Supplementary Material

(26 pages including this page)

Title: A DFT Study of Cycloaddition Reactions of [c]-Annelated Carbo and Heterocyclic Five Membered Dienes with Ethylene.

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Figure 1: The B3LYP/6-31G* optimized geometries (bond lengths in Å and angles in degrees) of the dienes **1X**; (X = CH_2, SiH_2, NH, PH, O and S).

Figure 2: The B3LYP/6-31G* optimized geometries (bond lengths in Å and angles in degrees) of the dienes **2X**; (X = CH_2, SiH_2, NH, PH, O and S).

Figure 3: The B3LYP/6-31G* optimized geometries (bond lengths in Å and angles in degrees) of the dienes **3X**; (X = CH_2, SiH_2, NH, PH, O and S).

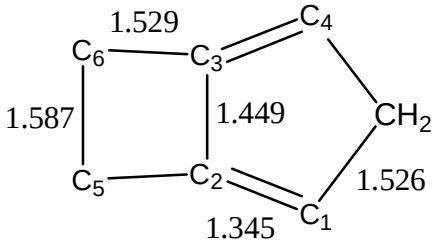
Table 1: The B3LYP/6-31G* geometries obtained for the transition states (**TS**) and products (**Pr**) of the cycloaddition reactions of dienes **1X** with ethylene. The bond lengths and angles are given in Å and degrees respectively (see Scheme 2 for designation).

Table 2: The B3LYP/6-31G* geometries obtained for the transition states (**TS**) and products (**Pr1** and **Pr2**) of the cycloaddition reactions of dienes **2CH_2, 2SiH_2** and **2NH** with ethylene. The bond lengths and angles are given in Å and degrees respectively (see Scheme 2 for designation).

Table 2 (contd.): The B3LYP/6-31G* geometries obtained for the transition states (**TS**) and products (**Pr1** and **Pr2**) of the cycloaddition reactions of dienes **2PH, 2O** and **2S** with ethylene. The bond lengths and angles are given in Å and degrees respectively (see Scheme 2 for designation).

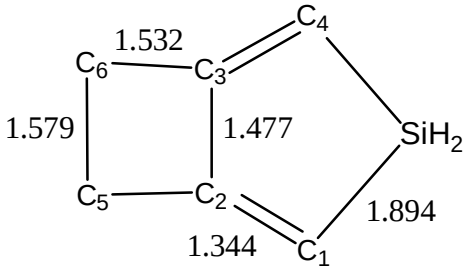
Table 3: The B3LYP/6-31G* geometries obtained for the transition states (**TS**) and products (**Pr**) of the cycloaddition reactions of dienes **3X** with ethylene. The bond lengths and angles are given in Å and degrees respectively (see Scheme 2 for designation).

Table 4: The B3LYP/6-31G* optimized Cartesian coordinates of all the reactants, transition states and products along with their total energies (in hartrees).



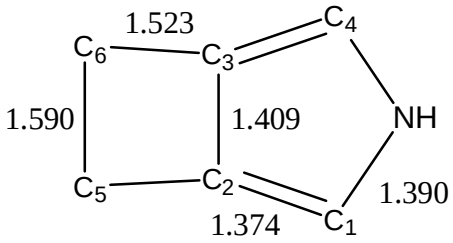
$\angle C_4\text{-}C\text{-}C_1$ 105.3 $\angle C_3\text{-}C_2\text{-}C_5$ 92.6
$\angle C\text{-}C_1\text{-}C_2$ 106.0 $\angle C_2\text{-}C_5\text{-}C_6$ 87.4
$\angle C_1\text{-}C_2\text{-}C_3$ 111.3

1CH$_2$



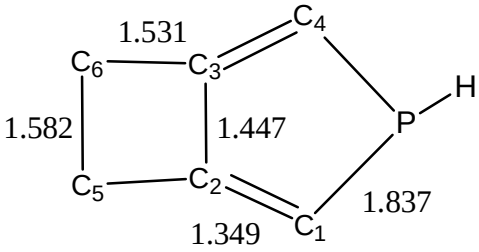
$\angle C_4\text{-Si-}C_1$ 95.5 $\angle C_3\text{-}C_2\text{-}C_5$ 91.9
$\angle Si\text{-}C_1\text{-}C_2$ 102.7 $\angle C_2\text{-}C_5\text{-}C_6$ 88.1
$\angle C_1\text{-}C_2\text{-}C_3$ 119.6

1SiH$_2$



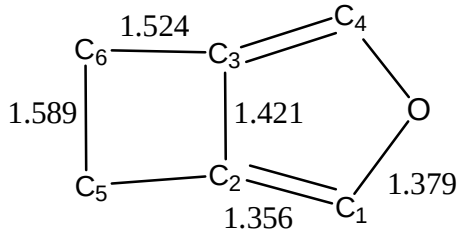
$\angle C_4\text{-N-}C_1$ 111.9 $\angle C_3\text{-}C_2\text{-}C_5$ 93.4
$\angle N\text{-}C_1\text{-}C_2$ 105.1 $\angle C_2\text{-}C_5\text{-}C_6$ 86.6
$\angle C_1\text{-}C_2\text{-}C_3$ 109.0

1NH



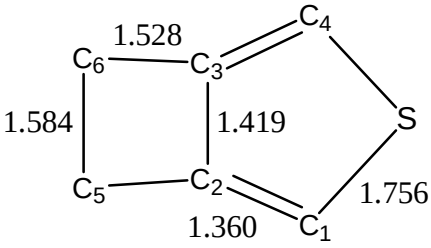
$\angle C_4\text{-P-}C_1$ 92.7 $\angle C_3\text{-}C_2\text{-}C_5$ 92.5
$\angle P\text{-}C_1\text{-}C_2$ 106.5 $\angle C_2\text{-}C_5\text{-}C_6$ 87.5
$\angle C_1\text{-}C_2\text{-}C_3$ 116.7

1PH



$\angle C_4\text{-O-}C_1$ 108.7 $\angle C_3\text{-}C_2\text{-}C_5$ 93.2
$\angle O\text{-}C_1\text{-}C_2$ 108.0 $\angle C_2\text{-}C_5\text{-}C_6$ 86.8
$\angle C_1\text{-}C_2\text{-}C_3$ 107.6

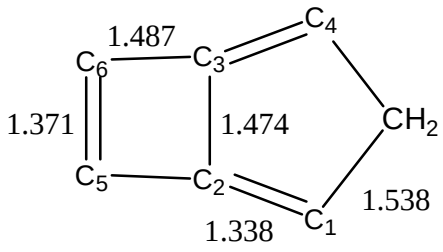
1O



$\angle C_4\text{-S-}C_1$ 93.5 $\angle C_3\text{-}C_2\text{-}C_5$ 93.1
$\angle S\text{-}C_1\text{-}C_2$ 108.5 $\angle C_2\text{-}C_5\text{-}C_6$ 86.9
$\angle C_1\text{-}C_2\text{-}C_3$ 114.8

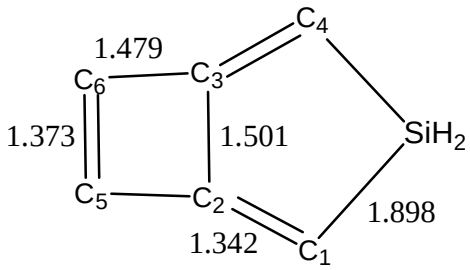
1S

Figure 1: The B3LYP/6-31G* optimized geometries (bond lengths in Å and angles in degrees) of the dienes **1X**; (X = CH_2, SiH_2, NH, PH, O and S).



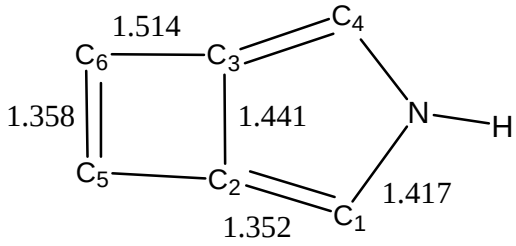
$\angle C_4\text{-}C\text{-}C_1$ 104.2 $\angle C_3\text{-}C_2\text{-}C_5$ 88.0
$\angle C\text{-}C_1\text{-}C_2$ 107.1 $\angle C_2\text{-}C_5\text{-}C_6$ 92.0
$\angle C_1\text{-}C_2\text{-}C_3$ 110.8

$2CH_2$



$\angle C_4\text{-}Si\text{-}C_1$ 95.1 $\angle C_3\text{-}C_2\text{-}C_5$ 87.5
$\angle Si\text{-}C_1\text{-}C_2$ 103.5 $\angle C_2\text{-}C_5\text{-}C_6$ 92.5
$\angle C_1\text{-}C_2\text{-}C_3$ 118.9

$2SiH_2$



$\angle C_4\text{-}N\text{-}C_1$ 108.8 $\angle C_3\text{-}C_2\text{-}C_5$ 88.4
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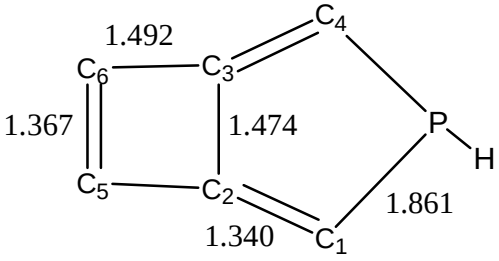
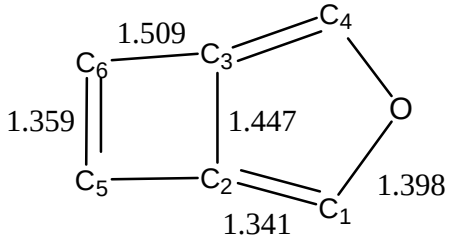
$\angle C_1\text{-}C_2\text{-}C_3$ 108.6

2NH



$\angle C_4\text{-}P\text{-}C_1$ 91.3 $\angle C_3\text{-}C_2\text{-}C_5$ 87.9
$\angle P\text{-}C_1\text{-}C_2$ 107.8 $\angle C_2\text{-}C_5\text{-}C_6$ 92.1
$\angle C_1\text{-}C_2\text{-}C_3$ 116.3

2PH



$\angle C_4\text{-}O\text{-}C_1$ 107.0 $\angle C_3\text{-}C_2\text{-}C_5$ 88.3
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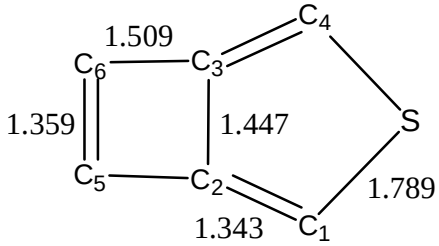
$\angle C_1\text{-}C_2\text{-}C_3$ 107.4

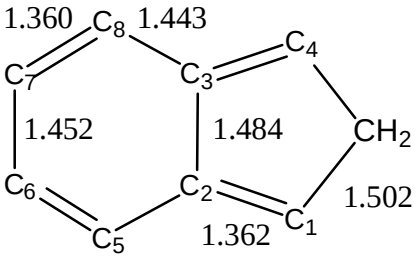
2O



$\angle C_4\text{-}S\text{-}C_1$ 91.9 $\angle C_3\text{-}C_2\text{-}C_5$ 88.3
$\angle S\text{-}C_1\text{-}C_2$ 109.3 $\angle C_2\text{-}C_5\text{-}C_6$ 91.7
$\angle C_1\text{-}C_2\text{-}C_3$ 114.8

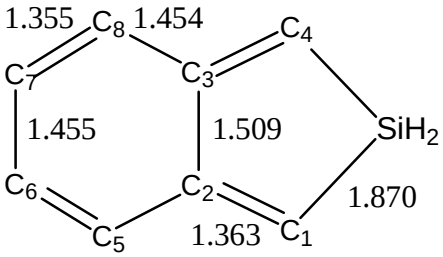
2S

Figure 2: The B3LYP/6-31G* optimized geometries (bond lengths in Å and angles in degrees) of the dienes **2X**; (X = CH_2, SiH_2, NH, PH, O and S).



