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Chem. Mater., 1996, 8(1), 189-196, DOI:10.1021/cm950314z

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I-196-M1

2

12

Ti	.0037226221	-.0034415729	-.0446697321
N	-1.5781281879	1.0101687816	-.0808798625
C	-2.9585030505	.5605003537	-.2930182192
N	1.5913044146	1.0204293905	.0589516128
H	-3.3991030930	1.0231708306	-1.1890307920
H	-3.5943983198	.7953718821	.5737227143
H	.0470174819	-1.0486032461	-1.3979702974
H	-.0550794515	-1.1403415653	1.2331062477
H	-2.9772314489	-.5278942624	-.4364588218
H	2.5044403810	.6135413914	.2473687885
H	-1.5431464252	2.0142505509	.0725187765
H	1.7048330772	2.0212574657	-.0720404147

2'

12

Ti	.0042746229	-.4747249538	.0121540466
N	1.5908542059	-.4612205942	1.0525725101
N	-1.5987592938	-.4437149896	1.0260580604
C	-.0048998278	1.0635349994	-1.3866853589
H	.0414806503	-1.8537604364	-1.0014425002
H	2.5266680751	-.5612085103	.6682727481
H	1.6637688031	-.3421022428	2.0582875807
H	-1.7786115765	-.9662299249	1.8784944184
H	-2.4413720627	.0654435288	.7739695391
H	-.8867290355	.9657120324	-2.0450723163
H	.8942147771	1.0314941015	-2.0255158111
H	-.0422834452	2.0547166397	-.9034125643

2‡

12

Ti	-.3122920731	-.8718428096	.5303072336
N	1.3156004098	-.6883049635	-.0854741706
C	.8483348313	1.1379428937	.1990746618
N	-1.8630785046	-.8459946602	-.6275643533
H	1.8666496293	1.3994318441	-.0907045138
H	.6775485447	1.4689069167	1.2301629207
H	.9446805049	-2.0143083032	-.0116221065
H	-.5867671456	-1.0106997223	2.2842241937
H	.1363357748	1.5857948405	-.4998884715
H	-2.8057951170	-.9860516489	-.2705755160
H	2.2543046757	-.6762033024	-.4502707656
H	-1.9238095300	-.7749000850	-1.6378611127

I-196-M2

3a

8

Ti	-1.3408423793	.2563860054	.0000000000
N	.3138883314	.2475831153	.0000000000
C	1.7554598914	.2463305561	.0000000000
H	-2.1286068695	.2570814374	1.5928105388
H	-2.1286068695	.2570814374	-1.5928105388
H	2.1454498530	.7552107362	-.8935798619
H	2.1454498530	.7552107362	.8935798619
H	2.1327841896	-.7868150240	.0000000000

3a-NH_3

12

Ti	.4396330295	.3493566300	-.0065657603
N	2.0365409586	-.1072113102	-.1633813337
N	.4423329639	2.3168541244	1.0412095552
C	3.3703944723	-.6089094707	-.3586630710
H	-.4750700961	-.6107115313	1.1855374171
H	-.3394341422	.8150461704	-1.5415552375
H	4.1002026013	-.0175359120	.2188953077
H	3.4518433630	-1.6566836285	-.0289399832
H	3.6620530159	-.5615749772	-1.4199843450
H	1.0338441717	2.9945024064	.5635721288
H	-.4786952262	2.7427464246	1.1297976664
H	.8143548884	2.2261210743	1.9850776556

3b

7

Ti	-.0251951969	-.0281425924	.0000000000
N	.0225845382	1.8911375692	.0000000000
N	1.4169354612	-.8618997312	.0000000000
H	.8304321161	2.5055966656	.0000000000
H	-.8130845411	2.4718751534	.0000000000
H	-1.5359360948	-.9614851544	.0000000000
H	2.3122637174	-1.3340819103	.0000000000

