	2.709941	-0.377526	1.340595
C	4.050478	-0.051893	1.986577
N	2.224874	0.417735	0.378426
C	-3.699216	2.248167	1.958002
C	-4.632618	1.210803	2.579459
H	-4.898042	1.503218	3.615825
H	-0.294835	-3.954055	1.854868
H	1.289347	-4.444155	1.176054
H	1.203164	-3.781087	2.831927
H	2.543390	-2.036758	2.678722
H	4.362536	-0.810335	2.730323
H	4.845988	0.015870	1.213878
H	4.001173	0.934215	2.494122
H	-2.757586	2.303067	2.553956
H	-4.158083	3.260417	2.012279
H	-4.152669	0.211304	2.639223
H	-5.581304	1.102626	2.011189
C	-3.101097	0.580194	-1.474771
C	-2.327678	1.557290	-2.125931
C	-2.027517	2.759325	-1.452383
C	-2.484738	2.967665	-0.141211
C	-3.268322	1.995019	0.528700
C	-3.563730	0.798549	-0.161483
H	-3.349329	-0.360356	-1.990338
H	-1.976024	1.395403	-3.156863
H	-1.432463	3.537349	-1.955934
H	-2.232939	3.903179	0.383721
H	-0.553302	1.378481	2.252560
H	-4.171343	0.023012	0.328015
Si	3.043625	1.687344	-0.530497
C	1.660123	2.396897	-1.626597
H	1.216432	1.623043	-2.290875
H	0.850371	2.855614	-1.015495
H	2.039789	3.205185	-2.287108
C	4.397706	0.984934	-1.651851
H	4.785113	1.762198	-2.345853
H	5.261446	0.598512	-1.070681
H	4.002668	0.145571	-2.262676
C	3.726600	3.112239	0.515205
H	4.661625	2.840481	1.047091
H	3.955064	3.991208	-0.126709
H	2.983088	3.433166	1.275470
Si	-0.760776	-2.812853	-0.886519
C	-0.679956	-1.852848	-2.522001
H	-0.888130	-0.769603	-2.402454
H	0.340079	-1.941931	-2.954334
H	-1.400368	-2.244295	-3.272279
C	-2.552562	-2.945226	-0.279491
H	-3.223469	-3.359177	-1.063371
H	-2.620951	-3.614452	0.604864
H	-2.957612	-1.959903	0.029786
C	-0.117870	-4.555888	-1.271126
H	-0.317523	-5.287293	-0.461728
H	-0.623293	-4.932512	-2.187786
H	0.973985	-4.552368	-1.475685

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Enthalpy: -2695.758020

Free energy: -2695.957242

C	4.510703	-1.702060	0.092781
C	4.707572	-1.603543	-1.326634
C	4.850890	-2.779912	-2.084036
C	4.791615	-4.045874	-1.479641
C	4.571162	-4.140171	-0.098659
N	4.218268	-0.521220	0.801833