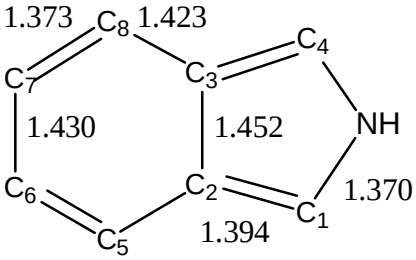
$\angle C_4\text{-}C\text{-}C_1$ 104.3 $\angle C_3\text{-}C_2\text{-}C_5$ 119.0
$\angle C\text{-}C_1\text{-}C_2$ 108.8 $\angle C_2\text{-}C_5\text{-}C_6$ 119.2
$\angle C_1\text{-}C_2\text{-}C_3$ 109.0 $\angle C_5\text{-}C_6\text{-}C_7$ 121.8

3CH$_2$



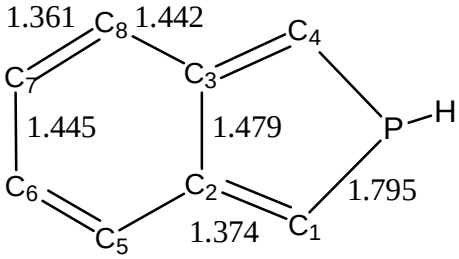
$\angle C_4\text{-}Si\text{-}C_1$ 92.9 $\angle C_3\text{-}C_2\text{-}C_5$ 117.8
$\angle Si\text{-}C_1\text{-}C_2$ 107.4 $\angle C_2\text{-}C_5\text{-}C_6$ 120.8
$\angle C_1\text{-}C_2\text{-}C_3$ 116.1 $\angle C_5\text{-}C_6\text{-}C_7$ 121.4

3SiH$_2$



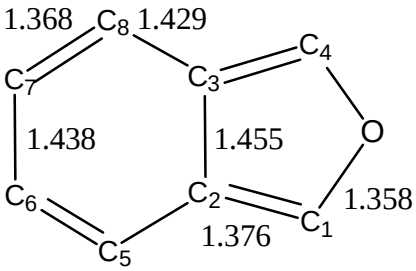
$\angle C_4\text{-}N\text{-}C_1$ 111.9 $\angle C_3\text{-}C_2\text{-}C_5$ 119.7
$\angle N\text{-}C_1\text{-}C_2$ 107.0 $\angle C_2\text{-}C_5\text{-}C_6$ 118.9
$\angle C_1\text{-}C_2\text{-}C_3$ 107.0 $\angle C_5\text{-}C_6\text{-}C_7$ 121.4

3NH



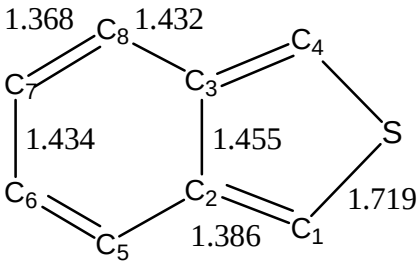
$\angle C_4\text{-}P\text{-}C_1$ 92.1 $\angle C_3\text{-}C_2\text{-}C_5$ 118.6
$\angle P\text{-}C_1\text{-}C_2$ 109.4 $\angle C_2\text{-}C_5\text{-}C_6$ 120.0
$\angle C_1\text{-}C_2\text{-}C_3$ 113.7 $\angle C_5\text{-}C_6\text{-}C_7$ 121.4

3PH



$\angle C_4\text{-}O\text{-}C_1$ 108.7 $\angle C_3\text{-}C_2\text{-}C_5$ 119.8
$\angle O\text{-}C_1\text{-}C_2$ 109.8 $\angle C_2\text{-}C_5\text{-}C_6$ 118.5
$\angle C_1\text{-}C_2\text{-}C_3$ 105.9 $\angle C_5\text{-}C_6\text{-}C_7$ 121.7

3O



$\angle C_4\text{-}O\text{-}C_1$ 93.2 $\angle C_3\text{-}C_2\text{-}C_5$ 119.3
$\angle O\text{-}C_1\text{-}C_2$ 111.3 $\angle C_2\text{-}C_5\text{-}C_6$ 119.5
$\angle C_1\text{-}C_2\text{-}C_3$ 112.1 $\angle C_5\text{-}C_6\text{-}C_7$ 121.3

3S

Figure 3: The B3LYP/6-31G* optimized geometries (bond lengths in Å and angles in degrees) of the dienes **3X**; (X = CH_2, SiH_2, NH, PH, O and S).

Table 1: The B3LYP/6-31G* geometries obtained for the transition states (**TS**) and products (**Pr**) of the cycloaddition reactions of dienes **1X** with ethylene. The bond lengths and angles are given in Å and degrees respectively (see Scheme 2 for designation).

Para	**1CH$_2$**		**1SiH$_2$**		**1NH**			**1PH**				**1O**		**1S**	
	TS	**Pr**	**TS**	**Pr**	**TS**	**Pr**		**TS**		**Pr**		**TS**	**Pr**	**TS**	**Pr**
					anti	***syn***	***anti***	***syn***	***anti***	***syn***	***anti***				
r1	1.529	1.558	1.886	1.928	1.414	1.493	1.498	1.866	1.850	1.915	1.917	1.384	1.447	1.787	1.874
r2	1.392	1.513	1.395	1.506	1.425	1.522	1.511	1.392	1.400	1.507	1.509	1.411	1.516	1.412	1.511
r3	1.395	1.340	1.407	1.334	1.369	1.342	1.337	1.396	1.392	1.340	1.339	1.376	1.338	1.377	1.337
r4	1.526	1.526	1.529	1.525	1.522	1.530	1.524	1.530	1.527	1.528	1.525	1.524	1.527	1.527	1.527
r5	1.586	1.584	1.579	1.586	1.587	1.579	1.585	1.580	1.582	1.581	1.586	1.584	1.581	1.580	1.581
r6	2.252	1.573	2.229	1.576	2.137	1.565	1.577	2.238	2.232	1.576	1.567	2.165	1.567	2.181	1.566
r7	1.388	1.564	1.400	1.570	1.408	1.561	1.561	1.397	1.394	1.566	1.564	1.398	1.560	1.404	1.563
a1	101.8	95.7	90.9	83.8	105.3	96.8	96.5	87.1	87.5	80.6	80.6	105.2	98.2	87.8	80.9
a2	103.8	98.1	100.8	93.8	103.1	101.1	97.6	106.8	102.2	101.5	95.5	105.8	99.7	106.3	100.4
a3	110.6	108.7	117.3	114.1	108.0	107.0	107.3	115.0	114.6	112.2	112.2	107.0	106.2	112.9	111.2
a4	93.6	94.6	93.2	94.6	94.1	94.4	94.7	93.4	93.6	94.5	94.6	93.9	94.6	93.8	94.6
a5	86.4	85.4	86.8	85.4	85.9	85.6	85.3	86.6	86.4	85.5	85.4	86.1	85.4	86.2	85.4
a6	89.1	99.5	86.3	99.1	94.2	98.6	102.6	86.2	95.7	97.8	103.4	91.2	100.6	93.8	101.0
a7	99.7	105.5	100.8	106.2	97.8	106.0	105.4	99.7	98.4	105.2	106.1	99.4	106.6	96.8	105.2
a8	102.6	103.7	106.8	108.6	101.3	102.4	102.3	105.2	105.1	106.8	107.0	100.7	101.5	104.3	106.1
ϕ	105.6	111.9	112.1	118.3	102.2	111.3	110.7	108.7	106.9	114.8	116.0	103.4	111.3	103.9	113.9

Table 2: The B3LYP/6-31G* geometries obtained for the transition states (**TS**) and products (**Pr1** and **Pr2**) of the cycloaddition reactions of dienes **$2CH_2$, $2SiH_2$** and **2NH** with ethylene. The bond lengths and angles are given in Å and degrees respectively (see Scheme 2 for designation).

Para	**$2CH_2$**			**$2SiH_2$**			**2NH**				
	TS	**Pr1**	**Pr2**	**TS**	**Pr1**	**Pr2**	**TS**	**Pr1**		**Pr2**	
							anti	***syn***	***anti***	***syn***	***anti***
r1	1.536	1.553	1.573	1.892	1.921	1.945	1.420	1.489	1.488	1.511	1.509
r2	1.395	1.508	1.493	1.400	1.497	1.480	1.422	1.518	1.509	1.498	1.495
r3	1.401	1.354	1.545	1.408	1.356	1.562	1.388	1.355	1.354	1.552	1.541
r4	1.539	1.573	1.339	1.545	1.577	1.342	1.564	1.576	1.570	1.342	1.337
r5	1.349	1.336	1.607	1.346	1.336	1.593	1.343	1.334	1.335	1.589	1.610
r6	2.123	1.574	1.561	2.089	1.586	1.569	2.082	1.565	1.579	1.551	1.565
r7	1.404	1.555	1.570	1.420	1.561	1.579	1.412	1.553	1.552	1.567	1.567
a1	99.7	95.3	97.2	88.9	83.5	85.7	103.4	96.3	96.3	98.4	97.9
a2	103.5	98.5	98.5	100.2	95.1	95.9	103.4	101.2	98.0	100.1	97.6
a3	109.9	108.2	105.8	116.4	113.6	111.5	107.2	106.5	106.6	104.2	104.2
a4	89.0	89.7	91.3	88.9	89.6	90.7	89.2	89.6	89.7	90.8	91.5
a5	91.0	90.3	88.7	91.1	90.4	89.3	90.8	90.4	90.3	89.2	88.5
a6	91.6	100.3	99.8	89.1	99.0	97.3	96.2	99.5	103.5	99.2	103.3
a7	101.2	105.1	106.4	102.6	106.1	106.3	98.7	105.8	105.0	108.3	106.6
a8	102.9	103.6	104.6	107.1	108.3	109.9	101.3	102.3	102.1	103.5	103.1
ϕ	107.2	111.2	112.2	114.1	117.6	117.6	102.9	110.8	109.9	113.2	111.2

Table 2 (contd.): The B3LYP/6-31G* geometries obtained for the transition states (**TS**) and products (**Pr1** and **Pr2**) of the cycloaddition reactions of dienes **2PH, 2O** and **2S** with ethylene. The bond lengths and angles are given in Å and degrees respectively (see Scheme 2 for designation).

