

Supporting Information

Reactivity in Friedel-Crafts Aromatic Benzylation: The Role of the Electrophilic Reactant

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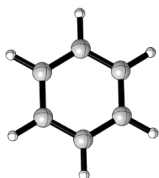
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Table S1. The change in the enthalpy and free energy, relative to the reactants of the reaction, catalyzed with two molecules TiCl_4 from CPCM/M06-2X/6-311+G(d,p) computations.

Structure	ΔH	ΔG
R	0.0	0.0
Pre-reaction complex	2.1	24.7
TS1	7.5	31.6
I2	-1.6	31.5
TS2	-0.8	30.6
I3 σ -complex	-3.8	29.9
P	-7.9	-6.3

Mechanism of benzylation

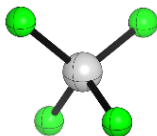
Optimized Cartesian coordinates, Electronic energies and the imaginary frequencies (all in atomic units). The computations are performed at CPCM//M06-2X/6-311+G(d,p) level of theory. Critical structures along the reaction path with two molecules TiCl_4 catalyst.



Benzene

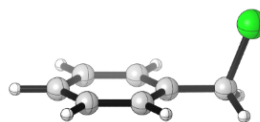
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C,0,-0.8375085627,1.1132409733,-0.0000615549
C,0,0.5453577429,1.2819404181,-0.0000956948
C,0,1.3828478647,0.1687193925,-0.0000591192
C,0,0.8374853023,-1.1132549492,0.0000120721
C,0,-0.5453347179,-1.281948618,0.0000607974
H,0,-2.4586688843,-0.2999785365,0.0000282944
H,0,-1.4890389314,1.9793259928,-0.0000945796
H,0,2.4586721503,0.2999386198,-0.000089595
H,0,1.4890711891,-1.9792980896,0.0000290025
H,0,-0.9695767801,-2.2792488993,0.0001091466
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E = -232.2017835
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TiCl_4

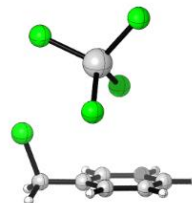
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Cl,0,-1.256423,1.256423,-1.256423
Cl,0,1.256423,-1.256423,-1.256423
E = -2690.474732
Nimag = 0
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Benzyl chloride

```
O 1
Cl,0,-2.5286001039,0.3652539288,-0.7330054374
C,0,1.7819075548,-1.3325598823,0.1691026473
C,0,0.4601383145,-1.0499152328,0.4976759522
C,0,-0.0308204842,0.2511907444,0.3834984831
C,0,0.8156260023,1.2675349296,-0.0609440245
C,0,2.1375892312,0.9861685502,-0.3898382783
C,0,2.621895425,-0.3147096218,-0.2760765724
H,0,2.1570200984,-2.3446074115,0.2634799001
H,0,-0.195740315,-1.8411725785,0.8456582571
H,0,0.4365019685,2.2804835368,-0.1478699963
H,0,2.7898814503,1.7811229513,-0.7310390987
H,0,3.652132341,-0.5339674489,-0.5300519082
C,0,-1.4546744247,0.5528115587,0.7286555548
H,0,-1.8531921382,-0.1344210333,1.4700139695
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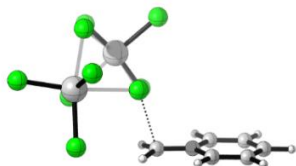


Pre-reaction complex

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H,0,-2.6293633262,3.067475105,0.0453340417
C,0,-2.5560426117,0.9316033172,0.3390409366
Cl,0,-0.3373287914,2.5208994351,0.143410795
C,0,-3.1647966104,0.6258783194,-0.8781390555
C,0,-2.3761423318,-0.0740722224,1.2888279246
C,0,-3.5873463659,-0.6725226315,-1.144279348
H,0,-3.3051189095,1.4069644135,-1.6183064358
C,0,-2.7925124734,-1.3737863281,1.0220365577
H,0,-1.9031126493,0.1631403871,2.2360595626
C,0,-3.3993280214,-1.6742452538,-0.1953414484
H,0,-4.0615289937,-0.902627425,-2.0910221439
H,0,-2.6464783438,-2.1504761916,1.7636014082
H,0,-3.7266590649,-2.686167436,-0.4029993282
Cl,0,1.106432724,-0.805801243,2.0352870968
Ti,0,1.7499109245,-0.8282521243,-0.0572752152
Cl,0,2.9314893383,0.9509126057,-0.5029897582
Cl,0,2.9651548405,-2.5983007868,-0.4374327721
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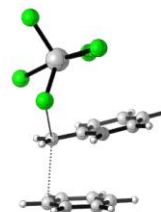


TS1

O 1
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H,0,1.5910473651,-0.693799971,-1.84329299
Cl,0,-2.1298181781,1.073557283,1.4315257243
Cl,0,-1.3996062015,-2.7478931633,-1.1389717397
Cl,0,-2.0185982361,-2.1895549006,2.1201841994
Cl,0,-4.1848814994,-1.0780207376,-0.2134216579
C,0,3.2159863231,-1.4164882539,-0.6069497278
C,0,4.0740637805,-0.3257962144,-0.8899504993
C,0,3.6732768219,-2.4913614361,0.1949514842
C,0,5.3597297375,-0.3218152664,-0.3909256817
H,0,3.7120491628,0.4891342389,-1.5050940809
C,0,4.9592523552,-2.4749495202,0.6909308879
H,0,3.0036812299,-3.3169897749,0.4074953142
C,0,5.7945898751,-1.3912801393,0.3984111115
H,0,6.0290800525,0.5005828967,-0.6057892947
H,0,5.3231146175,-3.2903246264,1.3018615943

H,0,6.8047703032,-1.3818063356,0.7909567086
Ti,0,-2.0371708602,-1.1061051589,0.2023482271
Cl,0,0.4814929678,-0.4901090601,0.584104423
Ti,0,-0.2845460106,1.9646549226,0.0132792178
