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A lead(II) toluene complex

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Contents

1. Additional Information

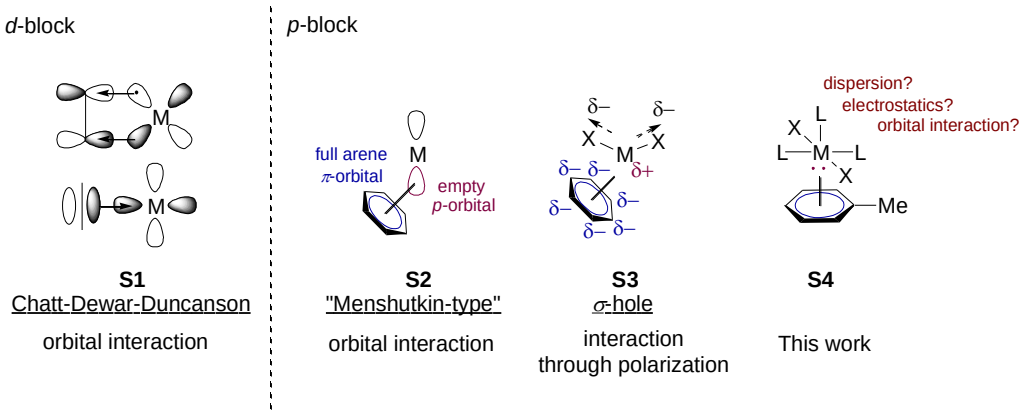

Figure S1. Representation of the Dewar-Chatt-Duncanson (DCD) model (**S1**), "Menshutkin-type" (**S2**), σ-hole (**S3**) and dispersive interactions (**S4**).

NOCV-EDA (Natural Orbitals for Chemical Valence - Energy Decomposition Analysis):

In general, the total energy (ΔE) of the formation of the molecule AB from the fragments A and B can be separated into two components (Eq. 1) [S1].

$$\Delta E_{\mathrm{tot}} = \Delta E_{\mathrm{geo,prep}} + \Delta E_{\mathrm{int}} \quad (1)$$

Where $E_{\mathrm{geo,prep}}$ is the energy penalty, sometimes referred to as "strain-energy", due to distorting the two fragments A and B. The interaction energy, ΔE_{int}, may be further separated into orbital (ΔE_{orb}), dispersive (ΔE_{disp}), Pauli- ($\Delta E_{\mathrm{Pauli}}$), as well as electrostatic ($\Delta E_{\mathrm{elstat}}$) contributions according to Eq. 2.

$$\Delta E_{\mathrm{int}} = \Delta E_{\mathrm{orb}} + \Delta E_{\mathrm{disp}} + \Delta E_{\mathrm{Pauli}} + \Delta E_{\mathrm{elstat}} \quad (2)$$

The latter two may be combined into $\Delta E_{\mathrm{Pauli+elstat}}$ (Eq. 3).

$$\Delta E_{\mathrm{tot}} = \Delta E_{\mathrm{geo,prep}} + \Delta E_{\mathrm{int}} = \Delta E_{\mathrm{geo,prep}} + \Delta E_{\mathrm{orb}} + \Delta E_{\mathrm{disp}} + \Delta E_{\mathrm{Pauli+elstat}} \quad (3)$$

Table S1 Energy contributions to the overall energy ΔE_{tot} of complex **7**·PhMe according to NOCV-EDA.

NOCV-EDA analysis in [kJ mol^{-1}]				
ΔE_{tot}	$\Delta E_{\mathrm{geo,prep}}$	ΔE_{orb}	ΔE_{disp}	$\Delta E_{\mathrm{Pauli+elstat}}$
−68	+2	+27	−58	−39

LED (local energy decomposition):

In LED analysis, the various contributions are separated into a Hartree-Fock (HF) and a correlated CCSD component as well as the perturbative triples correction (Eq. 4).

$$\Delta E_{\mathrm{int}} = \Delta E^{\mathrm{HF}} + \Delta E^{\mathrm{CCSD}} + \Delta E_{\mathrm{int}}^{(\mathrm{T})} \quad (4)$$

Therein, the coupled-cluster contributions may be further separated into dispersive- ($\Delta E_{\mathrm{disp}}^{\mathrm{CCSD}}$) as well as non-dispersive contributions ($\Delta E_{\mathrm{non-disp}}^{\mathrm{CCSD}}$).

$$\Delta E_{\mathrm{tot}} = \Delta E_{\mathrm{geo,prep}} + \Delta E_{\mathrm{int}} = \Delta E_{\mathrm{geo,prep}} + \Delta E^{\mathrm{HF}} + \Delta E_{\mathrm{disp}}^{\mathrm{CCSD}} + \Delta E_{\mathrm{non-disp}}^{\mathrm{CCSD}} + \Delta E_{\mathrm{int}}^{(\mathrm{T})} \quad (5)$$

Table S2 Energy contributions to the overall energy ΔE_{tot} of complex **7**·PhMe according to LED analysis.

LED analysis in [kJ mol^{-1}]				
ΔE_{tot}	$\Delta E_{geo,prep}$	ΔE^{HF}	ΔE_{disp}^{CCSD}	$\Delta E_{non-disp}^{CCSD} + \Delta E_{int}^{(T)}$
−73	+5	+44	−98	−24

2. General

All reactions were carried out under an atmosphere of dry dinitrogen, either in an MBraun dinitrogen filled glovebox or using standard Schlenk techniques. NMR spectra were recorded on a Bruker Avance III 300 NMR spectrometer (^{19}F = 282.40 MHz) and/or a Bruker Avance IV 400 NMR spectrometer (^{1}H = 400.13 MHz, ^{13}C = 100.60 MHz,^{207}Pb = 83.71 MHz). The solvent residual signals were used as an internal reference for the ^{1}H NMR and ^{13}C NMR spectra. ^{1}H NMR multiplicities are abbreviated as follows: d: doublet, t: triplet, q: quartet, spt: septet. All coupling constants *J* are given in Hz. Solvents were purified using a two-column solid-state purification system (MBraun; MB-SPS 5 / 7, Garching bei München, Germany). Hexane, toluene and benzene were stored over a mirror of potassium; all other solvents were stored over activated molecular sieves. Deuterated NMR solvents were obtained dry and packaged under argon and stored over activated molecular sieves or a mirror of potassium (C_6D_6). Elemental analyses were either obtained using Euro EA 3000 (Euro Vector) and EA 1108 (Carlo-Erba) elemental analyzers or performed in triplicate for each sample using Leco CHN-900 analyzer, the mean values are given below for each compound. Imidazolinium salt **4** [S2] and carbene **5** [S2(*a*)] were synthesized according to literature procedures. All other reagents were obtained from commercial sources and used as is without further purification.

3. Synthetic Procedures and NMR spectra

3.1 Lead(II) hexamethyldisilazide ($Pb[N(SiMe_3)_2]_2$)

$Pb[N(SiMe_3)_2]_2$ was synthesized according to a modified literature procedure [S3]. $PbBr_2$ (4.84 g; 13.2 mmol; 2.00 eq) and $LiN(SiMe_3)_2$ (4.20 g; 25.1 mmol; 1.90 eq.) were loaded in a Schlenk flask. The flask was cooled to 0 °C and Et_2O (20 mL) was slowly added. After the addition, the orange mixture was stirred at room temperature for 24 h. The solvent was removed *in vacuo*. The product was purified by distillation at 100–110 °C / 5.2×10^{-2} mbar to yield 6.61 g (95%) of the yellow product. The analytical data corresponded to the literature data [S3].

3.2 Lead(II) dibromide 6

Method A: Bis-imidazolinium dibromide salt **4** [S2] (580 mg; 0.83 mmol; 1.00 eq) and $Pb[N(SiMe_3)_2]_2$ (461 mg; 0.87 mmol; 1.05 eq) were loaded in a Schlenk flask. Toluene (10 mL) was added at −78 °C. The yellow mixture was stirred at room temperature. After 16 h, the volatiles were removed *in vacuo*. The residue was washed with pentane (3 × 20 mL) and dried *in vacuo* to yield 740 mg (quantitative yield) of the beige product.

Method B: The free carbene was prepared and isolated through deprotonation of **4** with $KN(SiMe_3)_2$ in toluene according to Ref. [S2(*a*)]. $PbBr_2$ (116 mg; 0.32 mmol; 0.90 eq.) was added to the carbene **5** dissolved in THF (2 mL). After 10 min, a thick, off-white precipitate formed. The mixture was vigorously stirred. After 16 h, the solvent was evaporated *in vacuo*. The residue was washed with C_6H_6 (3 × 2 mL) and pentane (5 mL). The residue was dried *in vacuo* to yield 222 mg (76%) of the beige product. M.p.: 273 °C (decomp.) Calculated for $C_{35}H_{45}Br_2N_5Pb$, %: C, 46.57; N, 7.76; H, 5.02. Found, %: C, 46.45; N, 7.58; H, 5.06.