Para	**2PH**						**2O**			**2S**		
	TS		**Pr1**		**Pr2**		**TS**	**Pr1**	**Pr2**	**TS**	**Pr1**	**Pr2**
	syn	***anti***	***syn***	***anti***	***syn***	***anti***						
r1	1.873	1.870	1.905	1.912	1.951	1.955	1.392	1.442	1.466	1.801	1.862	1.914
r2	1.395	1.398	1.500	1.501	1.471	1.479	1.410	1.513	1.495	1.408	1.507	1.474
r3	1.401	1.400	1.354	1.353	1.554	1.553	1.393	1.354	1.547	1.392	1.353	1.552
r4	1.546	1.542	1.578	1.575	1.345	1.341	1.544	1.573	1.339	1.547	1.577	1.343
r5	1.345	1.347	1.334	1.336	1.577	1.592	1.343	1.334	1.599	1.343	1.333	1.576
r6	2.112	2.116	1.579	1.572	1.559	1.556	2.098	1.569	1.552	2.104	1.568	1.550
r7	1.413	1.408	1.558	1.555	1.572	1.570	1.404	1.552	1.565	1.411	1.555	1.567
a1	85.5	85.2	80.5	80.2	82.0	81.5	103.2	97.7	99.3	86.0	80.7	81.9
a2	106.2	101.8	101.8	96.2	99.9	96.8	106.0	99.9	99.2	106.1	100.5	98.2
a3	114.2	113.8	111.6	111.7	110.0	109.7	106.2	105.7	103.3	112.2	110.6	109.0
a4	89.0	89.0	89.6	89.7	90.5	90.8	89.1	89.6	91.1	89.1	89.6	90.5
a5	91.0	91.0	90.4	90.3	89.5	89.2	90.9	90.4	88.9	90.9	90.4	89.5
a6	88.7	97.5	98.6	104.0	97.6	102.1	93.5	101.6	101.5	95.6	102.0	101.0
a7	101.5	100.1	105.0	105.8	107.8	106.8	100.3	106.4	108.6	98.4	105.2	108.3
a8	105.5	105.4	106.6	106.8	108.5	108.4	100.7	101.4	102.4	104.4	105.8	107.7
ϕ	110.5	108.7	114.2	115.2	117.7	116.3	104.2	110.8	112.8	105.5	113.4	117.2

Table 3: The B3LYP/6-31G* geometries obtained for the transition states (**TS**) and products (**Pr**) of the cycloaddition reactions of dienes **3X** with ethylene. The bond lengths and angles are given in Å and degrees respectively (see Scheme 2 for designation).

Para	**3CH$_2$**		**3SiH$_2$**		**3NH**			**3PH**				**3O**		**3S**	
	TS	**Pr**	**TS**	**Pr**	**TS**	**Pr**		**TS**		**Pr**		**TS**	**Pr**	**TS**	**Pr**
					anti	***syn***	***anti***	***syn***	***anti***	***syn***	***anti***				
r1	1.505	1.552	1.866	1.919	1.391	1.491	1.491	1.836	1.810	1.911	1.910	1.365	1.445	1.751	1.871
r2	1.399	1.518	1.401	1.515	1.437	1.525	1.516	1.402	1.416	1.512	1.516	1.421	1.520	1.429	1.515
r3	1.450	1.409	1.465	1.417	1.424	1.407	1.405	1.448	1.445	1.411	1.411	1.427	1.404	1.427	1.408
r4	1.425	1.388	1.433	1.393	1.405	1.387	1.386	1.427	1.422	1.388	1.390	1.410	1.386	1.412	1.386
r5	1.373	1.403	1.369	1.400	1.387	1.404	1.404	1.373	1.375	1.404	1.402	1.382	1.404	1.383	1.405
r6	1.432	1.396	1.432	1.396	1.414	1.396	1.396	1.428	1.424	1.394	1.396	1.419	1.396	1.416	1.394
r7	1.373	1.563	1.379	1.567	1.398	1.561	1.561	1.381	1.380	1.564	1.561	1.387	1.560	1.391	1.561
r8	2.391	1.564	2.404	1.565	2.211	1.558	1.569	2.380	2.356	1.562	1.556	2.257	1.559	2.274	1.555
a1	102.2	94.2	90.4	82.0	106.4	95.2	95.2	87.0	88.3	78.9	79.0	105.9	96.7	88.3	79.3
a2	107.1	100.1	105.9	97.3	105.5	103.1	99.3	111.0	105.8	103.3	98.1	108.3	101.5	109.6	102.0
a3	108.6	106.6	115.0	111.3	106.2	105.1	105.2	112.7	112.3	109.7	109.6	105.3	104.4	110.8	108.8
a4	119.6	120.8	118.6	120.1	120.4	120.9	121.0	119.2	119.3	120.5	120.5	120.4	121.1	119.9	120.7
a5	119.1	118.5	120.5	119.4	118.5	118.3	118.2	119.8	119.7	119.0	119.0	118.3	118.1	119.2	118.7
a6	121.3	120.7	120.9	120.4	121.1	120.8	120.8	121.0	120.9	120.5	120.6	121.3	120.8	120.9	120.6
a7	88.2	100.5	84.7	99.9	93.7	99.2	103.5	85.3	95.8	99.1	104.3	90.3	101.3	94.0	102.0
a8	97.7	106.8	99.0	107.5	96.6	107.3	106.8	97.4	96.4	107.2	107.5	97.9	108.0	94.9	107.3
a9	101.7	103.1	105.3	107.7	100.8	101.9	101.8	103.9	104.0	106.1	106.2	100.1	101.1	103.3	105.4
ϕ	102.4	112.3	107.9	117.6	100.2	111.8	111.3	104.3	103.2	115.5	115.9	101.1	112.0	100.6	114.8

Table 4: The B3LYP/6-31G* optimized Cartesian coordinates of all the reactants, transition states and products along with their total energies (in hartrees).

Ethylene			E= –78.58746
C	0.000000	0.000000	0.665422
C	0.000000	0.000000	-0.665422
H	0.000000	0.923450	1.239848
H	0.000000	-0.923450	1.239848
H	0.000000	0.923450	-1.239848
H	0.000000	-0.923450	-1.239848

$1CH_2$			E = -271.4690108
C	0.000000	0.724267	-0.215497
C	0.000000	-0.724267	-0.215497
C	0.000000	0.793644	-1.742711
C	0.000000	-0.793644	-1.742711
C	0.000000	-1.213783	1.037298
C	0.000000	1.213783	1.037298
H	0.000000	-2.237862	1.394306
H	0.000000	2.237862	1.394306
C	0.000000	0.000000	1.962909
H	-0.877929	0.000000	2.628370
H	0.877929	0.000000	2.628370
H	-0.888199	1.249996	-2.192973
H	-0.888199	-1.249996	-2.192973
H	0.888199	1.249996	-2.192973
H	0.888199	-1.249996	-2.192973

$1CH_2$-TS			E = -271.4690108
C	0.182401	-0.815963	0.697740
C	0.182401	-0.815963	-0.697740
C	-0.810940	-1.970867	0.793083
C	-0.810940	-1.970867	-0.793083
C	0.788089	0.337558	-1.186616
C	0.788089	0.337558	1.186616
H	1.038594	0.571698	-2.216931
H	1.038594	0.571698	2.216931
C	1.604556	0.850233	0.000000
H	2.584975	0.345068	0.000000
H	1.787091	1.927451	0.000000
C	-0.810940	1.844484	-0.694130
C	-0.810940	1.844484	0.694130
H	-1.602361	1.346663	-1.245054
H	-1.602361	1.346663	1.245054
H	-0.444151	-2.891419	1.261291
H	-0.444151	-2.891419	-1.261291
H	-1.780582	-1.719516	1.239421
H	-1.780582	-1.719516	-1.239421
H	-0.302864	2.634337	-1.240056
H	-0.302864	2.634337	1.240056

$1CH_2$-Pr			E = -271.4690108
C	0.178296	-0.767599	0.669859
C	0.178296	-0.767599	-0.669859
C	-0.667569	-2.032273	0.791990
C	-0.667569	-2.032273	-0.791990
C	0.551993	0.615465	-1.154994
C	0.551993	0.615465	1.154994
H	0.921193	0.747546	-2.174942
H	0.921193	0.747546	2.174942
C	1.526344	0.996094	0.000000
H	2.442807	0.398154	0.000000
H	1.782908	2.062748	0.000000
C	-0.667569	1.536600	-0.781837
C	-0.667569	1.536600	0.781837
H	-1.604223	1.162444	-1.206940
H	-1.604223	1.162444	1.206940
H	-0.201684	-2.897321	1.279340
H	-0.201684	-2.897321	-1.279340
H	-1.667825	-1.892330	1.221362
H	-1.667825	-1.892330	-1.221362
H	-0.510262	2.547768	-1.175056
H	-0.510262	2.547768	1.175056

$1SiH_2$			E = -271.4690108
C	0.000000	0.738552	-0.537831
C	0.000000	-0.738552	-0.537831
C	0.000000	0.789541	-2.068517
C	0.000000	-0.789541	-2.068517
C	0.000000	-1.401433	0.631138

C	0.000000	1.401433	0.631138
H	0.000000	-2.480135	0.753245
H	0.000000	2.480135	0.753245
Si	0.000000	0.000000	1.905113
H	-1.199473	0.000000	2.792672
H	1.199473	0.000000	2.792672
H	-0.887908	1.249558	-2.515225
H	-0.887908	-1.249558	-2.515225
H	0.887908	1.249558	-2.515225
H	0.887908	-1.249558	-2.515225

1SiH$_2$-TS E = -271.4690108

C	-0.036879	-0.932165	0.703552
C	-0.036879	-0.932165	-0.703552
C	-0.992014	-2.123602	0.789562
C	-0.992014	-2.123602	-0.789562
C	0.475541	0.196291	-1.344123
C	0.475541	0.196291	1.344123
H	0.515650	0.320955	-2.422698
H	0.515650	0.320955	2.422698
Si	1.606025	0.883907	0.000000
H	2.944926	0.221048	0.000000
H	1.831298	2.355544	0.000000
C	-0.992014	1.745791	-0.700142
C	-0.992014	1.745791	0.700142
H	-1.796393	1.256790	-1.238787
H	-1.796393	1.256790	1.238787
H	-0.589261	-3.027787	1.259698
H	-0.589261	-3.027787	-1.259698
H	-1.969114	-1.907002	1.238026
H	-1.969114	-1.907002	-1.238026
H	-0.518974	2.563509	-1.235773
H	-0.518974	2.563509	1.235773

1SiH$_2$-Pr E = -271.4690108

C	0.056366	-0.839375	0.672100
C	0.056366	-0.839375	-0.672100
C	-0.116939	-2.349370	0.793095
C	-0.116939	-2.349370	-0.793095
C	0.056366	0.535317	-1.287722
C	0.056366	0.535317	1.287722
H	0.219395	0.624214	-2.362663
H	0.219395	0.624214	2.362663
Si	1.300061	1.251915	0.000000
H	2.647688	0.624986	0.000000
H	1.450501	2.743717	0.000000
C	-1.258733	1.243370	-0.784873
C	-1.258733	1.243370	0.784873
H	-2.137797	0.716434	-1.173049
H	-2.137797	0.716434	1.173049
H	0.707806	-2.901766	1.259903
H	0.707806	-2.901766	-1.259903
H	-1.058815	-2.694642	1.238184
H	-1.058815	-2.694642	-1.238184
H	-1.302474	2.268344	-1.171651
H	-1.302474	2.268344	1.171651