Cl,0,-1.5588357864,0.5536769528,-1.6191330317
Cl,0,-1.4046683211,3.7707971173,-0.4967145479
Cl,0,0.7918206668,2.6441842544,1.8101531119
Cl,0,1.3716862231,2.1078304701,-1.4572044862

E = -6112.049714
Nimag = -183.72



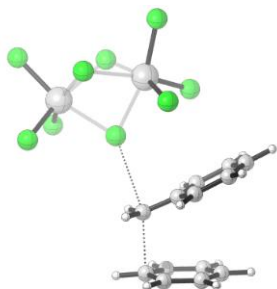
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H,0,-1.0421332052,-1.7740129774,-0.2397750352
H,0,-1.5074812448,-1.5840278345,1.5463890315
Cl,0,4.5058707814,-0.7556025643,0.3339161263
C,0,-4.1053173273,-0.3860863914,-1.6200759076
C,0,-3.792950122,-1.7007153838,-1.293789837
C,0,-3.9607901139,-2.1513714939,0.0185386969
C,0,-4.4687784623,-1.2916535782,0.9951063529
C,0,-4.7766654517,0.0241915997,0.6676978441
C,0,-4.5838342263,0.4799195623,-0.6365387792
H,0,-3.9653467562,-0.0293007144,-2.6338335548
H,0,-3.4108330714,-2.374597874,-2.0518042642
H,0,-4.6095496857,-1.6484047568,2.0087414614
H,0,-5.1580037772,0.6985339484,1.425458506
H,0,-4.8111900186,1.5096915342,-0.8881709881
C,0,-1.4735298591,0.2346570138,0.3990957986
C,0,-1.8094807173,1.0697366796,1.502844202
C,0,-1.2450455249,0.8160466696,-0.8818458393
C,0,-1.8715070938,2.434032478,1.3351415499
H,0,-1.9996594362,0.6133775912,2.467932556
C,0,-1.3043075126,2.1831749587,-1.0343371691
H,0,-1.0078475577,0.1681437968,-1.7183525845
C,0,-1.6098872843,2.982462933,0.0729929603
H,0,-2.1145233672,3.0815426385,2.1669425957
H,0,-1.1175867356,2.6386903164,-1.9977074828
H,0,-1.6501138249,4.0587536069,-0.0504223895
Cl,0,1.4907795068,-1.4915381766,-1.7253329887

Ti,0,2.4374648749,-0.1600923545,-0.1324827861
Cl,0,1.7464236201,1.5716720962,1.1509811888
Cl,0,3.0209117935,1.3263074733,-1.7912481578
Cl,0,1.4998263766,-1.611277536,1.4630633553

E = -3653.780961

Nimag = 0



TS2

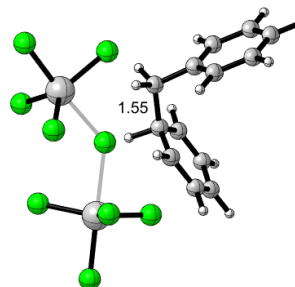
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H,0,2.0953967013,-1.7703920015,-0.5179723297
Cl,0,-2.7741703118,-0.1426399522,1.08369699
Cl,0,-2.4236151491,-2.0704779104,-3.173664744
Cl,0,-2.095340018,-3.2466719316,-0.0342353827
Cl,0,-4.9446529691,-1.7056580417,-0.9673004281
C,0,5.9188440532,-1.2511347301,1.035405635
C,0,5.1188951119,-2.3773343575,0.9976587546
C,0,4.4143942047,-2.6946861764,-0.1813192815
C,0,4.6406136227,-1.9514751594,-1.3575577583
C,0,5.4417655378,-0.8260279941,-1.3139703873
C,0,6.0521563035,-0.460254717,-0.1104200902
H,0,6.4302343749,-0.9716232446,1.9480602778
H,0,4.98873537,-2.9930362671,1.8798999915
H,0,4.1438580853,-2.2409127968,-2.2762593362
H,0,5.5872093816,-0.2211824354,-2.2002391197
H,0,6.657898156,0.4379173141,-0.070863685
C,0,2.9203590704,-0.0996360727,0.5782170085
C,0,2.824524077,0.8089900868,-0.5023233811
C,0,3.3134468494,0.3728282272,1.8527106384
C,0,3.0726708901,2.1524997132,-0.2999056241
H,0,2.5359690597,0.4408143691,-1.4814020634
C,0,3.5610137062,1.7177187197,2.0462544647
H,0,3.4019550955,-0.3304698701,2.6735384195
C,0,3.4370826255,2.6018444125,0.9716172753
H,0,2.9820598866,2.8537950513,-1.1189767607
H,0,3.8473586842,2.0857873388,3.0228154832
H,0,3.6295315711,3.6571133015,1.1269823127

Ti,0,-2.7584361914,-1.4150307198,-1.0868055469
Cl,0,-0.3989165466,-0.5001624192,-0.9715187671
Ti,0,-1.4077251554,1.6288893704,-0.0713266817
Cl,0,-3.0548687867,0.9579341456,-1.8616730479
Cl,0,-2.7889928606,3.2085753072,0.6275624823
Cl,0,0.0259781056,1.6358353079,1.6104564761
Cl,0,-0.2374441513,2.7973853516,-1.5445376661

E = -6344.266867

Nimag = -151.65



I3 σ - complex

0 1

Ti,0,-0.4322959768,2.6373674032,0.2339922322
Cl,0,-0.5108129514,1.3777813225,2.0901034788
Cl,0,-1.1774435122,0.524422647,-1.0008133155
Cl,0,1.0721337265,2.7581081074,-1.4249113717
Cl,0,-2.340923466,3.5584934885,-0.3154337222
C,0,5.8616549595,-0.4956332873,-1.5225519357
C,0,4.6743448931,-0.0134977386,-0.9782611239
C,0,4.2958053561,-0.3643232896,0.3185226506
C,0,5.1297257911,-1.1970513906,1.0665985275
C,0,6.3169225612,-1.6798751788,0.524569858
C,0,6.6832473109,-1.3329050787,-0.7733768414
H,0,6.1448738948,-0.2149067612,-2.5300425221
H,0,4.0409793182,0.6461780867,-1.5636549148
H,0,4.8547306862,-1.4635516175,2.0825793215
H,0,6.9564721066,-2.3237033511,1.1165970388
H,0,7.6072422765,-1.7088497784,-1.196161878
C,0,2.9731444761,0.1032581429,0.8813205158
H,0,2.6538705,1.0276111894,0.3965857608
H,0,3.0462814181,0.2941222975,1.9534237465
Cl,0,0.3977478702,4.4194789453,1.3019618706
Ti,0,-2.9416017793,-1.2103054032,-0.2354999752
Cl,0,-4.515737198,-2.6969329483,0.3099265872
Cl,0,-1.5115750621,-1.855495628,1.3246281061
Cl,0,-4.2405311564,0.5660537037,0.1252107324