3c

10

Ti	-.6902500088	.5797811285	.0000000000
N	.9715953600	.4779726680	.0000000000
N	-1.7078451505	-1.0595760044	.0000000000
C	2.4097889421	.4296497647	.0000000000
H	-1.4023938537	2.2147513687	.0000000000
H	-1.3639762174	-2.0143746465	.0000000000
H	-2.7251453234	-1.0966084888	.0000000000
H	2.7802957197	-.6074293011	.0000000000
H	2.8114147661	.9388957554	-.8896318137
H	2.8114147661	.9388957554	.8896318137

I-196-M3

3d

10

Ti	-.0822106720	-.1167632837	-.0554440267
N	-1.5864221321	-.0190096868	-.7708679889
N	.1418087384	.5729758295	1.7096512056
C	-.6897446457	1.2128863539	2.7318254674
H	1.2809274940	-.8106516329	-.9692377420
H	-2.4873633736	.0475730187	-1.2279797206
H	1.1036102040	.5113574425	2.0445546984
H	-.6253246367	.6819755732	3.6946006589
H	-1.7373547606	1.2028099532	2.4110670156
H	-.3929262157	2.2608464324	2.8978304324

3e

5

Ti	.0000000000	.0000000000	-.0279481644
N	.0000000000	.0000000000	1.6268262847
H	.0000000000	.0000000000	2.6402561173
H	-1.5767233533	.0000000000	-.8250770299
H	1.5767233533	.0000000000	-.8250770299

3e-NH_2Me

12

Ti	.2396147334	-1.4511604079	.0000000000
N	1.8494706297	-1.8979372019	.0000000000
N	.2285899585	.7620188942	.0000000000
C	-1.0932509342	1.4444510590	.0000000000
H	-.6151045436	-1.7621695719	-1.5272609567
H	-.6151045436	-1.7621695719	1.5272609567
H	2.7854554634	-2.2829667462	.0000000000
H	.7694373530	1.0670681102	-.8056826884
H	.7694373530	1.0670681102	.8056826884
H	-.9807153798	2.5363194394	.0000000000
H	-1.6498234291	1.1362475158	-.8904586403
H	-1.6498234291	1.1362475158	.8904586403

3a‡

12

Ti	-.0366817553	.2303333498	.0000000000
N	1.6926105623	.2453080930	.0000000000
C	3.0953339312	-.1043489626	.0000000000
N	.2210978149	2.3034102979	.0000000000
H	3.2254006426	-1.1951162956	.0000000000
H	-.6833702892	-.4558019998	-1.4583152082
H	-.6833702892	-.4558019998	1.4583152082
H	3.6004143154	.2995164247	-.8916023743
H	3.6004143154	.2995164247	.8916023743
H	1.3203253345	1.5541213734	.0000000000
H	.0670217086	2.8760121471	-.8258442971
H	.0670217086	2.8760121471	.8258442971

 I-196-my

3b‡

12			
Ti	-.5989615815	-.6611527135	-.2702973906
N	1.1095326951	-.9034627972	-.4304611756
C	1.1250878392	1.3517080821	-.5049106871
N	-1.3828380766	-1.1348208391	1.4170524852
H	1.0227250933	1.8330309216	.4660156599
H	.7798783611	1.9515580023	-1.3449876318
H	-1.5598011412	-1.0858073555	-1.6780227470
H	-.5492134425	1.0479173013	-.3880618715
H	2.1279149786	.9768191013	-.6755942395
H	-2.3833640043	-1.1292698295	1.5986210265
H	2.1001596586	-1.0659719270	-.5435296931
H	-.9123803799	-1.4935649466	2.2415352646

3b'‡

12			
Ti	-0.120758	-0.779526	-0.367523
N	1.605087	-0.652924	-0.367538
H	0.997665	0.605057	-0.367523
H	2.604568	-0.504623	-0.367508
C	-0.094986	1.523941	-0.367538
H	-0.859879	-1.290695	-1.777435
N	-0.969300	-1.366516	1.251129
H	-0.703979	1.690826	-1.266205
H	-0.703842	1.690704	0.531204
H	0.688263	2.295807	-0.367569
H	-0.509888	-1.532303	2.139969
H	-1.932953	-1.679733	1.326584

