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$(Al_{16}Ti)^{n\pm}$ (*n*=0-3)离子团簇中 Ti 原子对电子结构及其与 H_2O 分子相互作用的显著影响

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A Dramatic Influence of Ti Atom on the Electronic Structures of $(Al_{16}Ti)^{n\pm}$ (n=0−3) Ionic Clusters and Their Interaction with H_2O Molecules

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表 S1　$(Al_{16}Ti)^n$ (n= -3 – 3)离子团簇最稳定结构的笛卡尔坐标和振动频率

Table S1　Cartesian coordinates and vibrational frequencies of the $(Al_{16}Ti)^n$ (n= -3 – 3) clusters

		Coordinates /Å			Vibrational frequencies/cm^{-1}		
		X	Y	Z			
$(Al_{16}Ti)^{3-}$	Al	-0.624	0.977	4.146			
	Al	1.702	-2.122	0.279	46.5	163.6	222.5
	Al	1.949	-0.370	-1.838	72.3	168.0	230.9
	Al	0.015	0.035	-0.015	73.3	170.8	236.7
	Al	-1.612	2.125	-0.293	93.7	176.9	243.6
	Al	1.392	1.543	-3.738	105.9	186.5	248.9
	Al	0.813	-0.517	2.455	112.6	188.9	254.4
	Al	-1.845	0.398	1.837	116.3	191.4	263.2
	Al	0.572	-1.117	-4.151	130.8	194.8	272.2
	Al	-0.872	0.598	-2.488	134.6	197.0	275.6
	Al	1.036	2.283	-1.049	135.3	198.3	297.4
	Al	-1.426	-1.640	3.730	143.0	199.5	306.6
	Al	-2.561	-0.652	-0.702	144.2	201.7	313.7
	Al	2.502	0.698	0.661	147.3	212.3	353.2
	Al	-0.340	-2.100	-1.670	152.5	216.8	373.6
	Al	-1.023	-2.237	1.096	161.7	219.9	380.6
	Ti	0.321	2.098	1.741			
$(Al_{16}Ti)^{2-}$	Al	-0.635	0.941	4.149			
	Al	1.656	-2.095	0.280	49.8	168.5	231.7
	Al	1.952	-0.369	-1.816	71.6	179.5	242.6
	Al	0.020	0.050	-0.011	75.6	184.2	247.2
	Al	-1.604	2.103	-0.318	96.9	190.1	252.2
	Al	1.381	1.513	-3.727	112.8	190.8	252.7
	Al	0.829	-0.507	2.440	113.4	194.6	258.3
	Al	-1.846	0.414	1.821	115.0	195.7	277.2
	Al	0.578	-1.101	-4.119	132.9	203.8	282.3
	Al	-0.880	0.600	-2.472	138.2	204.4	288.3
	Al	1.030	2.298	-1.048	141.0	207.8	313.9
	Al	-1.406	-1.606	3.685	145.4	210.8	315.3
	Al	-2.512	-0.663	-0.681	149.2	211.9	325.2
	Al	2.493	0.697	0.630	152.2	218.2	357.5
	Al	-0.340	-2.116	-1.673	158.8	224.4	387.0
	Al	-1.027	-2.248	1.099	164.7	226.8	393.5
	Ti	0.311	2.089	1.763			
$(Al_{16}Ti)^{-}$	Al	-0.636	0.927	4.147	62.7	168.9	239.2
	Al	1.635	-2.082	0.280	72.5	185.0	251.5

