

Supporting Information

Transmetallation Between Metal-Only Lewis Pairs

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General Considerations

All manipulations were performed either under dry argon or *in vacuo* using standard Schlenk line and glovebox techniques. Solvents were purified by distillation under dry argon from sodium and stored under the same inert gas over molecular sieves. $[\text{Cp}(\text{Me}_3\text{P})_2\text{Rh}]$ (**5**) was prepared as described in previous publications.^[1] NMR spectra in solution were acquired on a BrukerAvance 400 (^1H : 400.1 MHz, $^{13}\text{C}\{^1\text{H}\}$: 100.6 MHz, $^{31}\text{P}\{^1\text{H}\}$: 162.0 MHz) NMR spectrometer. NMR spectra were referenced to external SiMe_4 (^1H , ^{13}C) and 85% H_3PO_4 (^{31}P). Microanalyses was performed on an EuroEA elemental analyser.

Crystal structure determination

The crystal data of **13** were collected on a Bruker X8APEX diffractometer with a CCD area detector and multi-layer mirror monochromated $\text{MoK}\alpha$ radiation. The structure was solved using direct methods, refined with the Shelx software package and expanded using Fourier techniques.^[2] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factors calculations. All hydrogen atoms were assigned to idealized geometric positions.

Theoretical Calculations

All geometries reported herein were computed using a Turbomole 5.10 package on a cluster of Linux workstations.^[3] The computations were performed using DFT methods, applying the three hybrid functional B3LYP using 6-31G(d,p) basis set for H, C, Al, Cl, N, P and Stuttgart Relativistic Small Core ECP Basis Set for Pd.^[4-7] The *Wiberg Bond Indexes* were obtained with the NBO 5.0 program.^[8,9] Drawings of the Kohn-Sham-Orbitals were performed with Molekel 4.3.^[10] Computation of the orbital interactions were carried out in the frozen core geometry using the Amsterdam density functional (ADF) software 2012 at the OLYP level of theory applying TZP basis sets for all atoms; relativistic effects were considered by the zeroth-order regular approximation (ZORA).^[11-25]

Cartesian coordinates of all calculated geometries listed below:

[Cp(Me₃P)₂Rh] (5)

Rh	-0.34923147586331	0.28979342213041	0.00601584307328
P	-0.29764541165160	-1.95427868551272	-0.00559503782723
P	1.87325848601438	0.59999029072213	-0.00330825864284
C	-1.93004225593816	1.57530441644928	1.22600061945403
C	-1.10971240000109	2.43310216363152	0.44562225123671
C	-2.60234880476270	0.71388416103169	0.31266874697866
H	-0.47128068729586	3.21764131176186	0.83115059909147
C	-1.39187134291913	2.20002016800866	-0.95448882746483
H	-3.31241217535308	-0.05708571318280	0.58262321161041
C	-2.31924788687126	1.14827650477347	-1.03596178172862
H	-0.96430324387629	2.74526389349000	-1.78484714661910
H	-2.74005915472209	0.72915968562634	-1.93970852615967
H	-1.99293512475814	1.54690381424466	2.30438812222249
C	0.78806572216225	-2.87228695888325	1.19499059060040
H	1.83783325952778	-2.61098064304066	1.03664650526343
H	0.51765031971409	-2.57718778250630	2.21226013809059
H	0.67816732978281	-3.95782036861759	1.09144436544747
C	0.12124313942205	-2.84860569676287	-1.58434282842478
H	-0.57777098761548	-2.52972252616591	-2.36212087318205
H	1.12835042496660	-2.57911751839688	-1.91023534833984
H	0.06139757424233	-3.93702589992662	-1.46737197556992
C	-1.92605306543181	-2.76049539438239	0.37997462745457
H	-1.84653326901327	-3.85272443202111	0.35469215495668
H	-2.26071482218086	-2.44725074192493	1.37206563530916
H	-2.67338412241850	-2.44098791432807	-0.35070900367326
C	3.01175390630160	-0.47161307588931	-1.01158204917943

