Supporting Information

for

Theoretical Elucidation of the Platinum-Mediated Arene C-H Activation Reactions

Ji-Lai Li,[†] Cai-Yun Geng,[†] Xu-Ri Huang,^{*,†} Xiang Zhang,[‡] and Chia-Chung Sun[†]

*State Key Laboratory of Theoretical and Computational Chemistry, Institute of Theoretical Chemistry,
Jilin UniVersity, Changchun 130023, People's Republic of China, and State Key Laboratory of Molecular
Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023,
People's Republic of China*

* Corresponding author

Fax: (+86) 431-8894-5942

E-mail: tcclab@gmail.com

The structures optimized at B1 basis set:

Aa

Pt	0.00000000	0.00000000	0.00000000
N	2.16113207	0.00000000	0.00000000
N	0.52220844	2.06323680	0.00000000
C	2.72487108	1.17959414	-0.02248494
C	1.79972678	2.34417546	-0.01641649
C	2.35981222	3.73804673	-0.03000034
C	4.20876296	1.41374848	-0.04831860
C	2.94742895	-1.21695004	-0.03449000
C	3.21361188	-1.88485667	1.17908213
C	3.93505745	-3.08678438	1.11857478
C	4.36975844	-3.60660896	-0.10308302
C	4.09025991	-2.92624501	-1.29034269
C	3.37658103	-1.71759765	-1.28216105
C	3.08470036	-0.98778354	-2.57519825
C	2.75844746	-1.31975332	2.50470848
C	-0.48670062	3.10136451	0.06380353
C	-0.81560330	3.65439135	1.32061593
C	-1.83524384	4.61838867	1.36254811
C	-2.49808375	5.01809423	0.19993777
C	-2.15218031	4.45411408	-1.03034303
C	-1.14394405	3.48275119	-1.12476090
C	-0.76758506	2.88446977	-2.46001869
C	-0.10982501	3.22738710	2.58975480
C	-0.72220195	-2.62533297	1.36614688
C	-0.54917486	-3.98341143	1.63250183

C	-0.02988166	-4.82726548	0.64008721
C	0.30833623	-4.31497046	-0.62231279
C	0.14673820	-2.95663310	-0.88700614
C	-0.37991625	-2.05786517	0.09473574
C	-2.00774948	0.08956482	-0.05932094
C	-2.82589431	0.68276389	0.92009378
C	-4.19623790	0.40733757	0.97925256
C	-4.81029513	-0.48869919	0.07736907
C	-4.04708145	-1.08426142	-0.91325856
C	-2.64040962	-0.83964716	-0.97698430
H	1.57047461	4.48097553	-0.14313758
H	2.90073188	3.95284915	0.90047653
H	3.07628151	3.86134686	-0.84963569
H	4.50959531	2.09974458	0.75117008
H	4.75859595	0.48011586	0.06928882
H	4.51623842	1.87449778	-0.99581294
H	4.15571286	-3.61228803	2.04205626
H	4.92626768	-4.53726079	-0.12941561
H	4.42831667	-3.32946594	-2.23973421
H	3.27851510	-1.63609558	-3.43405700
H	3.71698828	-0.09786516	-2.69695774
H	2.04231213	-0.65195105	-2.62854455
H	2.97892441	-2.01729572	3.31693190
H	3.26082527	-0.37239107	2.74078151
H	1.68016163	-1.12222989	2.50694004
H	-2.10577502	5.05442284	2.31893487
H	-3.28182626	5.76595819	0.25254315
H	-2.66566466	4.76547779	-1.93412577
H	-1.43490973	3.24650211	-3.24637330
H	0.25777312	3.14629837	-2.75258142
H	-0.82564954	1.78974486	-2.43675865
H	-0.64497826	3.59803493	3.46809581
H	-0.03867422	2.13607977	2.67054141
H	0.91270817	3.62388907	2.64696338
H	-0.82208874	-4.38850802	2.60135584
H	0.09629157	-5.88583218	0.84369563
H	0.70163339	-4.97618871	-1.38706885
H	0.41050489	-2.57178347	-1.86741180
H	-1.73743336	-1.77276880	-0.38416329
H	-2.39176945	1.36105053	1.64496814
H	-4.80126549	0.88616300	1.74363135
H	-5.87375708	-0.68672243	0.15119651
H	-4.50918064	-1.73464105	-1.64962984
H	-2.15117376	-1.04606551	-1.93010941
H	-1.15690382	-1.98145595	2.12524378

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C	1.74975769	2.32060169	-0.00032623
C	2.25930073	3.73294934	0.00025421
C	4.19784832	1.49774159	-0.00276359
C	3.03515623	-1.19034576	-0.00072522
C	3.39737215	-1.76813946	1.23631108
C	4.12590490	-2.96783997	1.20831637
C	4.48479793	-3.56599324	-0.00198154
C	4.12492828	-2.96714538	-1.21166222
C	3.39640054	-1.76742348	-1.23840352
C	3.04228436	-1.10720985	-2.55372891
C	3.04469013	-1.10844388	2.55227361
C	-0.54230781	3.04998906	0.00148985
C	-1.01509909	3.52966523	1.23935323
C	-2.01044486	4.51805403	1.21361290
C	-2.50906353	5.00761229	0.00450550
C	-2.01226379	4.51993964	-1.20611438
C	-1.01695714	3.53158619	-1.23491207
C	-0.46957683	3.02542689	-2.54961032
C	-0.46601059	3.02121422	2.55247705
C	-0.17522755	-2.33916514	0.71344719
C	-1.36234494	-2.68116447	1.41207511
C	-2.50869249	-3.02140336	0.70876050
C	-2.50858748	-3.02364446	-0.70470603
C	-1.36218797	-2.68552068	-1.40899790
C	-0.17520081	-2.34141610	-0.71137138
C	-2.01355693	0.29398990	-0.00309572
C	-2.72540529	0.41132603	1.20370657
C	-4.10970665	0.63517107	1.20110785
C	-4.80444778	0.74534154	-0.00819134
C	-4.10613517	0.63013712	-1.21494804
C	-2.72182951	0.40624995	-1.21251234
H	1.44412778	4.45426189	-0.00132643
H	2.88478946	3.91748100	0.88194471
H	2.88804983	3.91705391	-0.87914760
H	4.47847379	2.08954837	0.87652376
H	4.78568891	0.57996550	-0.00166346
H	4.47700936	2.08637620	-0.88467501
H	4.41225032	-3.42970133	2.14762739
H	5.04503854	-4.49441571	-0.00247670
H	4.41049091	-3.42849765	-2.15146169
H	3.19586602	-1.79903094	-3.38605830

H	3.67044426	-0.22688393	-2.74637477
H	2.00020003	-0.76718759	-2.57938810
H	3.19725402	-1.80121060	3.38400867
H	3.67449600	-0.22940315	2.74544882
H	2.00324902	-0.76653166	2.57845974
H	-2.39425127	4.89993266	2.15388786
H	-3.28223858	5.76804938	0.00567884
H	-2.39746811	4.90330335	-2.14520863
H	-1.05760412	3.41451235	-3.38466111
H	0.57056754	3.33976883	-2.71114109
H	-0.49012353	1.93111226	-2.60234401
H	-1.05351430	3.40811550	3.38891466
H	-0.48555476	1.92675261	2.60297472
H	0.57403581	3.33606061	2.71366560
H	-1.35514479	-2.70634110	2.49626942
H	-3.41053618	-3.29889273	1.24303584
H	-3.41035059	-3.30286064	-1.23822287
H	-1.35494792	-2.71402909	-2.49310594
H	0.76462690	-2.31377979	-1.25066122
H	-2.20975118	0.32258328	2.15478861
H	-4.64097636	0.72207277	2.14435079
H	-5.87560107	0.91899987	-0.01014154
H	-4.63460564	0.71308872	-2.16011957
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Ba'

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C	0.00325324	2.42884498	0.01143232
C	-0.70067661	1.23354119	-0.01569368
Pt	0.75135111	-0.87936851	-2.18275217
C	0.73569066	-2.65302630	-1.17851849
C	-0.47102534	-3.31457838	-0.89164582
C	-0.46855773	-4.54531798	-0.21935253
C	0.73900846	-5.13222000	0.17518583
C	1.94609249	-4.48235116	-0.10596089
C	1.94527689	-3.24989256	-0.77621517
N	0.58742224	-1.78620560	-4.02589802
C	0.31602224	-3.20850715	-4.15853323
C	1.35350006	-4.12987588	-4.02324140
C	1.08147305	-5.50347781	-4.14772255
C	-0.23556006	-5.90849394	-4.40923071
C	-1.28715810	-4.98483382	-4.54441218

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C	-2.69746042	-5.45895467	-4.81538561
N	0.86552538	0.82500797	-3.63471882
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C	2.35000619	2.74755376	-3.24830869
C	2.54218693	4.12008474	-3.01635269
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C	0.10754898	4.43948394	-2.99571395
C	-0.06520744	3.06442187	-3.22472494
C	3.93756658	4.69932248	-2.93608204
C	-1.08857249	5.35992544	-2.89034759
C	0.63997121	-1.02976430	-5.09638152
C	0.52982347	-1.56088958	-6.49753336
C	0.82171570	0.42715570	-4.87896773
C	0.94235463	1.32839638	-6.07744660
H	1.88096263	1.13480545	-6.61266095
H	0.92695859	2.37872429	-5.79312134
H	0.12636040	1.14637630	-6.78474537
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H	1.29439569	-1.11295051	-7.13923754
H	0.63906842	-2.64380490	-6.52379419
H	2.35902517	-3.78797410	-3.80668650
H	-0.45020723	-6.96914357	-4.50489392
H	-1.79019670	-2.88194827	-4.50638348
H	1.89347234	-7.50272447	-4.33387290
H	2.44721888	-6.61929924	-2.90471684
H	3.10058050	-6.21704299	-4.49576540
H	-3.38750180	-4.61977680	-4.94349701
H	-3.07237606	-6.07564228	-3.98954682
H	-2.74371319	-6.07332226	-5.72224838
H	3.20368858	2.08449703	-3.34571521
H	1.55485243	6.00881515	-2.71046385
H	-1.06216142	2.64351387	-3.30396964
H	-2.01059121	4.80376407	-2.69541808
H	-1.23567195	5.92325826	-3.82093478
H	-0.95891042	6.09516305	-2.08887881
H	4.25333053	5.10183144	-3.90756319
H	4.67270358	3.94392713	-2.64157599
H	3.98807581	5.52206565	-2.21568393
H	-1.41862324	-2.88342671	-1.20231327
H	-1.41020114	-5.04147764	-0.00478688
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Pt	0.00000000	0.00000000	0.00000000
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C	1.91034359	2.37432780	0.06889421
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C	4.29615932	1.37940091	0.07780609
C	3.00088896	-1.23207937	0.00745137
C	3.48829625	-1.73632622	1.23249437
C	4.16715508	-2.96457247	1.20650326
C	4.35827433	-3.65892437	0.01038560
C	3.86626099	-3.13555573	-1.18760884
C	3.17208367	-1.91752943	-1.21398439
C	2.64620834	-1.35600421	-2.51445644
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C	-1.03626037	3.61490786	1.10380333
C	-1.98669274	4.64193779	1.00080499
C	-2.23004281	5.28298604	-0.21549278
C	-1.51417959	4.91133382	-1.35529252
C	-0.54415797	3.89881321	-1.30382896
C	0.21654397	3.51133085	-2.55457810
C	-0.79021998	2.93121286	2.42856843
C	-0.32197693	-2.00715384	-0.11599486
C	0.14837161	-2.90476275	0.85606335
C	0.00351533	-4.28501863	0.66553001
C	-0.60995941	-4.77862340	-0.49147581
C	-1.09280163	-3.88670776	-1.45500328
C	-0.97144527	-2.50382420	-1.26049310
C	-2.02120853	0.21058501	-0.04807305
C	-2.90407544	-0.40573446	0.85627874
C	-4.28610064	-0.23359380	0.71501543
C	-4.79982088	0.53533084	-0.33647549
C	-3.92610354	1.14077608	-1.24570665
C	-2.54043028	0.99285675	-1.09437013
H	1.78284239	4.50701533	0.32273802
H	3.25709503	3.77581472	0.99095467
H	3.08988074	3.98202915	-0.74982941
H	4.61941877	1.77757093	1.04799554

H	4.82720920	0.44429128	-0.09845192
H	4.60120673	2.10632143	-0.68206216
H	4.54401567	-3.37464753	2.13790371
H	4.88700724	-4.60569814	0.01177694
H	4.01539608	-3.67419977	-2.11749147
H	2.88360364	-2.02429091	-3.34594994
H	3.07685529	-0.37393563	-2.74776031
H	1.55458368	-1.24093143	-2.48912905
H	3.50840455	-1.66344808	3.38518134
H	3.94084635	-0.13037234	2.63716887
H	2.25273455	-0.65149716	2.65995747
H	-2.53884364	4.93392899	1.88787939
H	-2.97409925	6.06960001	-0.27483172
H	-1.70467584	5.40747053	-2.30147105
H	-0.26084569	3.94103932	-3.43899786
H	1.25191356	3.87690526	-2.54211807
H	0.25891332	2.42428336	-2.69606733
H	-1.33134355	3.44132534	3.22939780
H	-1.13610806	1.89022955	2.40713770
H	0.27177773	2.91916262	2.70181452
H	0.63623030	-2.54565420	1.75538561
H	0.37211974	-4.97090222	1.42152414
H	-0.72183716	-5.84807208	-0.63487104
H	-1.58506169	-4.25958412	-2.34742554
H	-1.39865665	-1.82758185	-1.99414865
H	-2.52527323	-1.03680427	1.65189901
H	-4.95971879	-0.71188545	1.41866029
H	-5.87174375	0.65991677	-0.44708756
H	-4.31519606	1.73639321	-2.06512836
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H	-0.17801261	-0.10868259	1.51680336

Da

Pt	0.00000000	0.00000000	0.00000000
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N	0.64176481	2.17193821	0.00000000
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C	2.56049770	3.74311947	-0.02625364
C	4.31867291	1.40673184	-0.00687334
C	3.06286737	-1.21729796	0.00359245
C	3.15100072	-1.95329713	1.20754183
C	3.86718627	-3.15854501	1.18840455
C	4.46171567	-3.63033232	0.01630097
C	4.36589628	-2.88493553	-1.15899527
C	3.67761426	-1.66138685	-1.19001404

C	3.63654845	-0.86664122	-2.47834922
C	2.52315514	-1.46734865	2.49275433
C	-0.28617376	3.27049426	0.19907885
C	-0.42960410	3.79947192	1.50396595
C	-1.36267658	4.82989210	1.69554573
C	-2.11787906	5.32756154	0.63239116
C	-1.95691954	4.78947176	-0.64527704
C	-1.05060726	3.74594309	-0.88636251
C	-0.92613102	3.16070349	-2.27290464
C	0.36641435	3.27796001	2.68177479
C	-0.35913478	-2.01202637	0.21288085
C	-1.16239743	-2.52093692	1.24898406
C	-1.35339773	-3.90189246	1.38534004
C	-0.75329133	-4.79204117	0.48769377
C	0.04322217	-4.29221596	-0.54674803
C	0.24129457	-2.91059340	-0.68356455
C	-2.03856559	0.25037177	0.05160575
C	-2.63216661	1.02599659	1.06091908
C	-4.01676196	1.24626535	1.06835925
C	-4.82701852	0.68488477	0.07710448
C	-4.24524215	-0.10875074	-0.91735824
C	-2.86209590	-0.33386656	-0.92557314
H	1.81330172	4.52078826	-0.18116970
H	3.07086759	3.94731222	0.92317881
H	3.31509285	3.81763005	-0.81599804
H	4.59075361	2.12132437	0.77652175
H	4.85601307	0.47564711	0.17068600
H	4.66723053	1.82728064	-0.95832133
H	3.95246910	-3.72921077	2.10713681
H	5.00156141	-4.57091060	0.02120289
H	4.83396809	-3.24523284	-2.06970647
H	3.74134899	-1.53370283	-3.33939906
H	4.46525954	-0.14754707	-2.53553240
H	2.70574772	-0.30517154	-2.59351502
H	2.86725392	-2.07093621	3.33662591
H	2.77072254	-0.42142303	2.70862601
H	1.43098479	-1.54466601	2.45066652
H	-1.49093547	5.24078286	2.69174286
H	-2.82905045	6.12913765	0.79912205
H	-2.54240093	5.17488954	-1.47359744
H	-1.38187560	3.82653548	-3.01102080
H	0.11616481	2.99436502	-2.56610106
H	-1.44280286	2.19522412	-2.32527567
H	-0.07263465	3.62756459	3.61983738
H	0.39006353	2.18271276	2.71122458
H	1.40735708	3.62722235	2.66916584

H	-1.65600149	-1.84744510	1.93956570
H	-1.97729000	-4.27730823	2.19042352
H	-0.90618066	-5.86106795	0.59274530
H	0.51718272	-4.97221610	-1.24814708
H	0.87678863	-2.55080181	-1.48413172
H	-2.02818401	1.47023989	1.84295682
H	-4.45610206	1.85300204	1.85396607
H	-5.89907028	0.85130292	0.08682144
H	-4.86644719	-0.56898518	-1.67980078
H	-2.43926010	-0.98786515	-1.67853721
H	-0.07010723	0.03828736	1.53914930
N	0.02741119	-0.15313178	-2.26820198
C	-0.13431277	-0.32567700	-3.40912905
C	-0.35307540	-0.54999985	-4.83036477
H	0.59490832	-0.51873083	-5.37655303
H	-1.01701945	0.21820762	-5.23948804
H	-0.81480093	-1.52965359	-4.99093058