	Al	1.957	-0.372	-1.792	76.2	188.1	252.3
	Al	0.020	0.055	-0.004	97.2	190.6	254.4
	Al	-1.600	2.099	-0.331	105.8	194.3	260.1
	Al	1.369	1.485	-3.718	116.8	195.7	261.2
	Al	0.861	-0.515	2.428	119.8	201.0	288.6
	Al	-1.865	0.429	1.798	123.5	206.3	289.1
	Al	0.572	-1.081	-4.070	129.8	211.5	296.3
	Al	-0.896	0.606	-2.452	142.1	213.7	320.8
	Al	1.031	2.301	-1.044	147.1	216.3	327.3
	Al	-1.381	-1.563	3.634	149.6	218.7	334.7
	Al	-2.492	-0.660	-0.669	157.5	222.9	359.5
	Al	2.495	0.692	0.615	165.6	228.3	389.8
	Al	-0.349	-2.132	-1.672	166.9	229.6	402.6
	Al	-1.032	-2.268	1.079			
	Ti	0.311	2.078	1.771			
$Al_{16}Ti$	Al	-0.635	0.939	4.143			
	Al	1.643	-2.093	0.276	68.1	167.4	242.1
	Al	1.983	-0.376	-1.760	76.6	187.1	253.2
	Al	0.011	0.039	0.010	78.4	189.1	254.7
	Al	-1.594	2.116	-0.332	89.8	190.9	256.9
	Al	1.367	1.472	-3.706	94.9	196.0	267.8
	Al	0.938	-0.536	2.427	109.6	196.8	273.5
	Al	-1.934	0.456	1.763	113.8	201.4	292.1
	Al	0.555	-1.053	-3.971	116.3	209.0	292.7
	Al	-0.930	0.628	-2.433	120.0	211.0	308.3
	Al	1.029	2.278	-1.056	139.1	211.5	324.2
	Al	-1.343	-1.504	3.559	150.0	214.5	338.2
	Al	-2.500	-0.664	-0.677	154.9	221.7	339.3
	Al	2.501	0.706	0.613	158.4	225.5	363.3
	Al	-0.361	-2.152	-1.659	164.6	229.0	380.8
	Al	-1.025	-2.298	1.025	166.4	236.6	396.3
	Ti	0.295	2.041	1.778			
$(Al_{16}Ti)^+$	Al	-0.629	0.959	4.130	62.5	165.5	243.5
	Al	1.659	-2.105	0.278	66.2	178.4	254.1
	Al	2.032	-0.390	-1.732	74.6	187.7	255.7
	Al	0.002	0.017	0.013	82.0	191.2	259.5
	Al	-1.594	2.137	-0.329	87.7	191.6	270.7
	Al	1.367	1.482	-3.690	96.5	196.7	282.9
	Al	1.008	-0.555	2.429	106.9	203.4	293.2
	Al	-1.997	0.479	1.731	114.9	203.8	294.1
	Al	0.538	-1.026	-3.873	117.6	207.8	318.3
	Al	-0.982	0.654	-2.427	135.0	210.1	325.4
	Al	1.028	2.259	-1.066	139.7	214.5	339.5

	Al	-1.315	-1.468	3.500	156.2	221.0	344.8
	Al	-2.518	-0.669	-0.688	156.5	224.6	364.9
	Al	2.512	0.718	0.619	161.0	226.1	368.4
	Al	-0.374	-2.184	-1.641	162.5	239.1	383.0
	Al	-1.025	-2.326	0.987			
	Ti	0.290	2.016	1.760			
$(Al_{16}Ti)^{2+}$	Al	-0.612	0.884	3.978			
	Al	1.604	-2.110	0.474	35.4	160.4	243.3
	Al	1.992	-0.487	-1.643	56.3	163.4	255.9
	Al	-0.086	-0.050	0.307	58.9	166.4	259.2
	Al	-1.595	2.190	-0.344	77.7	171.1	271.7
	Al	1.340	1.474	-3.588	89.0	181.1	272.8
	Al	1.304	-0.351	2.600	102.6	182.2	288.0
	Al	-2.150	0.830	1.806	111.7	192.0	307.0
	Al	0.543	-1.019	-3.885	115.6	192.7	307.6
	Al	-1.046	0.569	-2.349	116.4	197.5	324.3
	Al	0.991	2.171	-1.062	124.5	202.7	337.6
	Al	-1.177	-1.509	2.898	140.1	208.7	343.1
	Al	-2.558	-0.667	-0.491	146.1	215.6	345.6
	Al	2.550	0.768	0.606	150.6	218.7	354.5
	Al	-0.346	-2.106	-1.681	154.4	233.8	367.8
	Al	-1.112	-2.763	0.669	159.9	236.6	401.4
	Ti	0.358	2.175	1.703			
$(Al_{16}Ti)^{3+}$	Al	-0.619	0.838	3.911			
	Al	1.627	-2.103	0.518	27.5	152.5	237.5
	Al	2.017	-0.518	-1.622	42.6	156.3	257.2
	Al	-0.097	-0.049	0.362	60.4	159.6	259.9
	Al	-1.602	2.231	-0.352	71.2	164.1	270.2
	Al	1.360	1.499	-3.630	82.7	168.3	273.2
	Al	1.371	-0.331	2.611	85.6	172.9	278.4
	Al	-2.197	0.880	1.786	104.4	178.6	302.5
	Al	0.534	-1.003	-3.850	107.3	182.8	304.8
	Al	-1.097	0.569	-2.347	111.7	192.5	320.4
	Al	0.996	2.152	-1.082	119.9	199.4	338.8
	Al	-1.172	-1.543	2.850	130.3	204.4	339.4
	Al	-2.584	-0.647	-0.458	139.1	204.7	344.3
	Al	2.584	0.789	0.610	140.6	217.4	348.4
	Al	-0.363	-2.114	-1.651	145.7	228.8	362.4
	Al	-1.127	-2.858	0.667	149.8	230.5	402.5
	Ti	0.369	2.209	1.677			

表 S2　$(Al_{16}TiH_2O)^n$ (n= -3–3)吸附体系稳定结构的笛卡尔坐标和振动频率

Table S2　Cartesian coordinates and vibrational frequencies of the $(Al_{16}TiH_2O)^n$ (n= -3–3) adsorption systems