Cl,0,-2.4091734643,-2.2039419572,-2.1562808461
C,0,1.6301112961,-3.3934187299,1.0414405006

C,0,1.9643366944,-2.1541806016,1.5056687124
C,0,1.8797863084,-0.9683952714,0.651626139
C,0,1.5352417443,-1.2078642423,-0.7492298793
C,0,1.1884697943,-2.4529798403,-1.1978715508
C,0,1.2414440985,-3.5332067654,-0.3036918293
H,0,1.6586124995,-4.2599728506,1.6878647
H,0,2.2473327087,-2.0076576174,2.5432347337
H,0,0.923794956,-0.5080956469,1.0334377662
H,0,1.5240417205,-0.3531517498,-1.4181178655
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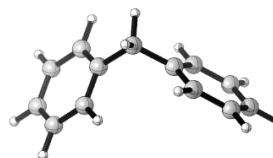
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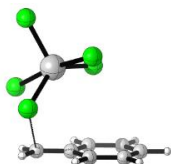


Diphenylmethane

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C,0,0.0000118408,-0.0000882157,1.5301971639
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C,0,3.1872852772,-1.2108043512,-0.1881062124
C,0,2.047875761,-1.1799378712,0.6150663984
C,0,1.254473394,-0.0354014734,0.6818703733
C,0,1.622435978,1.0824287448,-0.0727120244
C,0,2.7589076573,1.0567862131,-0.8727264503
C,0,3.5457693425,-0.0929625814,-0.9336349972
H,0,3.7935886211,-2.1083432159,-0.2280334038
H,0,1.7741267842,-2.0537049858,1.1974891077
H,0,1.0096010108,1.9779251621,-0.0307347222
H,0,3.033138823,1.9328541816,-1.449017821
H,0,4.4316977034,-0.1141838953,-1.5571502271
C,0,-1.2544554329,0.0353159729,0.6818765846
C,0,-1.6223213026,-1.0823545339,-0.0729896704
C,0,-2.0479706471,1.1797912098,0.6153808611
C,0,-2.7588130194,-1.0566173483,-0.8729721603
H,0,-1.00939611,-1.9778005856,-0.0312595824
C,0,-3.1874002063,1.2107534365,-0.1877600574
H,0,-1.7742918572,2.0534375807,1.1980175994
C,0,-3.5457904749,0.0930686456,-0.9335681498
H,0,-3.0329689936,-1.9325636352,-1.4494844604
H,0,-3.79379019,2.1082444949,-0.2274471161
H,0,-4.4317337813,0.114362027,-1.5570597103

E = -502.522613
Nimag = 0

Optimized Cartesian coordinates, Electronic energies and the imaginary frequencies (all in atomic units). The computations are performed at CPCM//M06-2X/6-311+G(d,p) level of theory. Critical structures with one molecule TiCl_4 .



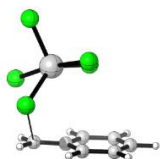
TS1 (with 1 molecule TiCl_4)

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C,0,1.6780042312,-2.1824230442,0.1334616383
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H,0,1.7707748003,-2.9237277224,-0.650482598
Cl,0,-3.6976739094,-0.4670610999,-0.2748112734
C,0,2.2121124343,-0.9127824713,-0.0208421655
C,0,2.7607867515,-0.5226738385,-1.2733804972
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C,0,3.2848807661,0.7409677766,-1.4250495869
H,0,2.7525354529,-1.2282963803,-2.0960866951
C,0,2.7361391224,1.2630474228,0.9036157924
H,0,1.7876430202,-0.3082728639,2.0188384484
C,0,3.2656666162,1.6264697628,-0.3407126363
H,0,3.7049857706,1.0536317446,-2.3715587135
H,0,2.7408359921,1.970669513,1.7218981434
H,0,3.6740515266,2.622550987,-0.4679134367
Cl,0,-0.8614040724,-2.1453667088,-0.7263111261
Ti,0,-1.6147320656,-0.1047949112,0.3151443188
Cl,0,-1.9951029771,1.8516659947,1.4197498553
Cl,0,-1.1013162202,-1.1136069742,2.2850266088
Cl,0,-0.4898785967,0.9874121864,-1.3071640196

E = -3421.565473

Nimag = -92.56



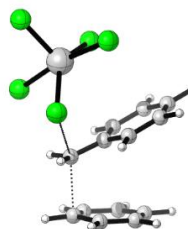
I2 (with 1 molecule TiCl_4)

0 1

C,0,1.9246140411,2.0086578301,-0.919957463
H,0,1.3273908331,2.0572827449,-1.8243085009
H,0,2.0829965156,2.9286131493,-0.3697174277
Cl,0,-3.2812338893,0.3546501003,0.8849131136
C,0,2.5295180466,0.8332300118,-0.5305525759
C,0,3.300566567,0.7932713158,0.6682292601
C,0,2.3634905576,-0.3507070769,-1.3104712444
C,0,3.8785369136,-0.3885204638,1.0669558782
H,0,3.4142244158,1.6992821156,1.2520977831
C,0,2.9443895496,-1.5255274946,-0.8963310862
H,0,1.7725675368,-0.3051295681,-2.2181818533
C,0,3.6939491912,-1.5384915851,0.2879429777
H,0,4.4657049673,-0.4383318292,1.9739296885
H,0,2.8261021288,-2.4337204791,-1.4718854878
H,0,4.1463530953,-2.4689668242,0.611827193
Cl,0,-0.5792131326,2.2068214687,0.4112873305
Ti,0,-1.2789552555,-0.0437787132,0.0639582056
Cl,0,-1.6843053368,-2.2479849432,-0.4153831338
Cl,0,-1.1601400618,0.4016362315,-2.1644535467
Cl,0,0.1735833167,-0.6429549907,1.6884858895

E = -3421.565590

Nimag = 0



TS2

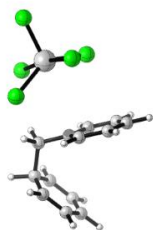
0 1

H,0,2.839298448,-3.153972601,-1.0519019982
C,0,2.0786993164,-0.765036175,-0.5907272735
H,0,1.5185833436,-1.3677197065,0.1149283289
H,0,1.8291260258,-0.8920694072,-1.6365903267