3c‡

12			
Ti	.1752000823	-.0215257800	.0287366692
N	1.8953204120	-.0642700819	-.0080925428
C	3.3384089755	-.0661232972	-.0394710222
N	-.6988355016	-.6224761012	1.6192015005
H	3.7628418985	.4934343589	.8086650451
H	3.7268423576	.3614099275	-.9764669568
H	-.6302641076	-.4105247839	-1.4745271598
H	.5094589616	1.8063107333	.0059081273
H	3.6903300262	-1.1052874812	.0316950460
H	-1.7061356198	-.7522044897	1.6906719270
H	1.3607006547	1.3104651643	-.0093445793
H	-.2767591395	-.9282471690	2.4893149459

I-196-MS

3d‡

12

Ti	-.3410750546	.3617904740	-.7495159332
N	1.3716474641	.5410073326	-.8487187531
H	2.3614471810	.7411637986	-.9100764178
N	-1.0759877645	-.6507489519	.6698087230
H	-1.2319769436	.2282356746	-2.2486169679
H	-.1992913691	2.1771297439	-.3503331828
H	-2.0588349163	-.8813298677	.5220611208
H	.6897839040	1.8167052852	-.5072491871
C	-.5889574789	-1.3028638516	1.8866724131
H	-.5759020917	-2.3991248808	1.7841160055
H	-1.2160529431	-1.0465800785	2.7549279755
H	.4345970127	-.9710206783	2.0973892038

3e‡

12

Ti	.0509113789	-.0534301183	.0038049592
N	1.7842105425	.0580101066	.0939906718
H	2.7661552019	-.1765797742	.1474092541
N	.2063486937	2.0150620317	.0005654962
H	-.5209757261	-.7707544615	-1.4655682620
H	-.6608674261	-.7335072346	1.4271508047
H	1.3598899797	1.3378256441	.0704275389
C	-.0162186622	2.8806530993	-1.1697416584
H	-.0126916568	2.5028522151	.8648018225
H	.3099008676	2.3566548400	-2.0776541759
H	.5639039828	3.8112968762	-1.0914172495
H	-1.0781421759	3.1401237754	-1.2915022017

3e'‡

12

Ti	-.7357035553	-1.1650616842	-.0213605999
H	-1.7403101794	-2.3083296743	-.9027769311
H	-.8960636032	-1.3283327839	1.7234248157
C	.9872374546	.9264172067	.8514856891
H	1.3995198239	1.3821948067	-.0423158041
H	.3035865880	1.5066241584	1.4571252418
H	1.5627699820	.1601768625	1.3557575408
N	.9301110202	-1.1952421167	-.4384902636
N	-1.1493828478	.7603693004	-.2224046178
H	-.8949897470	1.3254024390	-1.0255477568
H	-1.9384190785	1.2015818998	.2455595415
H	1.8916441425	-1.3248004144	-.7244568558

I-196-M6

4‡

10

Ti	.8695684393	1.3471946887	.0029401985
N	-.6857195671	1.9346429947	-.5323123077
N	.4160149292	-.3201182570	.1713833765
C	-.0922063725	-1.6687438838	.2691515680
H	2.4241679347	2.1760608337	.2896213471
H	-1.6376070324	2.1038957975	-.8257604101
H	-.6153797305	.5346871923	-.2656885080
H	-.9274713175	-1.7291705216	.9849421768
H	.7006135183	-2.3477976991	.6128711113
H	-.4520568014	-2.0306051453	-.7071635524