		Coordinates /Å			Vibrational frequencies /(cm^{-1})		
		X	Y	Z			
-3A	Al	-0.864	-0.434	4.364			
	Al	1.051	-2.761	-0.170	49.9	166.1	247.9
	Al	1.916	-0.641	-1.706	55.0	173.6	251.2
	Al	-0.043	-0.255	0.115	68.4	177.2	256.8
	Al	-1.117	2.165	0.393	75.0	179.0	266.2
	Al	1.994	1.770	-3.039	88.5	187.4	272.4
	Al	0.325	-1.653	2.324	96.3	191.0	276.8
	Al	-1.916	0.094	1.964	107.4	192.2	298.4
	Al	0.636	-0.411	-4.191	113.6	193.3	306.7
	Al	-0.519	1.121	-2.139	122.0	194.3	321.1
	Al	1.545	1.857	-0.252	128.2	198.3	354.2
	Al	-2.280	-2.440	3.146	132.9	204.2	373.8
	Al	-2.640	-0.032	-0.791	135.5	207.4	380.3
	Al	2.460	-0.460	1.002	139.2	211.5	387.3
	Al	-0.710	-1.727	-2.083	144.7	221.6	635.2
	Al	-1.719	-2.376	0.486	146.3	225.6	718.7
	Ti	0.644	1.123	2.381	153.2	233.1	1533.0
	O	2.072	1.495	4.173	156.1	234.4	3053.7
	H	1.438	0.869	4.641	163.2	240.9	3311.1
	H	2.665	0.884	3.659			
-3B	Al	-1.096	1.699	3.690	20.8	163.7	238.4
	Al	1.648	-1.922	0.650	25.8	170.3	243.9
	Al	2.109	-0.544	-1.681	47.3	172.0	249.6
	Al	-0.018	0.102	-0.163	71.1	177.0	255.6
	Al	-1.641	2.057	-0.951	74.6	187.1	263.9
	Al	1.726	1.014	-3.918	91.2	190.2	266.1
	Al	0.519	-0.014	2.429	93.2	191.1	273.8
	Al	-2.068	0.717	1.403	104.1	195.4	277.5
	Al	0.996	-1.698	-3.969	110.7	197.3	298.4
	Al	-0.642	0.223	-2.777	117.9	198.4	307.9
	Al	1.064	2.180	-1.454	132.4	200.9	313.8
	Al	-1.829	-0.992	3.617	133.9	203.0	354.7
	Al	-2.497	-0.762	-0.989	135.3	212.2	375.3
	Al	2.372	0.946	0.637	142.5	218.1	379.8
	Al	-0.172	-2.283	-1.472	145.7	221.2	592.1
	Al	-1.138	-1.996	1.188	148.7	222.3	1647.3
	Ti	0.086	2.434	1.242	153.5	225.2	3494.8
	O	-2.763	0.420	6.982	161.5	231.7	3538.3

	H	-2.353	1.110	6.415			
	H	-2.710	-0.326	6.342			
-3C	Al	-0.910	2.038	3.858			
	Al	2.355	-1.045	0.710	16.7	166.7	245.5
	Al	2.073	0.122	-1.776	23.5	169.7	250.1
	Al	0.085	0.369	0.008	57.4	172.8	255.2
	Al	-2.107	1.731	-0.652	72.1	180.1	261.1
	Al	1.002	1.265	-4.040	74.2	188.1	265.0
	Al	0.990	0.736	2.476	85.8	190.2	270.5
	Al	-1.813	0.551	1.846	96.1	193.0	280.7
	Al	1.021	-1.527	-3.772	110.6	195.6	299.5
	Al	-0.897	0.033	-2.475	114.1	197.7	307.3
	Al	0.388	2.496	-1.583	118.0	200.6	315.6
	Al	-0.721	-0.699	4.139	133.6	202.3	321.5
	Al	-2.127	-1.214	-0.350	134.4	205.3	353.3
	Al	2.231	1.891	0.358	136.5	212.8	375.4
	Al	0.417	-2.107	-1.084	143.7	217.8	381.1
	Al	-0.200	-1.766	1.677	144.6	222.8	506.3
	Ti	-0.336	2.781	1.202	151.4	225.6	1658.2
	O	2.275	-3.356	4.256	155.0	231.3	3531.2
	H	1.420	-2.897	4.406	163.1	239.9	3625.1
	H	2.503	-3.003	3.372			
-2A	Al	-0.988	-0.019	4.515			
	Al	1.800	-1.927	0.283	39.0	178.6	252.9
	Al	1.851	0.124	-1.533	53.9	182.4	256.0
	Al	-0.119	-0.008	0.273	66.8	185.4	274.3
	Al	-1.992	1.840	0.233	78.7	190.4	282.5
	Al	1.094	2.201	-3.144	85.7	193.0	285.3
	Al	0.734	-0.830	2.639	98.8	195.3	291.8
	Al	-2.023	-0.241	2.071	110.0	197.2	304.3
	Al	0.603	-0.396	-3.983	116.2	202.8	313.6
	Al	-1.057	0.832	-2.107	125.3	205.6	316.1
	Al	0.630	2.469	-0.365	134.2	208.8	329.8
	Al	-1.305	-2.506	3.568	135.8	215.2	360.2
	Al	-2.515	-0.912	-0.597	139.3	215.6	387.2
	Al	2.244	0.810	1.094	143.5	219.9	395.8
	Al	-0.182	-1.884	-1.741	152.1	228.3	553.0
	Al	-0.838	-2.579	0.929	153.1	235.3	684.4
	Ti	-0.168	1.779	2.346	159.2	242.6	1534.9
	O	-1.186	3.360	3.635	160.7	246.2	3134.0
	H	-1.934	3.409	2.997	169.5	251.8	3497.5
	H	-1.431	2.607	4.250			
-2B	Al	0.637	0.718	3.879	12.5	164.7	242.6