^{1}H NMR (400 MHz; DMSO-d_6): δ = 8.17 (t, *J* = 8.0 Hz, 1 H, Py–**H**^{para}), 7.38 (t, *J* = 8.0 Hz, 2 H, Dipp–**H**^{para}), 7.26 (d, *J* = 8.0 Hz, Dipp–**H**^{meta}), 7.01 (d, *J* = 8.0 Hz, 2 H, Py–**H**^{meta}), 4.32 (t, *J* = 10.0 Hz, 4 H, C**H**$_2$), 4.09 (t, *J* = 10.0 Hz, 4 H, C**H**$_2$), 3.14 (spt, *J* = 8.0 Hz, 4 H, C**H**) 1.19 (d, *J* = 8.0 Hz, 12 H, C**H**$_3$) 1.17 (d, *J* = 8.0 Hz, 12 H, C**H**$_3$) ppm.

^{13}C NMR (101 MHz; DMSO-d_6): δ = 246.2 (**C**^{Carbene}), 150.8 (Py–**C**^{ortho}H), 145.9 (N–**C**^{Dipp}), 143.5 (Py–**C**^{para}H), 134.2 (**C**^{Dipp}–*i*Pr), 129.3 (Py–**C**^{meta}H), 124.4 (Dipp–**C**^{meta}H), 105.0 (Dipp–**C**^{para}H), 56.9 (**C**H$_2$), 46.6 (**C**H$_2$), 27.4 (**C**H$_3$), 25.6 (**C**H), 24.7 (**C**H$_3$) ppm.

^{207}Pb NMR (83.7 MHz; DMSO-d_6): δ = 186.9 ppm.

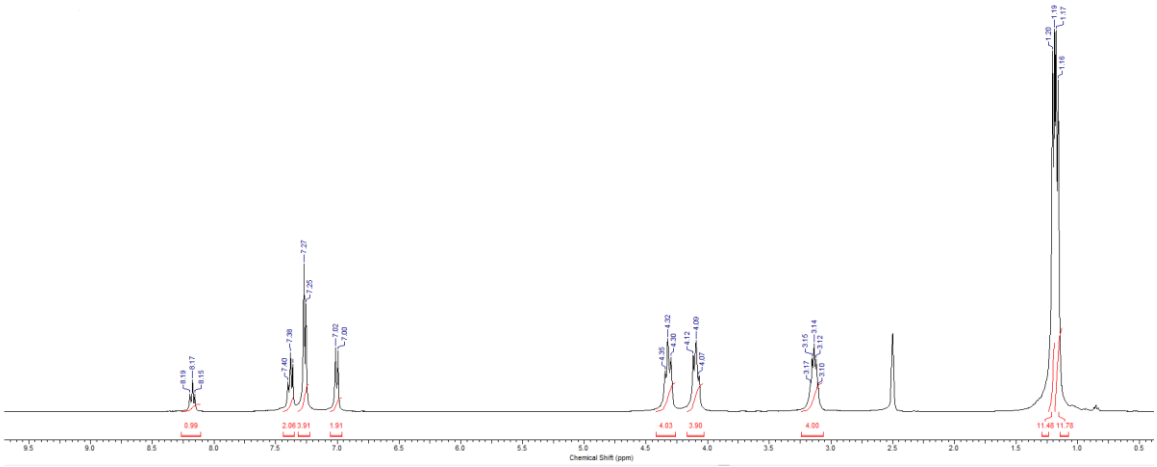

Figure S2. ^{1}H NMR spectrum of **6** (DMSO-d_6, 400.1 MHz).

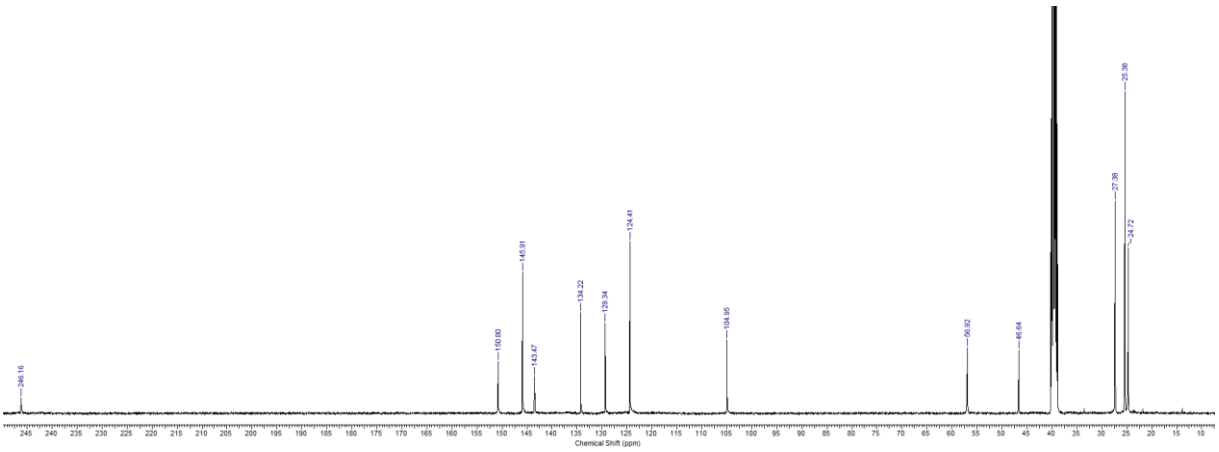

Figure S3. ^{13}C NMR spectrum of **6** (DMSO-d_6, 100.6 MHz).

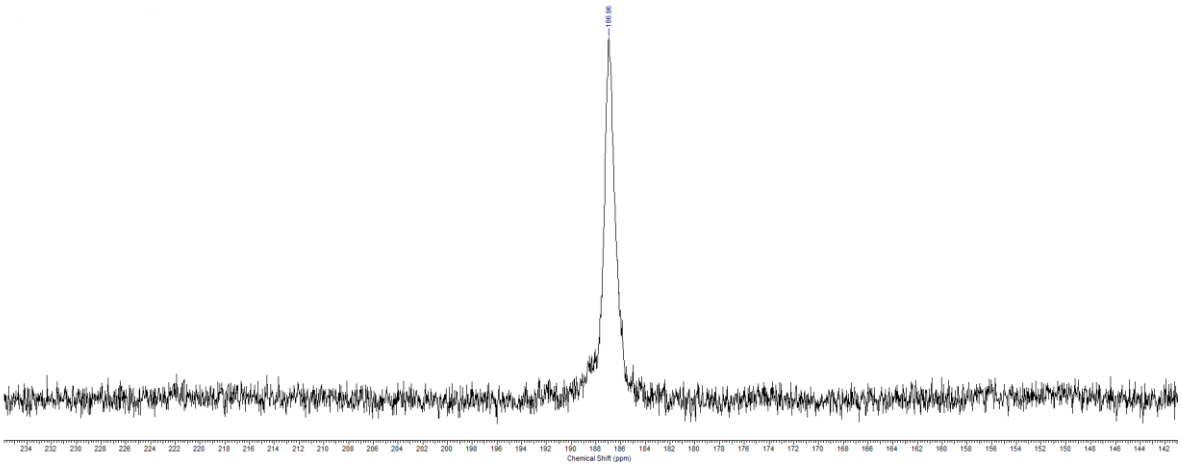

Figure S4. ^{207}Pb NMR spectrum of **6** (DMSO-d_6, 83.7 MHz).

3.3 Lead(II) ditriflate 7

Compound **6** (462 mg; 0.51 mmol; 1.00 eq.) was dissolved in THF (10 mL). Salt TlOTf (355 mg; 1.01 mmol; 1.98 eq.) was added. The mixture was stirred for 16 h. The suspension was filtered over diatomaceous earth. The solvent was removed *in vacuo*. The mixture was washed with cold (–30 °C) toluene (0.5 mL) and pentane (10 mL). The residue was dried *in vacuo* to yield 512 mg (97%) of the beige/yellow product. Single crystals suitable for X-Ray analysis were obtained by slow diffusion of hexane into a saturated toluene solution at room temperature. M.p. 261 °C (decomp.). Calculated for $C_{37}H_{45}F_6N_5O_6S_2Pb$, %: C, 42.69; N, 6.73; H, 4.36. Found, %: C, 41.94; N, 6.47; H, 4.51.

