THE JOURNAL OF PHYSICAL CHEMISTRY A
J. Phys. Chem. A, 1998, 102(11), 2055-2064, DOI:10.1021/jp973365n

Table I. Cartesian coordinates (in Å), calculated at the B3LYP/A level of theory for $(TiXH_6)^0$, X=B, Al, Ga, isomers.

Molecule/Isomers	Atom	X	Y	Z
M = B				
(2.3.1)	Ti	.168749	.300613	-.225889
	B	-.263273	-.464120	1.714940
	H	1.829706	.196135	-.686888
	H	-.674392	-1.166368	.743322
	H	-.760506	1.683907	-.679923
	H	.956034	-.302885	1.478935
	H	-.732160	.674636	1.487058
	H	-.523645	-.921919	2.779470
M = Al				
(2.3.1)	Ti	-1.182763	0.012022	-0.217840
	Al	1.293293	0.012317	-0.044503
	H	-1.910766	1.501437	-0.720533
	H	-1.966874	-1.463067	-0.679074
	H	0.113504	0.018254	1.270330
	H	2.841546	-0.039448	0.289623
	H	2.841546	-0.039448	0.289623
	H	0.355922	-1.141691	-0.746397
(2.2.2)	Ti	0.000000	0.000000	1.070661
	Al	0.000000	0.000000	-1.684522
	H	0.000000	-1.475167	1.966349
	H	0.000000	1.475167	1.966349
	H	1.163740	0.000000	-0.404071
	H	-1.163740	0.000000	-0.404071
	H	0.000000	1.415377	-2.390159
	H	0.000000	-1.415377	-2.390159

Table I. Continued.

Molecule/Isomers	Atom	X	Y	Z
M = Al				
(3,3,0)	Ti	-.000364	.000000	.118375
	Al	.000306	.000000	2.635813
	H	1.595507	.000000	-.469216
	H	-.797416	-1.382211	-.470202
	H	-.797416	1.382211	-.470202
	H	1.323026	.000000	1.560195
	H	-.661821	1.145983	1.560837
	H	-.661821	-1.145983	1.560837
M = Ga				
(2,3,1)	Ti	-.003098	-.000062	-.000588
	Ga	.024123	-.001251	2.491018
	H	.401733	1.484891	-.790422
	H	.401650	-1.484237	-.791961
	H	.717315	-1.151605	1.503419
	H	.717078	1.150296	1.504574
	H	-1.339997	-.000882	1.457334
	H	-.081128	-.002247	4.030286
(2,2,2)	Ti	.000000	.000000	.003994
	Ga	.000000	.000000	2.740950
	H	.000000	1.476658	-.889092
	H	.000000	-1.476658	-.889092
	H	1.180311	.000000	1.476039
	H	-1.180311	.000000	1.476039
	H	.000000	-1.403980	3.426725
	H	.000000	1.403980	3.426725

Table I. Continued.

Molecule/Isomers	Atom	X	Y	Z
M = Ga				
(3,3,0)	Ti	.000000	.000000	.118375
	Ga	.000000	.000000	2.635813
	H	1.595507	.000000	-.470202
	H	-.797416	-1.382211	-.470202
	H	-.797416	1.382211	-.470202
	H	1.323026	.000000	1.560837
	H	-.661821	1.145983	1.560837
	H	-.661821	-1.145983	1.560837

Table II. Cartesian coordinates (in Å), calculated at the B3LYP/A level of theory for $(TiXH_6)^-$, X=B, Al, Ga, isomers.

Molecule/Isomers	Atom	X	Y	Z
M = B				
(3,2,1)	Ti	-.003868	-.000507	.005513
	B	.017080	-.000127	2.032469
	H	1.676077	.002106	-.590334
	H	-.770024	-1.476836	-.622125
	H	-.773190	1.473894	-.622671
	H	.353209	-.000589	3.184863
	H	-.630045	-.983592	1.607656
	H	-.627285	.984880	1.607169
M = Al				
(3,2,1)	Ti	.837325	.000000	.000186
	Al	-1.500053	.000000	-.133790
	H	1.380294	1.421824	-.797122
	H	1.917146	-.142933	1.328358
	H	1.394004	-1.205402	-1.091195
	H	-2.810446	.000000	.671012
	H	-.405321	.946474	.921094
	H	-.396137	-1.126234	.703033
(2,2,2)	Ti	.000000	.000000	1.021123
	Al	.000000	.000000	-1.593973
	H	.000000	-1.515338	2.000464
	H	.000000	1.515338	2.000464
	H	1.317254	.000000	-.409805
	H	-1.317254	.000000	-.409805
	H	.000000	1.372534	-2.462187
	H	.000000	-1.372534	-2.462187

Table II. Continued.