	Al	1.973	-1.935	-0.656	20.5	170.1	247.4
	Al	1.618	-0.079	-2.630	52.7	177.9	252.7
	Al	0.226	0.117	-0.351	70.7	178.8	254.4
	Al	-1.500	2.094	-0.079	73.2	183.9	258.7
	Al	0.491	1.877	-4.176	74.7	190.2	279.2
	Al	1.674	-0.530	1.759	94.9	191.5	283.2
	Al	-1.114	0.252	1.918	110.0	195.3	288.1
	Al	-0.292	-0.747	-4.531	113.5	195.8	314.9
	Al	-1.325	0.769	-2.442	113.6	203.9	316.0
	Al	0.841	2.473	-1.451	131.7	205.7	325.8
	Al	-0.099	-1.858	3.431	135.7	209.1	359.1
	Al	-2.358	-0.702	-0.395	140.4	211.3	387.2
	Al	2.751	0.856	-0.332	141.8	214.0	394.6
	Al	-0.480	-1.957	-2.018	147.6	218.9	496.2
	Al	-0.397	-2.307	0.802	150.3	224.5	1643.7
	Ti	0.869	2.070	1.424	153.6	228.4	3581.9
	O	0.405	-1.341	7.221	159.7	232.9	3636.6
	H	0.162	-1.898	6.454			
	H	0.602	-0.507	6.751			
-2C	Al	-1.130	-0.157	4.021			
	Al	1.974	-2.038	0.021	7.2	164.6	245.8
	Al	2.099	0.025	-1.758	12.8	171.9	248.2
	Al	-0.009	-0.184	-0.122	53.8	179.4	252.8
	Al	-1.948	1.592	-0.293	71.9	184.5	254.7
	Al	1.350	2.071	-3.418	74.6	190.1	257.8
	Al	0.704	-0.992	2.286	82.2	191.9	281.7
	Al	-2.047	-0.452	1.532	96.3	195.9	284.3
	Al	1.056	-0.542	-4.272	111.9	196.1	288.9
	Al	-0.803	0.603	-2.555	114.0	203.0	315.1
	Al	0.657	2.337	-0.703	117.1	204.7	317.4
	Al	-1.385	-2.668	3.093	128.5	209.3	330.3
	Al	-2.305	-1.191	-1.155	132.3	212.8	359.8
	Al	2.247	0.754	0.865	140.4	213.9	387.5
	Al	0.163	-2.080	-2.109	141.5	218.9	395.0
	Al	-0.691	-2.778	0.509	145.0	224.7	472.4
	Ti	-0.246	1.557	1.950	149.8	227.7	1642.2
	O	-3.024	2.113	6.256	152.5	232.5	3462.5
	H	-3.678	1.994	5.548	158.3	242.4	3751.4
	H	-2.267	1.597	5.892			
-1A	Al	-0.801	0.040	4.535	52.4	178.4	260.3
	Al	1.861	-1.808	0.251	56.1	187.8	261.2
	Al	1.777	0.177	-1.591	66.0	189.3	277.3
	Al	-0.133	-0.012	0.271	77.6	193.8	285.6