^{1}H NMR (400 MHz; DMSO-d_6): δ = 8.31 (t, *J* = 8.0 Hz, 1 H, Py–**H**^{para}), 7.42 (t, *J* = 8.0 Hz, 2 H, Dipp–**H**^{para}), 7.31 (d, *J* = 8.0 Hz, Dipp–**H**^{meta}), 7.16 (d, *J* = 8.0 Hz, 2 H, Py–**H**^{meta}), 4.39 (t, *J* = 10.0 Hz, 4 H, C**H**$_2$) 4.12 (t, *J* = 10.0 Hz, 4 H, C**H**$_2$) 2.99 (spt, *J* = 8.0 Hz, 4 H, C**H**) 1.21 (d, *J* = 8.0 Hz, 12 H, C**H**$_3$) 1.16 (d, *J* = 8.0 Hz, 12 H, C**H**$_3$).

^{13}C NMR (101 MHz; DMSO-d_6): δ = 252.4 (**C**^{Carbene}), 151.1 (Py–**C**^{ortho}), 145.7 (N–**C**^{Dipp}), 144.9 (Py–**C**^{para}), 134.0 (**C**^{Dipp}–*i*Pr), 129.6 (Py–**C**^{meta}H), 124.5 (Dipp–**C**^{meta}H), 105.7 (Dipp–**C**^{para}H), 57.3 (**C**H$_2$), 47.1 (**C**H$_2$), 27.5 (**C**H$_3$), 25.0 (**C**H), 24.7 (**C**H$_3$) ppm.

^{19}F NMR (282 MHz; DMSO-d_6): δ = – 77.7 ppm.

^{207}Pb NMR (83.7 MHz; DMSO-d_6): δ = – 430.2 ppm.

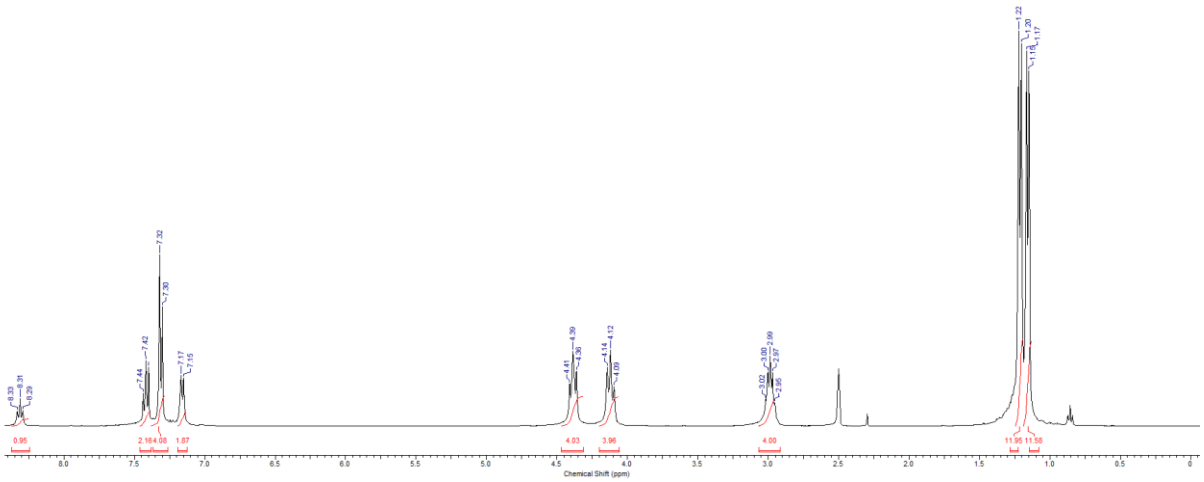

Figure S5. ^{1}H NMR spectrum of **7** (DMSO-d_6, 400.1 MHz).

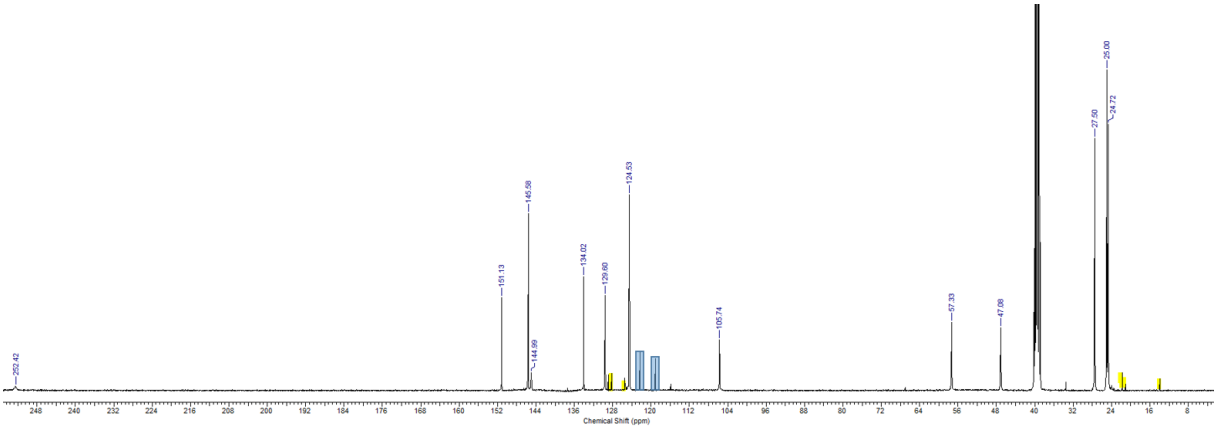

Figure S6. ^{13}C NMR spectrum of **7** (DMSO-d_6, 100.6 MHz). Two peaks of the quartet signal of the CF_3 group of the triflate anion are superimposed (blue). Signals marked yellow are assigned to small solvent (toluene; pentane) residues.

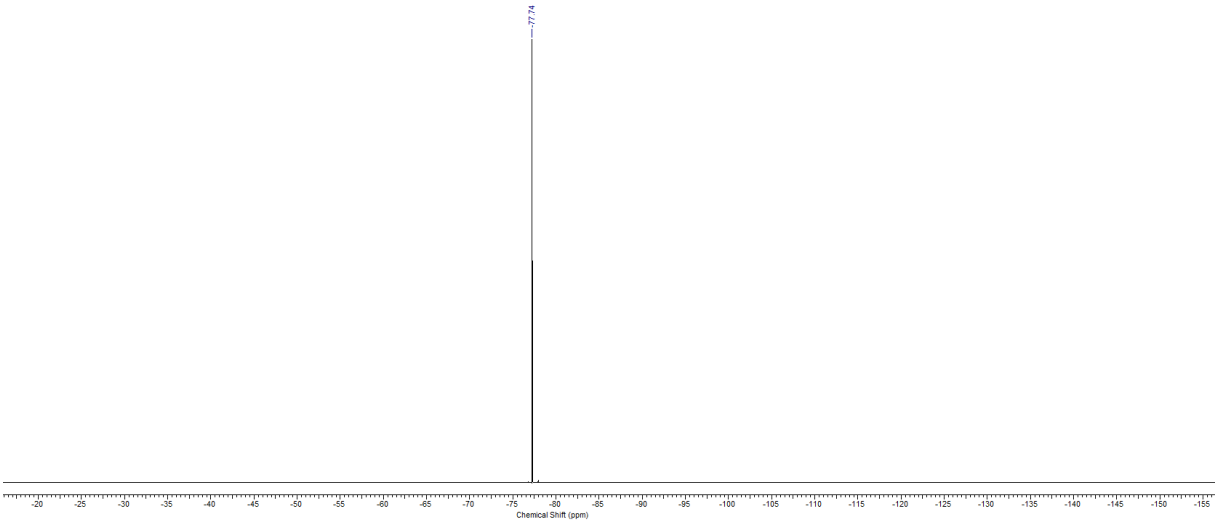

Figure S7. ^{19}F NMR spectrum of **7** (DMSO-d_6, 282.4 MHz).