1NH E = -271.4690108

C	0.000000	0.704716	-0.211940
C	0.000000	-0.704716	-0.211940
C	0.000000	0.795164	-1.732082
C	0.000000	-0.795164	-1.732082
C	0.000000	-1.151462	1.086901
C	0.000000	1.151462	1.086901
H	0.000000	-2.126541	1.553650
H	0.000000	2.126541	1.553650
N	0.000000	0.000000	1.865079
H	0.000000	0.000000	2.873718
H	-0.888886	1.246638	-2.187782
H	-0.888886	-1.246638	-2.187782
H	0.888886	1.246638	-2.187782
H	0.888886	-1.246638	-2.187782

***anti*-1NH-TS** E = -271.4690108

C	0.234245	-0.813879	0.684430
C	0.234245	-0.813879	-0.684430
C	-0.813787	-1.912069	0.793360
C	-0.813787	-1.912069	-0.793360
C	0.830494	0.402968	-1.124373
C	0.830494	0.402968	1.124373
H	1.192644	0.662682	-2.113475
H	1.192644	0.662682	2.113475
N	1.581455	0.817756	0.000000
H	1.897593	1.780686	0.000000

C	-0.813787	1.701878	-0.704220
C	-0.813787	1.701878	0.704220
H	-1.609718	1.194587	-1.242843
H	-1.609718	1.194587	1.242843
H	-0.502323	-2.847471	1.272379
H	-0.502323	-2.847471	-1.272379
H	-1.772014	-1.601831	1.227861
H	-1.772014	-1.601831	-1.227861
H	-0.415464	2.566154	-1.232291
H	-0.415464	2.566154	1.232291

***syn*-1NH-Pr** E = -271.4690108

C	0.204406	-0.769472	0.670858
C	0.204406	-0.769472	-0.670858
C	-0.665235	-2.022685	0.789268
C	-0.665235	-2.022685	-0.789268
C	0.572663	0.638640	-1.116357
C	0.572663	0.638640	1.116357
H	1.009493	0.803998	-2.103095
H	1.009493	0.803998	2.103095
N	1.467126	1.067484	0.000000
H	2.297724	0.470038	0.000000
C	-0.665235	1.535713	-0.780499
C	-0.665235	1.535713	0.780499
H	-1.588364	1.139238	-1.213891
H	-1.588364	1.139238	1.213891
H	-0.214549	-2.892759	1.280760
H	-0.214549	-2.892759	-1.280760
H	-1.661263	-1.859804	1.219067
H	-1.661263	-1.859804	-1.219067
H	-0.508713	2.544944	-1.172249
H	-0.508713	2.544944	1.172249

***anti*-1NH-Pr** E = -271.4690108

C	0.199859	-0.773336	0.668458
C	0.199859	-0.773336	-0.668458
C	-0.662544	-2.024020	0.792318
C	-0.662544	-2.024020	-0.792318
C	0.582784	0.617814	-1.117252
C	0.582784	0.617814	1.117252
H	1.020306	0.774244	-2.105171
H	1.020306	0.774244	2.105171
N	1.528902	0.933327	0.000000
H	1.709054	1.941577	0.000000
C	-0.662544	1.525388	-0.780576
C	-0.662544	1.525388	0.780576
H	-1.592722	1.140576	-1.211388
H	-1.592722	1.140576	1.211388
H	-0.207135	-2.893827	1.280090
H	-0.207135	-2.893827	-1.280090
H	-1.660709	-1.869321	1.221083
H	-1.660709	-1.869321	-1.221083
H	-0.510747	2.535817	-1.178360
H	-0.510747	2.535817	1.178360

1PH E = -271.4690108

C	-0.044962	-0.535042	0.723550
C	-0.044962	-0.535042	-0.723550
C	-0.015189	-2.064030	0.791038
C	-0.015189	-2.064030	-0.791038
C	-0.044962	0.670772	-1.329137
C	-0.044962	0.670772	1.329137
H	-0.013065	0.897655	-2.389204
H	-0.013065	0.897655	2.389204
P	0.161854	1.922535	0.000000
H	-1.118530	2.549496	0.000000
H	0.883085	-2.494503	1.246085
H	0.883085	-2.494503	-1.246085
H	-0.893975	-2.527114	1.252084
H	-0.893975	-2.527114	-1.252084

***syn*-1PH-TS** E = -271.4690108

C	-0.010345	-0.940600	0.697941
C	-0.010345	-0.940600	-0.697941
C	-1.019439	-2.087333	0.789854
C	-1.019439	-2.087333	-0.789854
C	0.531331	0.198831	-1.285560
C	0.531331	0.198831	1.285560
H	0.653341	0.379823	-2.349592
H	0.653341	0.379823	2.349592
P	1.619023	1.001903	0.000000
H	2.632827	-0.014507	0.000000
C	-1.019439	1.701422	-0.698599
C	-1.019439	1.701422	0.698599

H	-1.806651	1.188494	-1.241332
H	-1.806651	1.188494	1.241332
H	-0.658841	-3.008190	1.261521
H	-0.658841	-3.008190	-1.261521
H	-1.985261	-1.823884	1.237010
H	-1.985261	-1.823884	-1.237010
H	-0.554319	2.522815	-1.235041
H	-0.554319	2.522815	1.235041

***anti*-1PH-TS** E = -271.4690108

C	-0.036274	-0.908301	0.696164
C	-0.036274	-0.908301	-0.696164
C	-1.042280	-2.053143	0.791211
C	-1.042280	-2.053143	-0.791211
C	0.528448	0.232614	-1.279375
C	0.528448	0.232614	1.279375
H	0.679292	0.386318	-2.344732
H	0.679292	0.386318	2.344732
P	1.756976	0.758759	0.000000
H	1.593271	2.173533	0.000000
C	-1.042280	1.707732	-0.697239
C	-1.042280	1.707732	0.697239
H	-1.838455	1.206276	-1.238845
H	-1.838455	1.206276	1.238845
H	-0.682428	-2.975339	1.261020
H	-0.682428	-2.975339	-1.261020
H	-2.007898	-1.789247	1.238973
H	-2.007898	-1.789247	-1.238973
H	-0.570147	2.521123	-1.239477
H	-0.570147	2.521123	1.239477

***syn*-1PH-Pr** E = -271.4690108

C	0.315632	-0.829557	0.669837
C	0.315632	-0.829557	-0.669837
C	0.077818	-2.334622	0.790402
C	0.077818	-2.334622	-0.790402
C	0.077818	0.545016	-1.238783
C	0.077818	0.545016	1.238783
H	0.272950	0.730783	-2.296570
H	0.272950	0.730783	2.296570
P	1.041164	1.642360	0.000000
H	2.275667	0.928797	0.000000
C	-1.379165	0.935235	-0.783133
C	-1.379165	0.935235	0.783133
H	-2.101342	0.218064	-1.187753
H	-2.101342	0.218064	1.187753
H	0.865499	-2.921873	1.277620
H	0.865499	-2.921873	-1.277620
H	-0.888234	-2.628166	1.220488
H	-0.888234	-2.628166	-1.220488
H	-1.648064	1.922668	-1.173759
H	-1.648064	1.922668	1.173759

***anti*-1PH-Pr** E = -271.4690108

C	0.115677	-0.852668	0.669741
C	0.115677	-0.852668	-0.669741
C	-0.213539	-2.336854	0.792815
C	-0.213539	-2.336854	-0.792815
C	0.115677	0.544645	-1.239860
C	0.115677	0.544645	1.239860
H	0.349681	0.679489	-2.297389
H	0.349681	0.679489	2.297389
P	1.397635	1.247556	0.000000
H	0.960545	2.617125	0.000000
C	-1.230731	1.201647	-0.781798
C	-1.230731	1.201647	0.781798
H	-2.083095	0.639119	-1.181572
H	-2.083095	0.639119	1.181572
H	0.544349	-2.970149	1.268933
H	0.544349	-2.970149	-1.268933
H	-1.190837	-2.575814	1.230544
H	-1.190837	-2.575814	-1.230544
H	-1.305138	2.221498	-1.174212
H	-1.305138	2.221498	1.174212

1O E = -271.4690108

C	0.000000	0.710372	-0.195337
C	0.000000	-0.710372	-0.195337
C	0.000000	0.794491	-1.717192
C	0.000000	-0.794491	-1.717192
C	0.000000	-1.121052	1.096590
C	0.000000	1.121052	1.096590
H	0.000000	-2.060229	1.628414
H	0.000000	2.060229	1.628414

O	0.000000	0.000000	1.899992
H	-0.889297	1.248769	-2.166378
H	-0.889297	-1.248769	-2.166378
H	0.889297	1.248769	-2.166378
H	0.889297	-1.248769	-2.166378

1O-TS E = -271.4690108

C	0.246693	-0.817986	0.688118
C	0.246693	-0.817986	-0.688118
C	-0.807062	-1.913672	0.792219
C	-0.807062	-1.913672	-0.792219
C	0.837509	0.395492	-1.099933
C	0.837509	0.395492	1.099933
H	1.258884	0.695282	-2.051346
H	1.258884	0.695282	2.051346
O	1.531831	0.869464	0.000000
C	-0.807062	1.744909	-0.699194
C	-0.807062	1.744909	0.699194
H	-1.603349	1.246539	-1.245385
H	-1.603349	1.246539	1.245385
H	-0.495304	-2.847966	1.271644
H	-0.495304	-2.847966	-1.271644
H	-1.761299	-1.597665	1.229261
H	-1.761299	-1.597665	-1.229261
H	-0.346731	2.573494	-1.230237
H	-0.346731	2.573494	1.230237

1O-Pr E = -271.4690108

C	0.211184	-0.772267	0.669212
C	0.211184	-0.772267	-0.669212
C	-0.651807	-2.026294	0.790494
C	-0.651807	-2.026294	-0.790494
C	0.586073	0.634393	-1.093338
C	0.586073	0.634393	1.093338
H	1.086747	0.816607	-2.044408
H	1.086747	0.816607	2.044408
O	1.463581	0.992300	0.000000
C	-0.651807	1.542686	-0.779871
C	-0.651807	1.542686	0.779871
H	-1.577969	1.156439	-1.216598
H	-1.577969	1.156439	1.216598
H	-0.194179	-2.893627	1.279657
H	-0.194179	-2.893627	-1.279657
H	-1.648389	-1.869510	1.220903
H	-1.648389	-1.869510	-1.220903
H	-0.482394	2.549778	-1.172370
H	-0.482394	2.549778	1.172370

1S E = -271.4690108

C	0.000000	0.709527	-0.530220
C	0.000000	-0.709527	-0.530220
C	0.000000	0.792171	-2.055589
C	0.000000	-0.792171	-2.055589
C	0.000000	-1.279499	0.704901
C	0.000000	1.279499	0.704901
H	0.000000	-2.312567	1.026757
H	0.000000	2.312567	1.026757
S	0.000000	0.000000	1.908242
H	-0.889305	1.247962	-2.503625
H	-0.889305	-1.247962	-2.503625
H	0.889305	1.247962	-2.503625
H	0.889305	-1.247962	-2.503625