H	2.95277822822666	-1.51181073326065	-0.68146208672475
H	2.70837089887639	-0.42864032364622	-2.06089317357312
H	4.05167633108745	-0.13817129652687	-0.92434528293783
C	2.76377584958495	0.57260872487003	1.63117404034347
H	2.29292963522515	1.29897824211682	2.29913448986273
H	2.66051115279782	-0.41441906241969	2.08921515378448
H	3.82851449309462	0.81256094162583	1.52666843373347
C	2.40149544459447	2.26812124837828	-0.62820253166348
H	3.48917242970703	2.38968270202373	-0.58016148692833
H	2.07064025439988	2.38728327932971	-1.66303881300492
H	1.92954952111770	3.05020943829664	-0.02823045273315

[Cp(Me₃P)₂Rh→AlCl₃] (13)

Rh	-0.45940615347441	-0.02329390782978	0.69739068921385
Al	-0.02923792438310	0.11310032194726	-1.76061413493716
Cl	2.01326430038812	-0.39182703798269	-2.40252106047362
Cl	-1.32415013906169	-1.26624671414709	-2.86033395879498
Cl	-0.43118741245096	2.17190879271881	-2.39800255141664
P	0.88654545077638	-1.88422471839669	0.86168532346249
P	1.11376261493018	1.60814847620234	1.13500485188176
C	-2.28572383698469	-0.64967191927738	2.15192860791844
C	-2.18717931330005	0.74676333258017	2.19687491225171
C	-2.50966328772035	-1.03590268000876	0.77576114553117
H	-2.00017776528921	1.34614143179125	3.07849681632290
C	-2.36401830619640	1.25194880840495	0.85177741642872
H	-2.68067882322111	-2.04138181175577	0.41582249999727
C	-2.64628000981139	0.15177367435141	-0.00202219761683
H	-2.38695709190168	2.29164683722368	0.55830616944250
H	-2.90461697491469	0.19873529225577	-1.04921653400104
H	-2.18501875201284	-1.32341289083447	2.99192183150126
C	0.60645778056463	-2.74862971058160	2.47921364231628
H	0.81438943742947	-2.06748255741419	3.30828881210891
H	-0.43511648785741	-3.06941395926890	2.55091634551032
H	1.25438989117440	-3.62717594776540	2.56346787228826
C	2.72834527357754	-1.76713057445888	0.84461413316713
H	3.05564195194687	-1.38315509877721	-0.12280953057728
H	3.07938404040939	-1.10512525841490	1.63980148298579
H	3.15955472271199	-2.76082507350201	1.00212575020875
C	0.58818325821577	-3.25426933626537	-0.33779654580008
H	1.15587720155736	-4.14308754388931	-0.04265269068387
H	-0.47660085067422	-3.49424252827710	-0.36865493721113
H	0.89356647150223	-2.94121029614010	-1.33775385534109
C	2.65979310757053	1.86815861865024	0.16556243055864
H	3.26711110709278	0.96370473945153	0.14266948259139
H	2.40759537902423	2.12865152169349	-0.86380163179254
H	3.23403923066360	2.68280646025785	0.61876917448820
C	1.76279116182173	1.52296071982016	2.87083389873891
H	0.92340187846386	1.51066564552015	3.57101951611119
H	2.34212778168525	0.60817267663954	3.01738476210768
H	2.40286218342329	2.38368301566733	3.09088674198254
C	0.39479671905028	3.30917904288371	1.10278747643069
H	1.15770699348510	4.04793665696112	1.36852336556415
H	0.02391592126692	3.51412294870364	0.09608682160206
H	-0.43356883199331	3.38256548773484	1.81135126068271

[(Cy₃P)₂Pt] (12)

