

Supplementary information

Unveiling the potential of scandium complexes for methane C-H bond activation: A computational study

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DFT optimized geometries

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[MeHMe-Sc-CH₄]

Sc	-0.2221800000	-1.3286260000	-0.0155240000
C	-0.2033110000	-3.5849400000	-0.0085570000
H	-1.1974660000	-3.2276150000	-0.4058320000
H	0.6765320000	-3.2478340000	-0.6205180000
H	-0.2252190000	-4.6691000000	-0.0589030000
H	-0.0665960000	-3.3101710000	1.0646970000
N	-0.3401100000	0.2272400000	-1.4708770000
C	0.5436340000	1.1790100000	-1.2348700000
C	0.9939870000	1.5045530000	0.0558770000
H	1.7846560000	2.2422620000	0.1009820000
C	1.1086960000	1.9800050000	-2.3686180000
H	1.5358800000	1.3257370000	-3.1330240000
H	1.8791740000	2.6680800000	-2.0265690000
H	0.3223940000	2.5625340000	-2.8557190000
C	-0.8867050000	0.0832110000	-2.8015670000

H	-0.1220270000	-0.1725700000	-3.5467990000
H	-1.3963400000	0.9924940000	-3.1413120000
H	-1.6228970000	-0.7223220000	-2.7969800000
N	-0.5042710000	0.2259570000	1.4201900000
C	0.4014880000	1.1770640000	1.2872220000
C	0.8368740000	1.9745490000	2.4791530000
H	1.1681320000	1.3175790000	3.2875530000
H	1.6463150000	2.6573810000	2.2288500000
H	0.0034990000	2.5627970000	2.8720190000
C	-1.1977190000	0.0804900000	2.6803740000
H	-0.5246660000	-0.1962130000	3.5026860000
H	-1.7260860000	0.9957500000	2.9719200000
H	-1.9423070000	-0.7117510000	2.5859860000

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[MeHMe-Sc-TS]

Sc	-0.2678490000	6.8328000000	13.6170390000
C	-0.6859250000	4.7748660000	13.5929660000
H	-1.8375840000	5.7502940000	13.5160770000
H	0.0399560000	4.8040280000	12.7331880000
H	-1.2155790000	3.8288510000	13.5557080000
H	-0.0902780000	4.8054520000	14.5467460000
N	0.0396290000	8.3675970000	12.1453780000
C	0.6402980000	9.5173730000	12.4034030000
C	0.8998620000	10.0057780000	13.6913530000

H	1.4258310000	10.9509240000	13.7246680000
C	1.0631410000	10.3968750000	11.2648510000
H	1.7132290000	9.8561650000	10.5723150000
H	1.5901190000	11.2809290000	11.6168290000
H	0.1941160000	10.7241380000	10.6879170000
C	-0.2728090000	8.0300020000	10.7718280000
H	0.6219980000	7.9118260000	10.1476600000
H	-0.9221290000	8.7710390000	10.2918750000
H	-0.8125700000	7.0788990000	10.7477050000
N	-0.1481620000	8.3673040000	15.1163950000
C	0.4799070000	9.5172280000	14.9361540000
C	0.7551580000	10.3969690000	16.1189270000
H	1.3139590000	9.8569420000	16.8875420000
H	1.3208350000	11.2819020000	15.8360370000
H	-0.1799360000	10.7226320000	16.5822830000
C	-0.6325220000	8.0310600000	16.4394270000
H	0.1750450000	7.9213780000	17.1742370000
H	-1.3433790000	8.7688820000	16.8285580000
H	-1.1644620000	7.0762230000	16.3974800000

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[MeHMe-HScCH3]

Sc	-1.1612110000	-1.1283770000	-0.0729540000
C	-0.1971740000	-3.1116390000	-0.0125260000
H	-3.0275050000	-1.1533820000	-0.1947300000

H	0.4987990000	-3.2736070000	-0.8453450000
H	-0.9543710000	-3.9049580000	-0.0691670000
H	0.3765590000	-3.2821760000	0.9071510000
N	-0.2242260000	0.1820090000	-1.4477310000
C	0.5026140000	1.2633730000	-1.2277230000
C	0.7706700000	1.7671180000	0.0494520000
H	1.3804670000	2.6600170000	0.0879970000
C	1.0774780000	2.0075890000	-2.3919940000
H	1.7186240000	1.3553820000	-2.9908270000
H	1.6631500000	2.8654030000	-2.0691970000
H	0.2831670000	2.3614910000	-3.0545790000
C	-0.4614830000	-0.2808440000	-2.7980320000
H	0.4574580000	-0.5871210000	-3.3104970000
H	-0.9711090000	0.4610620000	-3.4219460000
H	-1.1151700000	-1.1637850000	-2.7741700000
N	-0.4071060000	0.1834310000	1.4095870000
C	0.3424180000	1.2642920000	1.2825680000
C	0.7656520000	2.0095220000	2.5095640000
H	1.3239410000	1.3572880000	3.1862380000
H	1.3895240000	2.8655920000	2.2626480000
H	-0.1057230000	2.3664040000	3.0650740000
C	-0.8132110000	-0.2775340000	2.7197610000
H	0.0335370000	-0.5842420000	3.3440840000
H	-1.3961910000	0.4658300000	3.2737720000