1S-TS E = -271.4690108

C	0.421619	-0.829481	0.688585
C	0.421619	-0.829481	-0.688585
C	-0.106458	-2.258514	0.789920
C	-0.106458	-2.258514	-0.789920
C	0.421619	0.470570	-1.238734
C	0.421619	0.470570	1.238734
H	0.543498	0.747425	-2.281003
H	0.543498	0.747425	2.281003
S	1.138491	1.540228	0.000000
C	-1.630214	0.979779	-0.701788
C	-1.630214	0.979779	0.701788
H	-2.119950	0.170838	-1.237149
H	-2.119950	0.170838	1.237149
H	0.554124	-2.988244	1.271049
H	0.554124	-2.988244	-1.271049
H	-1.107333	-2.352062	1.227948
H	-1.107333	-2.352062	-1.227948
H	-1.617665	1.926091	-1.233485
H	-1.617665	1.926091	1.233485

1S-Pr			E = -271.4690108
C	0.332022	-0.825669	0.668596
C	0.332022	-0.825669	-0.668596
C	0.085988	-2.327930	0.790743
C	0.085988	-2.327930	-0.790743
C	0.085988	0.561477	-1.215033
C	0.085988	0.561477	1.215033
H	0.330862	0.790059	-2.252651
H	0.330862	0.790059	2.252651
S	1.080009	1.584293	0.000000
C	-1.375412	0.921093	-0.781677
C	-1.375412	0.921093	0.781677
H	-2.082589	0.189111	-1.190131
H	-2.082589	0.189111	1.190131
H	0.872523	-2.916460	1.277154
H	0.872523	-2.916460	-1.277154
H	-0.881306	-2.615874	1.220940
H	-0.881306	-2.615874	-1.220940
H	-1.651078	1.904995	-1.172179
H	-1.651078	1.904995	1.172179

$2CH_2$			E = -271.4690108
C	0.000000	0.737032	-0.306946
C	0.000000	-0.737032	-0.306946
C	0.000000	0.685287	-1.793224
C	0.000000	-0.685287	-1.793224
C	0.000000	-1.213160	0.943947
C	0.000000	1.213160	0.943947
H	0.000000	-2.238853	1.297029
H	0.000000	2.238853	1.297029
C	0.000000	0.000000	1.888871
H	-0.877991	0.000000	2.554449
H	0.877991	0.000000	2.554449
H	0.000000	1.431112	-2.580748
H	0.000000	-1.431112	-2.580748

$2CH_2$-TS			E = -271.4690108
C	0.263335	-0.898037	0.700437
C	0.263335	-0.898037	-0.700437
C	-0.865048	-1.944962	0.674414
C	-0.865048	-1.944962	-0.674414
C	0.747608	0.320770	-1.174594
C	0.747608	0.320770	1.174594
H	0.965205	0.573808	-2.208720
H	0.965205	0.573808	2.208720
C	1.580252	0.856948	0.000000
H	2.587368	0.415660	0.000000
H	1.691042	1.944454	0.000000
C	-0.865048	1.618821	-0.702005
C	-0.865048	1.618821	0.702005
H	-1.656471	1.103184	-1.237874
H	-1.656471	1.103184	1.237874
H	-1.428891	-2.476666	1.432994
H	-1.428891	-2.476666	-1.432994
H	-0.444878	2.469218	-1.233022
H	-0.444878	2.469218	1.233022

$2CH_2$-Pr1			E = -271.4690108
C	0.473670	-0.802010	0.677079
C	0.473670	-0.802010	-0.677079
C	-0.470675	-2.060143	0.667892
C	-0.470675	-2.060143	-0.667892
C	0.473670	0.630575	-1.147226
C	0.473670	0.630575	1.147226
H	0.786995	0.851444	-2.170824
H	0.786995	0.851444	2.170824
C	1.318484	1.248043	0.000000
H	2.356104	0.900995	0.000000
H	1.296517	2.343454	0.000000
C	-0.952225	1.184579	-0.777472
C	-0.952225	1.184579	0.777472
H	-1.748106	0.562476	-1.200528
H	-1.748106	0.562476	1.200528
H	-0.891076	-2.695026	1.440748
H	-0.891076	-2.695026	-1.440748
H	-1.076211	2.196748	-1.179131
H	-1.076211	2.196748	1.179131

$2CH_2$-Pr2			E = -271.4690108
C	0.210317	-0.784826	0.772409
C	0.210317	-0.784826	-0.772409
C	0.210317	0.651119	1.179872

C	0.210317	0.651119	-1.179872
H	0.536508	0.914743	2.188739
H	0.536508	0.914743	-2.188739
C	1.076656	1.228244	0.000000
H	2.106404	0.857612	0.000000
H	1.087988	2.324669	0.000000
C	-1.188521	1.221293	0.784994
C	-1.188521	1.221293	-0.784994
H	-1.292121	2.239921	1.176279
H	-1.292121	2.239921	-1.176279
H	-2.003607	0.622944	1.201864
H	-2.003607	0.622944	-1.201864
C	0.344993	-2.116795	0.803296
C	0.344993	-2.116795	-0.803296
H	0.469425	-2.878226	1.567470
H	0.469425	-2.878226	-1.567470

$2SiH_2$ E = -271.4690108

C	0.000000	0.750460	-0.634167
C	0.000000	-0.750460	-0.634167
C	0.000000	0.686351	-2.112271
C	0.000000	-0.686351	-2.112271
C	0.000000	-1.399758	0.539991
C	0.000000	1.399758	0.539991
H	0.000000	-2.477800	0.669260
H	0.000000	2.477800	0.669260
Si	0.000000	0.000000	1.821464
H	-1.192631	0.000000	2.721031
H	1.192631	0.000000	2.721031
H	0.000000	1.430220	-2.901855
H	0.000000	-1.430220	-2.901855

$2SiH_2$-TS E = -271.4690108

C	0.349704	-0.949668	0.703835
C	0.349704	-0.949668	-0.703835
C	-0.320929	-2.341257	0.672942
C	-0.320929	-2.341257	-0.672942
C	0.349704	0.304430	-1.325180
C	0.349704	0.304430	1.325180
H	0.336865	0.440047	-2.403334
H	0.336865	0.440047	2.403334
Si	1.224562	1.333474	0.000000
H	2.710108	1.208511	0.000000
H	0.888559	2.784161	0.000000
C	-1.472597	1.119280	-0.709932
C	-1.472597	1.119280	0.709932
H	-2.093398	0.394116	-1.227412
H	-2.093398	0.394116	1.227412
H	-0.664995	-3.033327	1.433589
H	-0.664995	-3.033327	-1.433589
H	-1.385031	2.071809	-1.226227
H	-1.385031	2.071809	1.226227

$2SiH_2$-Pr1 E = -271.4690108

C	0.474279	-0.846299	0.678220
C	0.474279	-0.846299	-0.678220
C	0.065777	-2.369745	0.667885
C	0.065777	-2.369745	-0.667885
C	0.065777	0.463242	-1.278435
C	0.065777	0.463242	1.278435
H	0.191708	0.599484	-2.353764
H	0.191708	0.599484	2.353764
Si	1.011018	1.541041	0.000000
H	2.492156	1.446335	0.000000
H	0.596343	2.975416	0.000000
C	-1.415460	0.731645	-0.780484
C	-1.415460	0.731645	0.780484
H	-2.079380	-0.046959	-1.172724
H	-2.079380	-0.046959	1.172724
H	-0.101687	-3.112549	1.440270
H	-0.101687	-3.112549	-1.440270
H	-1.774253	1.688805	-1.175781
H	-1.774253	1.688805	1.175781

$2SiH_2$-Pr2 E = -271.4690108

C	-0.018918	-0.946626	0.780838
C	-0.018918	-0.946626	-0.780838
C	0.160858	-2.276308	0.796456
C	0.160858	-2.276308	-0.796456
C	-0.018918	0.430779	-1.322535
C	-0.018918	0.430779	1.322535
H	0.149453	0.578943	-2.390715
H	0.149453	0.578943	2.390715
Si	1.202482	1.165801	0.000000

H	2.580313	0.612657	0.000000
H	1.234005	2.655086	0.000000
C	-1.326193	1.114539	-0.789346
C	-1.326193	1.114539	0.789346
H	-2.204388	0.583864	-1.172247
H	-2.204388	0.583864	1.172247
H	0.328087	-3.032885	1.556396
H	0.328087	-3.032885	-1.556396
H	-1.378664	2.141295	-1.168238
H	-1.378664	2.141295	1.168238

2NH E = -271.4690108

C	0.084942	-0.287407	0.720557
C	0.084942	-0.287407	-0.720557
C	-0.010743	-1.797536	0.678811
C	-0.010743	-1.797536	-0.678811
C	-0.010743	0.990406	-1.152709
C	-0.010743	0.990406	1.152709
H	-0.059780	1.442217	-2.134489
H	-0.059780	1.442217	2.134489
N	-0.112451	1.808652	0.000000
H	0.292659	2.737632	0.000000
H	-0.073710	-2.574098	1.432120
H	-0.073710	-2.574098	-1.432120

***anti*-2NH-TS** E = -271.4690108

C	0.352042	-0.914165	0.693860
C	0.352042	-0.914165	-0.693860
C	-0.899377	-1.822429	0.671390
C	-0.899377	-1.822429	-0.671390
C	0.815756	0.362919	-1.114413
C	0.815756	0.362919	1.114413
H	1.132298	0.660485	-2.109587
H	1.132298	0.660485	2.109587
N	1.565704	0.824177	0.000000
H	1.829209	1.801872	0.000000
C	-0.899377	1.469474	-0.705812
C	-0.899377	1.469474	0.705812
H	-1.669371	0.911984	-1.233034
H	-1.669371	0.911984	1.233034
H	-1.500120	-2.297220	1.439353
H	-1.500120	-2.297220	-1.439353
H	-0.571634	2.364402	-1.231625
H	-0.571634	2.364402	1.231625

***syn*-2NH-Pr1** E = -271.4690108

C	0.478992	-0.794824	0.677406
C	0.478992	-0.794824	-0.677406
C	-0.449889	-2.067415	0.667097
C	-0.449889	-2.067415	-0.667097
C	0.478992	0.660116	-1.109055
C	0.478992	0.660116	1.109055
H	0.853780	0.926047	-2.099427
H	0.853780	0.926047	2.099427
N	1.245959	1.291359	0.000000
H	2.194848	0.907718	0.000000
C	-0.950585	1.204436	-0.776563
C	-0.950585	1.204436	0.776563
H	-1.735547	0.574750	-1.207411
H	-1.735547	0.574750	1.207411
H	-0.859494	-2.704903	1.443033
H	-0.859494	-2.704903	-1.443033
H	-1.062082	2.216612	-1.175953
H	-1.062082	2.216612	1.175953

***syn*-2NH-Pr2** E = -271.4690108

C	0.174411	-0.787776	0.776012
C	0.174411	-0.787776	-0.776012
C	0.470979	-2.096931	0.794738
C	0.470979	-2.096931	-0.794738
C	0.174411	0.663915	-1.144326
C	0.174411	0.663915	1.144326
H	0.571699	0.967043	-2.114731
H	0.571699	0.967043	2.114731
N	0.984099	1.228719	0.000000
H	1.920228	0.816558	0.000000
C	-1.211768	1.257693	-0.783461
C	-1.211768	1.257693	0.783461
H	-2.027936	0.665543	-1.206164
H	-2.027936	0.665543	1.206164
H	0.690320	-2.839657	1.556041
H	0.690320	-2.839657	-1.556041
H	-1.286741	2.276864	-1.173987
H	-1.286741	2.276864	1.173987