Pt	-0.00003978562367	0.00000899509695	0.00000035136047
P	0.06411005945519	2.29744236023098	0.14029119541180
P	-0.06415622838694	-2.29742297972801	-0.14027672622612
C	1.53321393007876	2.97316408585994	1.10822462995572
H	1.51374804190910	4.06975733968164	1.04155280234875
C	2.86064246997475	2.46992063739281	0.49818118956364
H	2.84341717912962	1.37224754464577	0.49548706027517
H	2.94641074044859	2.77848653386607	-0.54953060279889
C	4.08284474807599	2.97091831654575	1.28482361604637
H	5.00033715081439	2.57069431778307	0.83617740178721
H	4.14769270876121	4.06584524837526	1.20187815869521
C	3.99723213287614	2.58007507200602	2.76613885608878
H	4.85504268802425	2.98182669747274	3.31919165893991
H	4.05128705119097	1.48560008764662	2.85447450712677
C	2.68312939304798	3.07211371794335	3.38667678969452
H	2.68240919568113	4.17158947626007	3.40488254776360
H	2.60646019943497	2.74451391215510	4.43069549664059
C	1.45701665890751	2.57831641520697	2.59964701640377
H	1.38671739181533	1.48423435436892	2.66986395689884
H	0.54849629542920	2.98129732150379	3.06013321070656
C	-1.44024547631862	2.98262810550971	1.05258502693742
H	-1.35471796690813	2.50403431401382	2.03815590555947
C	-2.75305009672338	2.46316239422769	0.42701054294126
H	-2.87812052793292	2.88596471642007	-0.58058122532436
H	-2.69068918927673	1.37625340122461	0.30784161328352
C	-3.97209225326606	2.85003016086081	1.28112647658898
H	-4.89231156728324	2.50204310070284	0.79609377313396
H	-3.91226181752801	2.32797943013743	2.24656209101476
C	-4.03998625964440	4.36423560780046	1.52822861147558
H	-4.88609015988588	4.60805672723649	2.18195417671180
H	-4.22517784555505	4.87794903821436	0.57350137998672
C	-2.73018720018852	4.88833793781617	2.13423161652558
H	-2.77457708783661	5.97765462886558	2.25557615244703
H	-2.60140498089962	4.46719431767640	3.14152998475332
C	-1.51482427135786	4.50726155692028	1.26913584664824
H	-0.59719524036205	4.88499198574440	1.73475018848011
H	-1.60585799407708	5.01046470628064	0.29796366546460
C	0.06663625216897	3.22622146898701	-1.51317598670336
H	-1.00619602575696	3.34801327574653	-1.72380618022456
C	0.70480808184779	4.63223862858713	-1.53240815833736
H	0.28997490758740	5.26846324660873	-0.74499495452213
H	1.78045297145171	4.54909454166209	-1.33162117537596
C	0.51135739251623	5.31211554204743	-2.90068089408804
H	-0.56108904995893	5.48983163914761	-3.06611386798684
H	0.99258693278573	6.29780721185778	-2.89570598842283
C	1.06454023900550	4.45274696525776	-4.04631480127178
H	2.15687598169968	4.37968270444151	-3.94620279840652
H	0.87195513231532	4.93698940833928	-5.01156637035962
C	0.46137457297584	3.04110763196549	-4.02206231818977
H	0.90915889400631	2.42223128173806	-4.80928044785911
H	-0.61299541017743	3.10335876283200	-4.24882663602870
C	0.64922721547812	2.36370649499025	-2.65497093872991
H	0.18320162747601	1.37341513929757	-2.63877679620277
H	1.72054755395217	2.19725386114270	-2.47797019073335
C	-1.53316421730433	-2.97321366828390	-1.10831012825344