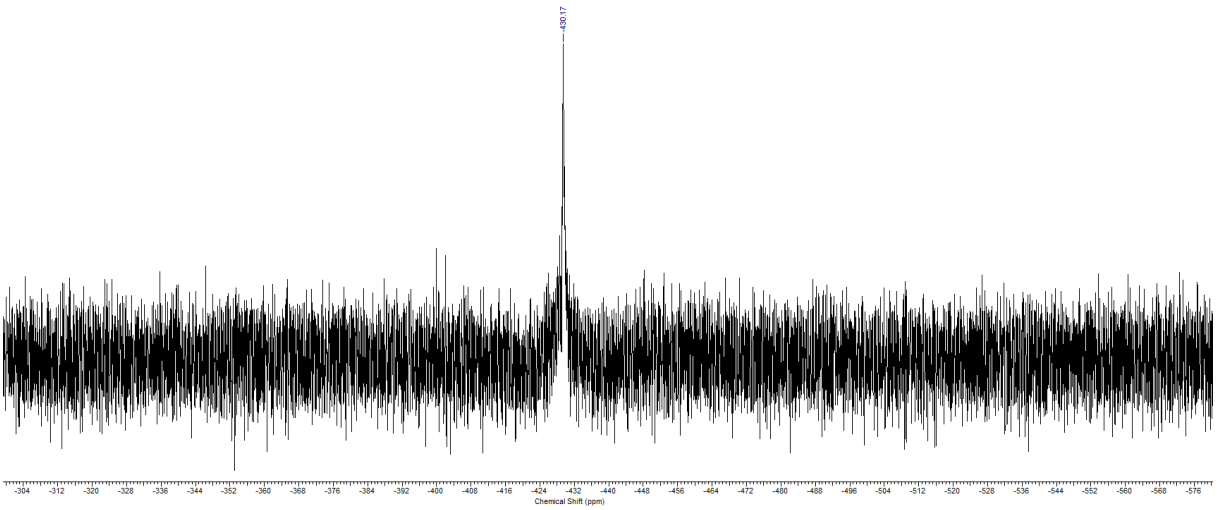

Figure S8. ^{207}Pb NMR spectrum of **7** (DMSO-d_6, 83.7 MHz).

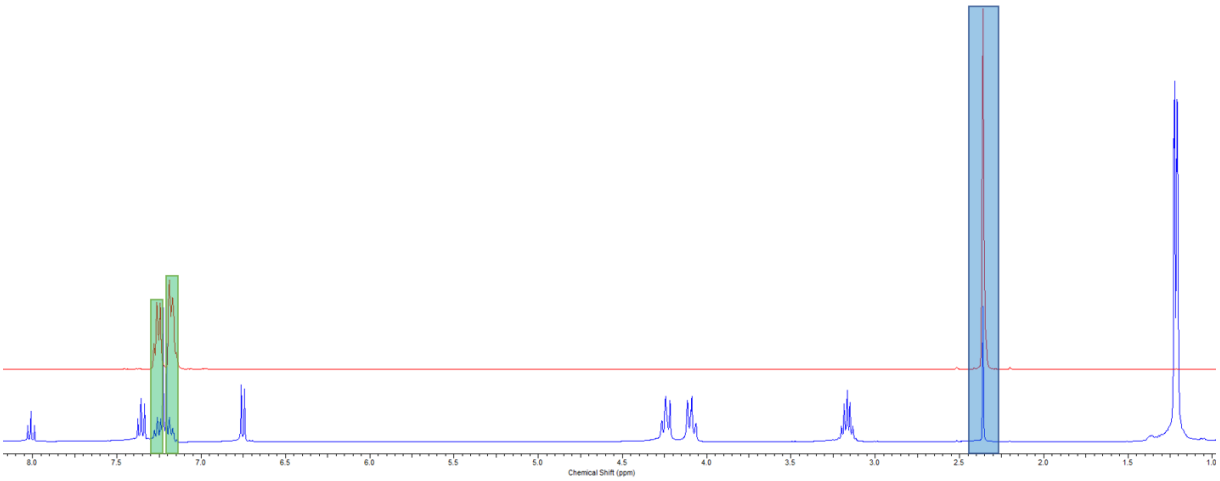

Figure S9. ^{1}H NMR (400.1 MHz) of single crystals of **7**·PhMe dissolved in $CDCl_3$ (bottom) and toluene dissolved in $CDCl_3$ top). No change was observed in the shift of either the Me-group (blue) or the aromatic protons (green) of the co-crystallized toluene molecule.

4. X-ray Crystallographic Data of **7**·PhMe

CCDC-2074842 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK (fax: ++33-1223-336-033; e-mail: deposit@ccdc.cam.ac.uk).

Single crystals of **7**·PhMe were obtained by vapor diffusion of *n*-hexane into a saturated toluene solution of **7**·PhMe. For the preparation, the sample was coated with protective perfluoropolyalkylether oil. A suitable single crystal was selected, mounted on a MiTeGen micro mount and transferred to the cold nitrogen gas stream of the diffractometer. Intensity data were collected at 100 K on a Bruker Kappa Photon 2 $I\mu S$ Duo diffractometer equipped with QUAZAR focusing Montel optics using Mo$K\alpha$ radiation (λ = 0.71073 Å). Data were corrected for Lorentz and polarization effects; semiempirical absorption corrections were performed on the basis of multiple scans using SADABS [S4]. The structure was solved by direct methods (*SHELXT*) [S5] and refined by full-matrix least-squares procedures on F^2 using *SHELXL 2018/3* [S6]. *OLEX2* was used to prepare material for publication [S7].

Identification code	**7**·PhMe
Empirical formula	$C_{37}H_{45}F_6N_5O_6PbS_2$ x C_7H_8 x 0.5 C_6H_{14}
Formula weight/g mol^{-1}	1176.31
Temperature/K	100
Crystal system	Monoclinic
Space group	$P2_1/c$
a/Å	20.6674(12)
b/Å	13.1044(7)
c/Å	18.8317(10)
α/°	90
β/°	98.208(2)
γ/°	90
Volume/Å^3	5050.5(5)
Z	4
ρ_{calc}g/cm^3	1.547
μ/mm^{-1}	3.50
F(000)	2372
Crystal size/mm^3	0.24×0.18×0.04
Radiation	Mo$K\alpha$, λ = 0.71073 Å
2Θ range for data collection/°	$3.6 \leq 2\Theta \leq 61.2$
Index ranges	$-29 \leq h \leq 29$, $-18 \leq k \leq 18$, $-26 \leq l \leq 21$
Reflections collected	224327
Independent reflections	15425
Observed reflections [I>=2σ(I)]	12732
Data/restraints/parameters	15425 / 0 / 614
Goodness-of-fit on F^2	1.062
Final R indexes [I>=2σ(I)]	R_1 = 0.0241, wR_2 = 0.0456
Final R indexes [all data]	R_1 = 0.0392, wR_2 = 0.0509
Largest diff. Peak/hole/eÅ^{-3}	1.415 / −1.429

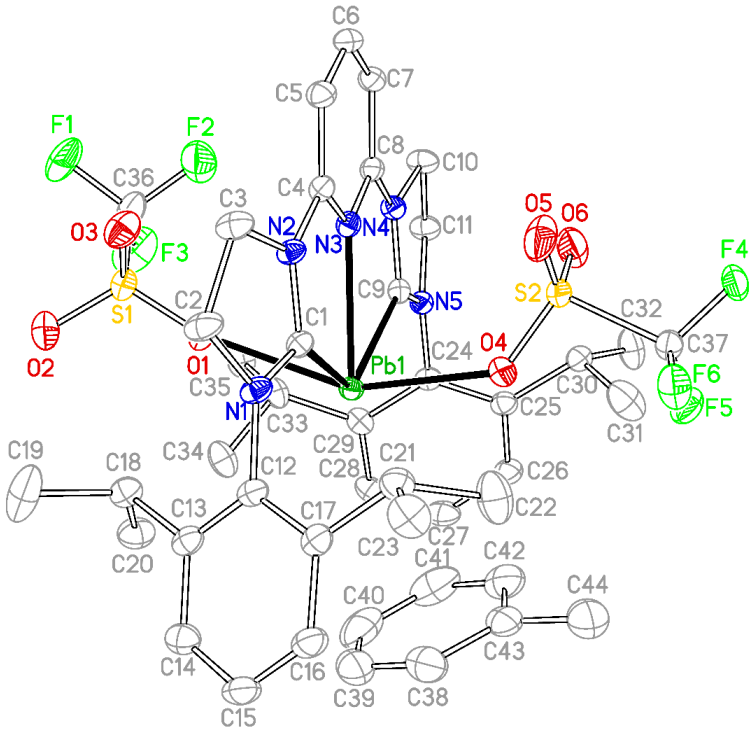

Figure S10. Thermal ellipsoid representation of the molecular structure of **7**·PhMe with the applied numbering scheme (50% probability ellipsoids, hydrogen atoms are omitted for clarity). Selected bond lengths [Å] and angles [°]: Pb-C1: 2.554(2); Pb-C9: 2.570(2); Pb-N3: 2.5416(18); Pb-C38: 4.398(3); Pb-C39: 4.253(3); Pb-C40: 3.932(3); Pb-C41: 3.728(4); Pb-C42: 3.889(3); Pb-C43: 4.253(3); C1-N1-C12: 125.07(18); C2-N1-C1: 113.79(18); C2-N1-C12: 121.13(17); C4-N2-C3: 123.36(17); C3-N2-C1 113.68(17); C4-N2-C1: 122.64(18); C9-N4-C8: 122.73(18); C8-N4-C10: 123.43(18); C9-N4-C10: 113.16(17); C9-N5-C11: 113.05(18); C9-N5-C24: 125.04(18); C24-N5-C11: 121.17(17); N1-C1-N2: 108.14(18); N1-C2-C3: 102.27(17); C2-C3-N2: 101.86(17); N4-C9-N5: 107.68(18); N5-C11-C10: 102.15(17); C11-C10-N4: 101.04(17).