5

12

N	-0.341812	-1.429993	-0.369202
C	0.660843	-2.203110	-0.436646
Ti	-0.528015	0.760818	0.188385
N	-0.460983	2.605713	0.593400
H	-1.208557	-1.893692	-0.626678
H	1.652206	-1.821457	-0.184586
H	0.570541	-3.252975	-0.741943
H	-1.652206	0.155746	1.343887
H	-1.320358	0.817810	-1.343903
H	1.190811	0.526932	0.401291
H	0.358398	3.108490	0.917709
H	-1.238388	3.252960	0.500397

5‡

12

Ti	0.496506	-0.235565	0.145874
N	1.829926	0.719391	1.086029
N	-1.538620	-0.940200	-0.221863
C	-2.018661	0.275558	-0.274933
H	1.168137	-0.508560	-1.396912
H	0.554321	-1.683777	1.066025
H	-0.519928	1.258347	0.224121
H	2.692932	0.274292	1.388809
H	1.825638	1.683792	1.396896
H	-1.833908	-1.422104	0.621033
H	-1.951843	0.830017	-1.209702
H	-2.692917	0.692993	0.480850

I-196-M7

H_3TiNH_2

7

Ti	-.0118027040	-.0159893195	-.0254591202
N	-.0879664639	.0820055074	1.8457887717
H	1.5988968297	.0758895563	-.5999364915
H	-.7349807992	-1.4551746367	-.5779926561
H	-.9446213629	1.2236751209	-.7278588196
H	.7154373095	.1697163436	2.4642212282
H	-.9355027955	.0562692848	2.4076397181

6a

8

Ti	.0640670344	-.0902141767	-.0813771961
C	-.5626954973	1.8700934381	-.0728153688
N	.8061922015	1.6674275769	-.2216924759
H	-.2650477913	-1.0227374532	-1.5556965124
H	.1225591332	-.7970330589	1.5520235552
H	-1.1178369493	2.1699735413	-.9672308177
H	-.9534068651	2.2827134860	.8650902517
H	1.3581687337	1.9587766466	.5816985640

6a-NH_3

12

Ti	-.6638238898	-.6101902754	-.1013157934
N	-1.8568115208	.8718892338	-.1040692496
C	-.5777454233	1.4471729232	-.1524439780
N	1.5827091136	-.8909396511	.0035704365
H	-.2963987909	1.9307728681	-1.0956623880
H	-.2002943241	1.9795460936	.7327946094
H	-.6898836925	-1.5816936386	-1.6013002194
H	-.7927254662	-1.3193410261	1.5402637727
H	2.0447265037	-.3690897287	.7439098411
H	-2.3908576345	1.0466929141	.7407741942
H	2.0400789312	-.6321178662	-.8678660848
H	1.8000261935	-1.8727018468	.1613448595

6b

10

Ti	.0395871978	-.1276924981	.1427605421
N	-.7563304698	-.0741760129	1.8705768173
N	.7370284874	1.5240440246	-.5622034097
C	-1.8321614576	.0040406360	.9624381872
H	.4399814587	-1.7272797729	-.5373431717
H	-2.3509518956	.9646978546	.9049575889
H	-2.4967677896	-.8630870349	.8540919525
H	-.7134684786	-.9415333277	2.4000848248
H	1.2048943625	1.6297396703	-1.4591146700
H	.7241885850	2.4332464610	-.1092486614

I-196-m8

6a‡

12

Ti	.0371844817	-.0387188410	.0000000000
N	-.1201881905	1.7655823857	.0000000000
C	1.3421446555	1.7591557210	.0000000000
N	1.9529930172	-.9147712460	.0000000000
H	1.7816744396	2.2101631515	-.9040730315
H	1.7816744396	2.2101631515	.9040730315
H	-.7544080848	-.6193159356	-1.4082366357
H	-.7544080848	-.6193159356	1.4082366357
H	1.9591104796	.3818785195	.0000000000
H	-.6463287609	2.6279022788	.0000000000
H	2.3321473039	-1.3693151249	-.8267926817
H	2.3321473039	-1.3693151249	.8267926817