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Pt	0.00000000	0.00000000	0.00000000
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N	0.45797545	1.99610384	0.00000000
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C	1.73095766	2.31753308	0.02965585
C	2.23719167	3.72941011	0.04306988
C	4.17869015	1.46755762	0.09418288
C	2.94489528	-1.22255476	0.00977619
C	3.31076489	-1.79037447	1.24900698
C	3.98924595	-3.01901870	1.22724095
C	4.28924374	-3.65666250	0.02069827
C	3.90703005	-3.07566097	-1.19137222
C	3.22253303	-1.85093718	-1.22306526
H	4.28290002	-3.47236981	2.16858235
H	4.14042990	-3.57025349	-2.12879009
C	-0.57022982	3.02627902	-0.07524132
C	-1.19876025	3.44556033	1.11404343
C	-2.20788466	4.41428060	1.00612264
C	-2.57723489	4.93595800	-0.23559351
C	-1.93504900	4.50090976	-1.39671382
C	-0.91519021	3.53874681	-1.34246919
H	-2.22416497	4.90486332	-2.36144926
H	-2.70624218	4.75361974	1.90805313
C	-2.03464130	0.17366517	0.06156996
C	-2.73153370	-0.13707441	1.24399002
C	-4.12905758	-0.03696014	1.29669415
C	-4.85000310	0.35629394	0.16378364

C	-4.16678634	0.64897228	-1.02166745
C	-2.76855115	0.55906312	-1.07291165
H	2.94547160	3.87742053	0.86573816
H	1.42314628	4.44519811	0.14871868
H	2.77579692	3.95787111	-0.88572861
H	4.48017980	2.14238550	-0.71474997
H	4.45222636	1.95733015	1.03720055
H	4.75335663	0.54476734	0.00951351
H	4.81943365	-4.60290460	0.02508354
H	-3.36461744	5.67907619	-0.29819351
H	-2.19102797	-0.45599273	2.13124396
H	-4.65060100	-0.26977617	2.22040546
H	-5.93196954	0.42921874	0.20303219
H	-4.71836792	0.94842395	-1.90774173
H	-2.25870692	0.79202264	-2.00247282
N	-0.31290618	-1.96712267	-0.02242122
C	-0.53878230	-3.10849143	-0.04542253
C	-0.82643892	-4.53350409	-0.07640185
H	-1.53376334	-4.79410432	0.71765719
H	0.09112442	-5.11296487	0.06590264
H	-1.27003063	-4.80932060	-1.03875842
C	2.80754196	-1.22533888	-2.53533549
H	2.99462826	-1.91056244	-3.36611766
H	1.74154473	-0.96569967	-2.53956841
H	3.36376621	-0.30175355	-2.74317814
C	-0.22375222	3.07960262	-2.60735020
H	-0.77212351	3.42287728	-3.48840992
H	0.79634954	3.47931235	-2.68856637
H	-0.14944750	1.98707900	-2.66025724
C	-0.80137645	2.88744416	2.46010252
H	-1.41811147	3.31984646	3.25187796
H	-0.92837523	1.79922668	2.48986194
H	0.24707209	3.10225131	2.70474796
C	2.98118155	-1.11005751	2.55908903
H	3.18799498	-1.77609599	3.40071342
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C	2.23966462	3.73216346	-0.01176054
C	4.17898197	1.48798222	-0.06933334

C	2.94610028	-1.21437291	-0.02583861
C	2.88213940	-2.06923275	1.08183774
C	3.59843765	-3.27631990	1.07714105
C	4.33702181	-3.61794947	-0.06830771
C	4.39184878	-2.77948798	-1.19434004
C	3.68961845	-1.56452413	-1.16253274
C	3.59337170	-4.17884843	2.29121252
C	5.20650097	-3.16952778	-2.40762507
C	-0.57663938	3.01259091	-0.02663291
C	-1.39687989	3.17860413	1.08946669
C	-2.41799475	4.14318065	1.06490452
C	-2.58967383	4.91193653	-0.09575625
C	-1.77582883	4.74313594	-1.23001702
C	-0.75560906	3.78346756	-1.18445976
C	-2.00594824	5.57411655	-2.47252342
C	-3.32950499	4.31431798	2.25865765
C	-2.02950662	0.18979990	-0.02567185
C	-2.78759007	-0.13968869	1.11290572
C	-4.18324973	-0.00282407	1.10536282
C	-4.84044803	0.44609425	-0.04618571
C	-4.09532271	0.75764285	-1.18923820
C	-2.69916832	0.63123031	-1.17985257
H	3.02621878	3.84651927	0.74100304
H	1.44321465	4.44230967	0.20426857
H	2.68075984	4.00427167	-0.97937127
H	4.45934932	2.03667915	-0.97650798
H	4.46012311	2.11584061	0.78402170
H	4.76719480	0.57233212	-0.02930031
H	2.28932841	-1.78406138	1.94487041
H	4.88056348	-4.55867171	-0.08439783
H	3.69912493	-0.90817425	-2.02696521
H	3.66063978	-5.23401085	2.00716285
H	2.68885109	-4.04279211	2.89273208
H	4.45116221	-3.96538955	2.94229366
H	4.93791385	-2.57122558	-3.28325174
H	5.06231532	-4.22481591	-2.66257809
H	6.27933801	-3.02593038	-2.22522409
H	-1.25339079	2.55227106	1.96225444
H	-3.38214543	5.65453650	-0.12207133
H	-0.12171035	3.61978154	-2.05037153
H	-2.97691736	5.34332529	-2.92770453
H	-1.23469929	5.39360798	-3.22719442
H	-2.00558102	6.64552502	-2.24086863
H	-3.95344069	5.20689866	2.16030547
H	-2.76071285	4.40108558	3.19139144
H	-3.99674109	3.44933810	2.36251836

H	-2.29581797	-0.49662442	2.01387719
H	-4.75355523	-0.25315250	1.99522186
H	-5.92109072	0.54577690	-0.05474528
H	-4.59771166	1.09959239	-2.08916477
H	-2.13874173	0.88531096	-2.07460922
N	-0.32727062	-1.96177380	-0.04886927
C	-0.56063330	-3.10006299	-0.11106582
C	-0.85439640	-4.52153882	-0.19657466
H	-1.56626948	-4.81021395	0.58352324
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Ee_b

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Pt	1.32580658	2.75545574	-1.51464932
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C	1.04987163	4.20166322	-4.18063473
C	0.61436701	3.25125100	-5.10334660
C	1.06918901	3.31441577	-6.43178376
C	1.95553806	4.33985608	-6.79196891
C	2.40303553	5.29872350	-5.86585695
C	1.93613725	5.22358055	-4.54638344
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N	0.05013416	3.98118888	-0.23471336
C	-0.59696530	4.90859006	-0.89149499
C	-0.27689367	4.99648455	-2.33807000
C	-0.94355471	6.03917982	-3.18823205
C	-0.13581599	3.74737182	1.17129648
C	-1.36134378	3.26902631	1.65788209
C	-1.52023171	3.01211781	3.02883036
C	-0.43785846	3.26107459	3.88894227
C	0.79164097	3.74841885	3.41449558
C	0.94151927	3.97074055	2.03684402
H	-2.17960387	3.07823615	0.97063812
H	1.88208029	4.33538720	1.63761601
C	-1.56904196	5.88126126	-0.28423898
C	2.43999033	1.70103432	-2.84741575
C	1.96708171	0.49473174	-3.40129647
C	2.75505260	-0.24691574	-4.29404154
C	4.03147418	0.20425234	-4.64875133
C	4.51221646	1.40311897	-4.10977024

C	3.72268303	2.14606140	-3.22043459
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H	-2.01157331	6.09522042	-2.95666654
H	-0.51927381	7.03395265	-2.99886438
H	-2.59943157	5.65374939	-0.58662810
H	-1.52745813	5.85243032	0.80444449
H	-1.35480881	6.90187041	-0.61709134
C	-2.83217060	2.49176226	3.57329585
H	-0.55517248	3.07205567	4.95258928
C	1.92114129	4.04970088	4.37490689
C	0.63063925	2.27126146	-7.43426509
H	2.31239733	4.39052330	-7.81679541
C	3.36577414	6.38583427	-6.28852532
H	0.97440828	0.12963220	-3.15014044
H	2.37062794	-1.17410836	-4.70916090
H	4.64277385	-0.36974285	-5.33751365
H	5.49941397	1.76426954	-4.38254674
H	4.11027237	3.08225609	-2.82808151
H	3.71759878	2.56807016	0.09745019
H	4.03469859	0.88588143	-0.37474889
H	1.90554946	-0.46421181	0.90780347
H	1.93556114	-0.49721152	-0.87901972
H	-0.35604073	-1.03634560	0.02574281
H	-0.40246897	0.47427714	-0.90118751
H	-0.39332328	0.52308408	0.87575575
H	3.65212642	0.14074980	2.01592777
H	3.12510036	1.78413842	2.44232985
H	4.81493302	1.46392080	2.00169463
H	0.89851452	2.55962486	-8.45443512
H	-0.45297884	2.11101601	-7.40217260
H	1.10931935	1.30638781	-7.22346004
H	3.61307017	7.05103218	-5.45599130
H	2.94443313	6.99925229	-7.09399779
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H	-3.54791827	2.28529318	2.77229907
H	-3.29351424	3.21761198	4.25401184
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N	2.09895711	-1.26535488	0.09495337
C	2.62416636	-1.88451631	-0.92547328
C	2.56250695	-1.40207627	-2.34597287
C	3.67980927	1.17694529	0.00465020
C	-0.78403644	-1.29231204	-0.01681733
Pt	2.43495935	-2.26964718	1.98932674
C	2.83823158	-3.28540826	3.70425429
C	2.01484518	-4.34412444	4.13507987
C	2.25325052	-4.99212010	5.35581881
C	3.32252734	-4.59727130	6.16737181
C	4.15277727	-3.55099684	5.75059704
C	3.91192549	-2.90053519	4.53158913
N	3.34090465	-3.50535103	0.67029160
C	3.31984030	-3.15745610	-0.59754024
C	3.94745882	-3.96509942	-1.69469714
C	3.97765848	-4.74525921	1.09749938
C	3.21376403	-5.92925193	1.10140357
C	3.83852375	-7.10153282	1.55324145
C	5.16869367	-7.09128270	1.97840068
C	5.90118706	-5.90235568	1.95778756
C	5.32174197	-4.70276901	1.51798336
C	1.77598460	-5.95262800	0.63378966
C	6.12217167	-3.42158278	1.48820564
H	4.49571510	-4.81954559	-1.30043461
H	3.18223446	-4.33790126	-2.38757911
H	4.63577657	-3.34825036	-2.28357717
H	2.14274394	-2.17116353	-3.00415696
H	1.94925019	-0.50394476	-2.42689597
H	3.56493062	-1.16894470	-2.72637295
H	-1.73928440	1.26246026	-0.02231708
H	-0.45511229	3.38696933	-0.02017648
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H	4.07386342	2.17178805	0.22866305
H	4.08966782	0.88264143	-0.97086050
H	4.08043758	0.47709595	0.74766154
H	-1.84781563	-1.10247915	0.14928287
H	-0.69333083	-1.81123148	-0.98047326
H	-0.43265002	-1.98936632	0.75384062
H	3.26957260	-8.02530375	1.57181873
H	5.63287313	-8.00731420	2.32701197
H	6.93422823	-5.89461641	2.28934959
H	7.09539818	-3.56599847	1.96401982
H	6.30838229	-3.07556424	0.46247473
H	5.60306326	-2.61326917	2.01570464

H	1.30599783	-6.90596080	0.88863987
H	1.18643356	-5.15054698	1.09274832
H	1.69439796	-5.83359306	-0.45528644
H	1.18494073	-4.67768894	3.51798400
H	1.60616782	-5.80677477	5.66729548
H	3.50852489	-5.10083663	7.11033910
H	4.98943238	-3.24094758	6.36977445
H	4.57769903	-2.09737750	4.22607301
O	1.42268480	-0.85417712	3.18272410
C	2.16113603	0.26298022	3.85888560
C	1.08553293	0.92886099	4.71286659
C	0.20527434	-0.26050266	5.16504233
C	0.16044608	-1.17937657	3.94120790
H	2.96035393	-0.18279872	4.45592910
H	2.56776632	0.88618398	3.06310111
H	0.50401379	1.63788038	4.11434135
H	1.51718290	1.46800939	5.56033710
H	-0.79615519	0.05759345	5.46673442
H	0.66787007	-0.77650085	6.01272445
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N	2.10620809	-1.27913666	0.01308603
C	2.41541619	-1.87799148	-1.11444381
C	2.09309993	-1.31989907	-2.47099506
C	3.68334395	1.15534457	-0.03135287
C	-0.79504665	-1.28500879	-0.03127647
Pt	2.62664900	-2.23352136	1.76305569
N	3.36904708	-3.60113591	0.19438629
C	3.12009520	-3.18124040	-1.01557734
C	3.49775677	-3.91789249	-2.26986616
C	1.81582585	-0.82410080	2.98406676
C	0.47673415	-0.93631174	3.40079565
C	-0.09786023	0.03977947	4.22698693
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C	2.56323793	0.28582482	3.41448481
C	4.05534876	-3.21815208	3.53441131
C	4.40782193	-2.36837667	4.61238455

C	3.52610248	-2.18928125	5.66939212
C	2.26766030	-2.83313284	5.67331678
C	1.89436733	-3.65314364	4.61960668
C	2.78543595	-3.86392443	3.53288592
C	4.05174413	-4.85213149	0.44765758
C	5.45758667	-4.84168271	0.58294754
C	6.09270206	-6.05110300	0.90688399
C	5.35842751	-7.22633341	1.08038403
C	3.97044963	-7.21256656	0.92351054
C	3.28556128	-6.02934732	0.60283421
C	6.26686775	-3.58282014	0.35492454
C	1.78476335	-6.03697616	0.40644768
N	-0.90766840	-4.61933347	2.60590599
C	-1.98804363	-5.03464323	2.78852906
C	-3.33161515	-5.55281160	3.01858608
H	1.63229289	-0.33606473	-2.40132874
H	2.99919166	-1.23925449	-3.08246857
H	1.40512027	-1.98521157	-3.00766036
H	4.20504642	-3.33217729	-2.86975421
H	3.95874103	-4.87791242	-2.03803570
H	2.61877110	-4.09768139	-2.89934662
H	7.17208122	-6.06353664	1.01863228
H	5.86635665	-8.15078851	1.33227073
H	3.40187779	-8.12848314	1.04723918
H	1.38179112	-7.03273354	0.60951692
H	1.50887667	-5.78038198	-0.62503096
H	1.26355738	-5.32864843	1.06161341
H	7.28768691	-3.70840362	0.72555645
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H	5.82697934	-2.71083920	0.85285281
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H	-0.43682924	3.38864065	0.03509122
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H	-0.71708362	-1.79086341	-1.00374888
H	-0.45790250	-1.99449019	0.73216879
H	4.08974614	2.15674396	0.13191187
H	4.09121329	0.49325310	0.74069942
H	4.06738035	0.80232595	-0.99833160
H	5.38189573	-1.89159570	4.62195017
H	3.80410255	-1.55588927	6.50480016
H	1.59384468	-2.68228469	6.50940108
H	0.93247798	-4.15151065	4.61037131
H	2.59593620	-4.69033691	2.85819947
H	3.60090205	0.39834799	3.11579830
H	2.58164862	2.11020996	4.56508250

H	0.20844744	1.89575560	5.29042020
H	-1.13252307	-0.06476903	4.54118626
H	-0.11838985	-1.79347890	3.10127064
H	4.82006825	-3.52935204	2.83290267
H	-3.39335147	-6.60638527	2.72782571
H	-4.06712627	-4.99073526	2.43412740
H	-3.59903863	-5.47201126	4.07695902

Ha'

C	0.00000000	0.00000000	0.00000000
C	1.42314568	0.00000000	0.00000000
C	2.12169022	1.23786073	0.00000000
C	1.41801135	2.43156734	0.01833793
C	0.00296609	2.42876023	0.00204293
C	-0.70084103	1.23283193	-0.02308950
Pt	0.81633979	-0.91429956	-2.17973077
N	1.00893117	0.77708389	-3.64449644
C	1.18844720	2.18828207	-3.36202697
C	2.49715560	2.68613608	-3.18833072
C	2.64287601	4.05932471	-2.93402715
C	1.53139964	4.90297573	-2.85845644
C	0.24727223	4.38228719	-3.03553822
C	0.04899683	3.01626072	-3.29389463
C	3.70846218	1.78644809	-3.28552970
C	-1.34077151	2.46537649	-3.51939312
C	0.72417034	-2.66923029	-1.13860924
C	-0.50400729	-3.30465142	-0.88156219
C	-0.55148563	-4.50792533	-0.16342787
C	0.62761805	-5.09513807	0.30786677
C	1.85414289	-4.47004385	0.06001009
C	1.90456036	-3.26369584	-0.65380941
N	0.73250124	-1.83904827	-4.02196139
C	0.52244265	-3.27486179	-4.15032965
C	-0.79765107	-3.75629105	-4.26238711
C	-0.97511771	-5.14423547	-4.36285048
C	0.11848511	-6.01276018	-4.35657468
C	1.41533787	-5.50448663	-4.25560461
C	1.64622521	-4.12448862	-4.15172492
C	-1.98884408	-2.82466046	-4.28446583
C	3.05202090	-3.57692752	-4.07286106
C	0.83042973	-1.09138701	-5.09441122
C	0.76779028	-1.63060869	-6.49532594
C	1.00589653	0.36617184	-4.88459144
C	1.17085634	1.25620900	-6.08616083
N	4.86852223	-0.79106591	-0.32081097
C	5.91140042	-1.12641991	0.09442710

