H-bridged $A_3H_3^+$ (A=Si and Ge): A π ligand in Organometallic Chemistry

Gantasala N. Srinivas, Liwen Yu and M. Schwartz*
Department of Chemistry, University of North Texas, Denton, Texas 76203, USA. Fax: 940-565-4318; Tel: 940-565-3542; E-mail: marty@unt.edu

Supplementary material

Cartesian coordinates (at the B3LYP/B1 level) of the Structures **9-11** shown in Figure 1.

9-si, $(Si_3H_3)Co(CO)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.000000	0.000000	0.362211
2	14	0	0.000000	-1.527171	-1.478551
3	14	0	-1.322569	0.763585	-1.478551
4	14	0	1.322569	0.763585	-1.478551
5	1	0	-1.207013	-0.696870	-2.318070
6	1	0	0.000000	1.393739	-2.318070
7	1	0	1.207013	-0.696870	-2.318070
8	6	0	0.000000	1.619922	1.120264
9	6	0	1.402893	-0.809961	1.120264
10	6	0	-1.402893	-0.809961	1.120264
11	8	0	0.000000	2.651419	1.629536
12	8	0	2.296196	-1.325709	1.629536
13	8	0	-2.296196	-1.325709	1.629536

9-Ge, $(Ge_3H_3)Co(CO)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	27	0	0.000000	0.000000	0.844974
2	32	0	0.000000	1.621674	-1.009813
3	32	0	1.404411	-0.810837	-1.009813
4	32	0	-1.404411	-0.810837	-1.009813
5	1	0	1.254682	0.724391	-1.902536
6	1	0	0.000000	-1.448782	-1.902536
7	1	0	-1.254682	0.724391	-1.902536
8	6	0	0.000000	-1.613342	1.601884
9	6	0	-1.397195	0.806671	1.601884
10	6	0	1.397195	0.806671	1.601884
11	8	0	0.000000	-2.639229	2.125059
12	8	0	-2.285639	1.319614	2.125059
13	8	0	2.285639	1.319614	2.125059

10-Si, $(Si_3H_3)Rh(CO)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.000000	0.000000	0.331478
2	14	0	0.000000	-1.551085	-1.646656
3	14	0	-1.343279	0.775543	-1.646656
4	14	0	1.343279	0.775543	-1.646656
5	1	0	-1.204939	-0.695672	-2.464114
6	1	0	0.000000	1.391344	-2.464114
7	1	0	1.204939	-0.695672	-2.464114
8	6	0	0.000000	1.775355	1.186727
9	6	0	1.537503	-0.887678	1.186727
10	6	0	-1.537503	-0.887678	1.186727
11	8	0	0.000000	2.812262	1.678096
12	8	0	2.435491	-1.406131	1.678096
13	8	0	-2.435491	-1.406131	1.678096

10-Ge, $(Ge_3H_3)Rh(CO)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.000000	0.000000	0.826635
2	32	0	0.000000	1.644359	-1.177114
3	32	0	1.424057	-0.822180	-1.177114
4	32	0	-1.424057	-0.822180	-1.177114
5	1	0	1.253314	0.723601	-2.043425
6	1	0	0.000000	-1.447203	-2.043425
7	1	0	-1.253314	0.723601	-2.043425
8	6	0	0.000000	-1.771935	1.663937
9	6	0	-1.534540	0.885967	1.663937
10	6	0	1.534540	0.885967	1.663937
11	8	0	0.000000	-2.805110	2.165992
12	8	0	-2.429296	1.402555	2.165992
13	8	0	2.429296	1.402555	2.165992

11-Si, $(Si_3H_3)Ir(CO)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.000000	0.000000	0.271176
2	14	0	0.000000	-1.568681	-1.712984
3	14	0	-1.358518	0.784341	-1.712984
4	14	0	1.358518	0.784341	-1.712984
5	1	0	-1.199703	-0.692649	-2.516400
6	1	0	0.000000	1.385297	-2.516400
7	1	0	1.199703	-0.692649	-2.516400
8	6	0	0.000000	1.756648	1.119818
9	6	0	1.521302	-0.878324	1.119818
10	6	0	-1.521302	-0.878324	1.119818
11	8	0	0.000000	2.800489	1.602385
12	8	0	2.425294	-1.400244	1.602385
13	8	0	-2.425294	-1.400244	1.602385

11-Ge, $(Ge_3H_3)Ir(CO)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	77	0	0.000000	0.000000	0.712731
2	32	0	0.000000	1.658488	-1.303481
3	32	0	1.436293	-0.829244	-1.303481
4	32	0	-1.436293	-0.829244	-1.303481
5	1	0	1.247681	0.720349	-2.157318
6	1	0	0.000000	-1.440698	-2.157318
7	1	0	-1.247681	0.720349	-2.157318
8	6	0	0.000000	-1.754520	1.544105
9	6	0	-1.519459	0.877260	1.544105
10	6	0	1.519459	0.877260	1.544105
11	8	0	0.000000	-2.794090	2.038832
12	8	0	-2.419753	1.397045	2.038832
13	8	0	2.419753	1.397045	2.038832