	Al	-2.111	1.706	0.246	85.3	197.7	290.0
	Al	0.812	2.122	-3.252	99.9	199.9	299.7
	Al	0.880	-0.738	2.594	109.5	201.9	311.9
	Al	-1.963	-0.267	2.134	116.4	208.3	325.0
	Al	0.469	-0.483	-3.949	120.3	212.0	326.8
	Al	-1.216	0.690	-2.078	129.9	215.8	336.9
	Al	0.419	2.486	-0.465	130.6	218.0	362.1
	Al	-1.066	-2.421	3.629	138.2	223.2	391.9
	Al	-2.493	-1.073	-0.468	147.3	226.3	405.2
	Al	2.203	0.973	0.950	147.9	229.4	515.3
	Al	-0.158	-1.967	-1.687	157.5	240.4	597.9
	Al	-0.705	-2.615	0.999	164.2	247.8	1550.1
	Ti	-0.173	1.814	2.311	166.9	251.9	3279.7
	O	-1.074	3.425	3.588	170.3	256.2	3642.5
	H	-1.896	3.637	3.103			
	H	-1.332	2.758	4.279			
-1B	Al	-0.423	0.731	4.028			
	Al	1.527	-2.161	-0.103	7.6	168.3	252.1
	Al	1.829	-0.351	-2.091	24.6	169.9	253.1
	Al	0.008	0.063	-0.185	62.1	181.3	254.8
	Al	-1.517	2.203	-0.305	66.7	185.1	260.2
	Al	1.239	1.639	-3.878	71.8	188.9	262.4
	Al	0.933	-0.685	2.164	78.0	190.3	289.0
	Al	-1.767	0.412	1.727	98.0	194.2	290.9
	Al	0.290	-0.858	-4.324	103.8	196.1	297.0
	Al	-1.002	0.809	-2.541	106.4	202.6	321.1
	Al	1.082	2.312	-1.147	118.3	207.1	328.7
	Al	-1.291	-1.702	3.422	122.2	212.2	334.7
	Al	-2.565	-0.497	-0.754	124.5	214.0	352.0
	Al	2.540	0.539	0.342	130.1	218.1	361.7
	Al	-0.554	-2.003	-1.948	143.9	220.1	392.0
	Al	-1.098	-2.273	0.819	147.8	224.1	404.2
	Ti	0.485	1.964	1.683	150.0	228.9	1635.6
	O	2.024	-1.251	6.124	157.5	230.3	3650.1
	H	1.116	-1.387	5.792	165.6	239.2	3767.7
	H	2.397	-0.667	5.444			
-1C	Al	-0.790	0.981	4.085	7.5	166.4	250.8
	Al	1.551	-2.018	0.233	24.5	168.0	253.3
	Al	1.903	-0.294	-1.822	57.8	169.0	255.1
	Al	-0.058	0.117	-0.056	63.3	184.7	260.4
	Al	-1.674	2.161	-0.402	72.0	188.7	262.6
	Al	1.338	1.568	-3.746	76.0	190.3	288.3
	Al	0.751	-0.445	2.388	83.2	194.7	289.3

	Al	-1.977	0.475	1.715	97.7	195.7	296.3
	Al	0.554	-0.997	-4.123	106.7	201.3	321.1
	Al	-0.941	0.674	-2.516	116.8	206.2	327.1
	Al	0.969	2.369	-1.073	119.4	212.3	331.5
	Al	-1.496	-1.516	3.556	124.4	214.0	335.2
	Al	-2.552	-0.612	-0.761	130.2	218.2	359.8
	Al	2.406	0.760	0.601	143.0	219.4	389.9
	Al	-0.399	-2.065	-1.746	147.4	223.6	402.8
	Al	-1.114	-2.216	1.004	149.9	229.6	1629.8
	Ti	0.184	2.141	1.727	157.5	230.5	3660.3
	O	3.930	-2.585	3.308	163.9	239.4	3770.5
	H	3.020	-2.881	3.478			
	H	3.802	-1.965	2.567			
0A	Al	0.748	-0.071	4.092			
	Al	0.853	-2.851	-0.543	46.5	175.1	257.4
	Al	1.457	-1.022	-2.412	55.9	189.1	268.1
	Al	0.234	-0.255	-0.149	68.4	193.5	273.4
	Al	-0.383	2.291	0.165	77.8	195.2	288.2
	Al	1.321	1.274	-3.918	83.3	198.5	296.2
	Al	1.249	-1.598	1.882	90.9	202.1	310.7
	Al	-0.996	0.488	2.073	98.1	204.2	321.7
	Al	-0.513	-0.626	-4.281	111.0	207.2	332.4
	Al	-0.812	1.134	-2.199	115.0	213.1	338.5
	Al	1.870	1.576	-1.190	117.4	216.4	341.0
	Al	-0.993	-1.891	3.419	124.9	220.9	366.5
	Al	-2.405	0.225	-0.240	136.3	222.5	385.2
	Al	2.819	-0.750	-0.134	146.9	229.6	401.0
	Al	-1.313	-1.724	-1.908	152.7	232.8	404.1
	Al	-1.465	-2.188	0.817	159.4	235.5	490.4
	Ti	1.699	1.113	1.716	161.6	240.7	1580.9
	O	3.538	1.931	2.642	166.6	250.7	3613.7
	H	3.622	1.522	3.525	168.2	254.1	3730.5
	H	4.344	1.707	2.142			
0B	Al	0.032	0.697	4.373	46.1	170.0	261.9
	Al	1.664	-2.147	0.106	57.8	173.0	271.6
	Al	1.824	-0.327	-1.859	68.5	188.6	276.8
	Al	0.069	0.032	0.176	77.7	189.9	284.3
	Al	-1.502	2.164	0.120	80.4	191.2	289.4
	Al	0.987	1.625	-3.614	91.7	197.9	293.1
	Al	1.327	-0.697	2.401	98.0	200.9	319.7
	Al	-1.704	0.435	2.225	106.1	207.5	328.0
	Al	0.106	-0.882	-3.878	110.8	209.7	335.4
	Al	-1.141	0.766	-2.118	119.4	214.1	343.4