C	7.20805096	-1.54435043	0.61440599
H	0.74452270	-2.71893494	-6.50627139
H	-0.12919688	-1.26362706	-7.01041846
H	1.63044301	-1.29191882	-7.07910794
H	0.33892362	1.12512360	-6.78703318
H	1.22102483	2.30570554	-5.80052095
H	2.08973996	1.00587312	-6.63094959
H	-0.61672499	5.03728344	-2.98377942
H	1.66611583	5.96227906	-2.66776322
H	3.64133414	4.46409086	-2.80247771
H	4.62110647	2.35055819	-3.07535638
H	3.81895085	1.35251435	-4.28807340
H	3.65793424	0.95206801	-2.57618140
H	-2.09783601	3.20492191	-3.24504929
H	-1.51117519	2.20478754	-4.57283630
H	-1.51673016	1.55935688	-2.92901796
H	-1.98249587	-5.53974847	-4.44246098
H	-0.03972029	-7.08313956	-4.43081630
H	2.26490334	-6.17938544	-4.25444788
H	3.77056009	-4.38613248	-3.91933993
H	3.33997982	-3.05594606	-4.99642022
H	3.16146735	-2.86395616	-3.24884097
H	-2.91811916	-3.38891088	-4.17041691
H	-1.94159795	-2.08243486	-3.47932770
H	-2.06208470	-2.27187054	-5.23116466
H	-1.78530193	1.23110370	0.00126633
H	-0.53091368	3.37238001	0.02788240
H	1.94761154	3.37659600	0.05026157
H	3.20442500	1.21766868	0.02976890
H	1.97416685	-0.89895211	0.24682660
H	-1.43206743	-2.86963946	-1.24096539
H	-1.50977421	-4.98196072	0.02654548
H	0.58999957	-6.02565424	0.86473567
H	2.77483602	-4.91489710	0.42608937
H	2.86646134	-2.78701151	-0.81980485
H	-0.54133751	-0.91388041	0.21067544
H	7.68002192	-0.72877121	1.17147373
H	7.87600772	-1.83499785	-0.20263872
H	7.09454936	-2.39964348	1.28809133

Hb

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C	2.12451337	1.19626564	0.00000000
C	1.44857142	2.42366603	0.00313958
C	0.04259653	2.41539075	-0.00463334

C	-0.69410608	1.22192360	-0.00328159
N	2.11482828	-1.26028423	0.01261398
C	2.74991185	-1.66862186	-1.06466631
C	2.70180827	-0.94761798	-2.38214266
H	3.20959156	1.16956891	0.01854361
H	-0.54043715	-0.93917785	0.01995075
Pt	2.28122265	-2.42542227	1.69989778
N	3.52716547	-3.49143439	0.22766708
C	3.55163835	-2.91217106	-0.94276648
C	4.31534925	-3.41843584	-2.13489496
C	1.11035146	-1.22472512	2.84690005
C	-0.26007231	-1.49090396	3.01995006
C	-1.06737685	-0.63085163	3.77898239
C	-0.51690835	0.50834156	4.37707817
C	0.84470548	0.78398950	4.20800447
C	1.65089827	-0.07386517	3.44630786
C	3.25418403	-3.60899839	3.54717187
C	3.31880021	-2.86970684	4.76114867
C	2.24572436	-2.87676978	5.63825203
C	1.07773289	-3.61257929	5.33241500
C	0.98587824	-4.32907188	4.14781560
C	2.07343184	-4.34606781	3.23893992
C	4.31398510	-4.67166728	0.50688003
C	5.68293072	-4.53192732	0.78469923
C	6.44883085	-5.66129869	1.11159606
C	5.81541224	-6.91561843	1.14907464
C	4.44889349	-7.06473517	0.86874911
C	3.69118446	-5.92270448	0.55145754
H	6.14295079	-3.54871528	0.75869434
H	2.62764676	-6.01164771	0.35628083
N	0.28432078	-6.64740079	1.27788281
C	-0.66190399	-7.32806642	1.16266581
C	-1.83754661	-8.17867887	1.01879574
H	1.89065186	-0.22145815	-2.40983092
H	3.63962393	-0.40882732	-2.57117781
H	2.56836297	-1.65821266	-3.20315790
H	4.98277358	-2.64624415	-2.53381104
H	4.91246444	-4.29281175	-1.88063691
H	3.62678757	-3.69664535	-2.94241903
C	7.92629542	-5.53509252	1.41029549
H	6.40045468	-7.79403729	1.40736191
C	3.79571343	-8.42847285	0.89109884
C	2.21089565	3.72971748	0.02757066
H	-0.48985290	3.36233858	-0.00408476
C	-2.20514917	1.23631255	0.03028848
H	4.22686772	-2.32986140	5.00707776

H	2.30150702	-2.32500109	6.57018385
H	0.25231067	-3.61817130	6.03610238
H	0.10093764	-4.91105737	3.91712658
H	2.05694927	-5.06701314	2.42994081
H	2.70375307	0.16230888	3.32290048
H	1.28226876	1.66579057	4.66692702
H	-1.14052033	1.17276148	4.96670980
H	-2.12286353	-0.85585352	3.90482595
H	-0.70700029	-2.37059465	2.56655232
H	4.17536894	-3.80569437	3.00855822
H	-1.59145188	-9.21808565	1.25819286
H	-2.21616858	-8.14190524	-0.00760100
H	-2.63562860	-7.85058245	1.69227532
H	-2.63260155	0.54713429	-0.70686515
H	-2.60019980	2.23544080	-0.17337527
H	-2.57138108	0.92695510	1.01766665
H	1.84321278	4.42052389	-0.73951046
H	3.28057206	3.57539536	-0.14276662
H	2.09876935	4.23320132	0.99601356
H	8.23733080	-4.48807921	1.47175728
H	8.53017275	-6.01654317	0.63096724
H	8.18244357	-6.01855594	2.35987066
H	2.73011477	-8.35277314	1.12676056
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Hb'

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C	0.00200475	2.42888378	0.00393335
C	-0.70165133	1.23359360	-0.02347826
Pt	0.76767381	-0.87420099	-2.17367723
N	0.96467931	0.82896274	-3.61913622
C	1.23936243	2.22195022	-3.33163951
C	2.56587454	2.64023504	-3.19071097
C	2.85049205	3.99552239	-2.95293667
C	1.78282930	4.90348592	-2.86808783
C	0.44661121	4.49206509	-3.00892670
C	0.18066762	3.13241911	-3.23868603
H	3.37045274	1.91543982	-3.26155637
H	-0.84139658	2.78524614	-3.34915302
C	0.69092083	-2.64887192	-1.17565724
C	-0.53119984	-3.30253751	-0.93853192
C	-0.56332630	-4.53731652	-0.27481040

C	0.62454537	-5.13584183	0.16025337
C	1.84532589	-4.49120472	-0.06911945
C	1.88059523	-3.25363193	-0.72897517
N	0.58445032	-1.76629037	-4.02450277
C	0.28075828	-3.18007789	-4.16492122
C	-1.03522584	-3.56276391	-4.45710144
C	-1.35097528	-4.92186479	-4.58779316
C	-0.32347223	-5.86829058	-4.42752073
C	0.99509041	-5.49149077	-4.13335806
C	1.29365926	-4.12430518	-4.00276370
H	-1.80902766	-2.80876423	-4.56313937
H	2.29973893	-3.80296303	-3.75909752
C	0.65605552	-1.00516497	-5.09110098
C	0.52715700	-1.52334288	-6.49604711
C	0.89532291	0.44068614	-4.86560533
C	1.05687109	1.34260667	-6.05936440
N	4.71007005	-0.92045881	0.38230180
C	5.67392996	-1.24970853	0.96048213
C	6.87266463	-1.65883947	1.68287196
H	0.60036092	-2.60908731	-6.52988835
H	-0.43953107	-1.23819692	-6.93162470
H	1.30586746	-1.09705024	-7.13543832
H	0.23292158	1.20244960	-6.76693247
H	1.08912686	2.39067315	-5.76826773
H	1.98563337	1.11003824	-6.59622948
C	-0.68126768	5.49871382	-2.94758195
H	1.99623603	5.95479536	-2.69525029
C	4.27936863	4.45977008	-2.77521816
C	-2.76601558	-5.36542123	-4.88554540
H	-0.55898359	-6.92405484	-4.52819157
C	2.07554974	-6.52758569	-3.92325459
H	-1.78614282	1.23071478	-0.00234398
H	-0.53272073	3.37219063	0.03145166
H	1.94623946	3.37702258	0.05684175
H	3.20413171	1.21655415	0.03670401
H	1.98128036	-0.89544087	0.24650188
H	-1.46340933	-2.86190374	-1.28083189
H	-1.51605862	-5.02750378	-0.09818941
H	0.59788198	-6.08978956	0.67698361
H	2.77215878	-4.94301988	0.27244426
H	2.83739993	-2.76328661	-0.88473416
H	-0.54226870	-0.91099460	0.22167047
H	7.23377965	-0.84554952	2.32043413
H	7.67089882	-1.92906202	0.98430264
H	6.66211477	-2.52513288	2.31806603
H	3.00069733	-6.25814202	-4.44492923

H	1.76082648	-7.51220196	-4.28027084
H	2.31743305	-6.62059581	-2.85667516
H	4.40667485	5.49493739	-3.10658862
H	4.97869190	3.83480124	-3.33965996
H	4.58250026	4.41617062	-1.72047738
H	-2.79959239	-6.03799771	-5.75039519
H	-3.41964813	-4.51383721	-5.09644998
H	-3.19536012	-5.91144645	-4.03635123
H	-1.64509479	5.01419794	-2.76350479
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H	-0.51582803	6.23771132	-2.15632830

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C	0.04487300	2.41255730	-0.00353854
C	-0.69493865	1.21681171	0.00238959
N	2.10029310	-1.27274801	0.01367908
C	2.13610157	-2.01896981	-1.06864363
C	1.57350799	-1.58980358	-2.39387733
C	2.22324877	3.71567271	0.03849170
C	-2.20699779	1.24767575	0.01848502
Pt	2.96280022	-2.04467428	1.71490134
O	-0.14743335	-6.55458029	1.58667774
C	-0.73300674	-7.12709018	0.37100048
C	-1.15158831	-8.58744125	0.52212865
N	3.23008734	-3.65617773	0.24105146
C	2.78063197	-3.35132829	-0.94604408
C	2.86561420	-4.25005361	-2.14796121
C	3.88792739	-4.91809727	0.50212763
C	5.25607671	-5.04938761	0.22588410
C	5.91486688	-6.25489493	0.51846352
C	5.17399198	-7.30538788	1.08443720
C	3.80248685	-7.18305393	1.35943847
C	3.15391190	-5.96969793	1.06525841
C	3.02849186	-8.33337150	1.96518506
C	7.38942125	-6.42212902	0.22527430
C	2.62377336	-0.38807600	2.84236511
C	1.36722565	-0.17442908	3.43490206
C	1.11528213	0.98494611	4.18205086
C	2.11383047	1.95257266	4.34207433
C	3.36577807	1.75433657	3.74892455
C	3.61898521	0.59256654	3.00454673
C	-1.10158077	-6.31466580	2.67021454

C	-0.37392569	-5.57057973	3.77805435
C	3.32132571	-3.48165714	3.63190819
C	4.60963159	-3.00478302	3.25150703
C	5.29264680	-2.09041172	4.09442666
C	4.71208922	-1.67486539	5.28384372
C	3.43514127	-2.14846278	5.66367773
C	2.74447548	-3.03393229	4.85080483
H	5.80357188	-4.21934844	-0.21051551
H	2.08949171	-5.86342229	1.26149640
H	3.21158463	1.16286499	0.02001762
H	-0.54242673	-0.94010866	0.01885263
H	1.38427145	-0.51748761	-2.41877463
H	2.26353272	-1.84607142	-3.20331264
H	0.62520330	-2.10207970	-2.60346278
H	3.57530484	-3.85252878	-2.88495367
H	3.19652891	-5.24961364	-1.86798365
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H	5.67688976	-8.24102970	1.31429309
H	-0.48561279	3.36060260	-0.00248402
H	6.28364736	-1.74777400	3.81725539
H	5.24264738	-0.98975307	5.93596353
H	3.00104723	-1.81984649	6.60150650
H	1.77551650	-3.41661175	5.15173279
H	2.89330709	-4.34474847	3.13326683
H	4.59689806	0.45840881	2.55194984
H	4.14832153	2.49868581	3.86632505
H	1.91837042	2.84978398	4.92063025
H	0.13948906	1.13012196	4.63632534
H	0.57622428	-0.90895792	3.31541839
H	5.15503212	-3.49637547	2.45333457
H	0.05800887	-7.02845984	-0.37778988
H	-1.58581738	-6.50554702	0.05738800
H	-1.49921698	-7.26798411	3.04062325
H	-1.94460816	-5.72216821	2.28323194
H	-1.05338887	-5.37745790	4.61556589
H	0.00623372	-4.61119347	3.41030760
H	0.46851464	-6.16334100	4.14920775
H	-1.96665893	-8.70966973	1.24280158
H	-0.30609620	-9.20022995	0.85061634
H	-1.50240451	-8.97706341	-0.44054750
H	1.58427920	4.57225479	-0.19342547
H	3.05499392	3.71098859	-0.67481757
H	2.65008281	3.87751112	1.03670158
H	-2.58316317	1.67910978	0.95428767
H	-2.63160094	0.24403506	-0.07836948
H	-2.60185019	1.86052317	-0.80011420

H	7.82497139	-5.50806364	-0.18894567
H	7.56088598	-7.23028043	-0.49601759
H	7.94828735	-6.67835424	1.13314476
H	1.97476396	-8.07246263	2.09313181
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C	0.06905582	2.43648734	0.04641868
C	-0.65409613	1.24177637	0.02813550
N	2.10624456	-1.26810067	0.06322378
C	2.47373904	-1.91389564	-1.00903916
C	2.23136534	-1.44274122	-2.41526680
C	3.68165366	1.17834287	-0.06060970
C	-0.79254404	-1.28802178	-0.06633911
Pt	2.74658267	-2.25257799	1.93407181
C	3.56470804	-3.29510480	3.47563645
C	2.86813923	-4.31138843	4.15015333
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C	4.77992138	-4.71119717	5.59583913
C	5.48354116	-3.70403332	4.92529360
C	4.88303708	-3.00105149	3.87126000
N	3.40090051	-3.54470580	0.47010105
C	3.17196852	-3.20452083	-0.77755895
C	3.56145460	-4.04931117	-1.95662764
C	4.05383173	-4.80885300	0.78333354
C	3.24475498	-5.93841116	1.02088517
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C	5.28132750	-7.21383946	1.42365435
C	6.05589177	-6.07879596	1.17545654
C	5.46051701	-4.85096057	0.84764878
C	1.73846556	-5.87041115	0.91938028
C	6.30936846	-3.63476263	0.55691151
C	2.33073738	-0.31081005	3.34464199
C	1.10560960	-1.03619977	3.31056826
C	0.65269144	-1.70336516	4.47674973
C	1.39343975	-1.63206538	5.64797440
C	2.60505081	-0.90483510	5.68830246
C	3.07276271	-0.25806350	4.55513095
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H	2.68365667	-4.28560551	-2.56968211
H	4.26509839	-3.51040123	-2.60282786