H	-1.51364560375901	-4.06980369582326	-1.04163062712224
C	-2.86066707987548	-2.47003965680160	-0.49837470623966
H	-2.84351606790860	-1.37236604196434	-0.49568209678690
H	-2.94651225240878	-2.77861561599283	0.54932794549216
C	-4.08276315081655	-2.97112515947927	-1.28513808122340
H	-5.00032984949812	-2.57097958009572	-0.83657538040582
H	-4.14752775479147	-4.06605798771764	-1.20219914109149
C	-3.99705220284349	-2.58028612358469	-2.76644987025035
H	-4.85478529428604	-2.98210496657982	-3.31957377408844
H	-4.05117440141648	-1.48581673466265	-2.85480271731733
C	-2.68286659009468	-3.07224194146883	-3.38687295664234
H	-2.68206616783901	-4.17171735435447	-3.40508480675370
H	-2.60611902611950	-2.74463060327442	-4.43088312653603
C	-1.45686788007404	-2.57836392761903	-2.59972736351629
H	-1.38663447137777	-1.48427719975385	-2.66994011367849
H	-0.54827975008852	-2.98128083412552	-3.06013446609998
C	1.44024131860972	-2.98258234574762	-1.05252441136351
H	1.35473768277959	-2.50399131721974	-2.03809706387054
C	2.75303233184548	-2.46311074929963	-0.42692780168641
H	2.87808763217027	-2.88590540167435	0.58066883960654
H	2.69066826824561	-1.37620096946074	-0.30776771676323
C	3.97208832568224	-2.84998507642223	-1.28102175114712
H	4.89229975418072	-2.50199673059842	-0.79597549140126
H	3.91227409421162	-2.32793708092903	-2.24646028985974
C	4.03999180374019	-4.36419218301593	-1.52811967185446
H	4.88611342028484	-4.60801450885478	-2.18182107073352
H	4.22516096162807	-4.87790158632576	-0.57338653691515
C	2.73020646524285	-4.88829489616717	-2.13414884333868
H	2.77459051334169	-5.97761220896902	-2.25549044918858
H	2.60146701310171	-4.46715126787480	-3.14145306626049
C	1.51483037157278	-4.50721513182376	-1.26907270588426
H	0.59721087471321	-4.88494517790774	-1.73470667144376
H	1.60585310063704	-5.01041327285360	-0.29789899864270
C	-0.06670753672462	-3.22619344266785	1.51319284671904
H	1.00612157561025	-3.34795062065969	1.72386083842917
C	-0.70483434625720	-4.63223122276645	1.53241609447438
H	-0.28996385870678	-5.26844593330035	0.74501529362586
H	-1.78047706377515	-4.54911997984368	1.33160537374029
C	-0.51139429841606	-5.31209580817274	2.90069780899885
H	0.56105389362794	-5.48977599792922	3.06615884611372
H	-0.99259155913789	-6.29780334694194	2.89571594019959
C	-1.06463493825436	-4.45274181037009	4.04631424051723
H	-2.15697113699605	-4.37971823171911	3.94617984900472
H	-0.87205210032501	-4.93697290289985	5.01157206713771
C	-0.46152037947439	-3.04108121394040	4.02206844015695
H	-0.90934345675507	-2.42221668298895	4.80927392147788
H	0.61284701966221	-3.10329451927771	4.24885722112623
C	-0.64936294780943	-2.36369407477806	2.65496733114625
H	-0.18337208701217	-1.37338619546817	2.63878147027670
H	-1.72068511789561	-2.19728131770221	2.47793636840627

[(Cy₃P)₂Pt→AlCl₃] (11)

Pt	-0.07376178738433	0.04709504819109	0.00728486177240
Al	-2.50041499084062	0.43590320783526	0.06822167690570
Cl	-3.18543037103219	1.59492915714562	1.77472827128140
Cl	-3.37180057110765	-1.55683936178545	0.15260355143251