C	5.050888	0.114654	1.625055	C	-4.576355	2.104049	0.751474
C	6.420240	-0.473209	1.932737	C	-4.633714	3.398194	1.299265
C	4.781979	-0.225362	-1.975701	C	-4.354085	4.530863	0.516891
C	6.208709	0.350753	-1.880574	C	-4.008505	4.368727	-0.831469
C	4.123047	-3.147928	2.193481	C	-3.920214	3.093622	-1.426095
C	5.270190	-3.855363	2.939549	C	-4.943656	0.869939	1.572039
C	4.743367	1.354127	2.252171	C	-6.369630	0.395715	1.227858
C	3.660431	2.252712	2.041688	C	-3.511342	2.978164	-2.892690
C	3.770427	3.587820	2.765866	C	-4.539236	3.656859	-3.819303
N	2.594880	1.997910	1.274389	C	-2.104195	3.551339	-3.141883
C	1.648110	2.981199	0.892516	C	-4.774289	1.039115	3.087484
C	0.476169	3.253823	1.667166	C	1.129176	-2.709482	-2.243000
C	-0.532079	4.075735	1.117268	C	-3.637888	-2.778597	3.091175
C	-0.389301	4.662262	-0.145761	C	0.219743	0.716580	-1.824234
C	0.776988	4.424527	-0.888504	C	-0.634793	0.290101	-3.033794
C	1.795118	3.585734	-0.401488	H	-0.624362	0.999659	-3.895945
C	0.316722	2.747284	3.097531	H	-3.105228	-3.850302	-3.366304
C	0.442946	3.910754	4.103495	H	-3.408724	-4.518818	-1.738904
C	3.047994	3.309464	-1.227707	H	-4.780974	-3.943131	-2.755450
C	4.215428	4.220823	-0.798115	H	-5.182816	-1.745049	-3.140912
C	-1.014469	2.007472	3.312047	H	-6.837214	-0.066174	-2.525851
C	2.822925	3.400549	-2.743738	H	-6.238436	1.559884	-2.041307
C	4.260778	-0.187386	-3.418957	H	-5.805045	0.866145	-3.638129
C	2.789593	-3.887642	2.415809	H	-0.974195	-2.696774	-2.699833
C	-0.128060	-1.093789	1.915256	H	-1.169758	-5.211413	-3.115916
C	0.803995	-0.993937	3.138367	H	0.025905	-4.407965	-4.188308
N	-2.628484	-2.104685	-0.962632	H	0.581772	-5.375921	-2.788934
C	-1.933646	-3.158893	-0.313427	H	1.878582	-3.275272	-1.650793
C	-0.737810	-3.728062	-0.846297	H	1.534964	-2.605705	-3.270656
C	-0.008274	-4.645161	-0.061104	H	1.032037	-1.680272	-1.836342
C	-0.446907	-5.028514	1.212857	H	0.923150	-5.074766	-0.464791
C	-1.631943	-4.481373	1.727298	H	0.135968	-5.747698	1.808900
C	-2.380215	-3.544747	0.992589	H	-1.969665	-4.777390	2.732117
C	-0.245877	-3.404094	-2.253551	H	-3.741705	-1.919797	1.109870
C	-0.203011	-4.669088	-3.133314	H	-5.831999	-3.246003	1.492214
C	-3.656353	-2.933352	1.563686	H	-4.980437	-3.745429	-0.000493
C	-4.902857	-3.714750	1.103670	H	-4.867968	-4.763052	1.470577
C	-3.572584	-2.338806	-1.882339	H	-2.739615	-2.225254	3.437132
C	-3.734284	-3.740561	-2.456212	H	-4.536667	-2.227216	3.436718
C	-4.476574	-1.363785	-2.387521	H	-3.648496	-3.759956	3.611106
C	-4.731143	-0.028603	-1.969691	H	-4.266721	0.048326	1.239116
C	-5.970384	0.623891	-2.567003	H	-7.115421	1.172845	1.499466
N	-3.977768	0.630054	-1.089479	H	-6.476033	0.184109	0.146479
C	-4.213040	1.939981	-0.630598	H	-6.624145	-0.533382	1.780124

H	-4.952120	0.073312	3.602908
H	-3.754641	1.380727	3.359402
H	-5.497990	1.767542	3.510338
H	-4.911191	3.528159	2.356355
H	-4.405994	5.537546	0.960483
H	-3.794177	5.259446	-1.444384
H	-3.479805	1.898721	-3.144125
H	-4.554014	4.756884	-3.664216
H	-4.289326	3.475637	-4.886226
H	-5.567135	3.282961	-3.641253
H	-1.339226	3.066260	-2.504057
H	-1.803032	3.407827	-4.200771
H	-2.069608	4.641479	-2.933262
H	3.171368	4.376045	2.270553
H	4.821656	3.929344	2.838331
H	3.391209	3.483364	3.805138
H	5.527447	1.733217	2.925027
H	7.199469	0.314251	1.961417
H	6.712945	-1.239999	1.189942
H	6.413820	-0.958857	2.932060
H	1.144560	2.032730	3.288617
H	1.372798	4.491322	3.946882
H	0.446092	3.532706	5.148029
H	-0.408842	4.617696	4.005526
H	-1.881985	2.661939	3.086637
H	-1.121396	1.669784	4.363892
H	-1.067477	1.102697	2.671385
H	-1.446877	4.274609	1.698515
H	-1.189291	5.298971	-0.551122
H	0.884784	4.886457	-1.881161
H	3.356873	2.268530	-0.981216
H	5.129267	3.996098	-1.387960
H	4.469125	4.089906	0.270844
H	3.959964	5.290234	-0.958649
H	1.971847	2.769008	-3.071672
H	3.730597	3.066532	-3.287572
H	2.622569	4.442236	-3.072866
H	4.143519	0.446277	-1.357054
H	6.926268	-0.277116	-2.450939
H	6.558588	0.394560	-0.830174
H	6.250483	1.380790	-2.293306
H	4.215910	0.857979	-3.786290
H	3.240811	-0.616903	-3.503861
H	4.918978	-0.746946	-4.116648
H	5.008363	-2.707180	-3.171118
H	4.906815	-4.957018	-2.087482
H	4.508285	-5.134121	0.373323
H	4.017749	-2.127691	2.617582
H	5.387172	-4.905779	2.596150
H	5.072771	-3.883322	4.032142
H	6.240773	-3.343820	2.780982
H	1.947248	-3.408747	1.876651
H	2.523629	-3.915681	3.493011
H	2.849938	-4.937685	2.059181
H	-0.000031	1.793761	-1.595983
H	1.285223	0.768339	-2.170636
H	-1.718000	0.151138	-2.791683
H	-1.176601	-1.129595	2.306750
H	-0.009330	-2.120475	1.479342
H	0.583841	-0.097038	3.754761
H	1.891337	-0.899387	2.880860
C	4.420429	-2.991926	0.705085
H	-0.308537	-0.691634	-3.437207
H	0.765868	-1.867332	3.833968
Sr	-1.705368	0.122940	-0.059256
Sr	1.769193	-0.210554	0.278497