***anti*-2NH-Pr1**			E = -271.4690108
C	0.505796	-0.807233	0.676892
C	0.505796	-0.807233	-0.676892
C	-0.477865	-2.030998	0.667711
C	-0.477865	-2.030998	-0.667711
C	0.505796	0.638876	-1.108191
C	0.505796	0.638876	1.108191
H	0.878115	0.905128	-2.099799
H	0.878115	0.905128	2.099799
N	1.335891	1.184564	0.000000
H	1.275377	2.205008	0.000000
C	-0.945624	1.165241	-0.775909
C	-0.945624	1.165241	0.775909
H	-1.728725	0.529341	-1.203086
H	-1.728725	0.529341	1.203086
H	-0.912169	-2.652083	1.443895
H	-0.912169	-2.652083	-1.443895
H	-1.079139	2.173819	-1.183638
H	-1.079139	2.173819	1.183638

***anti*-2NH-Pr2**			E = -271.4690108
C	0.254903	-0.781744	0.770513
C	0.254903	-0.781744	-0.770513
C	0.293105	-2.117926	0.804813
C	0.293105	-2.117926	-0.804813
C	0.254903	0.666994	-1.138353
C	0.254903	0.666994	1.138353
H	0.644539	0.970934	-2.111733
H	0.644539	0.970934	2.111733
N	1.113892	1.161579	0.000000
H	1.113173	2.185181	0.000000
C	-1.165778	1.218667	-0.783361
C	-1.165778	1.218667	0.783361
H	-1.969652	0.606800	-1.203603
H	-1.969652	0.606800	1.203603
H	0.324519	-2.885621	1.571690
H	0.324519	-2.885621	-1.571690
H	-1.277423	2.233824	-1.182151
H	-1.277423	2.233824	1.182151

2PH			E = -271.4690108
C	-0.045202	-0.628453	0.737130
C	-0.045202	-0.628453	-0.737130
C	-0.020103	-2.119511	0.683542
C	-0.020103	-2.119511	-0.683542
C	-0.020103	0.571830	-1.331381
C	-0.020103	0.571830	1.331381
H	0.020883	0.797525	-2.391642
H	0.020883	0.797525	2.391642
P	0.144288	1.862238	0.000000
H	-1.184484	2.395802	0.000000
H	0.001655	-2.905417	1.430070
H	0.001655	-2.905417	-1.430070

***syn*-2PH-TS**			E = -271.4690108
C	0.399671	-0.944860	0.700269
C	0.399671	-0.944860	-0.700269
C	-0.321897	-2.312306	0.672634
C	-0.321897	-2.312306	-0.672634
C	0.399671	0.327487	-1.271839
C	0.399671	0.327487	1.271839
H	0.429413	0.542400	-2.336474
H	0.429413	0.542400	2.336474
P	1.160403	1.473509	0.000000
H	2.477857	0.911504	0.000000
C	-1.506163	1.041238	-0.706436
C	-1.506163	1.041238	0.706436
H	-2.078573	0.282188	-1.231523
H	-2.078573	0.282188	1.231523
H	-0.683974	-2.992801	1.435029
H	-0.683974	-2.992801	-1.435029
H	-1.436510	1.991783	-1.228116
H	-1.436510	1.991783	1.228116

***anti*-2PH-TS**			E = -271.4690108
C	0.383988	-0.921980	0.700099
C	0.383988	-0.921980	-0.700099
C	-0.320428	-2.293858	0.673635
C	-0.320428	-2.293858	-0.673635
C	0.383988	0.356926	-1.265322

C	0.383988	0.356926	1.265322
H	0.437223	0.562807	-2.331684
H	0.437223	0.562807	2.331684
P	1.351798	1.335928	0.000000
H	0.588121	2.541925	0.000000
C	-1.548207	1.012562	-0.704087
C	-1.548207	1.012562	0.704087
H	-2.115027	0.248332	-1.228902
H	-2.115027	0.248332	1.228902
H	-0.669568	-2.982400	1.434908
H	-0.669568	-2.982400	-1.434908
H	-1.481230	1.958942	-1.233151
H	-1.481230	1.958942	1.233151

C	-0.024213	0.437138	1.280375
H	0.210340	0.630125	-2.329047
H	0.210340	0.630125	2.329047
P	1.197018	1.259649	0.000000
H	2.218423	0.265543	0.000000
C	-1.333834	1.123423	-0.785787
C	-1.333834	1.123423	0.785787
H	-2.205148	0.592703	-1.182794
H	-2.205148	0.592703	1.182794
H	0.386844	-3.023534	1.547393
H	0.386844	-3.023534	-1.547393
H	-1.372079	2.149282	-1.168055
H	-1.372079	2.149282	1.168055

***syn*-2PH-Pr1**	E = -271.4690108		
C	0.576505	-0.825357	0.677205
C	0.576505	-0.825357	-0.677205
C	0.098310	-2.329368	0.666997
C	0.098310	-2.329368	-0.666997
C	0.098310	0.484833	-1.230470
C	0.098310	0.484833	1.230470
H	0.252098	0.699492	-2.289848
H	0.252098	0.699492	2.289848
P	0.854093	1.727246	0.000000
H	2.190203	1.228242	0.000000
C	-1.410801	0.593177	-0.778754
C	-1.410801	0.593177	0.778754
H	-1.978197	-0.252899	-1.182227
H	-1.978197	-0.252899	1.182227
H	-0.089282	-3.063571	1.443055
H	-0.089282	-3.063571	-1.443055
H	-1.859365	1.508793	-1.177963
H	-1.859365	1.508793	1.177963

***anti*-2PH-Pr1**	E = -271.4690108		
C	0.522112	-0.834251	0.676349
C	0.522112	-0.834251	-0.676349
C	0.079789	-2.346000	0.667853
C	0.079789	-2.346000	-0.667853
C	0.079789	0.489049	-1.231059
C	0.079789	0.489049	1.231059
H	0.253513	0.690290	-2.290036
H	0.253513	0.690290	2.290036
P	1.066397	1.569084	0.000000
H	0.174831	2.691884	0.000000
C	-1.414732	0.664119	-0.777692
C	-1.414732	0.664119	0.777692
H	-2.026047	-0.154153	-1.177966
H	-2.026047	-0.154153	1.177966
H	-0.093179	-3.085884	1.441659
H	-0.093179	-3.085884	-1.441659
H	-1.821432	1.598164	-1.179159
H	-1.821432	1.598164	1.179159

***syn*-2PH-Pr2**	E = -271.4690108		
C	-0.024213	-0.944549	0.776805
C	-0.024213	-0.944549	-0.776805
C	0.197793	-2.270798	0.788584
C	0.197793	-2.270798	-0.788584
C	-0.024213	0.437138	-1.280375

***anti*-2PH-Pr2**	E = -271.4690108		
C	-0.137327	-0.938417	0.776486
C	-0.137327	-0.938417	-0.776486
C	-0.137327	-2.279498	0.796092
C	-0.137327	-2.279498	-0.796092
C	0.051085	0.440571	-1.275526

C	0.051085	0.440571	1.275526
H	0.310524	0.592567	-2.325165
H	0.310524	0.592567	2.325165
P	1.437382	0.961545	0.000000
H	1.130789	2.359497	0.000000
C	-1.172754	1.267327	-0.784825
C	-1.172754	1.267327	0.784825
H	-2.101496	0.838560	-1.178330
H	-2.101496	0.838560	1.178330
H	-0.079028	-3.051826	1.556360
H	-0.079028	-3.051826	-1.556360
H	-1.097829	2.289465	-1.170811
H	-1.097829	2.289465	1.170811

2O E = -271.4690108

C	0.000000	0.723282	-0.274918
C	0.000000	-0.723282	-0.274918
C	0.000000	0.679412	-1.782979
C	0.000000	-0.679412	-1.782979
C	0.000000	-1.123262	1.005224
C	0.000000	1.123262	1.005224
H	0.000000	-2.067594	1.528476
H	0.000000	2.067594	1.528476
O	0.000000	0.000000	1.836823
H	0.000000	1.434510	-2.559732
H	0.000000	-1.434510	-2.559732

2O-TS E = -271.4690108

C	0.351091	-0.912525	0.696542
C	0.351091	-0.912525	-0.696542
C	-0.885997	-1.835231	0.671547
C	-0.885997	-1.835231	-0.671547
C	0.817143	0.358599	-1.090948
C	0.817143	0.358599	1.090948
H	1.195760	0.693409	-2.049720
H	1.195760	0.693409	2.049720
O	1.517036	0.866922	0.000000
C	-0.885997	1.520013	-0.702043
C	-0.885997	1.520013	0.702043
H	-1.660770	0.977306	-1.237152
H	-1.660770	0.977306	1.237152
H	-1.481819	-2.312396	1.441097
H	-1.481819	-2.312396	-1.441097
H	-0.498754	2.388860	-1.227728
H	-0.498754	2.388860	1.227728

2O-Pr1 E = -271.4690108

C	0.502577	-0.802172	0.676768
C	0.502577	-0.802172	-0.676768
C	-0.462774	-2.044183	0.667040
C	-0.462774	-2.044183	-0.667040
C	0.502577	0.654199	-1.085324
C	0.502577	0.654199	1.085324
H	0.933585	0.956998	-2.040026
H	0.933585	0.956998	2.040026
O	1.266606	1.216822	0.000000
C	-0.934749	1.201553	-0.775874
C	-0.934749	1.201553	0.775874
H	-1.721352	0.575557	-1.209251
H	-1.721352	0.575557	1.209251
H	-0.885455	-2.669801	1.445417
H	-0.885455	-2.669801	-1.445417
H	-1.038990	2.213576	-1.177669
H	-1.038990	2.213576	1.177669

2O-Pr2 E = -271.4690108

C	0.222281	-0.783026	0.773728
C	0.222281	-0.783026	-0.773728
C	0.390421	-2.110833	0.799573
C	0.390421	-2.110833	-0.799573
C	0.222281	0.671718	-1.117179
C	0.222281	0.671718	1.117179
H	0.674224	1.006972	-2.050554
H	0.674224	1.006972	2.050554
O	1.025572	1.177595	0.000000
C	-1.175650	1.258245	-0.782501
C	-1.175650	1.258245	0.782501
H	-1.988648	0.661987	-1.206490
H	-1.988648	0.661987	1.206490
H	0.509139	-2.871642	1.564494
H	0.509139	-2.871642	-1.564494
H	-1.253003	2.275683	-1.177170
H	-1.253003	2.275683	1.177170

2S			E = -271.4690108
C	0.000000	0.723396	-0.614815
C	0.000000	-0.723396	-0.614815
C	0.000000	0.679453	-2.123558
C	0.000000	-0.679453	-2.123558
C	0.000000	-1.286234	0.604610
C	0.000000	1.286234	0.604610
H	0.000000	-2.321711	0.919184
H	0.000000	2.321711	0.919184
S	0.000000	0.000000	1.848284
H	0.000000	1.431920	-2.902879
H	0.000000	-1.431920	-2.902879