Cl	-3.20812391688934	1.51706401144677	-1.68033373025748
P	0.22434741833620	-0.22491259715170	-2.31825270898333
P	0.45847570923049	0.12733767687231	2.30922254239295
C	2.07591728319465	-0.65427660389778	-2.37010416075581
H	2.15822786106429	-1.38750064830836	-1.55308626058034
C	2.62181844203426	-1.34317427861248	-3.64092132417039
H	2.02782049165891	-2.22598901306914	-3.89472817849373
H	2.55345381389683	-0.66043687477653	-4.49561941268123
C	4.08927264069168	-1.76953452094183	-3.44838862374542
H	4.13707347480196	-2.54868650942837	-2.67373581090923
H	4.46054322648845	-2.22877276262597	-4.37204468471004
C	4.98408229395454	-0.59258713910296	-3.03878919175889
H	6.00984424060775	-0.93736758273087	-2.86386598087346
H	5.03516432354119	0.13011056618110	-3.86581642817084
C	4.43465762979717	0.10985170895451	-1.79011211856550
H	5.04914393856551	0.98340954056064	-1.54073377170579
H	4.49823729271601	-0.57314954441536	-0.93064875832038
C	2.97261466218484	0.54355050979618	-1.98631610698101
H	2.93387499135187	1.29813487220126	-2.78212404629760
H	2.59519295555756	1.02831399355701	-1.07868869071770
C	-0.57038107126140	-1.69985616650258	-3.17267762084481
H	-0.00810856908007	-1.83475384348165	-4.10706202973819
C	-0.40370302428081	-2.97649826563742	-2.31696645798836
H	0.65281966897502	-3.14893203335396	-2.07788561570244
H	-0.92595346589410	-2.82975645754650	-1.36369044462449
C	-0.97404899521455	-4.21268494269371	-3.03281000866646
H	-0.37639875131749	-4.42013875861222	-3.93307705648179
H	-0.87269441818651	-5.09013015614751	-2.38311185071379
C	-2.44103091367200	-4.00645959389869	-3.43207357464978
H	-3.05299027587469	-3.91674669471806	-2.52539021293491
H	-2.81157358681465	-4.88076827147642	-3.98059759683592
C	-2.60578621457154	-2.73670835820944	-4.27797429253987
H	-3.66256073204177	-2.57213102001157	-4.51723719328605
H	-2.08349778353154	-2.86711175481372	-5.23762945358800
C	-2.05132073592409	-1.49562074911248	-3.55703756130569
H	-2.64744984000440	-1.30616194679464	-2.65973780515316
H	-2.16721397155955	-0.62016168292839	-4.20308981946074
C	-0.13997545805912	1.24057080285252	-3.43006902711704
H	-1.23447731379381	1.19767865139120	-3.48261052015575
C	0.40635367706809	1.16739140355089	-4.87063277128835
H	1.50162927303108	1.23466110804117	-4.85716988780422
H	0.15334558486196	0.21041789926849	-5.34127420186692
C	-0.15002847686695	2.32583062671472	-5.71889059178217
H	0.26578643245311	2.27416857528721	-6.73241821964427
H	-1.23747948983014	2.20575622478317	-5.81957100026406
C	0.15445236380855	3.68940227819135	-5.08252010122504
H	-0.29094070957813	4.49310245553830	-5.68065890758012
H	1.24136711547998	3.85774606591159	-5.09463788179105
C	-0.35439098671418	3.75653503619794	-3.63544347793975
H	-1.45118421435950	3.70995177258746	-3.62810461915023
H	-0.07889754712392	4.71513043723916	-3.17963270579573
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H	2.66398454359808	-0.45911973119846	1.67403436784041
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H	2.93497641821667	0.00063214692838	4.13334512859017
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C	4.10354134780930	-1.74348610515802	3.59087777727163
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H	4.61271561257804	-1.78473296668064	4.56108072555782
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H	3.73319461256951	-2.63130623626798	0.93446248693101
C	1.78809943948996	-2.39527239349139	1.85863190683944
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H	3.06645146615648	1.62416286152505	1.92311221448492
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H	3.22508978856828	3.59941824655053	3.38960649424438
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H	0.40689694866750	-0.76731915307955	5.40065526784317
H	-0.05906476315857	0.92159401272299	5.23930313500275