Cl,0,-3.1922606781,1.6873532589,0.743375704
C,0,5.0335067012,-1.5106383269,0.9445196104
C,0,4.0010383284,-2.356593127,0.5868535116
C,0,3.5989365119,-2.4371793912,-0.7619896895
C,0,4.3426877747,-1.7713167091,-1.7579908058
C,0,5.3743714058,-0.9265268055,-1.3944010017
C,0,5.6962782909,-0.7741786994,-0.0426491892

H,0,5.3224060148,-1.406176842,1.9827623726
H,0,3.4634719248,-2.921907376,1.3391644901
H,0,4.0664433169,-1.8905704766,-2.7991381828
H,0,5.9229900716,-0.3752653342,-2.1476661858
H,0,6.488476583,-0.0915899166,0.2430280606
C,0,2.6897214889,0.434736354,-0.1583260512
C,0,3.1536317586,1.3726903954,-1.1069217871
C,0,2.7830432581,0.734126693,1.2208621542
C,0,3.6557713911,2.5908714222,-0.6890866438
H,0,3.0932593161,1.1315291576,-2.1627761825
C,0,3.2790981309,1.9574962971,1.6301396969
H,0,2.4433230144,0.0030818343,1.9463431452
C,0,3.7113123014,2.8811535732,0.6753390584
H,0,3.9986836974,3.3176215838,-1.4140446302
H,0,3.3351508983,2.1984530911,2.6838821046
H,0,4.1002855072,3.8391658096,1.0002007635
Cl,0,-0.5298670773,-0.556210478,1.9149352763
Ti,0,-1.0105436897,1.3977075248,0.8253421591
Cl,0,0.0410725271,3.1155487636,-0.2190633421
Cl,0,-0.7413175113,2.5103835579,2.8366796742
Cl,0,-0.9127313909,0.1982520556,-1.1745208203

E = -3653.778632

Nimag = -157.89



I3 (with 1 molecule TiCl₄)

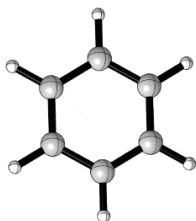
O 1

H,0,-3.1923859447,-2.8028423875,0.0957858241
C,0,-1.7465714551,-1.2539794422,0.310868945
H,0,-1.1231765348,-1.7894018053,-0.4054944204
H,0,-1.5105787435,-1.6176382469,1.3102330099
Cl,0,4.4316675916,-0.8455562365,0.5913204281
C,0,-4.5782800203,-0.3804237519,-1.5924738889
C,0,-3.6152117072,-1.315377154,-1.345081023
C,0,-3.2676108406,-1.7090362219,0.0174893278
C,0,-4.1200356951,-1.1807179339,1.0790438558
C,0,-5.0819711558,-0.2471296896,0.8234823768
C,0,-5.2859143004,0.1647133837,-0.5059305873
H,0,-4.8006956681,-0.0542291943,-2.5992504114
H,0,-3.0423298455,-1.7500853631,-2.157616189
H,0,-3.9270742237,-1.5152532997,2.0931681847
H,0,-5.6796531635,0.1778610955,1.6182070996
H,0,-6.033286117,0.9258943687,-0.7035878907
C,0,-1.5510749363,0.233939934,0.2016903769
C,0,-1.7766673861,1.0625773368,1.3017561574
C,0,-1.1587786153,0.8081987243,-1.0103109372
C,0,-1.6193845972,2.440161464,1.1938441118
H,0,-2.0690461383,0.6257585322,2.2521896178
C,0,-0.9967302737,2.1861058433,-1.1192851422
H,0,-0.969320517,0.1721088808,-1.8693727413
C,0,-1.2309297838,3.0042613577,-0.0180762266
H,0,-1.7917751733,3.0713511213,2.0575392173
H,0,-0.6841403349,2.6180463675,-2.0627105351
H,0,-1.103065101,4.0770551165,-0.1015768267
Cl,0,1.5034803612,-1.6176176211,-1.4463971997
Ti,0,2.3688582206,-0.207027615,0.1356512787
Cl,0,1.8664558453,1.6080226389,1.3971577115
Cl,0,2.99612177,1.2238089315,-1.5854040095
Cl,0,1.3936434835,-1.5489221337,1.7606375056

E = -3653.784348

Nimag = 0

Optimized Cartesian coordinates, Electronic energies and the imaginary frequencies (all in atomic units).
The computations are performed at CPCM//M06-2X/6-311+G(2df,2p) level of theory.



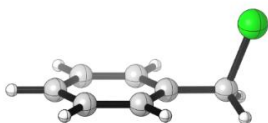
Benzene

0 1

H,0,-2.4708227422,-0.0257955091,0.0001343904
C,0,0.6820740293,1.21042776,-0.00003425
C,0,-0.707200184,1.1958996864,0.0000409977
C,0,-1.3892575579,-0.0145319206,0.0000780714
C,0,-0.6820861644,-1.210420896,0.0000395364
C,0,0.7072118914,-1.1958925134,-0.0000356297
C,0,1.3892575766,0.0145181335,-0.0000674761
H,0,1.2130208272,2.1527563656,-0.0000645023
H,0,-1.2577965942,2.1268840524,0.0000690039
H,0,-1.2130028436,-2.1527664484,0.0000660043
H,0,1.2577783903,-2.1268945823,-0.0000665759
H,0,2.4708223716,0.0258158718,-0.0001265701

E = -232.217545

Nimag = 0



Benzyl chloride

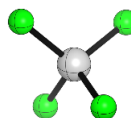
0 1

Cl,0,-2.5631102153,-0.0000028872,-0.5553229795
C,0,1.9700384149,-1.2027988658,-0.1567207793
C,0,0.6437403874,-1.201867341,0.2517822824
C,0,-0.0277053619,-0.0000155988,0.4576678695
C,0,0.6437193369,1.2018536334,0.2518140825
C,0,1.9700169821,1.2028198026,-0.156689513
C,0,2.6344666191,0.0000189848,-0.3625663222
H,0,2.4856862518,-2.1407115022,-0.3110005447
H,0,0.1243704868,-2.138256652,0.4143066753
H,0,0.1243327145,2.138229415,0.4143632056

H,0,2.4856477099,2.1407459495,-0.3109443375
H,0,3.6686409057,0.0000317709,-0.6786322824
C,0,-1.4586449507,-0.0000330873,0.8866622152
H,0,-1.7186038315,-0.8890131448,1.4509717283
H,0,-1.7186124498,0.8889165228,1.4510156997

E = -731.131908

Nimag = 0



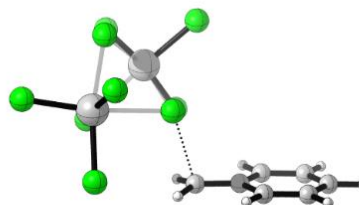
TiCl₄

0 1

Ti,0,0.,0.,0.