	Al	1.007	2.291	-0.926	128.0	217.6	367.9
	Al	-0.815	-1.668	3.727	135.5	222.6	371.5
	Al	-2.527	-0.551	-0.238	137.9	225.6	394.2
	Al	2.637	0.630	0.475	154.2	231.9	460.0
	Al	-0.585	-2.055	-1.540	155.4	238.9	562.8
	Al	-0.916	-2.324	1.160	159.0	243.6	1579.0
	Ti	0.593	1.910	1.989	164.1	249.5	3583.9
	O	-3.521	1.141	3.108	167.2	252.9	3703.2
	H	-3.837	1.898	2.575			
	H	-3.331	1.487	4.001			
0C	Al	-1.377	0.612	4.223			
	Al	1.451	-2.215	0.591	47.1	166.4	257.5
	Al	2.172	-0.382	-1.218	61.5	168.2	262.6
	Al	-0.101	-0.038	0.192	71.1	186.0	273.0
	Al	-1.533	2.126	-0.257	76.8	190.4	289.5
	Al	1.939	1.629	-3.102	81.7	193.3	293.5
	Al	0.415	-0.801	2.695	94.5	196.4	296.4
	Al	-2.282	0.331	1.620	99.9	198.4	311.9
	Al	1.143	-0.851	-3.682	106.4	201.5	325.0
	Al	-0.556	0.765	-2.311	110.8	209.1	339.5
	Al	1.184	2.234	-0.479	118.5	211.7	343.7
	Al	-2.048	-1.753	3.363	119.1	214.6	371.5
	Al	-2.511	-0.580	-0.974	126.5	218.4	381.6
	Al	2.271	0.508	1.290	140.6	222.9	396.0
	Al	-0.207	-2.069	-1.648	142.7	229.8	474.0
	Al	-1.329	-2.368	0.857	153.9	236.5	547.5
	Ti	-0.031	1.822	2.130	157.7	239.8	1596.0
	O	4.346	0.686	1.854	162.4	241.9	3580.3
	H	4.638	1.614	1.760	164.8	252.4	3700.3
	H	4.858	0.177	1.193			
1A	Al	-0.105	0.017	4.279	38.0	172.8	254.6
	Al	1.178	-2.695	-0.177	60.7	173.4	259.9
	Al	1.879	-0.805	-1.908	62.7	180.6	273.1
	Al	0.109	-0.229	0.066	64.3	192.1	283.4
	Al	-0.899	2.231	0.200	72.4	195.1	294.4
	Al	1.632	1.468	-3.459	85.7	196.1	298.6
	Al	1.039	-1.463	2.238	94.9	201.5	321.0
	Al	-1.618	0.401	2.000	100.0	202.2	332.8
	Al	0.214	-0.679	-4.061	105.2	208.8	335.9
	Al	-0.769	1.022	-2.172	108.1	210.0	344.1
	Al	1.607	1.836	-0.738	126.6	215.2	347.4
	Al	-1.422	-1.992	3.274	134.5	218.5	367.8
	Al	-2.525	-0.097	-0.514	140.7	219.6	371.0

	Al	2.727	-0.269	0.550	153.7	227.9	391.0
	Al	-0.869	-1.888	-1.918	155.7	234.2	439.4
	Al	-1.466	-2.388	0.662	159.0	239.0	1592.6
	Ti	1.007	1.341	2.125	160.6	242.9	3676.9
	O	2.022	3.008	3.092	164.2	253.5	3784.6
	H	2.023	3.169	4.051			
	H	2.525	3.722	2.664			
1B	Al	-1.437	1.141	4.072			
	Al	1.294	-2.291	0.466	31.8	166.2	274.7
	Al	2.784	-0.395	-0.955	50.7	171.3	277.5
	Al	-0.070	-0.101	-0.020	58.6	173.4	288.0
	Al	-1.428	2.244	-0.479	65.5	186.4	302.6
	Al	1.994	1.031	-3.192	76.0	188.5	309.4
	Al	0.296	-0.622	2.682	86.2	197.9	314.0
	Al	-2.348	0.595	1.456	88.9	198.9	326.8
	Al	0.988	-1.462	-2.468	96.5	206.1	338.4
	Al	-0.568	0.815	-2.533	98.6	208.9	344.9
	Al	1.288	2.080	-0.724	109.0	215.3	346.0
	Al	-2.243	-1.242	3.484	113.3	218.7	364.6
	Al	-2.539	-0.349	-1.036	121.9	224.5	374.5
	Al	2.240	0.557	1.369	126.6	225.1	380.5
	Al	-1.022	-2.507	-1.325	130.4	237.5	394.5
	Al	-1.371	-2.282	1.250	143.7	242.3	580.3
	Ti	-0.039	1.930	1.868	145.8	247.8	1598.1
	O	4.745	-0.885	-1.287	151.2	253.0	3613.0
	H	5.427	-0.635	-0.634	152.3	266.8	3725.8
	H	5.101	-0.700	-2.177			
1C	Al	-0.656	0.930	3.988	44.0	167.8	270.9
	Al	1.579	-2.064	0.479	48.2	170.3	279.9
	Al	1.922	-0.459	-1.703	59.9	173.3	288.8
	Al	-0.090	-0.042	0.247	66.4	176.4	299.8
	Al	-1.623	2.148	-0.373	81.5	182.7	305.6
	Al	1.311	1.435	-3.634	86.6	188.7	318.6
	Al	1.355	-0.266	2.654	93.5	193.9	328.2
	Al	-2.124	0.752	1.783	101.7	202.0	335.3
	Al	0.528	-1.057	-3.988	103.7	203.9	340.2
	Al	-1.015	0.547	-2.405	117.3	206.7	348.8
	Al	0.939	2.162	-1.102	126.9	211.4	356.5
	Al	-1.032	-1.488	2.892	132.1	222.7	368.3
	Al	-2.553	-0.641	-0.587	139.1	229.3	381.8
	Al	2.508	0.768	0.542	143.6	237.9	395.6
	Al	-0.290	-2.120	-1.718	148.4	242.2	558.5
	Al	-1.175	-2.668	0.625	156.2	243.2	1590.1