H -1.4598070000 -1.1596600000 2.6147310000

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[NHN-Sc-CH4]

Sc -1.7301560000 -0.1065510000 1.3156130000

C -3.4970640000 -0.2351300000 3.0323530000

H -3.9418580000 -0.5091090000 2.0580420000

H -2.6952010000 -0.9436100000 3.3102090000

H -4.2763250000 -0.2925820000 3.7882660000

H -3.1142130000 0.8017220000 3.0106460000

N 1.3988910000 -0.9333450000 -1.2706520000

N 0.8736380000 1.1471100000 -1.6527820000

C 0.5285890000 0.0613730000 -0.8743090000

N -0.3864270000 -0.0070310000 0.0107450000

C 2.2442080000 -0.4636100000 -2.2567080000

H 3.0009930000 -1.0863310000 -2.7028200000

C 1.3723550000 -2.2464420000 -0.6914620000

C 1.9201900000 0.8196130000 -2.4924710000

H 2.3401790000 1.5304910000 -3.1836810000

C 0.1965260000 2.4083730000 -1.5472590000

H -0.8681370000 2.2927040000 -1.7643610000

H 0.6378010000 3.1095890000 -2.2544090000

H 0.2839930000 2.8082860000 -0.5341070000

H 0.3928850000 -2.7091670000 -0.8342410000

H 2.1372070000 -2.8602010000 -1.1655080000

H 1.5591910000 -2.1970760000 0.3840710000

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[NHN-Sc-TS]

Sc 0.5677840000 -0.0590420000 -0.1033450000

C -1.4963830000 -0.0549100000 0.3000510000

H -0.6863260000 1.3495820000 0.0225690000

H -1.4477330000 -0.8701390000 -0.4770380000

H -2.5242500000 0.2811500000 0.3820960000

H -1.1708430000 -0.4813690000 1.2805960000

N 3.2527940000 -1.0179460000 -3.2762660000

N 2.4096830000 0.9649470000 -3.6172080000

C 2.3960450000 -0.0860710000 -2.7155340000

N 1.7535570000 -0.1716910000 -1.6210160000

C 3.7571810000 -0.5488180000 -4.4740270000

H 4.4452650000 -1.1260330000 -5.0682050000

C 3.5177300000 -2.2823810000 -2.6548550000

C 3.2368900000 0.6722750000 -4.6840220000

H 3.3845040000 1.3628330000 -5.4970870000

C 1.6263800000 2.1502050000 -3.4213840000

H 0.5612310000 1.9566550000 -3.5768660000

H 1.9565950000 2.9186690000 -4.1196330000

H 1.7455140000 2.5091610000 -2.3962020000

H 2.6271040000 -2.9162930000 -2.6508680000

H 4.3150760000 -2.7884300000 -3.1978770000

H 3.8234840000 -2.1349980000 -1.6165220000

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[NHN-HScCH3]