Cl,0,1.2574985755,1.2574985755,1.2574985755
Cl,0,-1.2574985755,-1.2574985755,1.2574985755
Cl,0,-1.2574985755,1.2574985755,-1.2574985755
Cl,0,1.2574985755,-1.2574985755,-1.2574985755

E = -2690.492504

Nimag = 0



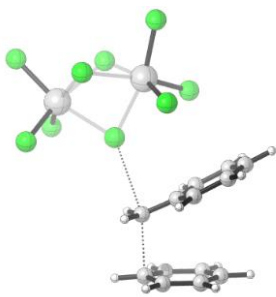
TS1 with 2 molecules TiCl₄

0 1

C,0,-2.2327332688,-1.1873990121,1.1481767699
H,0,-1.7358856583,-2.1479145589,1.1396760741
H,0,-1.8400270555,-0.4321944795,1.8173555451
Cl,0,2.2413526767,0.712875121,-1.3291094994
Cl,0,0.9094637003,-2.8602829624,1.356583802
Cl,0,1.7434636122,-2.5369264687,-1.889591293
Cl,0,3.9211593327,-1.5836506614,0.509471897
C,0,-3.4836288694,-1.0336245291,0.5527242443
C,0,-4.2168061359,0.1623649095,0.7354730101
C,0,-4.0293672415,-2.090053931,-0.2145358672

C,0,-5.4653342815,0.287964629,0.1731567305
H,0,-3.7870627062,0.9606197222,1.3249072367
C,0,-5.2767468681,-1.9518163257,-0.7748210028
H,0,-3.4540725644,-2.9964857534,-0.3491098259
C,0,-5.9869152455,-0.7652176594,-0.580168504
H,0,-6.0404064388,1.1915703968,0.3099897822
H,0,-5.7076023477,-2.749920519,-1.360698492
H,0,-6.9681787398,-0.660199467,-1.0232155771
Ti,0,1.8032732866,-1.3672327027,-0.0185317454
Cl,0,-0.583402128,-0.4803425384,-0.5650503749
Ti,0,0.4452093101,1.8695690404,-0.0573739993
Cl,0,1.4525964645,0.4121187433,1.7048688394
Cl,0,1.7513307031,3.5573085139,0.4406455845
Cl,0,-0.4460088517,2.5912038746,-1.9423305995
Cl,0,-1.2564386849,2.2924446178,1.3091922647

E = -6112.105938
Nimag = -175.07

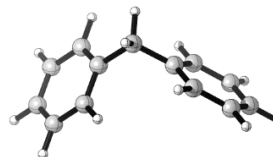


TS2 with 2 molecules

O 1
H,0,3.8779539788,-3.657450754,0.4243550344
C,0,2.7800375533,-1.3568246406,0.6220269649
H,0,2.7719165057,-1.7368973179,1.6343004558
H,0,2.1553785488,-1.8774290391,-0.0897380181
Cl,0,-2.3990171428,0.3925058564,1.759091786
Cl,0,-2.7722919207,-2.5895728939,-1.8332833706
Cl,0,-1.9597415672,-2.9238834662,1.4222121599
Cl,0,-4.898693205,-1.511396422,0.55355774
C,0,6.1732119757,-1.1843359584,0.6810583795
C,0,5.3556487753,-2.2242841493,1.0681334783
C,0,4.4705165564,-2.7990238688,0.1379758021
C,0,4.5214905366,-2.4094316843,-1.2128279094
C,0,5.341092804,-1.3685442234,-1.5940440374
C,0,6.1398882284,-0.7372723635,-0.6404270236
H,0,6.826239978,-0.7054414929,1.3967143838
H,0,5.3531829468,-2.5734241189,2.091850056
H,0,3.8805964208,-2.8996596496,-1.9331880926
H,0,5.3562246501,-1.0308313604,-2.6204904332
H,0,6.7607637854,0.0984129106,-0.9351508207

C,0,3.1576409051,-0.0241834276,0.3781666203
C,0,2.8982932581,0.5706883909,-0.8752491002
C,0,3.7493798702,0.7454378987,1.4025417553
C,0,3.1859715062,1.9026993089,-1.0799264449
H,0,2.4552591365,-0.0261378997,-1.6630403463
C,0,4.0357005794,2.0764023945,1.1896612539
H,0,3.9601189516,0.2802514107,2.3570310949
C,0,3.7508478124,2.6503544551,-0.0481635503
H,0,2.9720960205,2.3663521719,-2.0316840009
H,0,4.4754259347,2.6724796718,1.9758536863
H,0,3.9742865171,3.6960434161,-0.2119215324
Ti,0,-2.7517311501,-1.3890333096,0.030427586
Cl,0,-0.3986017172,-0.6272505762,-0.4657302462
Ti,0,-1.2186558517,1.7095093983,-0.0221483438
Cl,0,-3.1397831705,0.7031272469,-1.2946979242
Cl,0,-2.4422476613,3.498943174,0.4359419766
Cl,0,0.472525055,2.0748654229,1.3579020779
Cl,0,-0.2837084044,2.3895944886,-1.9151000973

E = -6344.337339
Nimag = -136.55

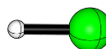


Diphenylmethane

O 1
C,0,-0.0000090224,0.0001980874,1.5244890802
H,0,-0.0433789483,0.8781395581,2.1701956313
H,0,0.043362873,-0.8775814315,2.1704149495
C,0,3.2468127145,-0.9854742201,-0.2092026298
C,0,2.1107853987,-1.0360614138,0.5919412334
C,0,1.2524959389,0.05510426,0.6783947888
C,0,1.5527719823,1.2030390438,-0.0545184238
C,0,2.6854345962,1.2588731219,-0.8527718445
C,0,3.5371238079,0.1617640216,-0.9334400047
H,0,3.9041673758,-1.8429276401,-0.2640755167
H,0,1.8903158136,-1.9326473819,1.1583828758
H,0,0.8897812234,2.0586238379,0.0034647646
H,0,2.9064834848,2.1580818657,-1.4121941677
H,0,4.4207549375,0.2040982371,-1.5555393583
C,0,-1.2525088588,-0.0549240572,0.6784045842
C,0,-1.5528318433,-1.2030885409,-0.054128932
C,0,-2.1107403442,1.0362575838,0.5915714344
C,0,-2.6854821774,-1.2591309505,-0.852385664

H,0,-0.8898875746,-2.058688974,0.0041549457
 C,0,-3.2467548694,0.9854611657,-0.2095769379
 H,0,-1.8902369447,1.933019883,1.1577207221
 C,0,-3.5371115907,-0.1620039222,-0.9334372333
 H,0,-2.9065677828,-2.1585152776,-1.4115110145
 H,0,-3.904065119,1.8429295078,-0.2647469676
 H,0,-4.420733071,-0.2044993641,-1.5555393151

E = -502.555649
 Nimag = 0

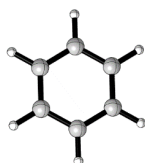


HCl

O 1
 H,0,0.,0.,-1.2113616997
 Cl,0,0.,0.,0.0693676997

E = -460.803141
 Nimag = 0

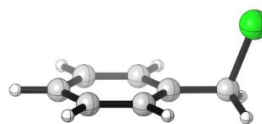
Optimized Cartesian coordinates, Electronic energies and the imaginary frequencies (all in atomic units).