H	1.61899207	-2.16287673	-2.97079213
H	1.72144506	-0.47936784	-2.42484712
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H	-0.45375202	3.38629661	0.07049505
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H	4.07338378	2.19484943	0.03421963
H	4.03923394	0.78426584	-1.02186295
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H	-0.76907012	-1.72398506	-1.07444633
H	-0.40514716	-2.05082072	0.61912182
H	3.28692626	-8.02439303	1.53376402
H	5.76138056	-8.15203809	1.67971772
H	7.13767341	-6.13552139	1.23737057
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H	6.28441104	-3.36526893	-0.50844762
H	5.98423388	-2.75633840	1.12447958
H	1.28709937	-6.80120867	1.27236827
H	1.33114840	-5.04600438	1.51650955
H	1.40201356	-5.71740812	-0.11524568
H	-0.29155878	-2.23653298	4.45477370
H	1.03767264	-2.12625345	6.54543146
H	3.16508337	-0.85117974	6.61524239
H	3.99151939	0.31590633	4.58872428
H	2.57118340	0.38714618	2.55085957
H	1.85129860	-4.56191392	3.86503761
H	2.91843835	-5.79765704	5.71286420
H	5.24634537	-5.25527826	6.41089129
H	6.50095952	-3.46339288	5.22076555
H	5.44123944	-2.21964708	3.36348104
H	0.42327119	-0.90256497	2.48002403
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C	7.44453235	0.04467231	0.89560499
C	8.44863936	1.03677182	1.50264378
C	8.28800027	0.80427617	3.02221247
C	6.78280566	0.54710087	3.16241765
H	7.89864445	-0.93493462	0.70888818
H	6.98007988	0.40532167	-0.02619209
H	8.17681078	2.06714364	1.24576981
H	9.47013330	0.86125199	1.15401181
H	8.62492813	1.65678445	3.61842075
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N	2.11965375	-1.25323756	0.05244997
C	2.22079848	-2.03214742	-0.99184169
C	1.67634357	-1.71558626	-2.35739056
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Pt	3.10802644	-2.06774618	1.84786610
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C	3.55333346	-4.06829198	4.05072338
C	4.29299217	-4.76411835	5.01809140
C	5.63507295	-4.44168341	5.24850925
C	6.23411072	-3.41813751	4.50502543
C	5.49348272	-2.72030886	3.53999067
N	3.43974146	-3.51836829	0.42568935
C	2.95401313	-3.30494681	-0.77803661
C	3.10799913	-4.27011952	-1.91935439
C	4.08616260	-4.78132460	0.73612310
C	3.29246243	-5.92564708	0.89483571
C	3.89430398	-7.15136837	1.20901851
C	5.29273835	-7.19625086	1.34933502
C	6.09228067	-6.05472152	1.19374483
C	5.47182966	-4.83287702	0.88153572
H	2.21384851	-5.85660137	0.79384082
H	6.06249411	-3.93093951	0.77140153
C	3.06489967	0.00842454	3.15650829
C	1.81439884	-0.65705160	3.31362518
C	1.48752351	-1.24784774	4.56472364
C	2.37490997	-1.16074838	5.62680674
C	3.61165710	-0.49197603	5.47478475
C	3.95768394	0.07610781	4.25815534
H	3.87320771	-5.01633085	-1.71027397
H	2.16698034	-4.80124826	-2.11454825
H	3.37344246	-3.73945873	-2.83824153
H	1.00748402	-2.50915250	-2.70952222
H	1.12574501	-0.77623323	-2.35878272
H	2.49228013	-1.63668939	-3.08646844
C	-2.21169278	1.24068258	0.00906554
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C	2.21327380	3.72265616	-0.05572892
C	3.06189709	-8.39996055	1.39786404

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C	7.58927081	-6.11557386	1.39404710
H	0.52553777	-1.73327002	4.68929701
H	2.11758244	-1.59640130	6.58618985
H	4.28777578	-0.42310882	6.32004681
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H	3.26194849	0.65017402	2.30517728
H	2.51621819	-4.34189145	3.88190336
H	3.81884730	-5.55809656	5.58766933
H	6.20623309	-4.98038862	5.99787714
H	7.27415089	-3.15604151	4.67812484
H	5.97542877	-1.92622768	2.97707039
H	1.02645956	-0.51401302	2.58198372
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C	6.31973903	2.42898027	1.36058255
C	6.96880641	3.77761468	1.69720156
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C	4.91969124	3.59823991	2.95075267
H	6.88580410	1.58841038	1.78010440
H	6.17532512	2.26403774	0.29000419
H	6.68123331	4.53724214	0.96108937
H	8.06079496	3.72269252	1.71716347
H	6.40314679	5.17889732	3.31229778
H	6.89489793	3.57151668	3.86931657
H	4.24897200	4.35792134	2.53388430
H	4.49772443	3.22514248	3.88699551
H	3.38014153	-9.19806111	0.71663867
H	2.00029055	-8.20792586	1.21625382
H	3.16023894	-8.78942693	2.41833343
H	8.12470397	-5.56766266	0.61065191
H	7.95205751	-7.14723883	1.39299266
H	7.86688249	-5.66493021	2.35575556
H	-2.63175895	0.23189185	-0.04123736
H	-2.60687556	1.81141812	-0.83943939
H	-2.59262027	1.71576636	0.92131833
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C	2.92959422	-1.23236674	-0.06083379
C	3.20263386	-1.91903080	1.13941329
C	3.90365968	-3.13111349	1.05171490
C	4.30893220	-3.64210500	-0.18322318
C	4.02070752	-2.94257814	-1.35688012
C	3.32747853	-1.72311829	-1.32165310
C	3.02128455	-0.97547238	-2.60067970
C	2.77005259	-1.36906613	2.47850289
C	-0.41613929	3.16531639	0.06893205
C	-0.77453208	3.68908377	1.32988170
C	-1.78800912	4.66013356	1.36967429
C	-2.41755087	5.09496958	0.20117627
C	-2.04325878	4.55992244	-1.03416311
C	-1.03904133	3.58426845	-1.12594147
C	-0.61971292	3.02619027	-2.46668985
C	-0.09997711	3.22860203	2.60414683
C	-0.60668934	-2.66718670	1.28360270
C	-0.75224767	-4.05937175	1.34015561
C	-0.56457638	-4.83738505	0.19058349
C	-0.22949182	-4.21349079	-1.01479902
C	-0.07639602	-2.81932158	-1.07079114
C	-0.25216507	-2.02373636	0.08004520
C	-1.96531195	0.12357952	-0.07872803
C	-2.74734212	0.72109435	0.93819430
C	-4.13372357	0.77129690	0.85466581
C	-4.86455281	0.24821143	-0.25896003
C	-4.18252100	-0.34084378	-1.28085271
C	-2.70505438	-0.47728575	-1.23388983
H	1.68589320	4.50287754	-0.04340580
H	2.99281602	3.90178508	0.99117172
H	3.17983092	3.86538926	-0.75935786
H	4.56160757	2.02940239	0.76737961
H	4.76675642	0.41741903	0.05284386
H	4.55178596	1.83754797	-0.98401509
H	4.12582142	-3.67464654	1.96414795
H	4.84502245	-4.58368512	-0.23099679
H	4.33094786	-3.34195849	-2.31716924
H	3.21978706	-1.60784769	-3.47012216
H	3.63904752	-0.07384833	-2.71155378
H	1.97290798	-0.65718557	-2.64466363
H	3.01499782	-2.07109627	3.27963987
H	3.26430997	-0.41702481	2.71324715
H	1.68874261	-1.19069266	2.50337422
H	-2.07851655	5.07566947	2.32941789
H	-3.19532726	5.84917795	0.25256585

H	-2.52773174	4.90161452	-1.94325626
H	-1.31967748	3.33081128	-3.24927322
H	0.37562504	3.38380277	-2.76263957
H	-0.56969865	1.93067572	-2.45108778
H	-0.66484319	3.56050590	3.47947062
H	-0.00982970	2.13669498	2.64950334
H	0.91358198	3.63970083	2.70331828
H	-1.01868408	-4.53445063	2.27964637
H	-0.68168951	-5.91522127	0.23484011
H	-0.07969896	-4.80690284	-1.91185585
H	0.19934421	-2.35891075	-2.01531505
H	-2.43719813	-1.55846107	-1.22847326
H	-2.26047610	1.14947946	1.80549617
H	-4.69150902	1.22997847	1.66676527
H	-5.94495171	0.33190161	-0.27492142
H	-4.70332502	-0.73910468	-2.14699426
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ts-BaBa

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C	3.40078614	-1.76816968	1.23700845
C	4.13923585	-2.96158802	1.21021511
C	4.50715388	-3.55496773	0.00007679
C	4.13895439	-2.96184659	-1.21009386
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C	3.01075622	-1.12692844	-2.55004127
C	3.01133402	-1.12637872	2.55002368
C	-0.53588454	3.04825174	0.00012386
C	-1.00904457	3.52952492	1.23728125
C	-2.00337462	4.51884577	1.21018824
C	-2.50069238	5.00806127	0.00037446
C	-2.00334456	4.51918719	-1.20956678
C	-1.00902632	3.52986393	-1.23691477
C	-0.46064560	3.02275628	-2.55080471
C	-0.46068151	3.02206016	2.55104334
C	-0.08453604	-2.35373083	0.00033584
C	-0.78334151	-2.54275468	1.22824077
C	-2.13730292	-2.87755106	1.22157159

C	-2.80533922	-3.05600231	0.00123028
C	-2.13812012	-2.87757705	-1.21953338
C	-0.78414413	-2.54276123	-1.22709821
C	-2.01205920	0.30600854	-0.00031855
C	-2.72278266	0.42601407	1.20760180
C	-4.10551877	0.65932492	1.20721082
C	-4.80131618	0.77679628	-0.00075611
C	-4.10512521	0.65939565	-1.20850820
C	-2.72239410	0.42608567	-1.20846522
H	1.44875574	4.45357621	-0.00036821
H	2.89064932	3.91742459	0.88099790
H	2.89154324	3.91724631	-0.88019211
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H	4.79086274	0.58058807	0.00004205
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H	4.42345456	-3.42395602	2.14991735
H	5.07571609	-4.47835454	0.00010816
H	4.42293811	-3.42442054	-2.14976561
H	3.17694540	-1.81707376	-3.38127782
H	3.60318254	-0.22498938	-2.75528127
H	1.95645994	-0.82534521	-2.55912869
H	3.17854596	-1.81602010	3.38147005
H	3.60314966	-0.22387249	2.75450967
H	1.95680286	-0.82561159	2.55959833
H	-2.38740746	4.90181261	2.14993729
H	-3.27319417	5.76920351	0.00047196
H	-2.38735481	4.90242015	-2.14921673
H	-1.05196149	3.40592387	-3.38630184
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H	-1.05233554	3.40455887	3.38660824
H	-0.47391793	1.92749387	2.59950425
H	0.57720657	3.34258956	2.71500349
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H	-2.66930287	-3.01880966	2.15527722
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H	-2.67073061	-3.01881891	-2.15289076
H	-0.24288667	-2.46673128	-2.16410613
H	-2.20715963	0.33406931	2.15845807
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C	3.11481116	-1.15962907	0.04136298
C	3.32600046	-1.80503393	1.27852299
C	4.11362938	-2.96780618	1.28248567
C	4.67222637	-3.46448899	0.10223857
C	4.45180906	-2.80172372	-1.10834483
C	3.67014657	-1.63717666	-1.16578698
C	3.42526814	-0.93170740	-2.48071029
C	2.73466607	-1.26652079	2.56210053
C	-0.52532412	3.02818790	-0.11726160
C	-1.08071493	3.57490977	1.05657158
C	-2.06969214	4.55868675	0.90586138
C	-2.48314088	4.97845512	-0.36047853
C	-1.90712857	4.42333625	-1.50547167
C	-0.91503401	3.43642450	-1.40940380
C	-0.29215485	2.84257057	-2.65267777
C	-0.62055331	3.14365925	2.42916981
C	-0.65654569	-2.36181735	-0.04267948
C	-1.93803385	-2.42232815	-0.66340170
C	-2.06606402	-2.88174466	-1.97136576
C	-0.93157951	-3.31603249	-2.67674759
C	0.33103438	-3.31044151	-2.07049699
C	0.46545057	-2.86608760	-0.75255518
C	-1.98673172	0.34298529	0.28029132
C	-2.52728476	0.14751432	1.56534483
C	-3.89117204	0.37083505	1.80857014
C	-4.73277591	0.78467361	0.77027091
C	-4.20366180	0.97496739	-0.51175593
C	-2.84109621	0.75366267	-0.75616626
H	1.44101444	4.44869882	0.00459103
H	2.89958636	3.93482301	0.87288372
H	2.87301185	3.90820495	-0.88808516
H	4.38098548	2.06003014	1.19351211
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H	4.55503056	2.17200907	-0.55574261
H	4.28673516	-3.48087137	2.22285757
H	5.27686022	-4.36439906	0.12540321
H	4.88838707	-3.18630317	-2.02445664
H	3.83830344	-1.51088312	-3.31071061
H	3.89744007	0.05893020	-2.51182231

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H	3.22973180	-0.33985098	2.88225996
H	1.66750845	-1.03652008	2.45483874
H	-2.51607845	4.99266378	1.79437403
H	-3.25195079	5.73754923	-0.45462133
H	-2.22714109	4.75186741	-2.48888630
H	-0.82390933	3.17907962	-3.54632074
H	0.75862814	3.14006516	-2.77020557
H	-0.31571927	1.74582732	-2.63458850
H	0.40709782	3.46994075	2.63978110
H	-1.26242008	3.57488866	3.20135323
H	-0.64882470	2.05433455	2.53645856
H	-2.81401071	-2.11927534	-0.10639970
H	-3.04350779	-2.92177830	-2.43852868
H	-1.03898095	-3.68079654	-3.69336956
H	1.19647543	-3.68246459	-2.60707724
H	1.42248809	-2.93560757	-0.25535558
H	-1.89440298	-0.18177004	2.38548624
H	-4.29045710	0.21867703	2.80683154
H	-5.78816711	0.95366238	0.95683173
H	-4.84998543	1.29100818	-1.32503197
H	-2.45550794	0.89521049	-1.76055628
H	-0.60485648	-2.27140992	1.04420828

ts-Ba'Ba'

Pt	0.00000000	0.00000000	0.00000000
N	2.12185495	0.00000000	0.00000000
N	0.50320806	2.06133090	0.00000000
C	2.69855264	1.17081205	0.00000000
C	1.77738113	2.34390759	0.00000000
C	2.34076207	3.73463779	-0.00007838
C	4.18321815	1.38832929	0.00030404
C	2.88716126	-1.23326558	0.00020338
C	3.22753631	-1.81845891	1.23694776
C	3.93611670	-3.02931103	1.21033144
C	4.28922606	-3.63143408	0.00055844
C	3.93604897	-3.02970790	-1.20938613
C	3.22743985	-1.81887326	-1.23635695
C	2.86119077	-1.16530117	-2.54946552
C	2.86124572	-1.16454765	2.54987691
C	-0.51334682	3.09730927	-0.00009543
C	-1.00155433	3.56658855	1.23652861
C	-2.00983743	4.54209529	1.20969331
C	-2.51063397	5.02807047	-0.00018838
C	-2.00932586	4.54251187	-1.21002447

C	-1.00101485	3.56703210	-1.23677418
C	-0.45257558	3.05635421	-2.54977680
C	-0.45354532	3.05552244	2.54955223
C	-0.39608827	-2.10533320	-0.00025981
C	-0.35701308	-2.81892680	1.21609291
C	-0.23250168	-4.21151198	1.21401573
C	-0.16428818	-4.90637317	-0.00063549
C	-0.23254795	-4.21119409	-1.21510179
C	-0.35704432	-2.81860613	-1.21680460
C	-2.13924512	0.11444634	-0.00017344
C	-2.82322896	0.32145528	1.21621113
C	-4.14657463	0.77263465	1.21421055
C	-4.80542978	1.00388866	-0.00040395
C	-4.14625892	0.77293035	-1.21490663
C	-2.82291367	0.32175562	-1.21668306
H	1.54857994	4.48274515	0.00175929
H	2.97493176	3.89805122	0.87957156
H	2.97168052	3.89919233	-0.88189522
H	4.49258037	1.96206788	0.88227189
H	4.72213717	0.44134412	-0.00162448
H	4.49247016	1.96582229	-0.87918958
H	4.20950708	-3.49737742	2.15039055
H	4.83693489	-4.56750705	0.00069966
H	4.20938950	-3.49807044	-2.14931355
H	3.06624609	-1.83983763	-3.38476306
H	3.43663645	-0.24655258	-2.72652015
H	1.79962957	-0.89341238	-2.58434435
H	3.06703902	-1.83856251	3.38541260
H	3.43606610	-0.24530222	2.72635192
H	1.79948787	-0.89342515	2.58496586
H	-2.40007486	4.91852490	2.14966968
H	-3.29015484	5.78210455	-0.00022397
H	-2.39918548	4.91925195	-2.15003429
H	-1.05849518	3.41632510	-3.38527146
H	0.57679042	3.39676628	-2.72612301
H	-0.44103312	1.96059568	-2.58509630
H	-1.05998475	3.41488992	3.38492885
H	-0.44158731	1.95975413	2.58437226
H	0.57561519	3.39624874	2.72650684
H	-0.43247233	-2.28792560	2.16002686
H	-0.19888073	-4.75373037	2.15318354
H	-0.07650692	-5.98781568	-0.00077799
H	-0.19896822	-4.75316500	-2.15441471
H	-0.43254774	-2.28736018	-2.16059340
H	-2.32529504	0.12200378	2.16010614
H	-4.66537142	0.93368553	2.15340143