Molecule/Isomers	Atom	X	Y	Z
M = Al				
(2.2.2)	Ti	.000000	.000000	1.140543
Ti planar	H	.000000	-1.167202	-.575773
	Al	.000000	.000000	-1.766600
	H	.000000	1.167202	-.575773
	H	-1.363225	.000000	-2.617983
	H	1.363225	.000000	-2.617983
	H	.000000	-1.493390	2.130685
	H	.000000	1.493390	2.130685
(3.3.0)	Ti	.000000	.000000	.000000
	Al	.000000	.000000	2.713734
	H	1.586760	.000000	-.730550
	H	-.793380	-1.374174	-.730550
	H	-.793380	1.374174	-.730550
	H	1.202825	.000000	1.394066
	H	-.601412	-1.041677	1.394066
	H	-.601412	1.041677	1.394066
(3.0.3)	Ti	.000000	.000000	1.085546
	Al	.000000	.000000	-1.692538
	H	.000000	1.713517	1.492813
	H	-1.483949	-.856758	1.492813
	H	1.483949	-.856758	1.492813
	H	.000000	-1.574076	-2.119153
	H	-1.363190	.787038	-2.119153
	H	1.363190	.787038	-2.119153
M = Ga				
(3.2.1)	Ga	-.005603	-.014987	-.009062
	Ti	-.003353	-.007773	2.459996
	H	1.528853	.009849	3.317081
	H	-1.015419	1.145393	3.313233
	H	-.703856	-1.575704	2.830802
	H	.298891	.667259	-1.442313

Table II Continued.

Molecule/Isomers	Atom	X	Y	Z
M = Ga				
	H	1.313367	.294926	1.129378
	H	-.654375	1.174483	1.127942
(2.2.2)	Ti	.000000	.000000	.000000
	Ga	.000000	.000000	2.525797
	H	.000000	1.519920	-.964041
	H	.000000	-1.519920	-.964041
	H	1.379318	.000000	1.306002
	H	-1.379318	.000000	1.306002
	H	.000000	-1.342408	3.392372
	H	.000000	1.342408	3.392372
(3,3,0)	Ti	.000000	.000000	.167628
	Ga	.000000	.000000	2.933992
	H	1.581027	-.000000	-.579081
	H	-.790256	-1.369380	-.581222
	H	-.790256	1.369381	-.581222
	H	1.217224	.000000	1.555059
	H	-.609520	1.053242	1.555641
	H	-.609520	-1.053242	1.555641
(3.0.3)	Ti	.000000	.000000	-1.540502
	Ga	.000000	.000000	1.135168
	H	.000000	-1.699903	-1.991336
	H	-1.472159	.849952	-1.991336
	H	1.472159	.849952	-1.991336
	H	.000000	1.556156	1.55827
	H	-1.347670	-.778078	1.558279
	H	1.347670	-.778078	1.558279

Table III. Harmonic Vibrational Frequencies (cm^{-1}), infrared intensities (km mol^{-1}) at the B3LYP/A level of theory for $(TiXH_6)^-$, X=B, Al, Ga, isomers.

Molecule /Isomer	Freq.	Intensity	Molecule /Isomer	Freq.	Intensity	Molecule /Isomer	Freq.	Intensity
X=B			X=Al			X=Al		
(3.2.1)	178	3.2	(3.2,1)	260	5.3	(3,3,0)	327	0.0
	303	23.0		283	16.1		347	75.7
	468	60.6		348	6.4		366	8.8
	505	27.6		380	115		366	8.8
	525	124.8		442	73.1		519	168.1
	592	76.6		488	44.7		519	168.1
	596	27.6		524	116.8		639	142.6
	651	124.8		539	622.2		792	12.2
	681	76.6		622	211.3		792	12.2
	960	70.1		773	43.8		1178	10.4
	1202	1.4		1080	32.6		1178	10.4
	1257	95.2		1180	465.1		1248	5.9
	1464	889.5		1357	20.9		1248	5.9
	1466	688.5		1436	18.4		1318	2109.2
	1533	575.5		1522	777.2		1398	73.5
	2198	19.2		1526	589.4		1546	632.9
	2227	50.6		1575	1106.4		1546	632.9
	2586.7	193.6		1738	491.4		1624	322.6

Table III . Continued.