 The computations are performed at CPCM//M06-2X/DEF2-TZVPP level of theory.



Benzene

O 1
 H,0,0.9674829836,2.2744084215,-0.0001565447
 C,0,-1.3794421714,-0.1682694636,0.0000077561
 C,0,-0.8354673138,1.1105288767,-0.000064442
 C,0,0.5439979393,1.2788376246,-0.0001001455
 C,0,1.379436978,0.1682989706,-0.000062639
 C,0,0.8354438186,-1.1105431407,0.0000094503
 C,0,-0.5439744649,-1.2788459007,0.0000462208
 H,0,-2.453369168,-0.2993004377,0.0000400528
 H,0,-1.4858804233,1.975084502,-0.0000929631
 H,0,2.4533721861,0.299262758,-0.000089893
 H,0,1.4859108933,-1.9750581252,0.0000427881
 H,0,-0.9675222574,-2.2743900856,0.0001073591

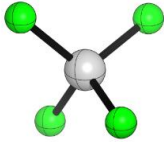
E = -232.230018
 Nimag = 0



Benzyl chloride

O 1
 Cl,0,-2.5154482781,0.3654048503,-0.7298479435
 C,0,1.7792407896,-1.3291588451,0.1686662015
 C,0,0.4608022041,-1.0466083776,0.4970267395
 C,0,-0.0294291817,0.2514111646,0.385197496
 C,0,0.8155574232,1.2642379158,-0.0596360117
 C,0,2.1342831158,0.9836180979,-0.3884707592
 C,0,2.6175929956,-0.3141188642,-0.2755223839
 H,0,2.1532175374,-2.339742788,0.2622145549
 H,0,-0.1939500604,-1.8364540268,0.8444179857
 H,0,0.4373099842,2.2755172822,-0.14613772
 H,0,2.7852332814,1.7772271291,-0.7295541833
 H,0,3.6458917625,-0.5331587198,-0.5295030159
 C,0,-1.4536330374,0.5517441786,0.7243665037
 H,0,-1.8499038967,-0.133043808,1.4668230967
 H,0,-1.5873246396,1.5761048112,1.0560644395

E = -731.144413
 Nimag = 0



TiCl₄

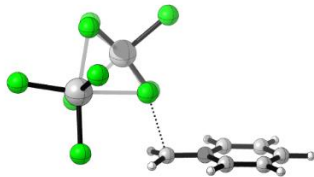
0 1

Ti,0,0.,0.,0.

Cl,0,1.2585013147,1.2585013147,1.2585013147
 Cl,0,-1.2585013147,-1.2585013147,1.2585013147
 Cl,0,-1.2585013147,1.2585013147,-1.2585013147
 Cl,0,1.2585013147,-1.2585013147,-1.2585013147

E = -2690.497310

Nimag = 0



TS1 with 2 molecules TiCl₄

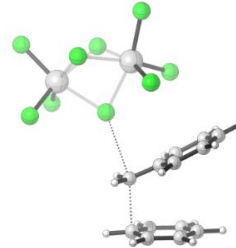
0 1

C,0,2.2151058849,-1.1821659829,-1.1245708894
 H,0,1.7203185081,-2.1439414455,-1.1164630646
 H,0,1.8122513795,-0.4219664114,-1.7816337251
 Cl,0,-2.2527636259,0.7432826551,1.2948246066
 Cl,0,-0.938468707,-2.8706010058,-1.3539176846
 Cl,0,-1.7911426772,-2.5009189296,1.9033008862
 Cl,0,-3.9419868234,-1.5588732294,-0.5188629374
 C,0,3.4730607339,-1.0344488127,-0.5390542541
 C,0,4.1988288671,0.1676051771,-0.7024060201
 C,0,4.0314483015,-2.1055001243,0.1969470086
 C,0,5.4530188867,0.2859934723,-0.1498446567
 H,0,3.7571220654,0.9782170803,-1.2660731214
 C,0,5.2856020104,-1.9759948044,0.7448463439
 H,0,3.4619195475,-3.0176823996,0.3169685462
 C,0,5.9886181524,-0.7824234541,0.5709387524
 H,0,6.0219045964,1.1961544744,-0.2698668236
 H,0,5.7265919782,-2.787059316,1.3053399938
 H,0,6.9746225265,-0.6837857044,1.0053041515
 Ti,0,-1.820695344,-1.3617004596,0.0117134352
 Cl,0,0.5959576243,-0.4823691794,0.5909298521
 Ti,0,-0.4133689167,1.8486889152,0.0546603877
 Cl,0,-1.4270093899,0.3978175147,-1.7139383726

Cl,0,-1.6885648017,3.5544281362,-0.4743414531
 Cl,0,0.4742744872,2.5744449376,1.9423651218
 Cl,0,1.3109148613,2.256196446,-1.2959445936

E = -6112.124908

Nimag = -172.74



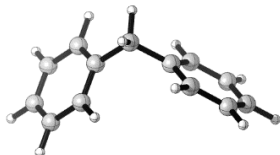
TS2 with 2 molecules TiCl₄

0 1

H,0,3.8779539788,-3.657450754,0.4243550344
 C,0,2.7800375533,-1.3568246406,0.6220269649
 H,0,2.7719165057,-1.7368973179,1.6343004558
 H,0,2.1553785488,-1.8774290391,-0.0897380181
 Cl,0,-2.3990171428,0.3925058564,1.759091786
 Cl,0,-2.7722919207,-2.5895728939,-1.8332833706
 Cl,0,-1.9597415672,-2.9238834662,1.4222121599
 Cl,0,-4.898693205,-1.511396422,0.55355774
 C,0,6.1732119757,-1.1843359584,0.6810583795
 C,0,5.3556487753,-2.2242841493,1.0681334783
 C,0,4.4705165564,-2.7990238688,0.1379758021
 C,0,4.5214905366,-2.4094316843,-1.2128279094
 C,0,5.341092804,-1.3685442234,-1.5940440374
 C,0,6.1398882284,-0.7372723635,-0.6404270236