7

Enthalpy: -2685.319950

Free energy: -2685.523766

C	4.100842	-2.603083	0.436873
C	4.286391	-2.835811	-0.972715
C	4.013176	-4.109288	-1.503598
C	3.568110	-5.159469	-0.682752
C	3.388488	-4.932770	0.688645
N	4.173448	-1.277776	0.889112
C	5.137546	-0.738652	1.630258
C	6.291032	-1.598764	2.129261
C	4.813616	-1.696844	-1.842727
C	6.340477	-1.549109	-1.680811
C	3.384111	-3.469966	2.762169
C	4.371582	-4.289376	3.616397
C	5.183658	0.636292	1.986495
C	4.381622	1.735185	1.565368
C	4.975284	3.104556	1.880399
N	3.220335	1.646188	0.908027
C	2.614160	2.773099	0.305018
C	1.388919	3.298541	0.840717

C	0.700778	4.298728	0.125137	C	-3.599535	-2.519453	2.744694
C	1.193020	4.796059	-1.092547	C	0.418957	1.020024	-2.139412
C	2.397397	4.295119	-1.602170	C	-0.496399	1.191351	-3.363041
C	3.122801	3.293316	-0.927551	H	-0.259311	2.064171	-4.021303
C	0.858164	2.782156	2.175057	H	-4.113578	-3.900679	-1.914041
C	1.706236	3.267952	3.367006	H	-5.747897	-3.436007	-1.336281
C	4.416819	2.766960	-1.546196	H	-5.305170	-3.151861	-3.035015
C	5.450859	3.893422	-1.736989	H	-6.295553	-1.029436	-2.339882
C	-0.619971	3.105388	2.435011	H	-7.567471	0.778760	-1.555154
C	4.155844	2.038591	-2.877895	H	-6.777309	2.265361	-0.910092
C	4.433721	-1.805126	-3.325594	H	-6.651007	1.851882	-2.646038
C	1.932655	-3.805734	3.155267	H	-1.296634	-1.282966	-2.809324
C	-0.411248	-0.601563	2.097385	H	-2.890008	-3.004248	-3.635433
C	0.534739	-0.551468	3.311377	H	-1.678323	-2.613047	-4.891046
N	-3.184491	-1.566933	-1.145640	H	-1.539610	-4.138867	-3.949952
C	-2.355239	-2.622901	-0.716130	H	0.913169	-3.352858	-3.470839
C	-1.150882	-2.920335	-1.446581	H	0.620784	-1.777148	-4.259509
C	-0.207902	-3.808003	-0.887166	H	1.184895	-1.828862	-2.572074
C	-0.433722	-4.426928	0.353070	H	0.716630	-4.042703	-1.437514
C	-1.628595	-4.172671	1.039362	H	0.319515	-5.111833	0.769456
C	-2.599119	-3.286162	0.531585	H	-1.810633	-4.667329	2.007174
C	-0.943765	-2.336362	-2.841664	H	-4.471065	-2.278585	0.793537
C	-1.814864	-3.064446	-3.885396	H	-5.710224	-4.135576	1.884798
C	-3.881137	-3.051168	1.327724	H	-4.932511	-4.753047	0.389738
C	-4.732718	-4.335063	1.396381	H	-4.220306	-5.124284	1.987433
C	-4.414892	-1.739989	-1.636711	H	-2.984819	-1.597755	2.725846
C	-4.908992	-3.136689	-1.998451	H	-4.549772	-2.298904	3.274860
C	-5.368709	-0.704021	-1.842878	H	-3.044800	-3.261899	3.357110
C	-5.391092	0.634813	-1.366189	H	-4.291820	0.363854	1.507458
C	-6.668325	1.422993	-1.620760	H	-6.870719	1.615833	2.627174
N	-4.376477	1.204238	-0.721494	H	-6.688813	0.765936	1.059220
C	-4.395649	2.454142	-0.083769	H	-6.478564	-0.138256	2.589691
C	-4.504937	2.474726	1.350773	H	-4.350119	0.134500	3.968368
C	-4.351948	3.695335	2.033503	H	-3.144171	1.391816	3.555204
C	-4.079832	4.887887	1.343360	H	-4.752832	1.856388	4.193533
C	-3.939026	4.860554	-0.050733	H	-4.439042	3.716206	3.130499
C	-4.079896	3.663819	-0.782777	H	-3.963956	5.833727	1.895465
C	-4.785532	1.171961	2.096085	H	-3.707874	5.793636	-0.589886
C	-6.290317	0.835498	2.089965	H	-3.933035	2.616064	-2.634186
C	-3.876390	3.672336	-2.294756	H	-4.955724	5.537077	-2.740673
C	-4.989866	4.460015	-3.012221	H	-4.879555	4.390087	-4.115182
C	-2.489589	4.223089	-2.681400	H	-5.996762	4.082833	-2.743588
C	-4.225729	1.143018	3.525325	H	-1.663836	3.699107	-2.157133
C	0.518794	-2.329058	-3.303305	H	-2.310177	4.118721	-3.771576