6b‡

12

Ti	-.0114578225	-.0087987679	-.0497994035
N	-.1169682891	1.9259121846	.1767303322
C	1.2642383427	1.7753493589	.1594000083
N	-.8240677055	-.8263395484	1.4753648407
H	1.7764787879	1.9407720809	1.1116250567
H	1.8340011789	2.1352618032	-.7070031961
H	1.5963660163	-.7775978031	-.1741352922
H	-.5920156992	-.4208638319	-1.6543722500
H	1.7489877765	.2273047964	-.0113063836
H	-.8664705486	-1.8167304324	1.6963178309
H	-.4909084630	2.3955013412	-.6430290377
H	-1.3370285746	-.3097951813	2.1838364943

NH_3

4

N	.0000000000	.0000000000	.0556088225
H	-.4679257536	.8104711794	.4524505797
H	-.4679257536	-.8104711794	.4524505797
H	.9358515072	.0000000000	.4524505797

NH_2Me

N	-.0325060971	-.0026625858	.0000000000
C	1.4308334542	.1052638966	.0000000000
H	-.3299637955	-.5406100920	-.8068383252
H	-.3299637955	-.5406100920	.8068383252
H	1.7543030563	.6692784521	.8855748059
H	1.7543030563	.6692784521	-.8855748059
H	1.9609941214	-.8639380311	.0000000000

I-196-m9

H_2

2

H	.0000000000	.0000000000	-.3740413020
H	.0000000000	.0000000000	.3740413020

$HN{=}CH_2$

5

C	.0246658717	-.0124891662	.0000000000
N	1.2894373933	.0477289341	.0000000000
H	-.5582267712	.9170153889	.0000000000
H	-.5540033672	-.9502339548	.0000000000
H	1.6811268733	-.8920212020	.0000000000