5. Determination of Average Lead(II)–NHC Bond Lengths

Average lead(II)–NHC bonds were determined through by mean of the following reported lead(II)–NHC compounds:

Table S3 Average Pb–NHC bond lengths.

Reference	Bond length [Å]
[S8]	2.411
[S9]	2.443
[S10]	2.541
[S11]	2.440
[S11]	2.418
[S12]	2.434
[S13]	2.725
[S13]	2.734
[S14]	2.584
[S15]	2.437
Average	**2.517**

6. Computational Details

All calculations were performed using ORCA 4.2.1 [S16] and the functionals BP86 [S17], B3LYP [S18], and PBE0 [S19] were evaluated. The geometry optimizations were performed at the PBE0-D3/ZORA-def2-SVP level of theory, applying Grimme's D3 dispersion correction [S20] with Becke-Johnson damping [S21]. For lead, the all-electron scalar relativistic basis set SARC-ZORA-TZVP was used [S22]. The RIJCOSX approximation [S23] and the related relativistically recontracted auxiliary basis set ("SARC/J") were used to speed up the calculations. Tighter than default convergence criteria were chosen for both the optimization (tightopt) of the structural parameters as well as the scf (tightscf) and more accurate than default grid values (Gridx9, Grid7, NoFinalGrid) were used. All PBE0-D3BJ/ZORA-def2-SVP optimized structures were verified as true minima by the absence of negative eigen values in the harmonic vibrational frequency analysis. The energies of all structures were corrected by single-point calculations at the PBE0-D3BJ/ZORA-def2-TZVPP level of theory. Electronic energies were corrected by single points calculations at the PBE0-D3BJ/ZORA-def2-TZVPP level of theory. Solvent effects were accounted for by using the implicit conductor-like polarizable continuum model (CPCM) [S24]. Energy decomposition analyses were carried out using either the natural orbitals for chemical valence (NOCV) [S25] scheme on the PBE0-D3BJ/ZORA-def2-TZVPP (lead: SARC-ZORA-TZVPP) level of theory or using the local energy decomposition (LED) [S26] scheme on the DLPNO-CCSD(T)/def2-TZVPP [S27 and S28, respectively] level of theory. For the LED scheme, tighter than normal "tightPNO" settings [S29], the RIJK approximation, as well as the auxiliary basis sets def2/JK and def2-TZVPP/C were used. For the visualization of the weak interactions, Yang's noncovalent interaction method [S30] in combination with MultiWFN [S31] was applied [S32].

Benchmark

Table S4 Screening of different functionals (BP86-D3; B3LYP-D3; PBE0-D3) showed that PBE0-D3 is in best agreement with the bond length obtained from the crystal structure according to their mean absolute deviation (MAD) and their root-mean-square deviation (RMSD).

Atom number	Crystal Structure [Å]	BP86-D3/ZORA-def2-SVP (lead: def2-TZVP) [Å]	B3LYP-D3/ZORA-def2-SVP (lead: def2-TZVP) [Å]	PBE0-D3/ZORA-def2-SVP (lead: def2-TZVP) [Å]
Pb1–N3	2.542	2.737	2.741	2.633
Pb1–C1	2.554	2.646	2.640	2.590
Pb1–C9	2.570	2.618	2.636	2.581
Pb1–C38	4.398	3.535	3.581	3.627
Pb1–C39	4.253	3.530	3.580	3.656
Pb1–C40	3.932	3.513	3.582	3.670
Pb1–C41	3.728	3.506	3.588	3.658
Pb1–C42	3.888	3.511	3.590	3.630
Pb1–C43	4.253	3.536	3.597	3.623
Pb1–C44	5.118	4.352	4.396	4.386
Pb1–O1	2.559	2.521	2.523	2.447
Pb1–O4	2.430	2.575	2.536	2.449
C27–C41	3.901	3.740	3.764	3.770
C26–C41	4.056	4.041	4.050	4.041
C28–C41	3.818	3.496	3.571	3.602
C28–C40	4.322	4.551	4.604	4.618
C27–C40	4.692	5.019	5.029	5.022
C26–C40	5.147	5.419	5.412	5.397
C26–C42	4.587	3.773	3.799	3.817
C27–C42	4.795	3.953	3.985	4.017
C14–C39	3.727	3.556	3.605	3.616
C15–C39	3.924	3.747	3.780	3.791
C15–C38	3.792	3.892	3.946	3.989
C16–C38	3.855	3.671	3.731	3.779
C22–C44	3.632	3.684	3.750	3.7909
MAD		**0.33**	**0.31**	**0.28**
RMSD		**0.43**	**0.40**	**0.38**

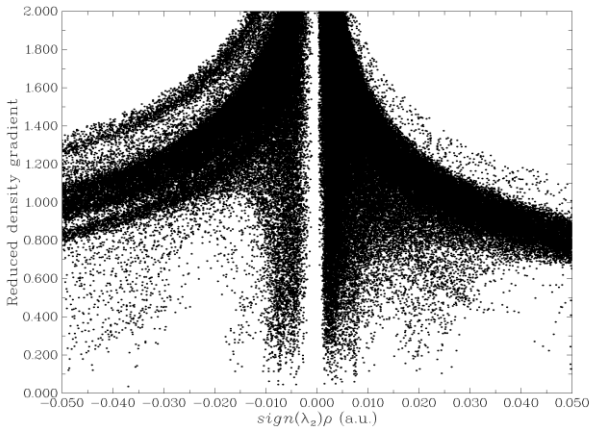

Figure S11 Scatter plot of **7**·PhMe.

The "strength" of the interaction correlates with the electron density ρ. Yet, this interaction could be either attractive or repulsive in nature. However, the product of ρ and the sign of λ_2 (an Eigenvector of the Hessian Matrix of electron density) gives rise to the "direction" of the interaction. At negative values, the interaction is attractive. At positive values, the interaction is repulsive. The interaction is weak at sign(λ_2)ρ close to zero [S30]. The scatter plot indicates weak interactions due to spikes observed in the negative region, close to 0.

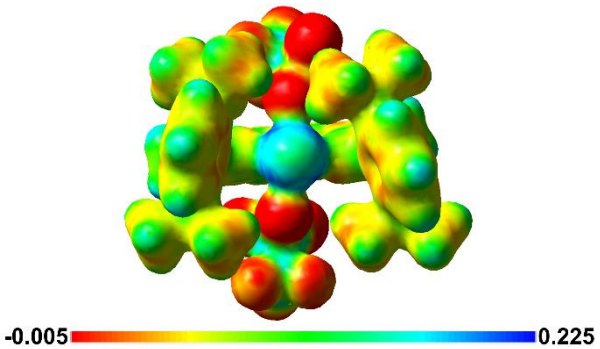

Figure S12. Electrostatic potential map (isovalue: 0.02) of **7**.