	Ti	0.332	2.133	1.715	158.8	251.5	3613.8
	O	2.752	-0.682	4.109	165.6	260.8	3728.6
	H	2.591	-0.335	5.008			
	H	3.696	-0.543	3.901			
2A	Al	-0.148	0.118	4.093			
	Al	1.141	-2.694	0.065	29.0	161.5	273.5
	Al	1.887	-0.900	-1.792	43.0	165.2	277.0
	Al	0.009	-0.298	0.342	55.3	166.3	288.6
	Al	-0.916	2.307	0.130	57.1	171.5	289.8
	Al	1.679	1.436	-3.362	64.0	177.2	306.4
	Al	1.346	-1.312	2.444	75.3	182.2	312.3
	Al	-1.724	0.806	2.080	91.1	189.1	325.0
	Al	0.279	-0.718	-3.992	105.1	195.6	331.3
	Al	-0.822	0.957	-2.137	109.4	196.1	341.8
	Al	1.551	1.789	-0.742	115.6	205.1	346.3
	Al	-1.351	-1.841	2.751	117.0	210.9	358.2
	Al	-2.547	-0.154	-0.393	125.8	217.3	371.8
	Al	2.773	-0.188	0.585	143.4	220.1	374.1
	Al	-0.785	-1.875	-1.908	145.6	236.3	404.3
	Al	-1.651	-2.682	0.363	149.8	239.2	478.1
	Ti	1.071	1.550	2.037	153.1	244.4	1622.7
	O	2.021	3.218	3.036	156.1	257.2	3661.7
	H	2.031	3.381	3.997	159.0	261.0	3758.4
	H	2.523	3.941	2.618			
2B	Al	-0.093	1.418	3.946			
	Al	2.004	-1.819	0.247	40.5	174.1	258.3
	Al	2.059	-0.294	-1.937	63.7	184.8	259.9
	Al	0.148	0.132	-0.026	71.5	187.9	272.0
	Al	-1.679	2.090	-0.382	74.0	190.4	282.3
	Al	0.979	1.355	-3.994	76.7	194.9	287.0
	Al	1.462	-0.122	2.291	88.4	196.7	296.4
	Al	-1.698	0.647	1.858	93.0	201.5	307.3
	Al	0.374	-1.237	-3.795	98.8	207.7	332.0
	Al	-1.181	0.442	-2.393	114.9	209.7	336.2
	Al	0.824	2.325	-1.441	118.8	211.8	343.9
	Al	-0.683	-1.121	3.688	122.7	218.7	358.0
	Al	-2.380	-0.766	-0.357	130.4	222.2	365.8
	Al	2.654	1.120	0.219	146.8	224.4	377.9
	Al	-0.187	-2.250	-1.392	151.2	228.3	432.9
	Al	-0.591	-2.161	1.270	154.3	231.0	568.9
	Ti	0.491	2.358	1.425	158.5	238.9	1612.6
	O	-1.195	-2.253	5.245	160.6	249.1	3609.0
	H	-1.252	-1.942	6.171	164.1	256.3	3714.3