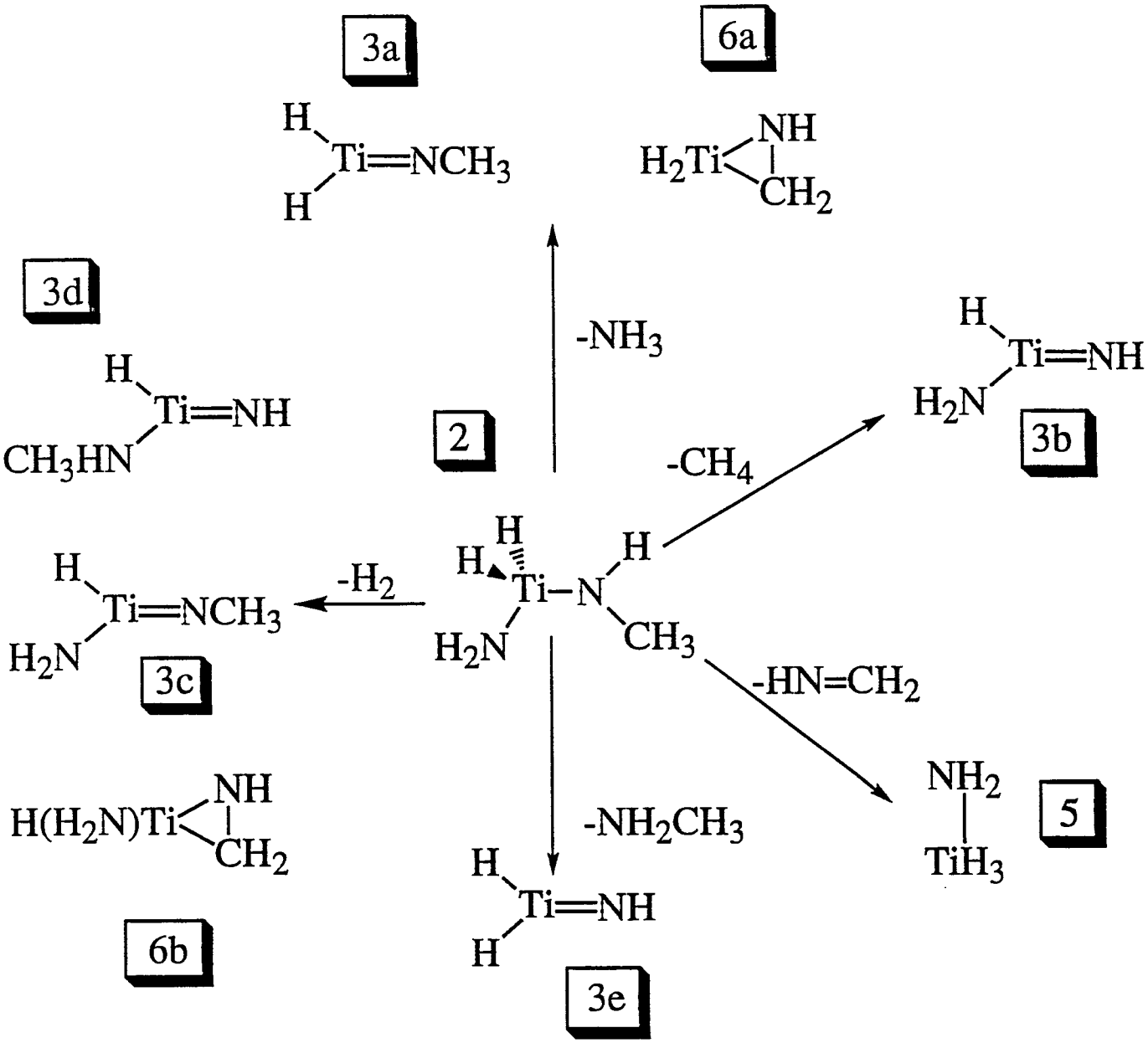
CH_4

5

C	.0000000000	.0000000000	.0000000000
H	.6345075036	-.6345075036	-.6345075036
H	-.6345075036	.6345075036	-.6345075036
H	-.6345075036	-.6345075036	.6345075036
H	.6345075036	.6345075036	.6345075036

x

I-196-M10



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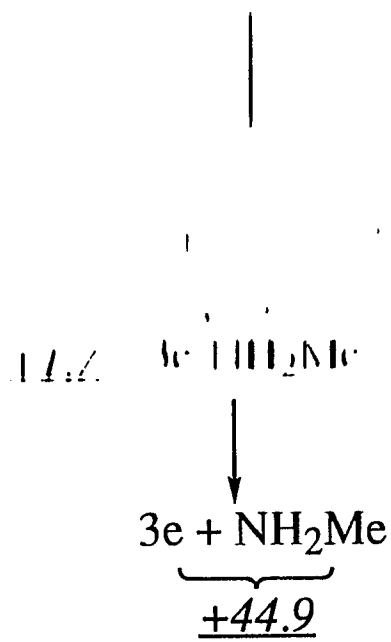
I-196-M11