Molecule /Isomer	Freq.	Intensity	Molecule /Isomer	Freq.	Intensity	Molecule /Isomer	Freq.	Intensity
X=Al			X=Al			X=Al		
(2.2.2)	228	8.3	(2,2,2)	165	0.0	(3,0,3)	130	0.0
	245	10.8	Ti pl.	186	11.9		157	11.1
	324	1.7		220	44.5		157	11.1
	379	0.0		259	1.6		222	2.3
	429	90.7		262	14.8		239	1.6
	552	185.9		491	44.0		239	1.6
	590	63.8		526	88.9		470	76.1
	671	529.0		704	0.0		585	97.8
	737	0.0		761	70.9		585	97.8
	753	251.1		765	346.8		667	995.6
	1013	169.4		915	312.8		750	158.7
	1046	136.1		1059	750.1		750	158.7
	1216	297.4		1458	404.4		1540	693.7
	1255	410.9		1469	251.3		1540	693.7
	1438	808.1		1597	214.1		1582	555.1
	1468	649.3		1696	461.6		1723	556.1
	1755	402.7		1820	276.9		1723	556.1
	1772	251.6		1842	187.3		1747	153.9

Table III . Continued.

Molecule /Isomer	Freq.	Intensity	Molecule /Isomer	Freq.	Intensity	Molecule /Isomer	Freq.	Intensity
X=Ga			X=Ga			X=Ga		
(3.2.1)	252	1.2	(2.2.2)	217	28.7	(3,3,0)	269	80.8
	278	6.8		223	23.7		338	0.0
	338	0.5		331	0.0		345	3.8
	386	9.4		400	0.0		354	2.4
	449	69.0		427	117.6		501	178.8
	494	49.7		559	74.7		501	178.8
	530	121.3		564	162.4		620	213.4
	540	83.7		612	305.4		745	20.6
	623	221.1		633	15.3		745	20.6
	757	36.0		727	0.3		1113	12.3
	1009	8.5		752	0.3		1113	12.3
	1119	446.4		782	7.3		1187	4.6
	1288	54.1		1257	490.4		1187	4.6
	1364	96.8		1324	447.3		1250	1334.9
	1524	690.1		1443	844.4		1356	1115.2
	1524	553.0		1478	697.8		1536	632.2
	1581	1013.5		1817	373.3		1536	632.2
	1729	529.8		1833	291.5		1619	279.7

Table III . Continued.

Molecule/ Isomer	Freq.	Intensity
X=Ga		
(3.0.3)	94	12.9
	94	12.9
	96	0
	197	0.0
	351	3.1
	351	3.1
	490	23.2
	580	96.6
	580	96.6
	609	770.8
	737	102.5
	737	102.5
	1543	682.1
	1543	682.1
	1589	633.6
	1746	535.4
	1746	535.4
	1760	136.0

Table IV. Bonding properties, in a.u., of the bond critical points of the $(TiXH_6)^0$, X=B, Al, Ga, at the B3LYP/A level of theory.

Bond	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$H(r_c)$	ε
Isomer (2,3,1)				
Ti - B	0.067	0.1933	-0.0152	0.123
Ti - H_t	0.098	0.0468	-0.0360	0.033
B - H_b	0.149	-0.0868	-0.1493	0.132
B - H_b	0.142	-0.0534	-0.1391	0.151
B - H_t	0.179	-0.2706	-0.1886	0.006
Ti - H_t	0.097	0.0490	-0.0348	0.047
Ti - H_b	0.049	0.1500	-0.0046	0.727
Ti - H_b	0.048	0.1248	-0.0054	0.545
Al - H_b	0.061	0.1975	-0.0154	0.053
Al - H_b	0.067	0.2175	-0.0183	0.031
Al - H_t	0.082	0.2742	-0.0249	0.001
r.c.p.	0.040	0.0555	-0.0455	-
Ti - Ga	0.045	0.1047	-0.0098	0.664
Ti - H_t	0.097	0.0479	-0.0353	0.044
Ti - H_b	0.045	0.1205	-0.0047	1.127
Ti - H_b	0.048	0.1471	-0.0045	1.007
Ga - H_b	0.090	0.1244	-0.0404	0.075
Ga - H_b	0.081	0.1159	-0.0347	0.095
Ga - H_t	0.117	0.1539	-0.0572	0.075
r.c.p.	0.045	0.1013	-0.0088	-
r.c.p.	0.044	0.1040	-0.0073	-
Isomer (2,2,2)				
Ti -H_t	0.099	0.03978	-0.0367	0.062
Ti -H_b	0.058	0.15843	-0.0084	0.682
Al -H_b	0.055	0.17863	-0.0123	0.189