H	-2.398506	5.301605	-2.432112
H	5.818299	3.326337	1.191867
H	5.391211	3.124437	2.908189
H	4.234110	3.919632	1.779676
H	6.062063	0.921535	2.585850
H	7.257451	-1.061515	2.051572
H	6.365002	-2.550179	1.567635
H	6.147780	-1.849032	3.202212
H	0.949927	1.673607	2.147548
H	2.750569	2.912518	3.298482
H	1.288117	2.888230	4.323375
H	1.719730	4.377604	3.418880
H	-0.787330	4.183593	2.638924
H	-0.985519	2.545928	3.319988
H	-1.282327	2.847147	1.583246
H	-0.240209	4.705140	0.526541
H	0.636138	5.572496	-1.639750
H	2.782734	4.683178	-2.559000
H	4.849795	2.025930	-0.844449
H	6.426729	3.482769	-2.072840
H	5.621239	4.454897	-0.795856
H	5.118866	4.625867	-2.503736
H	3.445199	1.196374	-2.753858
H	5.100799	1.635509	-3.299044
H	3.713564	2.720153	-3.635272
H	4.371741	-0.758725	-1.432797
H	6.864191	-2.453797	-2.057198
H	6.625723	-1.408992	-0.620308
H	6.715834	-0.672290	-2.249621
H	4.757144	-0.896475	-3.872896
H	3.339340	-1.912397	-3.472343
H	4.924880	-2.670119	-3.819439
H	4.154304	-4.288477	-2.580477
H	3.359505	-6.150804	-1.114625
H	3.038465	-5.757433	1.330852
H	3.552112	-2.394393	2.980052
H	4.210677	-5.379935	3.476389
H	4.237965	-4.068653	4.696674
H	5.425170	-4.072970	3.350990
H	1.189940	-3.254426	2.544472
H	1.746297	-3.551875	4.219355
H	1.719812	-4.889074	3.032819
H	0.628103	2.037912	-1.716020
H	1.423166	0.712536	-2.531108
H	-1.581638	1.322802	-3.108185
H	-1.407549	-0.224963	2.449916
H	-0.624135	-1.677956	1.859575
H	0.546604	0.457128	3.778782
H	1.608327	-0.756077	3.061577
C	3.634630	-3.671949	1.270140
H	-0.473640	0.296879	-4.022825
H	0.295021	-1.266452	4.136433
Ba	-1.765508	0.652005	-0.270393
Ba	1.690651	-0.536796	0.096916