2S-TS			E = -271.4690108
C	0.448017	-0.930649	0.696212
C	0.448017	-0.930649	-0.696212
C	-0.415578	-2.213530	0.671402
C	-0.415578	-2.213530	-0.671402
C	0.448017	0.372960	-1.228541
C	0.448017	0.372960	1.228541
H	0.551838	0.648396	-2.273736
H	0.551838	0.648396	2.273736
S	1.253519	1.414847	0.000000
C	-1.515432	0.918174	-0.705370
C	-1.515432	0.918174	0.705370
H	-2.065868	0.139363	-1.227419
H	-2.065868	0.139363	1.227419
H	-0.829732	-2.856292	1.439869
H	-0.829732	-2.856292	-1.439869
H	-1.474533	1.868025	-1.230141
H	-1.474533	1.868025	1.230141

2S-Pr1			E = -271.4690108
C	0.600366	-0.817348	0.676542
C	0.600366	-0.817348	-0.676542
C	0.101934	-2.313091	0.666714
C	0.101934	-2.313091	-0.666714
C	0.101934	0.502567	-1.205640
C	0.101934	0.502567	1.205640
H	0.297947	0.771371	-2.244405
H	0.297947	0.771371	2.244405
S	0.901527	1.674467	0.000000
C	-1.405307	0.573891	-0.777489
C	-1.405307	0.573891	0.777489
H	-1.954504	-0.284024	-1.184518
H	-1.954504	-0.284024	1.184518
H	-0.087867	-3.043354	1.445593
H	-0.087867	-3.043354	-1.445593
H	-1.861359	1.484161	-1.176759
H	-1.861359	1.484161	1.176759

2S-Pr2			E = -271.4690108
C	-0.144816	-0.929535	0.775890
C	-0.144816	-0.929535	-0.775890
C	-0.144816	-2.272832	0.788193
C	-0.144816	-2.272832	-0.788193
C	0.052985	0.450650	-1.254988
C	0.052985	0.450650	1.254988
H	0.377118	0.628939	-2.281164
H	0.377118	0.628939	2.281164
S	1.396429	0.984902	0.000000
C	-1.150675	1.305449	-0.783266
C	-1.150675	1.305449	0.783266
H	-2.083309	0.892335	-1.184390
H	-2.083309	0.892335	1.184390
H	-0.099996	-3.046794	1.547491
H	-0.099996	-3.046794	-1.547491
H	-1.041313	2.323913	-1.167575
H	-1.041313	2.323913	1.167575

3CH$_2$			E = -271.4690108
C	0.000000	0.741929	0.254105
C	0.000000	-0.741929	0.254105
C	0.000000	1.441900	-1.007729
C	0.000000	-1.441900	-1.007729
C	0.000000	-1.186251	1.541657
C	0.000000	1.186251	1.541657
H	0.000000	-2.217209	1.876528
H	0.000000	2.217209	1.876528

C	0.000000	0.000000	2.462807
H	-0.876262	0.000000	3.131735
H	0.876262	0.000000	3.131735
H	0.000000	2.529109	-1.020343
H	0.000000	-2.529109	-1.020343
C	0.000000	0.725954	-2.163727
C	0.000000	-0.725954	-2.163727
H	0.000000	1.238981	-3.122175
H	0.000000	-1.238981	-3.122175

$3CH_2$-TS E = -271.4690108

C	-0.401406	0.291689	0.725038
C	-0.401406	0.291689	-0.725038
C	-0.019656	1.470582	1.428965
C	-0.019656	1.470582	-1.428965
C	-0.733793	-0.991511	-1.171166
C	-0.733793	-0.991511	1.171166
H	-0.925201	-1.258335	-2.205350
H	-0.925201	-1.258335	2.205350
C	-1.326351	-1.727986	0.000000
H	-2.413765	-1.521955	0.000000
H	-1.204010	-2.812879	0.000000
C	1.354377	-2.050376	-0.686583
C	1.354377	-2.050376	0.686583
H	1.917493	-1.311578	-1.245721
H	1.917493	-1.311578	1.245721
H	-0.015250	1.479257	2.516378
H	-0.015250	1.479257	-2.516378
H	1.046224	-2.928783	-1.246018
H	1.046224	-2.928783	1.246018
C	0.327091	2.591002	0.715818
C	0.327091	2.591002	-0.715818
H	0.604999	3.502497	1.238863
H	0.604999	3.502497	-1.238863

$3CH_2$-Pr E = -271.4690108

C	-0.195437	0.271897	0.704529
C	-0.195437	0.271897	-0.704529
C	-0.009675	1.450120	1.414579
C	-0.009675	1.450120	-1.414579
C	-0.364745	-1.173257	-1.137119
C	-0.364745	-1.173257	1.137119
H	-0.704571	-1.327622	-2.164412
H	-0.704571	-1.327622	2.164412
C	-1.285539	-1.691091	0.000000
H	-2.273661	-1.219765	0.000000
H	-1.401465	-2.781821	0.000000
C	0.967463	-1.910526	-0.781750
C	0.967463	-1.910526	0.781750
H	1.839076	-1.403877	-1.206152
H	1.839076	-1.403877	1.206152
H	-0.004444	1.456481	2.502295
H	-0.004444	1.456481	-2.502295
H	0.951593	-2.932255	-1.177786
H	0.951593	-2.932255	1.177786
C	0.157193	2.645120	0.698059
C	0.157193	2.645120	-0.698059
H	0.283739	3.581215	1.236018
H	0.283739	3.581215	-1.236018

$3SiH_2$ E = -271.4690108

C	0.000000	0.754282	-0.073872
C	0.000000	-0.754282	-0.073872
C	0.000000	1.432898	-1.359809
C	0.000000	-1.432898	-1.359809
C	0.000000	-1.354788	1.149535
C	0.000000	1.354788	1.149535
H	0.000000	-2.435263	1.254382
H	0.000000	2.435263	1.254382
Si	0.000000	0.000000	2.438374
H	-1.203531	0.000000	3.317977
H	1.203531	0.000000	3.317977
H	0.000000	2.520034	-1.367268
H	0.000000	-2.520034	-1.367268
C	0.000000	0.727397	-2.516105
C	0.000000	-0.727397	-2.516105
H	0.000000	1.244351	-3.472202
H	0.000000	-1.244351	-3.472202

$3SiH_2$-TS E = -271.4690108

C	-0.291228	0.467698	0.732431
C	-0.291228	0.467698	-0.732431
C	-0.052712	1.703413	1.418506
C	-0.052712	1.703413	-1.418506

C	-0.435797	-0.794089	-1.324245
C	-0.435797	-0.794089	1.324245
H	-0.457755	-0.894745	-2.405873
H	-0.457755	-0.894745	2.405873
Si	-1.142140	-1.903343	0.000000
H	-2.636227	-1.831860	0.000000
H	-0.764024	-3.340365	0.000000
C	1.675565	-1.751841	-0.689722
C	1.675565	-1.751841	0.689722
H	2.155038	-0.953535	-1.243518
H	2.155038	-0.953535	1.243518
H	-0.048795	1.707022	2.505994
H	-0.048795	1.707022	-2.505994
H	1.487293	-2.664697	-1.246057
H	1.487293	-2.664697	1.246057
C	0.146339	2.861068	0.715948
C	0.146339	2.861068	-0.715948
H	0.306323	3.797973	1.243325
H	0.306323	3.797973	-1.243325

3NH E = -271.4690108

C	0.000000	0.726111	0.251082
C	0.000000	-0.726111	0.251082
C	0.000000	1.431176	-0.984498
C	0.000000	-1.431176	-0.984498
C	0.000000	-1.134851	1.583881
C	0.000000	1.134851	1.583881
H	0.000000	-2.117153	2.032363
H	0.000000	2.117153	2.032363
N	0.000000	0.000000	2.350549
H	0.000000	0.000000	3.360230
H	0.000000	2.518432	-0.995864
H	0.000000	-2.518432	-0.995864
C	0.000000	0.715217	-2.156256
C	0.000000	-0.715217	-2.156256
H	0.000000	1.238813	-3.108788
H	0.000000	-1.238813	-3.108788

3SiH$_2$-Pr E = -271.4690108

C	-0.008899	0.435907	0.708337
C	-0.008899	0.435907	-0.708337
C	-0.002593	1.640755	1.407287
C	-0.002593	1.640755	-1.407287
C	-0.021925	-0.975392	-1.258672
C	-0.021925	-0.975392	1.258672
H	-0.181553	-1.039409	-2.336681
H	-0.181553	-1.039409	2.336681
Si	-1.266311	-1.717145	0.000000
H	-2.620076	-1.104283	0.000000
H	-1.383125	-3.206973	0.000000
C	1.293277	-1.678172	-0.783610
C	1.293277	-1.678172	0.783610
H	2.166087	-1.144248	-1.176059
H	2.166087	-1.144248	1.176059
H	-0.005471	1.643930	2.495068
H	-0.005471	1.643930	-2.495068
H	1.337483	-2.701098	-1.174481
H	1.337483	-2.701098	1.174481
C	-0.001086	2.847889	0.698123
C	-0.001086	2.847889	-0.698123
H	-0.003417	3.790553	1.239337
H	-0.003417	3.790553	-1.239337

***anti*-3NH-TS** E = -271.4690108

C	-0.393199	0.272049	0.712193
C	-0.393199	0.272049	-0.712193
C	-0.042026	1.432304	1.423317
C	-0.042026	1.432304	-1.423317
C	-0.699623	-1.073535	-1.113463
C	-0.699623	-1.073535	1.113463
H	-0.997030	-1.391325	-2.105784
H	-0.997030	-1.391325	2.105784
N	-1.282537	-1.668875	0.000000
H	-1.412040	-2.673214	0.000000
C	1.298877	-1.923424	-0.699092
C	1.298877	-1.923424	0.699092
H	1.894370	-1.198031	-1.243787
H	1.894370	-1.198031	1.243787
H	-0.033393	1.438408	2.510561
H	-0.033393	1.438408	-2.510561
H	1.118492	-2.851218	-1.238001
H	1.118492	-2.851218	1.238001
C	0.281975	2.574499	0.706942
C	0.281975	2.574499	-0.706942
H	0.536434	3.488472	1.237251
H	0.536434	3.488472	-1.237251

***syn*-3NH-Pr**			E = -271.4690108
C	-0.196694	0.271384	0.703674
C	-0.196694	0.271384	-0.703674
C	0.002019	1.444824	1.416313
C	0.002019	1.444824	-1.416313
C	-0.388762	-1.188111	-1.101315
C	-0.388762	-1.188111	1.101315
H	-0.794993	-1.376979	-2.097373
H	-0.794993	-1.376979	2.097373
N	-1.236861	-1.728526	0.000000
H	-2.133217	-1.235154	0.000000
C	0.940676	-1.934343	-0.780716
C	0.940676	-1.934343	0.780716
H	1.809098	-1.429948	-1.212817
H	1.809098	-1.429948	1.212817
H	0.014443	1.451557	2.503981
H	0.014443	1.451557	-2.503981
H	0.899076	-2.953720	-1.174496
H	0.899076	-2.953720	1.174496
C	0.171067	2.639650	0.697978
C	0.171067	2.639650	-0.697978
H	0.298167	3.576083	1.235197
H	0.298167	3.576083	-1.235197