	NImag	**Δ*E*** (PBE0-D3/def2-SVP Lead: def2-TZVP)	**Δ*G*** (PBE0-D3/def2-SVP Lead: def2-TZVP)	**Δ*E*** (PBE0-D3/def2-TZVPP//PBE0-d3/def2-SVP)	**Δ*E*** (PBE0-D3/def2-TZVPP//PBE0-D3/def2-SVP) CPCM= Benzene	**Δ*E*** (PBE0-d3/def2-TZVPP//PBE0-D3/def2-SVP) CPCM= Chloroform	**Δ*E*** (PBE0-d3/def2-TZVPP//PBE0-D3/def2-SVP) CPCM= Toluene	**Δ*E*** (DLPNO-CCSD(T)/def2-TZVPP//PBE0-D3/def2-SVP)
7^{opt}	0	–25247.77213	–25247.048529	–25251.846144	–25251.865624	–25251.874956	–25251.866464	–3744.759329
7*	-			–25251.845463				–3744.757435
^{H}**7**$^{H\text{-}opt}$	-	–24314.925315						
7·PhMe	0	–25519.046583	–25518.200732	–25523.394742	–25523.415113	–25523.424887	–25523.415991	–4015.837783
^{H}**7**·PhMe$^{H\text{-}opt}$	-	–24586.188423						
PhMe^{opt}	0	–271.241873	–271.143030	–271.522496	–271.525193	–271.526452	–271.525307	–271.050771
PhMe*	-			–271.522399				–271.050760
PhMe$^{H\text{-}opt}$	-	–271.241852						

XYZ Coordinates

7^{opt}

Pb	-0.09481	0.07639	-0.20276
S	-1.67289	3.43046	0.41069
S	1.31797	-2.26249	2.09120
F	-1.26031	5.47803	1.97256
F	0.00823	3.79280	2.38592
F	0.38321	5.01887	0.66227
F	2.05470	-4.48612	3.20052
F	2.65577	-4.30289	1.14597
F	0.60623	-4.73054	1.62986
O	-0.69182	2.43577	-0.13977
O	-2.22582	4.32317	-0.60479
O	-2.62000	2.84916	1.37304
O	0.83401	-1.98082	0.68934
O	0.27446	-2.14464	3.10883
O	2.61528	-1.63259	2.37981
N	-3.44193	-0.43729	0.70658
N	-2.27180	0.21194	2.39857
N	-0.03730	0.72398	2.35024
N	2.17945	1.21209	2.04748
N	3.23108	1.05884	0.16773
C	-2.21291	-0.24766	1.14307
C	-4.47037	0.00936	1.65680
H	-5.18841	-0.79596	1.85235
H	-5.00808	0.86611	1.23383
C	-3.63864	0.39614	2.88584
H	-3.78452	1.44448	3.16706
H	-3.83360	-0.25241	3.74930
C	-1.14106	0.63222	3.07785
C	-1.16241	0.93460	4.44179
H	-2.07675	0.85850	5.02197
C	0.04199	1.29840	5.03230
H	0.07405	1.52075	6.09736
C	1.20712	1.38035	4.27694
H	2.15323	1.66769	4.72478
C	1.10350	1.09365	2.91473
C	2.04853	0.97299	0.73700
C	3.57415	1.34518	2.46544
H	3.84162	0.47217	3.07309
H	3.72986	2.26420	3.04172
C	4.30999	1.36411	1.11875
H	4.75232	2.33976	0.88307
H	5.09675	0.60486	1.05994
C	-3.76914	-1.03163	-0.55046
C	-3.90564	-0.22181	-1.69150
C	-4.25000	-0.85193	-2.89249
H	-4.36316	-0.25130	-3.79357
C	-4.43949	-2.22747	-2.95259
H	-4.70519	-2.69781	-3.89837
C	-4.28163	-3.00929	-1.81121
H	-4.41768	-4.08707	-1.87571
C	-3.94495	-2.42853	-0.58664
C	-3.68371	1.27412	-1.64570
H	-3.22708	1.51249	-0.67998
C	-5.00099	2.04950	-1.70774
H	-5.49716	1.91329	-2.67777
H	-4.80176	3.11774	-1.56285
H	-5.70024	1.72276	-0.92846
C	-2.72208	1.75070	-2.73497
H	-1.79525	1.16406	-2.73721
H	-2.45724	2.79799	-2.55584
H	-3.17031	1.67050	-3.73365
C	-3.70550	-3.27914	0.64568
H	-3.84720	-2.63784	1.52581
C	-2.25560	-3.76802	0.68083
H	-2.04050	-4.40401	-0.18760
H	-2.06309	-4.35280	1.58754
H	-1.53883	-2.94048	0.67439
C	-4.68689	-4.44180	0.77313
H	-5.72849	-4.10370	0.71113
H	-4.54670	-4.94603	1.73671
H	-4.52989	-5.19570	-0.00823
C	3.42999	0.97322	-1.24242
C	4.05122	-0.17425	-1.76324
C	4.30041	-0.21228	-3.13891
H	4.78758	-1.08616	-3.56920
C	3.90951	0.83496	-3.96411
H	4.10740	0.78747	-5.03407
C	3.23859	1.93278	-3.43225
H	2.90380	2.72860	-4.09417
C	2.97895	2.03051	-2.06264
C	4.39509	-1.36677	-0.89337
H	3.99748	-1.18731	0.11366
C	3.69990	-2.62920	-1.40521
H	2.61485	-2.48538	-1.44960
H	3.89133	-3.46537	-0.72620
H	4.05494	-2.91149	-2.40437
C	5.90736	-1.57116	-0.78712
H	6.34541	-1.80767	-1.76559
H	6.13475	-2.40257	-0.10885
H	6.41623	-0.67481	-0.41071
C	2.24744	3.23487	-1.49854
H	1.71054	2.91397	-0.59874
C	1.17856	3.78580	-2.43958
H	1.61357	4.30394	-3.30411
H	0.54639	4.49836	-1.90028
H	0.52127	2.98941	-2.80552
C	3.23135	4.33211	-1.08471
H	3.97576	3.96464	-0.36856
H	2.69320	5.16358	-0.61523
H	3.77465	4.71946	-1.95653
C	-0.56792	4.50230	1.42577
C	1.68298	-4.06750	2.00805

7*

Pb	-0.07296	-0.02656	-0.31796
S	-1.50010	3.37749	0.25338
S	1.19712	-2.38789	2.03537
F	-0.97358	5.41682	1.79142
F	0.25272	3.69682	2.18367
F	0.61491	4.89315	0.43726
F	2.13250	-4.56343	3.10897
F	2.29923	-4.50983	0.96531
F	0.39129	-4.86621	1.88440
O	-0.56891	2.36924	-0.35495
O	-2.06786	4.30882	-0.71815
O	-2.42195	2.80318	1.24506
O	0.65566	-2.15639	0.64697
O	0.20040	-2.22285	3.09326
O	2.51173	-1.76569	2.24532
N	-3.53261	-0.44859	0.65418
N	-2.27455	0.12421	2.30343
N	-0.02752	0.63504	2.22963
N	2.19437	1.16717	1.96114
N	3.33917	1.08849	0.14104
C	-2.27745	-0.26733	1.02045
C	-4.50804	-0.14090	1.70744
H	-5.09983	-1.03563	1.94074
H	-5.18999	0.64598	1.36549
C	-3.61377	0.31062	2.86276
H	-3.75416	1.36962	3.10948
H	-3.75263	-0.29908	3.76315
C	-1.12770	0.52470	2.96447
C	-1.14602	0.80087	4.33485
H	-2.05817	0.71083	4.91523
C	0.05399	1.15725	4.93346
H	0.08756	1.35422	6.00341
C	1.21274	1.26380	4.17516
H	2.15802	1.54237	4.62883
C	1.10955	1.00660	2.80609
C	2.14303	0.87174	0.65241
C	3.54751	1.45725	2.43148
H	3.90844	0.60777	3.02650
H	3.57101	2.36712	3.04067
C	4.30517	1.61561	1.11434
H	4.53263	2.66274	0.87496
H	5.23903	1.04419	1.08285
C	-3.97658	-0.98409	-0.58959
C	-4.38709	-0.10303	-1.60493
C	-4.90756	-0.66422	-2.77577
H	-5.23991	-0.00706	-3.57839
C	-4.98970	-2.04373	-2.93597
H	-5.38962	-2.46041	-3.85941
C	-4.55596	-2.89404	-1.92277
H	-4.61679	-3.97260	-2.06219
C	-4.05305	-2.38320	-0.72284
C	-4.26208	1.39931	-1.46346
H	-3.73538	1.61199	-0.52594
C	-5.63137	2.07599	-1.38295
H	-6.19297	1.95509	-2.31873
H	-5.50470	3.14932	-1.19870
H	-6.24523	1.66047	-0.57405
C	-3.41918	2.00012	-2.58919
H	-2.43040	1.53132	-2.63328
H	-3.26257	3.06813	-2.40693
H	-3.90209	1.87397	-3.56746
C	-3.58873	-3.31974	0.37573
H	-3.38700	-2.71744	1.26974
C	-2.26863	-3.99137	-0.00262
H	-2.38736	-4.61721	-0.89723
H	-1.90993	-4.62851	0.81298
H	-1.48699	-3.25085	-0.19891
C	-4.65725	-4.34769	0.74693
H	-5.60417	-3.86594	1.01981
H	-4.32115	-4.95053	1.59922
H	-4.86199	-5.03796	-0.08102
C	3.68616	0.95163	-1.23327
C	4.44912	-0.16794	-1.60851
C	4.85370	-0.26150	-2.94314
H	5.44022	-1.12058	-3.26669
C	4.51470	0.72769	-3.86140
H	4.84489	0.64400	-4.89593
C	3.74214	1.81632	-3.46700
H	3.46858	2.57499	-4.19864
C	3.29824	1.94990	-2.14748
C	4.79059	-1.26355	-0.61770
H	4.43785	-0.95335	0.37251
C	4.02218	-2.54372	-0.93938
H	2.94369	-2.35977	-0.92228
H	4.23115	-3.31423	-0.19010
H	4.29504	-2.94010	-1.92683
C	6.29621	-1.51066	-0.53272
H	6.69703	-1.89624	-1.47887
H	6.51568	-2.25251	0.24462
H	6.84547	-0.59133	-0.29326
C	2.45367	3.14019	-1.73646
H	1.97975	2.90878	-0.77673
C	1.30871	3.41685	-2.70982
H	1.67103	3.78851	-3.67720
H	0.63541	4.16808	-2.28377
H	0.71151	2.51573	-2.88201
C	3.32275	4.38525	-1.54125
H	4.13500	4.20828	-0.82551
H	2.71322	5.21505	-1.16547
H	3.78172	4.69736	-2.48858
C	-0.33060	4.41410	1.23252
C	1.52775	-4.20285	1.99639