H	-5.83521266	1.34560757	-0.00049531
H	-4.66481374	0.93421458	-2.15419121
H	-2.32473642	0.12254703	-2.16050149
H	-1.44383154	-1.13372565	-0.00017450

ts-BaCa

Pt	0.00000000	0.00000000	0.00000000
N	2.26196959	0.00000000	0.00000000
N	0.57241532	2.10142337	0.00000000
C	2.79033783	1.18926748	0.07760226
C	1.85266458	2.35693411	0.02648423
C	2.42752307	3.74459738	0.00419612
C	4.26222950	1.45584519	0.23016830
C	3.08729859	-1.19275349	-0.02278066
C	3.18550876	-1.98202634	1.14354879
C	3.95320406	-3.15549688	1.07562193
C	4.58563058	-3.53998894	-0.10761047
C	4.47144134	-2.74314049	-1.24876115
C	3.72957134	-1.55246338	-1.23128785
C	3.62668244	-0.70749955	-2.48410675
C	2.51204195	-1.59854324	2.44192751
C	-0.41261854	3.16972829	-0.01534778
C	-0.77654575	3.78627068	1.19983901
C	-1.76541388	4.78089041	1.15154000
C	-2.36118566	5.14922398	-0.05634612
C	-1.97833874	4.52296039	-1.24459144
C	-1.00040139	3.51780806	-1.24904420
C	-0.57811901	2.85405716	-2.53905796
C	-0.14120496	3.40210745	2.51803218
C	-0.47008243	-2.00079732	-0.38935679
C	-1.60146172	-2.67181285	0.11225669
C	-1.92651881	-3.94601154	-0.36703915
C	-1.13104670	-4.55869767	-1.34150102
C	0.00422986	-3.89966745	-1.82772008
C	0.35115697	-2.63450868	-1.33896212
C	-2.00303823	0.33604624	0.10833503
C	-2.59509120	0.74191266	1.31523401
C	-3.96316320	1.04436785	1.36273359
C	-4.74807925	0.94487677	0.20860899
C	-4.16371022	0.52948257	-0.99286769
C	-2.79976489	0.20940013	-1.04233445
H	1.65803914	4.48685310	-0.20552148
H	2.88433833	3.99266444	0.97084629
H	3.21594110	3.82788911	-0.75092387
H	4.44631353	2.14963417	1.05730052
H	4.81169398	0.53409280	0.41899701

H	4.67589470	1.92042722	-0.67354776
H	4.05103514	-3.76772984	1.96611408
H	5.16795031	-4.45414578	-0.13990577
H	4.96314141	-3.04033239	-2.16933459
H	3.96532184	-1.27606326	-3.35407312
H	4.25367750	0.19218305	-2.42937192
H	2.60015158	-0.37730436	-2.68213005
H	2.99661929	-2.09747026	3.28566369
H	2.53766909	-0.52055311	2.63010172
H	1.45677430	-1.90424502	2.45187537
H	-2.06836736	5.26330648	2.07508760
H	-3.12374805	5.92008248	-0.07134888
H	-2.44023191	4.80972541	-2.18349046
H	-1.18538065	3.21341662	-3.37360075
H	0.47227538	3.05746952	-2.78532634
H	-0.69650947	1.76380257	-2.49141364
H	-0.71651009	3.81196908	3.35220757
H	-0.09069781	2.31517494	2.64852652
H	0.88143393	3.79162902	2.61467216
H	-2.23464769	-2.20201167	0.85374395
H	-2.80265841	-4.45431328	0.02136013
H	-1.38734516	-5.54521247	-1.71266711
H	0.62755177	-4.36924372	-2.58153145
H	1.24475647	-2.15334015	-1.71172529
H	-2.00209833	0.82649359	2.22026728
H	-4.41093319	1.35615424	2.30116724
H	-5.80670814	1.17891398	0.24764532
H	-4.76829623	0.43560804	-1.88952417
H	-2.37335278	-0.15032500	-1.97315664
H	-0.03638542	-1.10828522	1.10785648

ts-Ba'Ca'

Pt	0.00000000	0.00000000	0.00000000
N	2.25333662	0.00000000	0.00000000
N	0.58069860	2.11405072	0.00000000
C	2.79376878	1.18343839	0.05333755
C	1.86225256	2.35902079	0.04147225
C	2.44728725	3.74134029	0.08782825
C	4.27377527	1.43628527	0.12961790
C	3.07127191	-1.19607547	0.03978835
C	3.45887511	-1.71462609	1.29450331
C	4.20540743	-2.90348115	1.30391987
C	4.56002559	-3.54145729	0.11238558
C	4.16419044	-3.00304868	-1.11434762
C	3.40500016	-1.82462725	-1.17793907
C	2.96132443	-1.25799383	-2.50628952

C	3.08191665	-1.03064923	2.59089343
C	-0.38841323	3.19639012	-0.05219532
C	-1.03152785	3.58453824	1.14126162
C	-1.99348745	4.60222221	1.05895855
C	-2.30620290	5.20307611	-0.16239504
C	-1.65301136	4.79844825	-1.32846915
C	-0.67784918	3.78985258	-1.29941454
C	0.02051911	3.36406698	-2.57317506
C	-0.69149371	2.94760993	2.46816530
C	-0.34225760	-1.97385283	-0.63588165
C	0.43823525	-3.06218499	-0.21246292
C	0.29618585	-4.30753276	-0.83932776
C	-0.62819763	-4.47528035	-1.87424560
C	-1.42667421	-3.39645928	-2.27217475
C	-1.30984417	-2.15186899	-1.64085634
C	-2.01420261	0.32837914	0.10682825
C	-2.78775125	-0.06546095	1.21223271
C	-4.16134507	0.21242570	1.25048643
C	-4.78052478	0.86750769	0.18115813
C	-4.01867852	1.25045746	-0.92812848
C	-2.64329857	0.98445536	-0.96453064
H	1.67255151	4.49483422	0.22337740
H	3.17306475	3.82888519	0.90299410
H	2.98495209	3.96659232	-0.84222394
H	4.54712929	1.85552554	1.10649562
H	4.83807186	0.51529386	-0.01244862
H	4.58842597	2.16119592	-0.62818362
H	4.50915997	-3.32460813	2.25674817
H	5.14159262	-4.45638790	0.14044244
H	4.43703304	-3.50052831	-2.03912496
H	3.29811380	-1.89494528	-3.32789577
H	3.36342304	-0.25235569	-2.68458251
H	1.86795378	-1.18871211	-2.56228253
H	3.28547698	-1.68470079	3.44253245
H	3.65419869	-0.10702089	2.75127944
H	2.01919421	-0.76175941	2.61896566
H	-2.49891991	4.91894341	1.96514566
H	-3.05699269	5.98440776	-0.20531809
H	-1.89825025	5.26399913	-2.27754309
H	-0.48490062	3.78728894	-3.44501718
H	1.06289469	3.70791309	-2.61042360
H	0.03590406	2.27382933	-2.69454555
H	-1.30344881	3.37431093	3.26669446
H	-0.87166341	1.86634804	2.44895014
H	0.36037981	3.10004070	2.74302438
H	1.15593153	-2.95457556	0.59018892

H	0.90625998	-5.14121537	-0.50835427
H	-0.73988162	-5.44123298	-2.35491326
H	-2.15623470	-3.52028799	-3.06572681
H	-1.96248109	-1.34267879	-1.93688413
H	-2.33740228	-0.59020535	2.04868492
H	-4.74462517	-0.09582340	2.11238906
H	-5.84529841	1.07297443	0.20900498
H	-4.48863212	1.75713669	-1.76505119
H	-2.07292168	1.29494163	-1.83482653
H	-0.37238271	-1.15076137	0.99170512

ts-BaIa

Pt	0.00000000	0.00000000	0.00000000
N	2.13007884	0.00000000	0.00000000
N	0.54126035	2.10120610	0.00000000
C	2.71707525	1.16971420	0.00986383
C	1.81967486	2.35956326	0.01674258
C	2.40711621	3.74207401	0.03568097
C	4.20582094	1.37091895	0.00894062
C	2.90103290	-1.23071650	-0.04597954
C	3.15946974	-1.91323411	1.15974988
C	3.86602888	-3.12287369	1.08488495
C	4.29046908	-3.63533782	-0.14296507
C	4.01691941	-2.93944530	-1.32214879
C	3.31835829	-1.72279567	-1.29962847
C	3.02854078	-0.97801458	-2.58394166
C	2.70294246	-1.36354817	2.49087562
C	-0.47923884	3.12275891	0.00676574
C	-0.93591035	3.63015700	1.24245739
C	-1.99870876	4.54714093	1.22088592
C	-2.58924575	4.94133660	0.01734359
C	-2.12156004	4.42223015	-1.19248575
C	-1.05859023	3.50388647	-1.22446323
C	-0.52492802	2.98141582	-2.54051221
C	-0.30413758	3.20714989	2.54992176
C	-0.66241412	-2.69919643	1.18524251
C	-0.83192662	-4.09080369	1.19078005
C	-0.66171497	-4.82666686	0.01287428
C	-0.32016568	-4.16137428	-1.16959667
C	-0.14358494	-2.77050953	-1.17301495
C	-0.30018999	-2.01659002	0.00659354
C	-2.02724961	0.09840237	0.01239822
C	-2.77769759	0.24349862	1.24247627
C	-4.14896609	0.08302213	1.28477414
C	-4.88914844	-0.19374227	0.10450986
C	-4.24626662	-0.30317114	-1.11430993

C	-2.83243933	-0.16243417	-1.17551985
H	1.62770284	4.50234502	-0.02622602
H	2.98043863	3.91200584	0.95554307
H	3.10057660	3.88537944	-0.80090872
H	4.51301498	2.01406399	0.84139852
H	4.73330489	0.42108320	0.09081687
H	4.53234042	1.86600747	-0.91442096
H	4.07672764	-3.66377018	2.00160524
H	4.82988371	-4.57545549	-0.18090946
H	4.34173909	-3.34006918	-2.27704904
H	3.23491384	-1.61330223	-3.44937910
H	3.64965452	-0.07791523	-2.68966269
H	1.98127032	-0.65884264	-2.63914098
H	2.95503398	-2.05507128	3.29893032
H	3.17359727	-0.39929025	2.72404701
H	1.61773967	-1.20865900	2.50304164
H	-2.36101076	4.95157711	2.16059762
H	-3.40897190	5.65140837	0.02234890
H	-2.57336554	4.73465975	-2.12863724
H	-1.22854936	3.18385872	-3.35268745
H	0.42480927	3.46356991	-2.80851651
H	-0.33195198	1.90225951	-2.50564257
H	-0.91274455	3.53510139	3.39675435
H	-0.18662154	2.11859679	2.61115239
H	0.69421576	3.64510052	2.68188706
H	-1.10000711	-4.59653598	2.11389232
H	-0.79692144	-5.90339837	0.01575234
H	-0.18770776	-4.72247784	-2.09010450
H	0.12923235	-2.27868057	-2.10264078
H	-2.31015936	-0.31844015	-2.11257782
H	-2.22970778	0.44681726	2.15461968
H	-4.67379936	0.16395662	2.23082407
H	-5.96518321	-0.31515411	0.16551514
H	-4.79916296	-0.51297079	-2.02256184
H	-2.35298372	1.08824067	-0.76078091
H	-0.80800378	-2.14952539	2.11140763

ts-HaEa

C	0.00000000	0.00000000	0.00000000
C	1.40942002	0.00000000	0.00000000
C	2.17146605	1.18546655	0.00000000
C	1.47517005	2.40333506	0.01314930
C	0.07904332	2.43555366	0.02409365
C	-0.64869893	1.24344948	0.01419097
N	2.10875023	-1.27741564	0.00508962
C	2.41959718	-1.86932148	-1.13083581

C	2.09391477	-1.29656059	-2.48132900
C	3.68170014	1.15877663	-0.03548392
C	-0.79481375	-1.28525016	-0.03063629
Pt	2.52993576	-2.25318009	1.73363849
N	3.36021987	-3.59930831	0.17047877
C	3.15053234	-3.14951511	-1.03939447
C	3.61530303	-3.82928815	-2.29722996
C	1.84917898	-0.79050525	2.97142843
C	0.51920088	-0.75806494	3.42741894
C	0.08508481	0.24732967	4.30256552
C	0.97061059	1.24242329	4.73038730
C	2.29335256	1.22455411	4.27627081
C	2.72767697	0.21951029	3.40088490
C	5.27579661	-2.64281720	3.49148601
C	5.78048300	-1.66122938	4.35088908
C	5.10764838	-1.36575409	5.54317275
C	3.92810484	-2.04650435	5.87858984
C	3.41761103	-3.02072167	5.02035054
C	4.08169179	-3.32215283	3.81266688
C	4.18135396	-4.76602603	0.41595286
C	5.58918352	-4.62617272	0.39508850
C	6.36429049	-5.74697856	0.73303029
C	5.76797420	-6.96737589	1.05584227
C	4.37707156	-7.09122852	1.02907072
C	3.55708790	-5.99945060	0.70536304
C	6.26627169	-3.33365146	-0.01134084
C	2.05959725	-6.16794602	0.59611672
N	1.02244844	-3.97699872	3.03473904
C	0.11593370	-4.45281776	3.59986353
C	-1.01325685	-5.03688426	4.31249713
H	1.61954634	-0.32001058	-2.40151999
H	3.00113303	-1.19368585	-3.08778991
H	1.41768295	-1.96387692	-3.03036278
H	4.37018636	-3.22681647	-2.81772597
H	4.04974967	-4.80500951	-2.07893592
H	2.78145600	-3.96722199	-2.99414589
H	7.44564997	-5.65447664	0.73510747
H	6.38453436	-7.82055925	1.31666607
H	3.91309072	-8.04654710	1.25247750
H	1.73935242	-7.09525312	1.07956189
H	1.74307999	-6.22488003	-0.45478320
H	1.52271560	-5.33461705	1.05491107
H	7.29485227	-3.30571908	0.35961245
H	6.32216110	-3.23819309	-1.10441153
H	5.74402587	-2.44931141	0.36717263
H	2.03986320	3.32981243	0.01803765

H	-0.44062601	3.38733283	0.04014645
H	-1.73348409	1.26921727	0.01961437
H	-1.85605528	-1.08287340	0.13620415
H	-0.71048947	-1.79736720	-0.99886951
H	-0.45491144	-1.98865462	0.73783251
H	4.08734855	2.15766265	0.14411781
H	4.09005902	0.48344725	0.72385352
H	4.06231360	0.82314017	-1.00990896
H	6.70293714	-1.14519715	4.10563475
H	5.50498520	-0.61241637	6.21563914
H	3.41588696	-1.81660005	6.80639073
H	2.51389736	-3.55620113	5.28373727
H	3.77494260	-4.18433668	3.22775564
H	3.76126636	0.22014980	3.07137986
H	2.99065312	1.99209510	4.59932311
H	0.63306113	2.02299835	5.40455931
H	-0.94629549	0.25403768	4.64373671
H	-0.18818465	-1.51396701	3.10449606

ts-Ha'Ea

C	0.00000000	0.00000000	0.00000000
C	1.40745710	0.00000000	0.00000000
C	2.07331715	1.24152047	0.00000000
C	1.35141283	2.44398218	-0.01569533
C	-0.04700699	2.42843518	-0.02955863
C	-0.72063488	1.20211250	-0.02166190
Pt	2.48314951	-1.73026732	-0.04658420
N	4.62198898	-0.39324904	-1.40108611
C	5.37743451	0.34806398	-1.89976252
C	6.31203032	1.27660046	-2.52327658
N	2.12550995	-2.27352815	1.86782296
C	2.70894527	-3.36543176	2.31577417
C	3.57180249	-4.09872627	1.36536777
N	3.64526934	-3.59097775	0.16357206
C	4.46906262	-4.20378325	-0.85785285
C	5.83219683	-3.84834845	-0.94497419
C	6.59284704	-4.42936253	-1.97185874
C	6.02576666	-5.34567029	-2.86087325
C	4.68016438	-5.69900722	-2.73450755
C	3.87322996	-5.13462180	-1.73475951
C	6.47407475	-2.90902345	0.05134280
C	2.42238484	-5.53223714	-1.59209235
C	1.22835277	-1.51237681	2.72349958
C	-0.12096021	-1.91321672	2.80951438
C	-0.97176931	-1.15084970	3.62362478
C	-0.49449992	-0.04108260	4.32456372

C	0.85000668	0.32510755	4.22617075
C	1.74128154	-0.40111914	3.42299940
C	-0.64629995	-3.11859911	2.06221971
C	3.19667797	-0.00943446	3.33033591
C	2.53623516	-3.88118982	3.71542512
C	4.28605227	-5.34136468	1.81787316
C	1.96640263	-1.57044048	-2.80940445
C	2.90174011	-2.31445467	-3.55224927
C	2.46218984	-3.31559712	-4.42340636
C	1.09182441	-3.58359942	-4.54915723
C	0.15595371	-2.85283584	-3.80306100
C	0.58957369	-1.84418505	-2.93775235
H	1.99534449	-3.17357946	4.34172405
H	1.98236457	-4.82903644	3.71428624
H	3.51048692	-4.08252387	4.17367499
H	3.58594023	-6.05463939	2.26658199
H	4.79195082	-5.82914505	0.98498763
H	5.03680146	-5.10533527	2.58265415
H	4.24215945	-6.42338866	-3.41357262
H	6.63275301	-5.79030082	-3.64220773
H	7.64241548	-4.16687720	-2.05935234
H	7.46253002	-2.59764612	-0.29824101
H	6.61870503	-3.39258867	1.02740219
H	5.86958855	-2.01170419	0.21267336
H	2.12797669	-6.20810969	-2.39854361
H	2.23236168	-6.05172494	-0.64344414
H	1.76038989	-4.65985389	-1.62587534
H	-2.01645201	-1.43390662	3.70119937
H	-1.16880398	0.53725574	4.94669905
H	1.22030236	1.18535424	4.77371865
H	3.38315229	0.90929173	3.89207499
H	3.85842841	-0.78486541	3.73853741
H	3.49652758	0.16068478	2.29015941
H	-1.73941412	-3.12533924	2.06816656
H	-0.31134430	-3.13128673	1.01850029
H	-0.31714372	-4.06147981	2.51984383
H	-0.90392411	-3.05732050	-3.91220946
H	0.75260271	-4.35493871	-5.23337840
H	3.18181407	-3.88095217	-5.00525979
H	3.95950940	-2.09927125	-3.45657215
H	2.28692974	-0.67180703	-2.28317781
H	-0.54623507	-0.93759867	0.02124528
H	-1.80619367	1.17741719	-0.02760643
H	-0.60488644	3.35902000	-0.04233999
H	1.88484090	3.39010798	-0.01475719
H	3.15720317	1.27761283	0.00864740