Sc -1.2103780000 0.4818060000 2.0196090000

C -3.0101460000 -0.7616610000 2.3692920000

H -0.9848470000 2.0917420000 2.9615470000

H -2.8010500000 -1.8140960000 2.5962310000

H -3.6932310000 -0.7658240000 1.5114040000

H -3.5747990000 -0.3590290000 3.2216200000

N 1.2617810000 -0.9095660000 -1.1230530000

N 0.6723470000 1.1385640000 -1.5781950000

C 0.5173600000 0.1442110000 -0.6330850000

N -0.1580350000 0.1942380000 0.4477450000

C 1.8519670000 -0.5614710000 -2.3237990000

H 2.4778340000 -1.2462780000 -2.8703140000

C 1.3758900000 -2.1592100000 -0.4280320000

C 1.4844050000 0.6992030000 -2.6063690000

H 1.7280520000 1.3259680000 -3.4473150000

C 0.0528600000 2.4261280000 -1.4460630000

H -1.0263360000 2.3685120000 -1.6131990000

H 0.4877870000 3.1099840000 -2.1736050000

H 0.2174860000 2.8166530000 -0.4389720000

H 0.3869180000 -2.5032680000 -0.1190460000

H 1.8236660000 -2.8987810000 -1.0904150000

H 1.9955920000 -2.0625710000 0.4677740000

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[NHC-Sc-CH4]+

Sc -0.2236610000 -1.6478060000 0.5038500000

C -0.4918990000 -3.7945450000 1.2250360000

H -1.3592020000 -3.5599490000 0.5659890000

H 0.4762380000 -3.7525520000 0.6748980000

H -0.6193990000 -4.8217890000 1.5546610000

H -0.4798330000 -3.1602190000 2.1393160000

N 1.1942160000 1.0824190000 -0.7422190000

N -0.9244200000 1.3333320000 -0.7763850000

C 0.0398430000 0.4497470000 -0.4336210000

C 0.9552230000 2.3280710000 -1.2632490000

H 1.7502060000 2.9853810000 -1.5749700000

C 2.5307160000 0.5530020000 -0.5422030000

C -0.3846860000 2.4867330000 -1.2849730000

H -0.9938920000 3.3101750000 -1.6197110000

C -2.3535430000 1.1301770000 -0.6254380000

H -2.5450230000 0.0876450000 -0.3702070000

H -2.8617680000 1.3603010000 -1.5613020000

H -2.7478410000 1.7677270000 0.1659560000

H 2.4670580000 -0.5103270000 -0.3099680000

H 3.1181210000 0.6775720000 -1.4512750000

H 3.0260600000 1.0676590000 0.2812410000

[NHC-Sc-TS]+

Sc	-0.3247510000	6.9017880000	13.8290900000
C	-0.6232440000	4.9314560000	13.4307700000
H	-1.8696280000	5.9419420000	13.5796370000
H	0.0481360000	5.1595580000	12.5573010000
H	-1.1548340000	4.0090920000	13.2253850000
H	0.0254820000	4.7830180000	14.3392960000
N	1.0718310000	9.3039620000	11.9439010000
N	-1.0537030000	9.4702590000	11.8549450000
C	-0.0633440000	8.7473920000	12.4235260000
C	0.7953280000	10.3497080000	11.0979930000
H	1.5698230000	10.9189090000	10.6108790000
C	2.4165680000	8.8808060000	12.2815460000
C	-0.5483970000	10.4543060000	11.0421260000
H	-1.1823410000	11.1337000000	10.4964810000
C	-2.4738970000	9.2643190000	12.0773510000
H	-2.6307290000	8.2774330000	12.5179570000
H	-3.0060500000	9.3142060000	11.1281840000
H	-2.8714670000	10.0248340000	12.7496890000
H	2.3813690000	7.8800170000	12.7152700000
H	3.0317340000	8.8456930000	11.3832240000
H	2.8711470000	9.5651910000	12.9983480000

[NHC-HScCH3]+

Sc	-0.7569190000	-1.3216650000	1.2959850000
C	0.4115300000	-3.0289270000	0.8486300000
H	-2.5105690000	-1.6447220000	1.0607980000
H	0.6962420000	-3.0096710000	-0.2114730000
H	-0.2735950000	-3.8795110000	0.9767120000
H	1.3115160000	-3.2342230000	1.4363780000
N	1.0393760000	0.7664210000	-0.5732540000
N	-1.0261350000	1.3068780000	-0.6626390000
C	-0.1749930000	0.4314280000	-0.0861760000
C	0.9485640000	1.8307540000	-1.4318510000
H	1.8095420000	2.2460160000	-1.9295880000
C	2.2919410000	0.1115560000	-0.2388630000
C	-0.3575840000	2.1717090000	-1.4884590000
H	-0.8628000000	2.9428970000	-2.0466560000
C	-2.4645420000	1.3514950000	-0.4480680000
H	-2.7847260000	0.4490380000	0.0750820000
H	-2.9771990000	1.3925340000	-1.4081440000
H	-2.7324180000	2.2299690000	0.1389050000
H	2.0866570000	-0.8199610000	0.2879290000
H	2.8403620000	-0.1243860000	-1.1499290000
H	2.9048360000	0.7578380000	0.3896180000

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CH4

C	1.6358490000	0.2976690000	0.0767480000
H	1.1652310000	0.3069180000	1.0581350000
H	1.4069620000	-0.6398580000	-0.4266970000
H	2.7139220000	0.3948360000	0.1903360000
H	1.2570360000	1.1290360000	-0.5149230000