***anti*-3NH-Pr**			E = -271.4690108
C	-0.219085	0.274735	0.702457
C	-0.219085	0.274735	-0.702457
C	-0.017233	1.445233	1.417008
C	-0.017233	1.445233	-1.417008
C	-0.395663	-1.177602	-1.101248
C	-0.395663	-1.177602	1.101248
H	-0.799912	-1.365887	-2.097981
H	-0.799912	-1.365887	2.097981
N	-1.297631	-1.622376	0.000000
H	-1.352072	-2.645183	0.000000
C	0.958347	-1.903095	-0.780342
C	0.958347	-1.903095	0.780342
H	1.823803	-1.390031	-1.210085
H	1.823803	-1.390031	1.210085
H	-0.010333	1.451750	2.504397
H	-0.010333	1.451750	-2.504397
H	0.944012	-2.923315	-1.181067
H	0.944012	-2.923315	1.181067
C	0.166101	2.636879	0.698088
C	0.166101	2.636879	-0.698088
H	0.305364	3.571496	1.235187
H	0.305364	3.571496	-1.235187

3PH			E = -271.4690108
C	-0.028672	-0.068973	0.739541
C	-0.028672	-0.068973	-0.739541
C	-0.007560	-1.334927	1.430629
C	-0.007560	-1.334927	-1.430629
C	-0.064343	1.188229	-1.292028
C	-0.064343	1.188229	1.292028
H	-0.044871	1.396040	-2.355649
H	-0.044871	1.396040	2.355649
P	0.163102	2.413499	0.000000
H	-1.053461	3.147950	0.000000
H	-0.000664	-1.341354	2.517565
H	-0.000664	-1.341354	-2.517565
C	-0.007560	-2.497368	0.722436
C	-0.007560	-2.497368	-0.722436
H	-0.002192	-3.451671	1.242564
H	-0.002192	-3.451671	-1.242564

***syn*-3PH-TS**			E = -271.4690108
C	-0.308679	0.452833	0.723758
C	-0.308679	0.452833	-0.723758
C	-0.066367	1.674323	1.420754
C	-0.066367	1.674323	-1.420754
C	-0.460582	-0.831906	-1.264138
C	-0.460582	-0.831906	1.264138
H	-0.540386	-1.014116	-2.331780
H	-0.540386	-1.014116	2.331780
P	-1.084081	-2.008570	0.000000
H	-2.422766	-1.484131	0.000000
C	1.695452	-1.661697	-0.690337
C	1.695452	-1.661697	0.690337
H	2.156389	-0.851566	-1.243507
H	2.156389	-0.851566	1.243507
H	-0.060707	1.677858	2.508020
H	-0.060707	1.677858	-2.508020
H	1.541078	-2.582997	-1.243038
H	1.541078	-2.582997	1.243038

C	0.132624	2.834096	0.714210
C	0.132624	2.834096	-0.714210
H	0.290933	3.771263	1.241478
H	0.290933	3.771263	-1.241478

***anti*-3PH-TS**		E = -271.4690108	
C	-0.298611	0.426015	0.722610
C	-0.298611	0.426015	-0.722610
C	-0.080935	1.646694	1.419345
C	-0.080935	1.646694	-1.419345
C	-0.418988	-0.877854	-1.260758
C	-0.418988	-0.877854	1.260758
H	-0.524328	-1.049464	-2.328227
H	-0.524328	-1.049464	2.328227
P	-1.274319	-1.855135	0.000000
H	-0.601888	-3.106044	0.000000
C	1.749339	-1.600954	-0.689907
C	1.749339	-1.600954	0.689907
H	2.203860	-0.786051	-1.242455
H	2.203860	-0.786051	1.242455
H	-0.080093	1.651068	2.506592
H	-0.080093	1.651068	-2.506592
H	1.615214	-2.523219	-1.246148
H	1.615214	-2.523219	1.246148
C	0.112751	2.810447	0.712146
C	0.112751	2.810447	-0.712146
H	0.262349	3.748108	1.240996
H	0.262349	3.748108	-1.240996

***syn*-3PH-Pr**		E = -271.4690108	
C	-0.049508	0.443593	0.705390
C	-0.049508	0.443593	-0.705390
C	-0.013847	1.639274	1.410037
C	-0.013847	1.639274	-1.410037
C	-0.053260	-0.980310	-1.214856
C	-0.053260	-0.980310	1.214856
H	-0.275087	-1.099105	-2.277509
H	-0.275087	-1.099105	2.277509
P	-1.223632	-1.878964	0.000000
H	-2.285464	-0.926840	0.000000
C	1.299487	-1.630295	-0.782175
C	1.299487	-1.630295	0.782175
H	2.139417	-1.057419	-1.188325
H	2.139417	-1.057419	1.188325
H	-0.010815	1.643858	2.497661
H	-0.010815	1.643858	-2.497661
H	1.375346	-2.649565	-1.175448
H	1.375346	-2.649565	1.175448
C	-0.001435	2.848796	0.696825
C	-0.001435	2.848796	-0.696825
H	0.002486	3.791535	1.237750
H	0.002486	3.791535	-1.237750

***anti*-3PH-Pr**		E = -271.4690108	
C	-0.042923	0.439312	0.705574
C	-0.042923	0.439312	-0.705574
C	-0.015028	1.637137	1.410729
C	-0.015028	1.637137	-1.410729
C	-0.044500	-0.988781	-1.214895
C	-0.044500	-0.988781	1.214895
H	-0.272958	-1.096979	-2.277224
H	-0.272958	-1.096979	2.277224
P	-1.332075	-1.705823	0.000000
H	-0.887345	-3.070307	0.000000
C	1.299447	-1.642470	-0.780743
C	1.299447	-1.642470	0.780743
H	2.146920	-1.075301	-1.183098
H	2.146920	-1.075301	1.183098
H	-0.016463	1.641174	2.498209
H	-0.016463	1.641174	-2.498209
H	1.370043	-2.660842	-1.176665
H	1.370043	-2.660842	1.176665
C	0.002427	2.843738	0.697947
C	0.002427	2.843738	-0.697947
H	0.010155	3.787161	1.237563
H	0.010155	3.787161	-1.237563

3O		E = -271.4690108	
C	0.000000	0.727741	0.265606
C	0.000000	-0.727741	0.265606

C	0.000000	1.438213	-0.974300
C	0.000000	-1.438213	-0.974300
C	0.000000	-1.103808	1.589079
C	0.000000	1.103808	1.589079
H	0.000000	-2.052338	2.103055
H	0.000000	2.052338	2.103055
O	0.000000	0.000000	2.380302
H	0.000000	2.524651	-0.985817
H	0.000000	-2.524651	-0.985817
C	0.000000	0.719145	-2.138001
C	0.000000	-0.719145	-2.138001
H	0.000000	1.238051	-3.092748
H	0.000000	-1.238051	-3.092748

3O-TS E = -271.4690108

C	-0.402378	0.279549	0.713319
C	-0.402378	0.279549	-0.713319
C	-0.024507	1.435556	1.427636
C	-0.024507	1.435556	-1.427636
C	-0.732692	-1.050715	-1.088915
C	-0.732692	-1.050715	1.088915
H	-1.078535	-1.420742	-2.044821
H	-1.078535	-1.420742	2.044821
O	-1.253935	-1.687330	0.000000
C	1.279567	-1.992705	-0.693321
C	1.279567	-1.992705	0.693321
H	1.885527	-1.282045	-1.245943
H	1.885527	-1.282045	1.245943
H	-0.013414	1.441112	2.514445
H	-0.013414	1.441112	-2.514445
H	1.010397	-2.894267	-1.236101
H	1.010397	-2.894267	1.236101
C	0.317150	2.566373	0.709725
C	0.317150	2.566373	-0.709725
H	0.588921	3.476914	1.236995
H	0.588921	3.476914	-1.236995

3O-Pr E = -271.4690108

C	-0.212177	0.275068	0.702141
C	-0.212177	0.275068	-0.702141
C	-0.004763	1.443566	1.417888
C	-0.004763	1.443566	-1.417888
C	-0.407076	-1.184027	-1.079113
C	-0.407076	-1.184027	1.079113
H	-0.873986	-1.398352	-2.041045
H	-0.873986	-1.398352	2.041045
O	-1.247073	-1.649921	0.000000
C	0.923770	-1.939677	-0.779939
C	0.923770	-1.939677	0.779939
H	1.796370	-1.444514	-1.215150
H	1.796370	-1.444514	1.215150
H	0.005075	1.450506	2.505220
H	0.005075	1.450506	-2.505220
H	0.871152	-2.958268	-1.175200
H	0.871152	-2.958268	1.175200
C	0.178959	2.635117	0.698060
C	0.178959	2.635117	-0.698060
H	0.317397	3.570024	1.234734
H	0.317397	3.570024	-1.234734

3S E = -271.4690108

C	0.000000	0.727349	-0.068160
C	0.000000	-0.727349	-0.068160
C	0.000000	1.427121	-1.317059
C	0.000000	-1.427121	-1.317059
C	0.000000	-1.248699	1.215772
C	0.000000	1.248699	1.215772
H	0.000000	-2.287297	1.516910
H	0.000000	2.287297	1.516910
S	0.000000	0.000000	2.397219
H	0.000000	2.513846	-1.322223
H	0.000000	-2.513846	-1.322223
C	0.000000	0.717179	-2.486269
C	0.000000	-0.717179	-2.486269
H	0.000000	1.241378	-3.438147
H	0.000000	-1.241378	-3.438147

3S-TS			E = -271.4690108
C	-0.311069	0.416784	0.713416
C	-0.311069	0.416784	-0.713416
C	-0.097285	1.621608	1.417848
C	-0.097285	1.621608	-1.417848
C	-0.422414	-0.914688	-1.219763
C	-0.422414	-0.914688	1.219763
H	-0.588961	-1.154001	-2.264426
H	-0.588961	-1.154001	2.264426
S	-1.136472	-1.947729	0.000000
C	1.711000	-1.502285	-0.695663
C	1.711000	-1.502285	0.695663
H	2.172198	-0.684434	-1.239015
H	2.172198	-0.684434	1.239015
H	-0.090188	1.624654	2.504912
H	-0.090188	1.624654	-2.504912
H	1.643350	-2.438645	-1.240334
H	1.643350	-2.438645	1.240334
C	0.077261	2.795365	0.707784
C	0.077261	2.795365	-0.707784
H	0.210422	3.733551	1.239816
H	0.210422	3.733551	-1.239816

3S-Pr			E = -271.4690108
C	-0.069262	0.443164	0.703887
C	-0.069262	0.443164	-0.703887
C	-0.023846	1.634210	1.412211
C	-0.023846	1.634210	-1.412211
C	-0.064134	-0.991036	-1.193381
C	-0.064134	-0.991036	1.193381
H	-0.343155	-1.144229	-2.236569
H	-0.343155	-1.144229	2.236569
S	-1.247918	-1.812728	0.000000
C	1.298470	-1.615853	-0.780511
C	1.298470	-1.615853	0.780511
H	2.126760	-1.027063	-1.190712
H	2.126760	-1.027063	1.190712
H	-0.020437	1.639122	2.499574
H	-0.020437	1.639122	-2.499574
H	1.379824	-2.633039	-1.173685
H	1.379824	-2.633039	1.173685
C	-0.002337	2.843007	0.696807
C	-0.002337	2.843007	-0.696807
H	0.007006	3.786070	1.236793
H	0.007006	3.786070	-1.236793