H	-0.12688395	-1.24753175	-2.38588804
H	6.66974146	0.87810188	-3.47790688
H	7.17614072	1.44753152	-1.87351147
H	5.82515111	2.23870506	-2.71198397

ts-HbEb

C	0.00000000	0.00000000	0.00000000
C	1.39433573	0.00000000	0.00000000
C	2.12388327	1.19633998	0.00000000
C	1.44695667	2.42350330	0.00098865
C	0.04105669	2.41494516	-0.00582460
C	-0.69491399	1.22088647	-0.00261695
N	2.11055562	-1.26242050	0.01216302
C	2.74124897	-1.68270778	-1.06933783
C	2.70282613	-0.96216214	-2.38854808
H	3.20889841	1.16999535	0.01777280
H	-0.53990034	-0.93975766	0.02279180
Pt	2.22220999	-2.41523335	1.67832938
N	3.46062582	-3.51894019	0.22748149
C	3.51133270	-2.93543015	-0.94535787
C	4.26682762	-3.45832149	-2.13716402
C	1.11005994	-1.18240025	2.84851419
C	-0.22898658	-1.47816054	3.16300642
C	-0.98163703	-0.61960277	3.97712032
C	-0.40998109	0.55198526	4.48636851
C	0.91815204	0.85990643	4.17259316
C	1.66964176	0.00247981	3.35697467
C	4.62811706	-2.57119592	3.58505024
C	4.86344676	-1.53797730	4.49854536
C	4.02295939	-1.38419986	5.60814151
C	2.94101210	-2.25477147	5.80880356
C	2.69710579	-3.28239677	4.89827632
C	3.53288030	-3.44645582	3.77144350
C	4.23124571	-4.69543014	0.53321837
C	5.63378692	-4.63014345	0.55873632
C	6.38663000	-5.76143592	0.90911681
C	5.70720306	-6.95213639	1.21437059
C	4.30539734	-7.03337845	1.18613696
C	3.56752543	-5.88592456	0.85491441
H	6.13553866	-3.69671898	0.32255285
H	2.48477667	-5.91140133	0.84082973
N	0.82254751	-4.51727748	2.39278758
C	-0.08204184	-5.22845991	2.60154654
C	-1.21720414	-6.10229997	2.87087613
H	1.99266121	-0.13763572	-2.37703868
H	3.68968125	-0.55622039	-2.64505200

H	2.42168357	-1.65188110	-3.19175272
H	5.06776745	-2.77026522	-2.43436263
H	4.71409902	-4.42953940	-1.93087264
H	3.59858964	-3.56103188	-2.99933045
C	7.89682878	-5.69982435	0.96668975
H	6.28241768	-7.83411482	1.48254700
C	3.60552542	-8.33952421	1.48929788
C	2.20870452	3.73003419	0.02174215
H	-0.49191462	3.36160763	-0.00556669
C	-2.20613401	1.23534742	0.03551351
H	5.70620243	-0.86923085	4.35860922
H	4.21286686	-0.58935784	6.32210842
H	2.29715835	-2.12755509	6.67193868
H	1.86985260	-3.96519291	5.05397976
H	3.44902658	-4.34428218	3.16871003
H	2.69609638	0.26397226	3.12003331
H	1.37147928	1.76870936	4.55782496
H	-0.99282401	1.21729824	5.11539053
H	-2.01304535	-0.86799393	4.21190347
H	-0.69481943	-2.37659293	2.77289159
H	5.30658456	-2.73382716	2.75503454
H	-0.88707731	-7.02356563	3.36116954
H	-1.72765316	-6.36845599	1.93991246
H	-1.93515466	-5.60080128	3.52787070
H	3.64880027	-9.01984166	0.62886943
H	2.54975852	-8.18265020	1.73086846
H	4.07390405	-8.85640988	2.33351355
H	8.27747959	-4.75449778	0.56890011
H	8.35013210	-6.51424239	0.39042204
H	8.25754994	-5.79546495	1.99841368
H	1.85938566	4.40834280	-0.76502326
H	3.28197628	3.57321534	-0.12157403
H	2.07415713	4.24943301	0.97876037
H	-2.63534011	0.51675458	-0.67170574
H	-2.60307784	2.22520299	-0.20664494
H	-2.56921077	0.96643334	1.03592256

ts-He_bEe_b

C	0.00000000	0.00000000	0.00000000
C	1.40159892	0.00000000	0.00000000
C	2.13029617	1.19035990	0.00000000
C	1.45087991	2.41920443	-0.01201857
C	0.04710381	2.41235068	-0.01609507
C	-0.69419031	1.21786610	-0.00380970
N	2.10621096	-1.26640247	0.01378357
C	2.09811516	-2.07485160	-1.02955498

C	1.43629159	-1.72292345	-2.33217874
C	2.22284682	3.71863206	0.01743326
C	-2.20617010	1.25009165	0.00901152
Pt	3.10699201	-1.86485063	1.64725798
O	1.83603183	-3.95476135	3.86763238
C	0.52781504	-4.25032807	3.26882382
C	-0.01524869	-5.61879949	3.67225018
N	3.43712619	-3.51815378	0.25733133
C	2.81752350	-3.35668600	-0.88829468
C	2.75174361	-4.36854475	-2.00020769
C	4.25629904	-4.64624581	0.57683613
C	5.26354765	-5.09103165	-0.29862864
C	6.08409245	-6.16900416	0.06216357
C	5.85949581	-6.80015742	1.29762831
C	4.86044386	-6.36374375	2.18452390
C	4.06906943	-5.26214760	1.82525844
C	4.64462805	-7.06491763	3.50737308
C	7.19284503	-6.64030079	-0.85227944
C	2.69146449	-0.36052803	2.91328887
C	1.41628461	-0.25949889	3.50577604
C	1.16708874	0.68842721	4.50610004
C	2.18008349	1.56923708	4.90715270
C	3.44152603	1.49705469	4.30455719
C	3.69510610	0.54673948	3.30570745
C	1.77651270	-3.56648107	5.28493427
C	3.19075146	-3.29567064	5.76375450
C	6.05508661	-2.40916748	3.07293589
C	6.40922680	-1.85212513	1.83090766
C	7.11483299	-0.64019943	1.78078088
C	7.47380534	0.00773283	2.96799179
C	7.12701605	-0.55092802	4.20867142
C	6.41836126	-1.75433184	4.26127877
H	5.43644911	-4.57762552	-1.23857141
H	3.30855413	-4.88994645	2.50704392
H	3.21381389	1.16005976	0.02693252
H	-0.54411268	-0.93895031	0.01971147
H	1.24436987	-0.65289394	-2.40541062
H	2.06573810	-2.02773594	-3.17322501
H	0.47486631	-2.24165800	-2.44134197
H	3.42402438	-4.11204025	-2.82893733
H	3.03221789	-5.36037431	-1.64344490
H	1.73912633	-4.41854654	-2.41184882
H	6.48501049	-7.64314270	1.57924472
H	-0.48287087	3.36067733	-0.02134201
H	7.39995347	-0.21683066	0.82299089
H	8.03283603	0.93723838	2.93096533

H	7.41813526	-0.05168449	5.12694511
H	6.16200842	-2.19100856	5.22051941
H	5.56085686	-3.37463450	3.11402059
H	4.67691393	0.50901325	2.84553671
H	4.22881596	2.18138918	4.60629453
H	1.98388613	2.31143395	5.67433813
H	0.18366468	0.74652357	4.96301208
H	0.61716793	-0.92249482	3.18765304
H	6.17707199	-2.38280648	0.91436466
H	0.70885131	-4.20441757	2.19136927
H	-0.17694762	-3.44883727	3.53341994
H	1.31394650	-4.37421545	5.86573331
H	1.15120582	-2.66831419	5.37664409
H	3.18091831	-3.01504797	6.82278632
H	3.63734644	-2.47439185	5.19590832
H	3.81703309	-4.18710293	5.65202089
H	-0.22209083	-5.67937309	4.74542685
H	0.69824044	-6.40799034	3.41419032
H	-0.95458460	-5.82025621	3.14408656
H	1.60998676	4.55583620	-0.32855243
H	3.11771024	3.67077887	-0.61206507
H	2.55380578	3.95012929	1.03822594
H	-2.58343710	1.72253897	0.92402658
H	-2.63149726	0.24361187	-0.04498221
H	-2.59922333	1.82663647	-0.83652161
H	7.19706760	-6.09028285	-1.79781373
H	7.08969989	-7.70665981	-1.08459874
H	8.17558712	-6.50578188	-0.38446262
H	3.86209740	-6.57396019	4.09251501
H	5.56273801	-7.07615942	4.10686242
H	4.34675237	-8.10990522	3.35755916

ts-Ht_aEt_a

C	0.00000000	0.00000000	0.00000000
C	1.41826033	0.00000000	0.00000000
C	2.15701542	1.20332753	0.00000000
C	1.44903352	2.41477958	0.02018669
C	0.05356159	2.43834998	0.04483014
C	-0.65963719	1.23876681	0.03379514
N	2.10331762	-1.27843009	0.03830562
C	2.12394872	-2.05853166	-1.01454158
C	1.68993498	-1.64645221	-2.39414511
C	3.66447142	1.20425656	-0.05495840
C	-0.81527587	-1.27660540	-0.03174023
Pt	2.92266407	-2.31270343	1.84320003
C	3.51563331	-3.47127389	3.39941709

C	2.56525695	-4.22606441	4.10968723
C	2.93875910	-4.97884086	5.23112132
C	4.27213703	-5.00287860	5.65420903
C	5.22943529	-4.26755682	4.94784062
C	4.85535936	-3.51150615	3.82743520
N	2.81084528	-3.79459711	0.46825157
C	2.54830094	-3.45332340	-0.77857709
C	2.57228564	-4.42662784	-1.92357753
C	3.05551620	-5.18791120	0.81587349
C	1.94443967	-5.98475557	1.16205452
C	2.18783680	-7.32016550	1.51572782
C	3.48389395	-7.84001209	1.51914374
C	4.56322786	-7.02981389	1.15997703
C	4.37272149	-5.68767180	0.79918693
C	0.53520801	-5.43795180	1.14624530
C	5.54178903	-4.82396750	0.39211008
C	1.81076785	-0.41102851	3.81244725
C	0.54115254	-0.91678465	3.46975010
C	-0.21021850	-1.63202790	4.41185897
C	0.29590811	-1.83387224	5.69987197
C	1.55214727	-1.31774110	6.05317810
C	2.30447427	-0.60763688	5.11696321
H	2.92508469	-5.40780138	-1.61030233
H	1.57212145	-4.54627214	-2.35847483
H	3.22540545	-4.05996025	-2.72389566
H	0.81204902	-2.21234887	-2.72829487
H	1.44491576	-0.58501060	-2.42852153
H	2.48858646	-1.84209874	-3.11892372
H	-1.74465917	1.25270888	0.04886428
H	-0.47471012	3.38512886	0.06784639
H	2.00693522	3.34541617	0.01053974
H	4.04531805	2.22875581	-0.08910754
H	4.03858905	0.68453490	-0.94669153
H	4.08653470	0.70371618	0.82251059
H	-1.83923936	-1.07954649	0.29756566
H	-0.88421078	-1.69309782	-1.04546665
H	-0.39685179	-2.05413076	0.61581541
H	1.34886565	-7.95050213	1.79176804
H	3.65250443	-8.87378914	1.80020647
H	5.56979258	-7.43481425	1.15897902
H	6.48564682	-5.34536273	0.57087096
H	5.50910060	-4.56204251	-0.67423176
H	5.55600103	-3.88744699	0.95891505
H	-0.15550409	-6.14611325	1.61126154
H	0.46361907	-4.48674736	1.68598619
H	0.17593358	-5.25942705	0.12352230

H	-1.19351763	-2.00863763	4.14913048
H	-0.28962871	-2.37798362	6.43382933
H	1.93385742	-1.46365654	7.05784784
H	3.26134625	-0.19008395	5.40516888
H	2.34555503	0.22957652	3.11605386
H	1.52500733	-4.22217899	3.80244164
H	2.18661123	-5.54805466	5.76928859
H	4.56211398	-5.59171366	6.51839419
H	6.26920977	-4.28412927	5.26186733
H	5.61445698	-2.95091829	3.29586313
H	0.12773051	-0.70497648	2.49286834
O	4.93711582	-0.68064459	2.33528226
C	6.10169786	-0.88884498	1.43191355
C	7.07686872	0.22395820	1.81285668
C	6.90768035	0.30877996	3.34817139
C	5.41573943	0.00587548	3.57879083
H	6.52768161	-1.88125507	1.61839446
H	5.72090375	-0.83947431	0.41179241
H	6.78578232	1.16709739	1.33722185
H	8.10492823	-0.00351586	1.51755459
H	7.19143957	1.28721340	3.74467869
H	7.53295404	-0.44459237	3.83958784
H	4.81073603	0.90937052	3.68783166
H	5.24038088	-0.66736575	4.41877220

ts-Ht_bEt_b

C	0.00000000	0.00000000	0.00000000
C	1.40692624	0.00000000	0.00000000
C	2.11451985	1.21084742	0.00000000
C	1.42154332	2.43026413	-0.04744474
C	0.01714772	2.41236762	-0.05335798
C	-0.70848543	1.20986473	-0.01777136
N	2.13731697	-1.23344138	0.07116574
C	1.91649053	-2.23735890	-0.74775557
C	1.01998485	-2.19160820	-1.95712579
H	3.19688375	1.19254737	0.05510575
H	-0.54219292	-0.93888250	0.04585247
Pt	3.61650168	-1.73136898	1.63418464
C	4.92477449	-2.41508112	3.02125440
C	4.48507128	-3.23900675	4.07161836
C	5.37961064	-3.69374230	5.05009757
C	6.73277779	-3.34220550	4.98897182
C	7.18567030	-2.53290142	3.94106278
C	6.28963888	-2.07594491	2.96332737
N	3.41571669	-3.47738436	0.63089500
C	2.63730621	-3.48588672	-0.43671433

C	2.45956239	-4.68737691	-1.32369232
C	4.08976021	-4.68761010	1.06551490
C	3.34253324	-5.69080954	1.69635895
C	3.97916978	-6.86077490	2.13375760
C	5.36170228	-6.99407000	1.91743456
C	6.11647783	-5.99086096	1.29113279
C	5.46240958	-4.82470212	0.86081959
H	2.27805822	-5.55274875	1.85803318
H	6.02171977	-4.02309087	0.39196118
C	2.72110681	0.20945344	3.43023287
C	1.56254626	-0.59065685	3.54118852
C	1.28613051	-1.26395970	4.73920850
C	2.15238498	-1.13143125	5.82895778
C	3.29877244	-0.32639674	5.73069381
C	3.57992658	0.34385653	4.54101022
H	3.05575594	-5.53189655	-0.98487661
H	1.40895293	-5.00022112	-1.35594891
H	2.75435821	-4.44824795	-2.35249017
H	0.09745003	-2.76514777	-1.80151044
H	0.73821020	-1.16836136	-2.20395497
H	1.52520828	-2.63129022	-2.82263337
C	-2.22078420	1.22408059	0.00959641
H	-0.52410477	3.35442634	-0.07354188
C	2.17173680	3.74262766	-0.09880860
C	3.20133980	-7.95028967	2.83765274
H	5.86267796	-7.89813987	2.25198111
C	7.61058937	-6.13580426	1.11202514
H	0.39035071	-1.86991008	4.82668589
H	1.93252750	-1.64347809	6.76015341
H	3.96053927	-0.22139283	6.58337130
H	4.45216519	0.98394866	4.47588785
H	2.86768801	0.83031965	2.55248878
H	3.44160439	-3.53080113	4.13209900
H	5.01825419	-4.32553711	5.85628088
H	7.42596142	-3.69818414	5.74442008
H	8.23511607	-2.25840244	3.87982033
H	6.66451833	-1.46004629	2.15270354
H	0.86161129	-0.63869520	2.71614894
O	5.11465214	0.35022576	1.05023757
C	5.82407730	0.12959115	-0.24093968
C	6.73512775	1.34852675	-0.39568082
C	7.15375150	1.64975769	1.06221686
C	5.89352645	1.32385567	1.87895319
H	6.39039858	-0.80562142	-0.17155204
H	5.05704390	0.03496675	-1.01164623
H	6.17894703	2.19241087	-0.81985232