H7H-opt

Pb	-0.07406	-0.03514	-0.33366
S	-1.50542	3.36761	0.23491
S	1.20001	-2.39251	2.02148
F	-0.98095	5.40912	1.77074
F	0.24774	3.69111	2.16420
F	0.60769	4.88620	0.41647
F	2.13863	-4.56578	3.09685

F	2.30446	-4.51407	0.95307
F	0.39734	-4.87203	1.87325
O	-0.57315	2.35998	-0.37280
O	-2.07476	4.29725	-0.73731
O	-2.42613	2.79307	1.22751
O	0.65770	-2.16308	0.63307
O	0.20348	-2.22774	3.07960
O	2.51388	-1.76839	2.23031
N	-3.53279	-0.46073	0.64024
N	-2.27483	0.11533	2.28844
N	-0.02849	0.62901	2.21326
N	2.19260	1.16377	1.94338
N	3.33679	1.08480	0.12291
C	-2.27772	-0.27748	1.00584
C	-4.50820	-0.15327	1.69359
H	-5.10078	-1.04199	1.94278
H	-5.18833	0.63977	1.36310
C	-3.61408	0.30054	2.84811
H	-3.75323	1.36058	3.09081
H	-3.75311	-0.30979	3.74759
C	-1.12824	0.51796	2.94864
C	-1.14639	0.79545	4.31876
H	-2.05770	0.70363	4.90012
C	0.05339	1.15397	4.91655
H	0.08726	1.35175	5.98624
C	1.21171	1.26129	4.15769
H	2.15672	1.54132	4.61096
C	1.10831	1.00262	2.78891
C	2.14113	0.86699	0.63496
C	3.54554	1.45607	2.41291
H	3.90618	0.60567	3.00647
H	3.56825	2.36771	3.01892
C	4.30248	1.61412	1.09532
H	4.53288	2.66331	0.86750
H	5.23521	1.04084	1.07771
H	-3.79680	-0.73318	-0.29300
H	3.54639	0.95682	-0.85410
C	-0.33689	4.40670	1.21257
C	1.53298	-4.20707	1.98415

7·PhMe **[**PBE0-D3/ZORA-def2-SVP (lead: SARC-ZORA-TZVP)]

Pb	-0.07296	-0.02656	-0.31796
S	-1.50010	3.37749	0.25338
S	1.19712	-2.38789	2.03537
F	-0.97358	5.41682	1.79142
F	0.25272	3.69682	2.18367
F	0.61491	4.89315	0.43726
F	2.13250	-4.56343	3.10897
F	2.29923	-4.50983	0.96531
F	0.39129	-4.86621	1.88440
O	-0.56891	2.36924	-0.35495
O	-2.06786	4.30882	-0.71815
O	-2.42195	2.80318	1.24506
O	0.65566	-2.15639	0.64697
O	0.20040	-2.22285	3.09326
O	2.51173	-1.76569	2.24532
N	-3.53261	-0.44859	0.65418
N	-2.27455	0.12421	2.30343
N	-0.02752	0.63504	2.22963
N	2.19437	1.16717	1.96114
N	3.33917	1.08849	0.14104
C	-2.27745	-0.26733	1.02045
C	-4.50804	-0.14090	1.70744
H	-5.09983	-1.03563	1.94074
H	-5.18999	0.64598	1.36549
C	-3.61377	0.31062	2.86276
H	-3.75416	1.36962	3.10948
H	-3.75263	-0.29908	3.76315
C	-1.12770	0.52470	2.96447
C	-1.14602	0.80087	4.33485
H	-2.05817	0.71083	4.91523
C	0.05399	1.15725	4.93346
H	0.08756	1.35422	6.00341
C	1.21274	1.26380	4.17516
H	2.15802	1.54237	4.62883
C	1.10955	1.00660	2.80609
C	2.14303	0.87174	0.65241
C	3.54751	1.45725	2.43148
H	3.90844	0.60777	3.02650
H	3.57101	2.36712	3.04067
C	4.30517	1.61561	1.11434
H	4.53263	2.66274	0.87496
H	5.23903	1.04419	1.08285
C	-3.97658	-0.98409	-0.58959
C	-4.38709	-0.10303	-1.60493
C	-4.90756	-0.66422	-2.77577
H	-5.23991	-0.00706	-3.57839
C	-4.98970	-2.04373	-2.93597
H	-5.38962	-2.46041	-3.85941
C	-4.55596	-2.89404	-1.92277
H	-4.61679	-3.97260	-2.06219
C	-4.05305	-2.38320	-0.72284
C	-4.26208	1.39931	-1.46346
H	-3.73538	1.61199	-0.52594
C	-5.63137	2.07599	-1.38295
H	-6.19297	1.95509	-2.31873
H	-5.50470	3.14932	-1.19870
H	-6.24523	1.66047	-0.57405
C	-3.41918	2.00012	-2.58919
H	-2.43040	1.53132	-2.63328
H	-3.26257	3.06813	-2.40693
H	-3.90209	1.87397	-3.56746
C	-3.58873	-3.31974	0.37573
H	-3.38700	-2.71744	1.26974
C	-2.26863	-3.99137	-0.00262
H	-2.38736	-4.61721	-0.89723
H	-1.90993	-4.62851	0.81298
H	-1.48699	-3.25085	-0.19891
C	-4.65725	-4.34769	0.74693
H	-5.60417	-3.86594	1.01981
H	-4.32115	-4.95053	1.59922

H	-4.86199	-5.03796	-0.08102
C	3.68616	0.95163	-1.23327
C	4.44912	-0.16794	-1.60851
C	4.85370	-0.26150	-2.94314
H	5.44022	-1.12058	-3.26669
C	4.51470	0.72769	-3.86140
H	4.84489	0.64400	-4.89593
C	3.74214	1.81632	-3.46700
H	3.46858	2.57499	-4.19864
C	3.29824	1.94990	-2.14748
C	4.79059	-1.26355	-0.61770
H	4.43785	-0.95335	0.37251
C	4.02218	-2.54372	-0.93938
H	2.94369	-2.35977	-0.92228
H	4.23115	-3.31423	-0.19010
H	4.29504	-2.94010	-1.92683
C	6.29621	-1.51066	-0.53272
H	6.69703	-1.89624	-1.47887
H	6.51568	-2.25251	0.24462
H	6.84547	-0.59133	-0.29326
C	2.45367	3.14019	-1.73646
H	1.97975	2.90878	-0.77673
C	1.30871	3.41685	-2.70982
H	1.67103	3.78851	-3.67720
H	0.63541	4.16808	-2.28377
H	0.71151	2.51573	-2.88201
C	3.32275	4.38525	-1.54125
H	4.13500	4.20828	-0.82551
H	2.71322	5.21505	-1.16547
H	3.78172	4.69736	-2.48858
C	-0.33060	4.41410	1.23252
C	1.52775	-4.20285	1.99639
C	-1.00630	-2.23553	-3.03864
H	-1.76934	-2.95411	-2.74454
C	-1.39917	-1.01124	-3.57933
H	-2.45882	-0.79468	-3.69247
C	-0.44110	-0.07544	-3.96916
H	-0.74622	0.88141	-4.39045
C	0.91169	-0.38259	-3.82276
H	1.67468	0.32997	-4.12754
C	1.29900	-1.60903	-3.28320
H	2.35958	-1.83262	-3.18436
C	0.34854	-2.55678	-2.87715
C	0.76716	-3.86338	-2.26926
H	1.71868	-4.21171	-2.68564
H	0.01314	-4.64027	-2.43602
H	0.89910	-3.75287	-1.18569