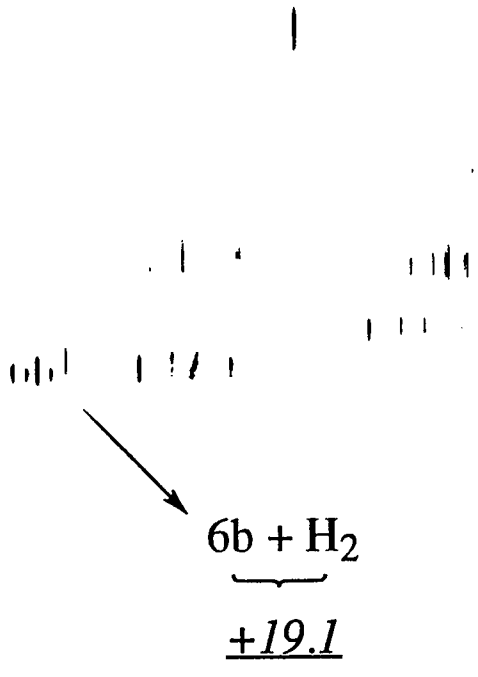


Figure 3

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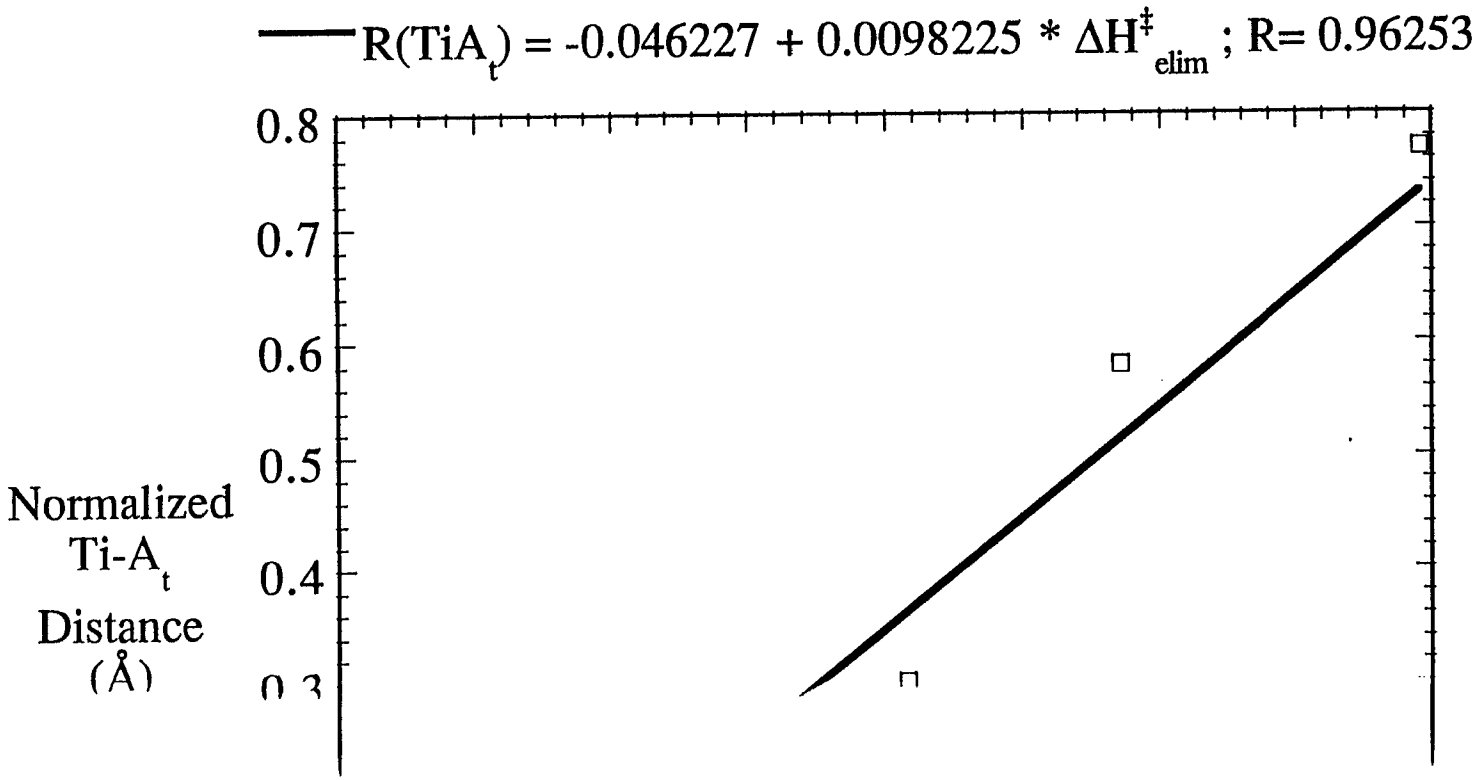
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