 H,0,6.826239978,-0.7054414929,1.3967143838
 H,0,5.3531829468,-2.5734241189,2.091850056
 H,0,3.8805964208,-2.8996596496,-1.9331880926
 H,0,5.3562246501,-1.0308313604,-2.6204904332
 H,0,6.7607637854,0.0984129106,-0.9351508207
 C,0,3.1576409051,-0.0241834276,0.3781666203
 C,0,2.8982932581,0.5706883909,-0.8752491002
 C,0,3.7493798702,0.7454378987,1.4025417553
 C,0,3.1859715062,1.9026993089,-1.0799264449
 H,0,2.4552591365,-0.0261378997,-1.6630403463
 C,0,4.0357005794,2.0764023945,1.1896612539
 H,0,3.9601189516,0.2802514107,2.3570310949
 C,0,3.7508478124,2.6503544551,-0.0481635503
 H,0,2.9720960205,2.3663521719,-2.0316840009
 H,0,4.4754259347,2.6724796718,1.9758536863
 H,0,3.9742865171,3.6960434161,-0.2119215324
 Ti,0,-2.7517311501,-1.3890333096,0.030427586
 Cl,0,-0.3986017172,-0.6272505762,-0.4657302462

Ti,0,-1.2186558517,1.7095093983,-0.0221483438
Cl,0,-3.1397831705,0.7031272469,-1.2946979242
Cl,0,-2.4422476613,3.498943174,0.4359419766
Cl,0,0.472525055,2.0748654229,1.3579020779
Cl,0,-0.2837084044,2.3895944886,-1.9151000973

E = -6344.366673
Nimag = -138.72



Diphenylmethane

O 1
C,0,0.0000247458,0.0000174075,1.524966496
H,0,0.0162765385,0.8790807586,2.1707031418
H,0,-0.016233754,-0.879011945,2.1707522121
C,0,3.1719086793,-1.2034317549,-0.2088528749
C,0,2.034670225,-1.177257274,0.5915218197
C,0,1.2531444903,-0.029960133,0.6795144079
C,0,1.6321647475,1.0957429048,-0.0512831951
C,0,2.7664227366,1.0750717337,-0.8487682538
C,0,3.5407844544,-0.0776721761,-0.9308580743
H,0,3.7689955202,-2.1040277601,-0.2648885341
H,0,1.7528170878,-2.0576037299,1.156399676

H,0,1.0292435982,1.9946870685,0.0079131525
H,0,3.0491336746,1.958055393,-1.4066004042
H,0,4.4258819484,-0.0949999775,-1.5524008437
C,0,-1.2531097431,0.0299649577,0.6795249905
C,0,-1.6319462726,-1.0956265503,-0.0515409577
C,0,-2.0348515652,1.1771367709,0.5918443383
C,0,-2.7662428757,-1.0749690987,-0.8489702571
H,0,-1.0288520549,-1.9944710326,0.0074012863
C,0,-3.1721296339,1.203298363,-0.208475588
H,0,-1.7531306725,2.0574001412,1.1569174906
C,0,-3.5408264733,0.0776485578,-0.9307413843
H,0,-3.048811504,-1.9578672696,-1.407010137
H,0,-3.7693825744,2.1037991957,-0.2642698698
H,0,-4.4259533231,0.094962449,-1.5522426379

E = -502.582121
Nimag = 0



HCl

O 1
H,0,0.,0.,-1.2200749806
Cl,0,0.,0.,0.0596529806

E = -460.802097
Nimag = 0

Optimized Cartesian coordinates, Electronic energies and the imaginary frequencies (all in atomic units).
The computations are performed at SDM//M06-2X/6-311+G(d,p) level of theory.

Benzene

0 1

H,0,-2.47677,-0.025845,0.000139
C,0,0.683895,1.213682,-0.000034
C,0,-0.709136,1.199103,0.000038
C,0,-1.393044,-0.014589,0.000072
C,0,-0.683919,-1.213669,0.000036
C,0,0.709159,-1.199089,-0.000035
C,0,1.393044,0.014562,-0.000084
H,0,1.215992,2.157869,-0.000052
H,0,-1.260849,2.131952,0.000071
H,0,-1.215955,-2.15789,0.000066
H,0,1.260812,-2.131974,-0.000052
H,0,2.47677,0.025888,-0.000132

E = -232.2071976

Nimag = 0

Benzyl chloride

0 1

Cl,0,-2.5311610226,0.3647352935,-0.7335915501
C,0,1.7822895619,-1.3328266702,0.1691909475
C,0,0.460100606,-1.0505136182,0.4978488659
C,0,-0.0308243128,0.2510665777,0.3832397268
C,0,0.8155085924,1.2682230874,-0.0609695697
C,0,2.1378397634,0.9867250643,-0.3898079535
C,0,2.6222009319,-0.3145929774,-0.2765192713
H,0,2.1578503348,-2.3453078396,0.2632600339
H,0,-0.1975536345,-1.8405641017,0.8465919636
H,0,0.4341819146,2.280918903,-0.1466942561
H,0,2.7904873435,1.7819537831,-0.7313867745
H,0,3.6527270307,-0.533938467,-0.5312640487
C,0,-1.4537454336,0.5526626699,0.7296768895
H,0,-1.8517685969,-0.1362352211,1.4703591035
H,0,-1.5886930787,1.5806735163,1.0561708932

E = -731.1185821

Nimag = 0

TiCl₄

0 1

Ti,0,0.,0.,0.