References

- [1] H. Werner, R. Feser, V. Harder, W. Hofmann, H. Neukomm *Inorg. Synth.* **1989**, 25, 158-164.
- [2] G. M. Sheldrick, *Acta Crystallogr., Sect. A: Found. Crystallogr.* **2008**, A64, 112–122.
- [3] R. Ahlrichs *et al.*, Quantum Chemistry Group, Universitaet Karlsruhe, **Turbomole**, ver. 5.10.
- [4] A. D. Becke *J. Chem. Phys.* **1993**, 98, 5648.
- [5] S. H. Vosko, L. Wilk, M. Nusair *Can. J. Phys.* **1980**, 58, 1200.
- [6] C. Lee, W. Yang, R. G. Parr *Phys. Rev.* **1988**, B37, 785.
- [7] Stuttgart RSC 1997 ECP Basis Set was obtained from the Extensible Computational Chemistry Environment Basis Set Database, Version 02/25/04, as developed and distributed by the Molecular Science Computing Facility, Environmental and Molecular Sciences Laboratory which is part of the Pacific Northwest Laboratory, P.O. Box 999, Richland, Washington 99352, USA, and funded by the U.S. Department of Energy.
- [8] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian 98, g03, Revision E.01, Gaussian, Inc., Wallingford CT, **2004**.
- [9] E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, and F. Weinhold, *NBO5.0*, Theoretical Institute, Univeristy of Wisconsin, Madison, **2001**.
- [10] P. Flükinger, H. P. Lüthi, S. Portmann, and J. Weber, *Molekel 4.3*, Swiss Center for Scientific Computing, Manno, **2000**.
- [11] Amsterdam Density Functional, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, <http://www.scm.com>.

- [12] G. Te Velde, F. M. Bickelhaupt, E. J. Baerends, C. Fonseca Guerra, S. J. A. Van Gisbergen, J. G. Snijders, T. Ziegler *J. Comput. Chem.* **2001**, 22, 931-967.
- [13] N. C. Handy, A. J. Cohen *Mol. Phys.* **2001**, 99, 403-412.
- [14] D. P. Chong *Mol. Phys.* **2005**, 103, 749-761.
- [15] D. P. Chong, E. Van Lenthe, S. Van Gisbergen, E. J. Baerends *J. Comput. Chem.* **2004**, 25, 1030-1036.
- [16] E. Van Lenthe, E. J. Baerends *J. Comput. Chem.* **2003**, 24, 1142-1156.
- [17] R. Bouten, E. J. Baerends, E. Van Lenthe, L. Visscher, G. Schreckenbach, T. Ziegler *J. Phys. Chem. A* **2000**, 104, 5600-5611.
- [18] R. C. Raffenetti *J. Chem. Phys.* **1973**, 59, 5936-5949.
- [19] F. M. Bickelhaupt, E. J. Baerends *Rev. Comput. Chem.* **2000**, 15, 1-86.
- [20] K. Morokuma *Acc. Chem. Res.* **1977**, 10, 294-300.
- [21] T. Ziegler, A. Rauk, E. J. Baerends *Theor. Chim. Acta* **1977**, 43, 261-271.
- [22] P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch *J. Phys. Chem.* **1994**, 98, 11623-11627.
- [23] E. Van Lenthe, E. J. Baerends, J. G. Snijders *J. Chem. Phys.* **1993**, 99, 4597-4610.
- [24] E. Van Lenthe, A. Ehlers, E. J. Baerends *J. Chem. Phys.* **1999**, 110, 8943-8953.
- [25] C. Goedecke, P. Hillebrecht, T. Uhlemann, R. Haunschild, G. Frenking *Can. J. Chem.* **2009**, 87, 1470-1479.