	H	-1.412	-3.206	5.222			
2C	Al	-0.584	1.506	3.864			
	Al	1.860	-1.588	0.985	28.7	163.0	266.6
	Al	2.085	-0.321	-1.435	64.8	166.7	276.2
	Al	0.034	0.269	0.464	67.4	170.0	279.7
	Al	-1.770	2.113	-0.526	71.4	175.1	296.9
	Al	1.114	1.153	-3.657	86.8	182.5	316.3
	Al	1.529	0.550	2.709	88.9	185.8	317.6
	Al	-2.143	1.108	1.835	95.5	190.9	330.3
	Al	0.690	-1.426	-3.508	106.7	197.9	339.2
	Al	-1.084	0.160	-2.159	110.0	199.2	346.7
	Al	0.781	2.292	-1.320	112.1	207.4	354.6
	Al	-0.758	-1.000	2.983	116.1	210.4	359.8
	Al	-2.271	-0.975	0.036	125.0	221.8	376.3
	Al	2.538	1.424	0.495	141.5	224.1	400.2
	Al	0.023	-2.170	-1.104	142.5	228.8	431.6
	Al	-0.605	-2.875	1.280	147.2	231.7	574.7
	Ti	0.189	2.725	1.406	149.7	237.9	1616.7
	O	-0.983	-4.784	1.716	155.9	249.3	3620.1
	H	-1.226	-5.116	2.603	157.5	261.0	3724.6
	H	-0.906	-5.546	1.109			
3A	Al	-0.872	0.676	2.780			
	Al	1.246	-2.643	0.810	24.3	153.7	267.9
	Al	1.832	-0.695	-2.028	46.8	158.6	279.2
	Al	0.004	-0.235	0.266	52.9	162.9	284.8
	Al	-0.731	2.450	0.700	63.3	170.7	288.0
	Al	0.967	1.647	-3.526	80.3	172.0	300.8
	Al	1.531	-0.889	2.838	83.6	178.2	305.4
	Al	-2.632	0.505	0.662	88.7	181.6	313.1
	Al	-0.485	-0.505	-3.409	97.1	188.8	317.8
	Al	-1.204	1.540	-1.717	102.0	198.4	323.6
	Al	1.536	1.814	-0.903	109.4	203.7	331.9
	Al	-0.869	-1.988	3.160	119.6	209.4	338.2
	Al	-2.304	-0.998	-1.455	127.9	216.1	345.4
	Al	2.750	-0.316	0.405	130.3	217.9	393.5
	Al	-0.034	-2.557	-1.501	134.1	229.7	395.4
	Al	-1.713	-2.423	0.710	140.7	245.4	526.1
	Ti	1.537	1.627	1.900	142.1	249.0	1641.8
	O	2.587	3.080	3.061	146.8	258.8	3626.6
	H	2.195	3.847	3.526	151.6	263.5	3713.0
	H	3.540	3.087	3.278			
3B	Al	-0.279	0.744	3.898	6.4	160.1	272.7
	Al	1.710	-2.123	0.414	57.0	164.1	276.1

	Al	1.927	-0.531	-1.761	64.9	168.0	285.0
	Al	0.014	-0.035	0.380	68.9	173.5	303.5
	Al	-1.479	2.267	-0.235	73.8	176.5	317.7
	Al	1.144	1.497	-3.762	82.5	178.3	320.1
	Al	1.631	-0.321	2.519	87.3	184.1	324.5
	Al	-1.960	0.982	1.947	91.5	187.4	338.4
	Al	0.320	-0.987	-3.901	107.9	193.2	344.2
	Al	-1.171	0.570	-2.223	116.3	196.2	354.1
	Al	1.028	2.105	-1.166	124.0	209.4	356.4
	Al	-0.980	-1.535	2.765	125.7	210.7	370.8
	Al	-2.513	-0.668	-0.195	132.1	224.4	409.6
	Al	2.703	0.757	0.429	135.9	229.7	474.8
	Al	-0.444	-2.082	-1.638	142.3	234.8	626.6
	Al	-0.955	-2.965	0.687	145.7	240.1	1639.2
	Ti	0.614	2.205	1.661	152.7	262.4	3592.1
	O	-0.514	0.941	5.836	154.6	265.8	3683.6
	H	-1.329	1.237	6.293			
	H	0.165	0.758	6.519			
3C	Al	-0.583	1.145	3.818			
	Al	1.731	-1.807	0.877	31.0	162.2	273.4
	Al	2.058	-0.422	-1.467	59.0	165.1	280.1
	Al	0.002	0.211	0.464	70.5	170.3	295.5
	Al	-1.709	2.197	-0.491	74.0	174.3	312.0
	Al	1.244	1.252	-3.680	86.5	184.2	318.5
	Al	1.551	0.256	2.702	90.0	186.9	323.1
	Al	-2.205	1.063	1.811	92.8	189.7	338.2
	Al	0.658	-1.309	-3.615	95.9	197.2	344.0
	Al	-1.095	0.275	-2.198	103.4	201.8	351.5
	Al	0.895	2.232	-1.260	105.5	208.6	353.2
	Al	-0.868	-1.262	2.751	112.7	210.2	360.3
	Al	-2.332	-0.909	-0.097	121.3	221.8	376.0
	Al	2.564	1.216	0.566	135.1	229.9	393.7
	Al	-0.113	-2.163	-1.241	138.1	231.7	469.1
	Al	-0.851	-3.123	1.025	141.4	237.3	628.5
	Ti	0.289	2.590	1.510	146.7	248.5	1633.8
	O	-1.344	-4.993	1.341	149.0	255.7	3557.2
	H	-1.650	-5.363	2.199	156.7	262.8	3647.3
	H	-1.314	-5.727	0.688			