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[NHO-Sc-CH4]+

Sc	-0.5388290000	-0.3023400000	2.0251990000
C	-2.2814050000	-0.4775100000	3.5412470000
H	-2.1117420000	0.6060710000	3.3599060000
H	-2.5845740000	-1.0118360000	2.6141650000
H	-3.1168040000	-0.5536090000	4.2320890000
H	-1.4080240000	-0.9579670000	4.0298100000
N	0.3049650000	-0.8071300000	-1.8762760000
N	0.3787260000	1.3262890000	-1.5380630000
C	0.5853010000	0.1313310000	-0.9512020000
C	0.9795180000	-0.0963890000	0.3996580000
H	1.5150300000	-1.0439570000	0.5324930000
H	1.5753460000	0.7260110000	0.8130130000
C	-0.0918910000	-0.1920450000	-3.0511210000
H	-0.3614060000	-0.7610390000	-3.9241550000
C	0.3928550000	-2.2317900000	-1.6512730000
C	-0.0460540000	1.1324670000	-2.8411660000
H	-0.2671490000	1.9601390000	-3.4928270000

C	0.5608620000	2.6022840000	-0.8849050000
H	-0.0650640000	2.6638720000	0.0092800000
H	0.2717220000	3.3935040000	-1.5723320000
H	1.6039170000	2.7470320000	-0.5995480000
H	-0.2477900000	-2.5246350000	-0.8151980000
H	0.0610590000	-2.7503150000	-2.5475090000
H	1.4200120000	-2.5277310000	-1.4329160000

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[NHO-Sc-TS]+

Sc	0.5881380000	-0.0464310000	-0.0573370000
C	-1.4322120000	-0.0481120000	0.2494490000
H	-0.6427770000	1.3230640000	0.0118510000
H	-1.3460300000	-0.8651880000	-0.5319400000
H	-2.4527680000	0.3187910000	0.2444800000
H	-1.2156670000	-0.5036370000	1.2473530000
N	0.7921970000	-0.5847220000	-3.9769110000
N	0.8314660000	1.5386240000	-3.5749880000
C	1.2457320000	0.3434440000	-3.1103330000
C	1.9600580000	0.0979300000	-1.8985030000
H	2.5568590000	-0.8159250000	-1.9436450000
H	2.5910320000	0.9477690000	-1.6196560000
C	0.0877710000	0.0372920000	-4.9932490000
H	-0.3570830000	-0.5221690000	-5.7981060000
C	1.0225870000	-2.0065990000	-3.8519580000

C	0.1127010000	1.3556310000	-4.7429520000
H	-0.3072310000	2.1859760000	-5.2841280000
C	1.1062690000	2.8105180000	-2.9402140000
H	0.7019550000	2.8225420000	-1.9245180000
H	0.6323150000	3.5990510000	-3.5195910000
H	2.1804970000	2.9976630000	-2.9034140000
H	0.6203350000	-2.3790610000	-2.9066800000
H	0.5208650000	-2.5168600000	-4.6705250000
H	2.0890210000	-2.2320170000	-3.8974410000

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[NHO-HScCH3]+

Sc	-0.0203370000	0.2021560000	2.3393140000
C	-1.6454150000	-1.1508650000	2.0764490000
H	-0.6050600000	1.8900360000	2.0636490000
H	-1.4291280000	-2.2219400000	2.0148910000
H	-2.1438210000	-0.8461230000	1.1448490000
H	-2.3816950000	-1.0108990000	2.8780840000
N	-0.0785210000	-0.7333000000	-1.3764650000
N	0.3145310000	1.3830780000	-1.1859540000
C	0.5760750000	0.1820490000	-0.6370090000
C	1.3455480000	-0.0709490000	0.5493040000
H	1.7699290000	-1.0768650000	0.5550900000
H	2.1421220000	0.6666610000	0.6788610000
C	-0.7564840000	-0.0984670000	-2.3990720000

H	-1.3457270000	-0.6468430000	-3.1138150000
C	-0.0448290000	-2.1630630000	-1.1478820000
C	-0.5112800000	1.2172740000	-2.2801140000
H	-0.8438340000	2.0544380000	-2.8694360000
C	0.8379880000	2.6494630000	-0.7102360000
H	0.4932590000	2.8392630000	0.3085240000
H	0.4744260000	3.4403800000	-1.3614070000
H	1.9284410000	2.6444370000	-0.7387320000
H	-0.4279200000	-2.3995620000	-0.1541850000
H	-0.6734430000	-2.6489240000	-1.8899250000
H	0.9728530000	-2.5432360000	-1.2459380000