Cl,0,1.2531658158,1.2531658158,1.2531658158

Cl,0,-1.2531658158,-1.2531658158,1.2531658158
Cl,0,-1.2531658158,1.2531658158,-1.2531658158
Cl,0,1.2531658158,-1.2531658158,-1.2531658158

E = -2690.4715174

Nimag = 0

TS1 with 2 molecules TiCl₄

0 1

C,0,2.2150391812,-1.4118722878,-1.0364390628
H,0,1.8315906023,-2.415185294,-0.8863590354
H,0,1.8047387002,-0.8360648378,-1.861104688
Cl,0,-2.1782640164,0.5576999639,1.3629033559
Cl,0,-0.9740748377,-2.6612624346,-1.7697489548
Cl,0,-1.867879818,-2.7652591012,1.4625587778
Cl,0,-3.949210143,-1.3892284914,-0.8029069037
C,0,3.4715557022,-1.067840963,-0.4936954626
C,0,4.1527914811,0.0780054992,-0.9602631946
C,0,4.0630920518,-1.8973984779,0.4863015936
C,0,5.4036381887,0.3813241678,-0.4580355253
H,0,3.6949189953,0.6927587698,-1.7259923063
C,0,5.3088523806,-1.5800897711,0.988175829
H,0,3.5247552183,-2.7734064991,0.8323440714
C,0,5.972160874,-0.4423302407,0.516798019
H,0,5.9415078485,1.2501084662,-0.8159186223
H,0,5.7733804973,-2.2059274007,1.7396174273
H,0,6.9515557533,-0.197756514,0.9126443508
Ti,0,-1.8414386893,-1.3427951559,-0.2201694735
Cl,0,0.6018032876,-0.6517785455,0.4933965936
Ti,0,-0.3076238052,1.8175212926,0.2722422535
Cl,0,-1.3565791193,0.6445285324,-1.6702333421
Cl,0,-1.5312813901,3.6101154527,0.002339183
Cl,0,0.5687337965,2.2344151626,2.2516242796
Cl,0,1.4318262602,2.3300537074,-0.9864341633

E = -6112.066698

Nimag = -198.14

TS2 with 2 molecules TiCl₄

0 1

H,0,-3.9228981511,-3.3371537986,1.5741279644
C,0,-2.7520832472,-1.1318088138,1.0116529572
H,0,-2.2075057237,-1.8793689717,0.4448460439
H,0,-2.6878054268,-1.1909519467,2.0916610606

Cl,0,2.5673779019,1.5814711851,-1.2969613232
Cl,0,2.4242603787,-3.0533963415,-2.0314947292
Cl,0,1.9770108818,-0.3557279478,-3.9905386285
Cl,0,4.8433614314,-0.7217615488,-2.266912849
C,0,-5.5316306876,-1.6812642526,-0.9118726
C,0,-4.6997907324,-2.6038416262,-0.3048388279
C,0,-4.5280352792,-2.5766574049,1.0933767491
C,0,-5.3044082323,-1.702984248,1.8802861845
C,0,-6.1338967389,-0.7812634542,1.267942819
C,0,-6.222549411,-0.7524822526,-0.1269779137
H,0,-5.6391843401,-1.6646381149,-1.9898034133
H,0,-4.1387404203,-3.317165678,-0.8978208236
H,0,-5.2060607062,-1.7273095477,2.9596170763
H,0,-6.70280275,-0.0754535657,1.8611368189
H,0,-6.8534834228,-0.0120687415,-0.6067648166
C,0,-3.123389499,0.0848877232,0.4028967783
C,0,-3.5712735793,1.1652219716,1.1980929218
C,0,-3.0119959414,0.2474032357,-0.9972690806
C,0,-3.8552264788,2.3838327317,0.6115247247
H,0,-3.6711498987,1.0237676146,2.269449589
C,0,-3.2977617646,1.4699302279,-1.5761084489
H,0,-2.6962511939,-0.5959726155,-1.6019329251
C,0,-3.7143330454,2.5325383569,-0.7709064547
H,0,-4.1834821695,3.2194738941,1.217084618
H,0,-3.2003185566,1.6043041382,-2.6462547188
H,0,-3.9360659778,3.4906338163,-1.2279906823
Ti,0,2.6598945798,-0.8543391158,-1.9431670763
Cl,0,0.2996941797,-0.6071048389,-1.0787941625
Ti,0,1.253979514,0.866354836,0.7196874414
Cl,0,2.9928858791,-0.9543097259,0.5434693494
Cl,0,2.5823009692,2.0380523203,2.0471903281
Cl,0,-0.283852566,2.3978740983,0.3209843889
Cl,0,0.1739592251,-0.3037545987,2.2728416608

E = -6344.290945
Nimag = -179.42

Diphenylmethane

O 1

C,0,-0.0000040047,0.0001538507,1.5281125977
H,0,0.0406064788,-0.8812760241,2.1729827033
H,0,-0.0406244698,0.8817159053,2.1728008518
C,0,-3.2485542727,1.0038379537,-0.2078828909
C,0,-2.1092855714,1.0488748256,0.595291442
C,0,-1.2539509367,-0.0496970547,0.6803093425
C,0,-1.5600399023,-1.1987274642,-0.0556751369
C,0,-2.6959830383,-1.2480175151,-0.8563156126
C,0,-3.5449083736,-0.1441931494,-0.9355215726
H,0,-3.9038118078,1.8661652396,-0.2615818152
H,0,-1.882927651,1.9451938931,1.1641877961
H,0,-0.8996810528,-2.0592730849,0.0017439315
H,0,-2.9217416691,-2.1475790204,-1.4181704369
H,0,-4.4307369874,-0.1816016059,-1.5592658423
C,0,1.2539507724,0.0498325108,0.680312584
C,0,1.5600951032,1.1987522304,-0.0558213712
C,0,2.1092323308,-1.0487922872,0.5954377297
C,0,2.6960391183,1.2478826915,-0.8564705585
H,0,0.8997786813,2.0593378333,0.0014878523
C,0,3.2485013305,-1.0039156546,-0.2077450532
H,0,1.882833215,-1.9450249877,1.1644536571
C,0,3.5449097939,0.1440060745,-0.9355344549
H,0,2.9218410946,2.1473600427,-1.4184425052
H,0,3.9037174723,-1.8662813919,-0.2613313113
H,0,4.4307393464,0.181290189,-1.5592849261

E = -502.533512
Nimag = 0

HCl

O 1

H,0,0.,0.,-1.216036397
Cl,0,0.,0.,0.074042397

E = -460.801855
Nimag = 0