Bond	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$H(r_c)$	ε
Al -H_t	0.079	0.2669	-0.0235	0.010
r.c.p.	0.039	0.04028	-0.0073	-
Ti -H_t	0.099	0.0398	-0.0367	0.061
Ti -H_b	0.057	0.1544	-0.0082	0.073
Ga-H_b	0.075	0.1239	-0.0305	0.057
Ga -H_t	0.111	0.1509	-0.0539	0.023
r.c.p.	0.039	0.0539	-0.0071	-
Isomer (3,3,0)				
Ti -$H_{(t)}$	0.105	0.0245	-0.0407	0.019
Ti -H_b	0.051	0.1436	-0.0054	0.027
Al -H_b	0.064	0.2019	-0.01758	0.069
c.c.p.	0.038	0.0824	-0.00879	-
r.c.p.	0.039	0.0808	-0.0076	-
Ti -$H_{(t)}$	0.105	0.025	-0.0407	0.021
Ti -H_b	0.050	0.1373	-0.0054	0.064
Ga -H_b	0.083	0.1083	-0.0360	0.073
c.c.p.	0.040	0.1190	-0.0068	-
r.c.p.	0.040	0.1185	-0.0067	-

Table V. Bonding properties, in a.u., of the bond critical points of the $(TiXH_6)^{-1}$, X=B, Al, Ga, at the B3LYP/A level of theory.

Bond	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$H(r_c)$	ε
		Isomer (3,2,1)		
Ti - B	0.103	0.0109	-0.0469	0.166
Ti -H_t	0.085	0.0500	-0.0283	0.038
Ti -H_t	0.083	0.0765	-0.0255	0.130
B -H_b	0.149	-0.1101	-0.1496	0.244
B -H_t	0.166	-0.1727	-0.1689	0.021
Ti -Al	0.042	0.0244	-0.0135	1.309
Ti - H_t	0.089	0.0577	-0.0297	0.052
Ti - H_t	0.091	0.0494	-0.0313	0.019
Ti - H_b	0.057	0.0529	-0.0080	0.264
Al - H_b	0.058	0.1564	-0.0166	0.058
Al - H_t	0.070	0.2222	-0.0197	0.027
r.c.p.	0.042	0.0419	-0.0121	-
Ti - Ga	0.048	0.0782	-0.0119	0.397
Ti - H_t	0.090	0.0572	-0.0314	0.044
Ti - H_t	0.091	0.0497	-0.0312	0.013
Ti - H_b	0.057	0.1443	-0.0086	0.243
Ga - H_b	0.073	0.0940	-0.0293	0.102
Ga - H_t	0.098	0.1247	-0.0455	0.013
		Isomer (2,2,2)		
Ti -H_t	0.079	0.0725	-0.0230	0.166
Ti -H_b	0.051	0.0690	-0.0106	4.071
Al -H_b	0.059	0.1342	-0.0185	0.421
Al -H_t	0.072	0.2433	-0.0195	0.005
r.c.p.	0.049	-0.0194	-0.0184	-
Ti - Ga	0.059	0.0138	-0.0215	0.707
Ti - H_t	0.079	0.0728	-0.0233	0.154
Ti - H_b	0.053	0.1505	-0.0081	2.102
Ga - H_b	0.069	0.0552	-0.0267	0.262
Ga - H_t	0.101	0.1435	-0.0472	0.029
r.c.p.				
		Isomer (2,2,2) Ti planar		
Ti-H_t	0.084	0.0511	-0.0274	0.116
Ti-H_b	0.039	0.0857	-0.0040	0.493
Al-H_b	0.063	0.2170	-0.0151	0.121
Al-H_t	0.073	0.2503	-0.0200	0.007
r.c.p.	0.028	0.0575	-0.0021	-

Bond	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$H(r_c)$	ε
Isomer (3,3,0)				
Ti -H_t	0.092	0.0515	-0.0317	0.012
Ti -H_b	0.066	0.1374	-0.0134	0.073
Al -H_b	0.049	0.1484	-0.0116	0.247
c.c.p.	0.040	0.0721	-0.0074	-
Isomer (3,3,0)				
Ti - H_t	0.092	0.0509	-0.0314	0.008
Ti - H_b	0.065	0.1288	-0.0135	0.108
Ga - H_b	0.070	0.0925	-0.0217	0.126
c.c.p.	0.036	0.0814	-0.0055	-
Isomer (3,0,3)				
Ti-Al	0.045	-0.0296	-0.0199	0.000
Ti-H	0.089	0.0579	-0.0298	0.062
Al-H	0.068	0.2302	-0.0179	0.045
Ti-Ga	0.055	-0.0114	-0.0187	0.000
Ti-H	0.090	0.0563	-0.0302	0.043
Ga-H	0.096	0.1398	-0.0443	0.049