H	7.59194797	1.14776513	-1.04475840
H	7.47523919	2.68561147	1.19994574
H	7.98386197	0.99940080	1.36007957
H	5.25314572	2.19767357	2.03259986
H	6.10844727	0.84639362	2.83573248
H	3.43978932	-8.93835208	2.42869662
H	2.12163097	-7.79888213	2.74597823
H	3.44217027	-7.97741804	3.90798312
H	7.93426203	-5.79392135	0.12272316
H	7.92895159	-7.17534007	1.23078574
H	8.14863047	-5.53601326	1.85764188
H	-2.63483999	0.21291030	-0.04297828
H	-2.62753494	1.79747425	-0.83141392
H	-2.59594935	1.69024760	0.92880897
H	2.14652034	4.17249806	-1.10846503
H	3.22269022	3.61513635	0.17842044
H	1.73022956	4.48253642	0.57745291

tsIaBa'

Pt	0.00000000	0.00000000	0.00000000
N	2.16113207	0.00000000	0.00000000
N	0.52220844	2.06323680	0.00000000
C	2.72487108	1.17959414	-0.02248494
C	1.79972678	2.34417546	-0.01641649
C	2.35981222	3.73804673	-0.03000034
C	4.20876296	1.41374848	-0.04831860
C	2.94742895	-1.21695004	-0.03449000
C	3.21361188	-1.88485667	1.17908213
C	3.93505745	-3.08678438	1.11857478
C	4.36975844	-3.60660896	-0.10308302
C	4.09025991	-2.92624501	-1.29034269
C	3.37658103	-1.71759765	-1.28216105
C	3.08470036	-0.98778354	-2.57519825
C	2.75844746	-1.31975332	2.50470848
C	-0.48670062	3.10136451	0.06380353
C	-0.81560330	3.65439135	1.32061593
C	-1.83524384	4.61838867	1.36254811
C	-2.49808375	5.01809423	0.19993777
C	-2.15218031	4.45411408	-1.03034303
C	-1.14394405	3.48275119	-1.12476090
C	-0.76758506	2.88446977	-2.46001869
C	-0.10982501	3.22738710	2.58975480
C	-0.72220195	-2.62533297	1.36614688
C	-0.54917486	-3.98341143	1.63250183
C	-0.02988166	-4.82726548	0.64008721
C	0.30833623	-4.31497046	-0.62231279

C	0.14673820	-2.95663310	-0.88700614
C	-0.37991625	-2.05786517	0.09473574
C	-2.00774948	0.08956482	-0.05932094
C	-2.82589431	0.68276389	0.92009378
C	-4.19623790	0.40733757	0.97925256
C	-4.81029513	-0.48869919	0.07736907
C	-4.04708145	-1.08426142	-0.91325856
C	-2.64040962	-0.83964716	-0.97698430
H	1.57047461	4.48097553	-0.14313758
H	2.90073188	3.95284915	0.90047653
H	3.07628151	3.86134686	-0.84963569
H	4.50959531	2.09974458	0.75117008
H	4.75859595	0.48011586	0.06928882
H	4.51623842	1.87449778	-0.99581294
H	4.15571286	-3.61228803	2.04205626
H	4.92626768	-4.53726079	-0.12941561
H	4.42831667	-3.32946594	-2.23973421
H	3.27851510	-1.63609558	-3.43405700
H	3.71698828	-0.09786516	-2.69695774
H	2.04231213	-0.65195105	-2.62854455
H	2.97892441	-2.01729572	3.31693190
H	3.26082527	-0.37239107	2.74078151
H	1.68016163	-1.12222989	2.50694004
H	-2.10577502	5.05442284	2.31893487
H	-3.28182626	5.76595819	0.25254315
H	-2.66566466	4.76547779	-1.93412577
H	-1.43490973	3.24650211	-3.24637330
H	0.25777312	3.14629837	-2.75258142
H	-0.82564954	1.78974486	-2.43675865
H	-0.64497826	3.59803493	3.46809581
H	-0.03867422	2.13607977	2.67054141
H	0.91270817	3.62388907	2.64696338
H	-0.82208874	-4.38850802	2.60135584
H	0.09629157	-5.88583218	0.84369563
H	0.70163339	-4.97618871	-1.38706885
H	0.41050489	-2.57178347	-1.86741180
H	-1.73743336	-1.77276880	-0.38416329
H	-2.39176945	1.36105053	1.64496814
H	-4.80126549	0.88616300	1.74363135
H	-5.87375708	-0.68672243	0.15119651
H	-4.50918064	-1.73464105	-1.64962984
H	-2.15117376	-1.04606551	-1.93010941
H	-1.15690382	-1.98145595	2.12524378

The structures optimized at B2 basis set:

Ba			
Pt	0.07811000	0.31894300	0.00304400
N	1.80639200	-1.09158600	-0.00260300
N	-0.80920400	-1.55015000	-0.01045600
C	1.45021900	-2.33330600	-0.01720500
C	-0.02309100	-2.58781500	-0.01962000
C	-0.51005700	-4.00858000	-0.03052500
C	2.39770800	-3.50041800	-0.03053600
C	3.19118900	-0.70288100	0.00100800
C	3.83562200	-0.47751900	-1.23168600
C	5.15339100	-0.00454500	-1.19925500
C	5.80557500	0.23096200	0.00995900
C	5.14845700	-0.01379600	1.21465000
C	3.83048200	-0.48643200	1.23796500
C	3.13881700	-0.78499000	2.54916600
C	3.14934100	-0.76423500	-2.54843300
C	-2.24780900	-1.73356800	-0.00426000
C	-2.92285300	-1.79480000	-1.23578500
C	-4.31430100	-1.94004900	-1.20070000
C	-4.99977700	-2.02173500	0.00996900
C	-4.29889800	-1.96887700	1.21337500
C	-2.90709700	-1.82462200	1.23402000
C	-2.15301300	-1.79376000	2.54202900
C	-2.18467400	-1.73636400	-2.55168500
C	1.41499500	2.21737700	-0.70038300
C	0.72514000	3.24138300	-1.39841500
C	0.05065300	4.22430300	-0.69654500
C	0.03534500	4.21489000	0.71600400
C	0.69526800	3.22276400	1.41798900
C	1.40053600	2.20771100	0.72038000
C	-1.67001700	1.34682400	0.00095000
C	-2.28241200	1.72322700	-1.20311200
C	-3.50475400	2.40660100	-1.20633600
C	-4.13572100	2.72846000	-0.00309200
C	-3.53431200	2.36043600	1.20228800
C	-2.31285600	1.67603700	1.20308600
H	-1.59696000	-4.06262200	-0.05383200
H	-0.11134200	-4.54132000	-0.90169900
H	-0.15068700	-4.54108600	0.85820000
H	2.24596900	-4.11206500	-0.92766000
H	3.43455400	-3.16487800	-0.00955000
H	2.22197900	-4.15273200	0.83258800
H	5.66937800	0.17639700	-2.13829300
H	6.82620300	0.60111100	0.01339900
H	5.66063000	0.15965500	2.15715500
H	3.69970900	-0.36239800	3.38718700

H	3.05897600	-1.86602000	2.72652800
H	2.11928200	-0.38222600	2.58275900
H	3.71191500	-0.33087700	-3.37983300
H	3.07369800	-1.84347600	-2.73821400
H	2.12876200	-0.36407900	-2.58144200
H	-4.86051000	-1.98840900	-2.13863900
H	-6.08019700	-2.12928000	0.01558200
H	-4.83310500	-2.03907800	2.15684100
H	-2.84641100	-1.71541800	3.38355900
H	-1.55942400	-2.70539000	2.69505700
H	-1.46125500	-0.94514600	2.59274300
H	-2.88815400	-1.64379900	-3.38331000
H	-1.49605700	-0.88488100	-2.59390000
H	-1.59026400	-2.64315300	-2.72871300
H	0.75917000	3.26467000	-2.48376000
H	-0.46459800	5.01623400	-1.23198300
H	-0.49132900	4.99962900	1.25043000
H	0.70594800	3.23026500	2.50393700
H	2.11249000	1.59439000	1.26319100
H	-1.81088700	1.49219800	-2.15480400
H	-3.95890200	2.68604800	-2.15426200
H	-5.08374100	3.25862700	-0.00464800
H	-4.01155000	2.60404700	2.14869500
H	-1.86535600	1.40780300	2.15657900
H	2.13257800	1.60579300	-1.23747800

Ba'

Pt	-0.09241000	-0.48017600	-0.00055900
N	1.57709500	1.07501200	-0.00213000
N	-1.07564400	1.34401800	-0.00534600
C	1.11868000	2.28387400	-0.00898100
C	-0.36765900	2.43298800	-0.01190800
C	-0.95668100	3.81561800	-0.01943500
C	1.96048300	3.53199800	-0.01193700
C	3.00332300	0.87198000	0.00637900
C	3.66659800	0.78280800	1.24409300
C	5.05375800	0.58965600	1.22671800
C	5.75338400	0.49184000	0.02472900
C	5.06964400	0.58702800	-1.18637900
C	3.68308900	0.78138700	-1.22231100
C	2.95652600	0.92571600	-2.53868800
C	2.92241900	0.92751000	2.55057600
C	-2.52329000	1.43196400	-0.00290400
C	-3.19110400	1.47147900	1.23339000
C	-4.58900800	1.53184400	1.20863700
C	-5.28770000	1.55467000	0.00296800

C	-4.59442600	1.52545900	-1.20570000
C	-3.19665200	1.46476400	-1.23637900
C	-2.45232500	1.46909500	-2.55048200
C	-2.44107300	1.48255000	2.54421000
C	0.88144500	-2.59962400	0.70401800
C	2.12103400	-2.53548500	1.39353300
C	3.30625000	-2.49907900	0.68314500
C	3.29604100	-2.49860600	-0.73133400
C	2.10030200	-2.53739700	-1.42380900
C	0.87192700	-2.60191400	-0.71506500
C	-1.81722800	-1.55723500	0.00511600
C	-2.41662900	-1.94734800	1.21215000
C	-3.59781700	-2.69972700	1.21808600
C	-4.19749600	-3.08018300	0.01620200
C	-3.60769400	-2.70167300	-1.19121900
C	-2.42658100	-1.94923000	-1.19632800
H	-2.04466300	3.79120200	-0.03294200
H	-0.62857200	4.37410200	0.86509200
H	-0.60584300	4.37439800	-0.89471900
H	1.73004200	4.15395900	0.86064100
H	3.02365400	3.29764000	-0.00074900
H	1.74584500	4.13842500	-0.89951300
H	5.58635200	0.52450300	2.17191700
H	6.82958900	0.34711400	0.03203900
H	5.61442600	0.51913200	-2.12436300
H	3.60475500	0.64041500	-3.37184900
H	2.64110900	1.96259100	-2.71747700
H	2.05452100	0.30449600	-2.57746400
H	3.56082600	0.64634900	3.39278200
H	2.60000100	1.96326300	2.72332100
H	2.02266000	0.30235300	2.57873300
H	-5.12990300	1.56108600	2.15050300
H	-6.37264500	1.59708800	0.00528800
H	-5.13956700	1.54967300	-2.14525800
H	-3.13888400	1.28844900	-3.38190000
H	-1.96297300	2.43461300	-2.73891400
H	-1.67177600	0.70055600	-2.58121100
H	-3.12413800	1.30667100	3.37952000
H	-1.66074900	0.71381800	2.57569100
H	-1.95041300	2.44879800	2.72535700
H	2.12920000	-2.57464700	2.47907600
H	4.25561000	-2.48994300	1.20897200
H	4.23819400	-2.48695600	-1.26962400
H	2.09085200	-2.57772400	-2.50919000
H	-0.02674800	-2.89324400	-1.24732000
H	-1.97067200	-1.66813500	2.16399700

H	-4.04239000	-2.98874400	2.16736400
H	-5.11080500	-3.66775900	0.02043000
H	-4.06002800	-2.99233000	-2.13631700
H	-1.98865200	-1.67131500	-2.15224600
H	-0.00961100	-2.88977400	1.24969700
Ca			
Pt	0.00154500	0.37037500	-0.09542000
N	1.31007400	-1.46774800	0.04439200
N	-1.39070200	-1.43173800	-0.02211000
C	0.70034200	-2.60566500	0.04989700
C	-0.80979400	-2.58523200	-0.00273900
C	-1.53709600	-3.90149200	-0.03426300
C	1.39335300	-3.93843600	0.12384800
C	2.74775400	-1.38082700	0.06201000
C	3.46255500	-1.54128300	-1.14025500
C	4.85251100	-1.37825300	-1.09390600
C	5.50413300	-1.07157500	0.09896100
C	4.76979000	-0.91950200	1.27401000
C	3.37837700	-1.06247000	1.27976600
C	2.58901500	-0.90491600	2.55706800
C	2.77524900	-1.87034900	-2.44615300
C	-2.82761900	-1.32067700	-0.00234000
C	-3.50462500	-1.04748600	-1.20639900
C	-4.89317300	-0.88352700	-1.14789000
C	-5.58091500	-0.97348800	0.06075200
C	-4.88534500	-1.24202900	1.23754300
C	-3.49767100	-1.42483500	1.23297200
C	-2.76444500	-1.71755600	2.52330100
C	-2.77585600	-0.95320600	-2.52528600
C	1.43421400	1.80432700	-0.01501200
C	2.46285600	1.90175900	-0.96102000
C	3.49071900	2.83443900	-0.78723700
C	3.50307200	3.67308300	0.32964100
C	2.47390500	3.58544300	1.26889200
C	1.43000700	2.67052100	1.08820000
C	-1.35037700	1.87528300	-0.17272400
C	-1.34717500	2.89820800	-1.13255200
C	-2.29764600	3.91986400	-1.06732500
C	-3.24038300	3.94358600	-0.03636800
C	-3.23883000	2.93364000	0.92716900
C	-2.30799300	1.89182200	0.85037000
H	-2.60516400	-3.75863500	-0.19545700
H	-1.13904700	-4.54087400	-0.82952900
H	-1.39875400	-4.44388600	0.90904500
H	1.24390800	-4.50418200	-0.80395600

H	2.46426300	-3.81720900	0.28467000
H	0.97792700	-4.54428200	0.93619600
H	5.42498100	-1.49480700	-2.01015400
H	6.58315400	-0.95178800	0.11310700
H	5.27716500	-0.68383700	2.20527100
H	3.24963200	-0.65373500	3.39096300
H	2.05072700	-1.82261300	2.82717800
H	1.84629400	-0.10047400	2.47441300
H	3.46612600	-1.74715300	-3.28436200
H	2.41667300	-2.90769400	-2.47765200
H	1.90833000	-1.22435700	-2.63097200
H	-5.43572000	-0.68172100	-2.06719700
H	-6.65772100	-0.83669800	0.08492300
H	-5.42096400	-1.31291600	2.18033200
H	-3.41874500	-1.54769800	3.38244200
H	-2.42555900	-2.76027000	2.58112000
H	-1.87751900	-1.08439800	2.65178800
H	-3.48472500	-0.82985400	-3.34814300
H	-2.09411700	-0.09389800	-2.54417700
H	-2.17845900	-1.84929200	-2.73484700
H	2.48297600	1.25517500	-1.83288300
H	4.28311500	2.89863500	-1.52837500
H	4.30204000	4.39681000	0.46069500
H	2.46245300	4.24268900	2.13444400
H	0.61459900	2.65427400	1.80644600
H	-0.59656300	2.91845500	-1.91589200
H	-2.28976500	4.70683100	-1.81633000
H	-3.97060800	4.74577900	0.01699200
H	-3.96560700	2.94440300	1.73470300
H	-2.34113600	1.10323400	1.59771200
H	0.03626700	0.47808400	-1.62329000

ts-Ba'Ba'

Pt	0.00003100	0.29323600	-0.00013800
N	1.31064900	-1.39150500	-0.00001700
N	-1.31064500	-1.39146900	0.00011600
C	0.74968100	-2.55684000	0.00031500
C	-0.74970800	-2.55682200	0.00023600
C	-1.48896200	-3.86328000	0.00020500
C	1.48892100	-3.86330500	0.00091100
C	2.74669700	-1.24607300	0.00024300
C	3.41450800	-1.15274500	-1.23406600
C	4.80136200	-0.96515500	-1.20653700
C	5.49186300	-0.87195200	0.00061900
C	4.80108600	-0.96561500	1.20757600
C	3.41422400	-1.15326000	1.23473300

C	2.67346600	-1.27207300	2.54571200
C	2.67397800	-1.27118400	-2.54519600
C	-2.74669300	-1.24600600	-0.00016200
C	-3.41421500	-1.15362800	-1.23470100
C	-4.80107100	-0.96599100	-1.20762700
C	-5.49186400	-0.87190800	-0.00070300
C	-4.80137500	-0.96466100	1.20648600
C	-3.41450900	-1.15221900	1.23409700
C	-2.67404700	-1.27026800	2.54530500
C	-2.67341300	-1.27288200	-2.54561400
C	1.41413200	1.88493100	-0.00059600
C	1.98888400	2.31022000	-1.21320900
C	3.14123100	3.09776300	-1.21253000
C	3.72086100	3.48719900	-0.00122900
C	3.14210400	3.09745600	1.21039500
C	1.98974500	2.30993600	1.21171300
C	-1.41404900	1.88497800	0.00028800
C	-1.99006000	2.30969200	-1.21193400
C	-3.14252800	3.09705600	-1.21043500
C	-3.72100700	3.48692800	0.00127900
C	-3.14099500	3.09777800	1.21249000
C	-1.98854200	2.31039200	1.21298900
H	-2.56751500	-3.70825000	0.00237300
H	-1.22034000	-4.45714900	-0.88154000
H	-1.21688200	-4.45927100	0.87940600
H	1.21643700	-4.45994400	-0.87771600
H	2.56747400	-3.70827900	-0.00183700
H	1.22069900	-4.45651800	0.88322800
H	5.33987000	-0.89389700	-2.14759600
H	6.56784500	-0.72610000	0.00077200
H	5.33937900	-0.89466200	2.14878200
H	3.32836300	-1.01648500	3.38304900
H	2.30829700	-2.29322600	2.72005100
H	1.80152800	-0.60799600	2.58057100
H	3.32928700	-1.01634100	-3.38243600
H	2.30789800	-2.29203300	-2.71937600
H	1.80262900	-0.60634400	-2.58035800
H	-5.33936100	-0.89539000	-2.14886100
H	-6.56784700	-0.72607000	-0.00092100
H	-5.33988400	-0.89303900	2.14751700
H	-3.32889800	-1.01343900	3.38230100
H	-2.30962400	-2.29152200	2.72064700
H	-1.80164800	-0.60678200	2.57965400
H	-3.32858400	-1.01862800	-3.38314200
H	-1.80210100	-0.60800800	-2.58107500
H	-2.30725800	-2.29382500	-2.71908400

H	1.53048200	2.03332800	-2.15894800
H	3.57938400	3.41537800	-2.15476200
H	4.61191100	4.10834500	-0.00147300
H	3.58095600	3.41481500	2.15238800
H	1.53205700	2.03276900	2.15771600
H	-1.53258500	2.03243900	-2.15801400
H	-3.58168000	3.41419200	-2.15236300
H	-4.61214300	4.10794900	0.00165900
H	-3.57893700	3.41549800	2.15478600
H	-1.52985200	2.03372400	2.15865200
H	-0.00003400	2.11241800	-0.00032700

ts-BaCa

C	-1.93064600	2.38511300	0.90840900
C	-1.58422000	1.61861900	-0.21238200
C	-2.37249400	1.69605400	-1.36714400
C	-3.50970600	2.51202800	-1.39065800
C	-3.86850800	3.25418300	-0.26326500
C	-3.07858900	3.18609900	0.88617900
Pt	0.00710200	0.36698700	-0.12129700
C	1.20475500	2.06800600	-0.00697800
C	0.89193100	3.30929200	-0.58698200
C	1.67024800	4.43344900	-0.29799200
C	2.76491300	4.33210400	0.56250500
C	3.09229600	3.09395600	1.12146700
C	2.33358400	1.95970200	0.82075200
N	1.51610200	-1.36083300	-0.06271700
C	2.94873800	-1.21905600	-0.12725700
C	3.55289000	-0.93348400	-1.36744100
C	4.93851400	-0.73423200	-1.38512200
C	5.69492800	-0.80690700	-0.21739700
C	5.07267400	-1.09700000	0.99518600
C	3.69134100	-1.31371200	1.06798500
C	2.75906300	-0.87597000	-2.65092500
C	3.04058500	-1.62685000	2.39745300
N	-1.17510800	-1.47294600	0.10550100
C	-2.61648100	-1.45339400	0.20382300
C	-3.38480200	-1.68037700	-0.95265600
C	-4.77693600	-1.60016000	-0.82810500
C	-5.37698600	-1.31050200	0.39562000
C	-4.58851900	-1.09310000	1.52415900
C	-3.19288100	-1.15456600	1.45190100
C	-2.75293200	-2.00290900	-2.28734700
C	-2.34326200	-0.94341500	2.68167100
C	0.97385200	-2.53165000	-0.01383600
C	1.73280500	-3.82844700	-0.09616300

C	-0.52483500	-2.59143700	0.12936500
C	-1.17260300	-3.93709700	0.29841500
H	-2.22831400	-3.83932300	0.54889200
H	-1.09005200	-4.52188600	-0.62610700
H	-0.66909900	-4.51113800	1.08327900
H	1.28726600	-4.48719300	-0.84908900
H	2.77855000	-3.65718800	-0.34974300
H	1.69294000	-4.36488100	0.85963300
H	5.42435300	-0.52170000	-2.33330600
H	6.76775300	-0.64412300	-0.25311300
H	5.66189300	-1.16079000	1.90594800
H	3.74571800	-1.45992400	3.21594900
H	2.71649800	-2.67361600	2.46425600
H	2.15899500	-1.00232200	2.58630000
H	3.42434700	-0.73964500	-3.50737300
H	2.18084800	-1.79226100	-2.82255200
H	2.04468300	-0.04274100	-2.65564600
H	-5.39223900	-1.76654400	-1.70805600
H	-6.45868100	-1.25322900	0.46966000
H	-5.05577900	-0.87167300	2.47964700
H	-2.96075700	-0.63600900	3.52969100
H	-1.81036200	-1.85716400	2.97675800
H	-1.58626800	-0.16383600	2.52575200
H	-3.48836600	-1.91050300	-3.09102300
H	-1.91663400	-1.33373500	-2.52037100
H	-2.36768500	-3.03089600	-2.32476400
H	0.03818900	3.40988600	-1.24647900
H	1.41327400	5.38808400	-0.74872600
H	3.36568200	5.20813500	0.78831300
H	3.94500300	3.00131500	1.78864000
H	2.62382000	1.00899200	1.24870000
H	-2.11203900	1.12665500	-2.25506800
H	-4.11221400	2.56282900	-2.29407700
H	-4.75061800	3.88735300	-0.28374400
H	-3.33887400	3.76996400	1.76543700
H	-1.30747400	2.37938700	1.79855900
H	0.70244800	1.02518300	-1.36396200

Ts-Ba'Ca'

C	-2.44571300	1.87143600	0.60136600
C	-1.57249300	1.64683000	-0.47069000
C	-1.82067600	2.28759000	-1.69265200
C	-2.93523400	3.12167200	-1.84152000
C	-3.80244300	3.34009000	-0.76989800
C	-3.55296400	2.71413600	0.45337900
Pt	0.00026400	0.38095200	-0.19985400

C	1.28038400	1.99530700	0.16250900
C	2.61026300	2.02177900	-0.27895000
C	3.47365800	3.02790100	0.16858200
C	3.01519400	4.01389000	1.04225700
C	1.68023200	4.00284300	1.45435000
C	0.80125500	3.01667000	0.99719400
N	1.47819400	-1.34255800	0.01167900
C	2.90808600	-1.21709000	-0.10460900
C	3.49996600	-1.33767400	-1.37682300
C	4.88415500	-1.14543500	-1.46732000
C	5.64711700	-0.85569000	-0.33667500
C	5.03204300	-0.74628800	0.90969300
C	3.64993000	-0.91423400	1.05237800
C	2.68435900	-1.65949400	-2.60861600
C	2.98568600	-0.77718500	2.40105800
N	-1.21634300	-1.43582200	0.13161800
C	-2.65658600	-1.40787600	0.25382900
C	-3.43109900	-1.38275700	-0.92038900
C	-4.82064800	-1.30462800	-0.77620200
C	-5.41317100	-1.24707500	0.48398100
C	-4.61932600	-1.27504600	1.62901300
C	-3.22467500	-1.35785400	1.54058500
C	-2.79857100	-1.46442600	-2.28845000
C	-2.37873900	-1.39081000	2.79357300
C	0.93397700	-2.50486700	0.14284200
C	1.69435100	-3.80128400	0.21112200
C	-0.57091400	-2.55276000	0.23278300
C	-1.22894900	-3.88943100	0.42768200
H	-2.31310000	-3.81329500	0.35735000
H	-0.87069400	-4.60600800	-0.31893200
H	-0.97203200	-4.30160000	1.41147100
H	1.47507000	-4.42123000	-0.66711700
H	2.76894600	-3.62636900	0.24791700
H	1.39853000	-4.38070000	1.09201400
H	5.36357200	-1.23037500	-2.43869300
H	6.72020200	-0.71672400	-0.42713000
H	5.62640100	-0.52069000	1.79072300
H	3.71941300	-0.51482600	3.16757700
H	2.49711200	-1.70746200	2.71877500
H	2.21887400	0.00737900	2.38920900
H	3.28432500	-1.52556000	-3.51253000
H	2.33112000	-2.69930500	-2.60761600
H	1.79811500	-1.01907500	-2.69499200
H	-5.43981800	-1.28906600	-1.66868900
H	-6.49334700	-1.18324200	0.57372900
H	-5.08152600	-1.23255400	2.61149800

H	-2.98901500	-1.17063600	3.67340000
H	-1.92056600	-2.37483800	2.95963200
H	-1.56255500	-0.65781900	2.76443200
H	-3.56082300	-1.39759300	-3.06900800
H	-2.08257800	-0.64984800	-2.44900400
H	-2.25820400	-2.40875600	-2.43688800
H	2.98783300	1.26995800	-0.96125000
H	4.50297000	3.03531000	-0.17891800
H	3.68614100	4.79585100	1.38519900
H	1.30655600	4.77212200	2.12481600
H	-0.23652400	3.05080500	1.30136600
H	-1.15385200	2.15252900	-2.53973300
H	-3.11206200	3.60831100	-2.79725800
H	-4.66078000	3.99542600	-0.88411700
H	-4.21701500	2.87627500	1.29852800
H	-2.27508000	1.39866000	1.56515200
H	0.61012900	1.24993000	-1.34764200

ts-HaEa

C	-3.09369000	-1.86324700	1.10377600
C	-2.38275300	-1.78091200	-0.11046800
C	-3.01876200	-1.77316000	-1.36810200
C	-4.42023200	-1.83761500	-1.38565300
C	-5.15329500	-1.90858100	-0.19873300
C	-4.49327900	-1.92510200	1.03246900
N	-0.93033700	-1.68644500	-0.06444500
C	-0.18915600	-2.77555900	-0.07622200
C	-0.75736200	-4.16497800	-0.13742000
C	-2.23084000	-1.72115800	-2.65652200
C	-2.38558800	-1.90153300	2.43862200
Pt	0.00860300	0.10420500	0.11428200
N	1.68805800	-1.35046700	0.03916100
C	1.27713100	-2.58797700	-0.04780800
C	2.18136200	-3.78551000	-0.13539200
C	-1.66910400	1.23824700	0.03070700
C	-2.36190200	1.62197200	1.19012900
C	-3.49875400	2.43834700	1.11672700
C	-3.97040600	2.88108800	-0.12491600
C	-3.29382700	2.49715700	-1.28795800
C	-2.15725000	1.68088600	-1.20766200
C	1.55094000	2.03058700	-2.09623800
C	0.88648000	2.88635900	-2.97909600
C	0.24448700	4.03171800	-2.48811500
C	0.26407200	4.31953500	-1.11504900
C	0.92110900	3.46108000	-0.23380200

C	1.56316700	2.30369400	-0.71449700
C	3.09002000	-0.99973000	-0.04428400
C	3.69913400	-0.91826300	-1.31840400
C	5.02619000	-0.46321100	-1.38244800
C	5.73096000	-0.12626900	-0.22497600
C	5.12240100	-0.26138500	1.02522500
C	3.79616900	-0.70482100	1.14299600
C	2.98368600	-1.34310700	-2.58405500
C	3.18071700	-0.93666100	2.50378600
N	0.72647300	1.43904300	2.29446300
C	0.68709200	1.98492600	3.31691700
C	0.63299400	2.68177900	4.60082000
H	-1.84200300	-4.15373800	-0.22947300
H	-0.34166100	-4.71643300	-0.98850300
H	-0.49470400	-4.72884300	0.76659100
H	2.08261400	-4.28619200	-1.10661700
H	3.22507300	-3.49908500	-0.00427000
H	1.92388600	-4.52382000	0.63187400
H	5.50584600	-0.38190800	-2.35263100
H	6.75388600	0.22675600	-0.29594400
H	5.68011800	-0.03141400	1.92742100
H	3.75871100	-0.42803600	3.28069600
H	3.17215100	-2.00656300	2.75588300
H	2.14926300	-0.57963300	2.55237300
H	3.44900400	-0.88553300	-3.46198900
H	3.04053600	-2.43102300	-2.72782900
H	1.92363700	-1.07018900	-2.57990300
H	-4.93374900	-1.82825600	-2.34144900
H	-6.23640700	-1.95117100	-0.23303400
H	-5.06356200	-1.98444800	1.95372200
H	-3.10280500	-1.78949800	3.25593100
H	-1.85877200	-2.85273100	2.59662900
H	-1.64167500	-1.10129700	2.52385900
H	-2.89165000	-1.51689000	-3.50280400
H	-1.46265200	-0.94085800	-2.62784300
H	-1.72244000	-2.67331200	-2.86314200
H	0.88270800	2.67533200	-4.04408900
H	-0.26415900	4.70240100	-3.17288200
H	-0.23274100	5.20873700	-0.74080500
H	0.94448600	3.68699000	0.82667600
H	2.20394600	1.72608800	-0.05302400
H	-1.64653800	1.40592100	-2.12643600
H	-3.64729000	2.82973400	-2.26051200
H	-4.85274900	3.50965000	-0.18472700
H	-4.01685600	2.72169100	2.02941100
H	-2.02052400	1.28940100	2.16617100

H	2.08978200	1.17156900	-2.47786100
H	0.55796000	1.96347000	5.42323200
H	-0.23773300	3.34435900	4.63529800
H	1.53522300	3.28431800	4.74559800

ts-Ha'Ea

C	-2.38418200	1.91277600	-0.94175300
C	-1.63184000	1.54380100	0.18546500
C	-1.89272700	2.20683500	1.39793700
C	-2.85959600	3.21935700	1.47626300
C	-3.58918300	3.58720000	0.34003300
C	-3.34766200	2.92804000	-0.87112800
Pt	-0.16454000	0.14501000	0.09479700
N	1.28455200	1.50238700	2.18351200
C	1.65348300	2.24342200	2.99642900
C	2.11523400	3.18344000	4.01645900
N	-1.37386600	-1.46853300	-0.04137700
C	-0.81017100	-2.65757100	-0.06045200
C	0.66727600	-2.69792200	0.01421300
N	1.25863600	-1.53451300	0.06713400
C	2.69975900	-1.42511700	0.16020100
C	3.30806900	-1.45114200	1.43379900
C	4.70189600	-1.29452800	1.49308600
C	5.46186900	-1.14288500	0.33018000
C	4.83527800	-1.14748800	-0.91876900
C	3.44296000	-1.28366400	-1.03074400
C	2.50369300	-1.67827600	2.69411500
C	2.77129300	-1.29983200	-2.38447900
C	-2.81788000	-1.32792200	-0.14737900
C	-3.39913100	-1.30805500	-1.43202900
C	-4.79020800	-1.14268700	-1.50981500
C	-5.56527500	-1.00709100	-0.35547300
C	-4.96042400	-1.03968400	0.90369100
C	-3.57337500	-1.20059000	1.03641200
C	-2.57020000	-1.46124100	-2.68781500
C	-2.92593900	-1.25294500	2.39988700
C	-1.58689600	-3.93889800	-0.15281300
C	1.37531300	-4.02325000	0.02373000
C	1.38439900	2.32318100	-0.95961500
C	2.76674000	2.12684500	-0.81412700
C	3.60576900	2.23116200	-1.92716500
C	3.06447100	2.51621600	-3.18902200
C	1.68158200	2.69841000	-3.33963500
C	0.84277100	2.60538000	-2.22579500
H	-2.65816500	-3.76861700	-0.05846400
H	-1.40303500	-4.43521200	-1.11457900

H	-1.27162200	-4.63640400	0.63064500
H	1.06261200	-4.64158200	-0.82493000
H	2.45601900	-3.89097500	-0.02313600
H	1.13935000	-4.58705200	0.93513100
H	5.42592400	-1.04790400	-1.82369900
H	6.53906800	-1.03405700	0.39652300
H	5.19010600	-1.30855500	2.46235300
H	3.11442500	-1.48004600	3.57934400
H	2.15640600	-2.71802900	2.77112100
H	1.62305700	-1.03007900	2.73623600
H	3.50054200	-1.12058100	-3.17810900
H	2.29165800	-2.26566400	-2.59247100
H	1.99739600	-0.52727100	-2.45802400
H	-5.26210900	-1.11786400	-2.48666900
H	-6.63884200	-0.87669600	-0.43679000
H	-5.56398700	-0.93765700	1.79934000
H	-3.66318600	-1.05663700	3.18231600
H	-2.48126400	-2.23588200	2.60624100
H	-2.12712800	-0.50821200	2.49138700
H	-3.15383000	-1.17986100	-3.56823300
H	-1.66993700	-0.83609000	-2.66272100
H	-2.24122700	-2.49861700	-2.83905100
H	1.26626200	2.92791600	-4.31614300
H	3.71833700	2.60401300	-4.05075800
H	4.67643300	2.09490400	-1.81341400
H	3.18176000	1.90747800	0.16463200
H	0.75697400	2.42588000	-0.07294400
H	-2.22962400	1.40884600	-1.89235100
H	-3.91023800	3.19773300	-1.76082900
H	-4.33732100	4.37065000	0.39803300
H	-3.04180000	3.71581800	2.42574500
H	-1.33890300	1.94151300	2.29410200
H	-0.22347300	2.77962500	-2.32586100
H	3.19602900	3.33490000	3.93402100
H	1.89111400	2.80175700	5.01741300
H	1.61806600	4.15065600	3.89214600