7·PhMe **[**B3LYP-D3/ZORA-def2-SVP (lead: SARC-ZORA-TZVP)]

Pb	-0.08750	0.01164	-0.38362
S	-1.65074	3.39982	0.11389
S	1.33433	-2.36918	1.96835
F	-0.83674	5.23571	1.81945
F	0.58924	3.64010	1.50898
F	0.31544	5.15189	-0.00905
F	2.25871	-4.54781	3.09778
F	2.37266	-4.56816	0.93779
F	0.47087	-4.85380	1.92049
O	-0.83549	2.40280	-0.67830
O	-2.38666	4.35503	-0.72325
O	-2.38725	2.79415	1.24434
O	0.78562	-2.17009	0.56970
O	0.34504	-2.14788	3.03511
O	2.67113	-1.76417	2.15529
N	-3.55469	-0.39867	0.65651
N	-2.29806	0.16833	2.32448
N	-0.04695	0.70707	2.26699
N	2.20122	1.17306	2.00689
N	3.36055	1.05433	0.18377
C	-2.29818	-0.22986	1.03832
C	-4.54350	-0.08346	1.70967
H	-5.12854	-0.98073	1.94946
H	-5.22850	0.69570	1.35937
C	-3.65086	0.38541	2.86881
H	-3.77880	1.45130	3.08859
H	-3.80781	-0.20088	3.78120
C	-1.15046	0.57588	2.99712
C	-1.16844	0.82874	4.37681
H	-2.07854	0.72589	4.95792
C	0.03488	1.17961	4.98258
H	0.06718	1.36324	6.05506
C	1.20066	1.28870	4.22639
H	2.14567	1.55364	4.68814
C	1.10008	1.04727	2.84973
C	2.14587	0.91454	0.68628
C	3.57661	1.36263	2.49742
H	3.86535	0.48319	3.08628
H	3.65834	2.26431	3.11359
C	4.36638	1.47484	1.18502
H	4.69464	2.49934	0.96868
H	5.24080	0.81791	1.15641
C	-3.98484	-0.96621	-0.58566
C	-4.42499	-0.10906	-1.61446
C	-4.93234	-0.70238	-2.77931
H	-5.28678	-0.06766	-3.58940
C	-4.97008	-2.08925	-2.92323
H	-5.35801	-2.52960	-3.84087
C	-4.50326	-2.91479	-1.89955
H	-4.52703	-3.99555	-2.02774
C	-4.01354	-2.37241	-0.70370
C	-4.34425	1.40454	-1.49123
H	-3.78241	1.63985	-0.58266
C	-5.73741	2.03990	-1.34645
H	-6.33631	1.89861	-2.25639
H	-5.63572	3.11712	-1.16658
H	-6.29961	1.60380	-0.51043
C	-3.57555	2.03234	-2.66522
H	-2.56771	1.61321	-2.74012
H	-3.46503	3.10810	-2.49882
H	-4.09380	1.87142	-3.62000
C	-3.51343	-3.28638	0.40752

H	-3.33036	-2.67224	1.29583
C	-2.16652	-3.92430	0.03185
H	-2.26940	-4.56791	-0.85211
H	-1.78202	-4.53523	0.85580
H	-1.41058	-3.16387	-0.18180
C	-4.55226	-4.35063	0.79510
H	-5.51338	-3.89497	1.06580
H	-4.19375	-4.93254	1.65362
H	-4.73709	-5.05582	-0.02537
C	3.69534	0.91804	-1.20047
C	4.44049	-0.21229	-1.59075
C	4.84473	-0.29670	-2.93041
H	5.41957	-1.15953	-3.26294
C	4.51350	0.70581	-3.84117
H	4.84170	0.62948	-4.87698
C	3.74128	1.79629	-3.43643
H	3.46676	2.55649	-4.16437
C	3.30007	1.92307	-2.11228
C	4.76206	-1.33536	-0.61421
H	4.36574	-1.06658	0.36924
C	4.02577	-2.62532	-1.00260
H	2.94557	-2.45825	-1.01209
H	4.22441	-3.41208	-0.26763
H	4.33602	-2.98899	-1.99168
C	6.27565	-1.56334	-0.47866
H	6.71815	-1.90868	-1.42243
H	6.47779	-2.32754	0.28250
H	6.79954	-0.64318	-0.18760
C	2.44267	3.10877	-1.68610
H	1.87954	2.81348	-0.79641
C	1.39323	3.50261	-2.73527
H	1.85010	3.92572	-3.63936
H	0.71777	4.25124	-2.31117
H	0.78020	2.64120	-3.01891
C	3.31722	4.31425	-1.29699
H	4.05138	4.04967	-0.52594
H	2.68826	5.12153	-0.90489
H	3.87157	4.69331	-2.16607
C	-0.31465	4.42583	0.91320
C	1.63041	-4.20755	1.98316
C	-1.02805	-2.18940	-3.04808
H	-1.78956	-2.90887	-2.75701
C	-1.42311	-0.95014	-3.56304
H	-2.48131	-0.72622	-3.65875
C	-0.46276	-0.00835	-3.94614
H	-0.76860	0.95933	-4.33999
C	0.89409	-0.32420	-3.81896
H	1.65556	0.39159	-4.11494
C	1.28385	-1.56493	-3.30409
H	2.34346	-1.79177	-3.21547
C	0.33080	-2.51933	-2.90613
C	0.75135	-3.84470	-2.32362
H	1.68762	-4.19804	-2.77080
H	-0.01687	-4.61005	-2.48251
H	0.91334	-3.75091	-1.24279

7·PhMe **[**BP86-D3/ZORA-def2-SVP (SARC-ZORA-TZVP)]

Pb	-0.09468	0.01753	-0.38364
S	-1.69359	3.38508	0.02455
S	1.55301	-2.30622	1.93901
F	-0.88566	5.10097	1.88949
F	0.61001	3.60148	1.37622
F	0.20731	5.24891	0.00869
F	2.42271	-4.50067	3.13321
F	2.47592	-4.60904	0.95543
F	0.57657	-4.77553	2.00752
O	-0.86003	2.38655	-0.78275
O	-2.40984	4.37012	-0.82196
O	-2.46649	2.76196	1.14234
O	0.99973	-2.13065	0.52068
O	0.57304	-2.00621	3.01713
O	2.93372	-1.75506	2.10982
N	-3.57816	-0.35912	0.63413
N	-2.33098	0.21778	2.31534
N	-0.07213	0.74787	2.25448
N	2.19577	1.15064	2.00462
N	3.36114	0.96257	0.18059
C	-2.31613	-0.21965	1.03481
C	-4.58030	0.02205	1.66242
H	-5.21171	-0.85206	1.90699
H	-5.22867	0.82553	1.27339
C	-3.69274	0.48442	2.83272
H	-3.79027	1.56570	3.03174
H	-3.88267	-0.08465	3.75966
C	-1.18321	0.63596	2.98892
C	-1.20510	0.91303	4.37174
H	-2.12549	0.82449	4.95476
C	0.00540	1.26524	4.97937
H	0.03503	1.47053	6.05576
C	1.18203	1.34331	4.22374
H	2.13628	1.60566	4.68749
C	1.08380	1.07541	2.84417
C	2.12873	0.90688	0.67503
C	3.58253	1.26695	2.50597
H	3.80462	0.37743	3.12202
H	3.71355	2.18681	3.10135
C	4.39585	1.28697	1.19868
H	4.83889	2.27442	0.97304
H	5.19953	0.53310	1.18662
C	-4.00153	-0.95317	-0.59994
C	-4.45942	-0.11229	-1.64263
C	-4.95576	-0.73341	-2.80630
H	-5.32245	-0.10991	-3.63095
C	-4.96504	-2.12940	-2.93332
H	-5.34413	-2.59228	-3.85277
C	-4.48364	-2.93723	-1.89233
H	-4.48989	-4.02806	-2.00575
C	-4.00653	-2.36815	-0.69582
C	-4.40309	1.40475	-1.53333
H	-3.84176	1.65854	-0.61677
C	-5.81161	2.01785	-1.40460

H	-6.40473	1.85653	-2.32427
H	-5.73178	3.10588	-1.23344
H	-6.37907	1.57647	-0.56474
C	-3.63385	2.03193	-2.71083
H	-2.61033	1.62801	-2.76666
H	-3.54018	3.11913	-2.55501
H	-4.14216	1.84919	-3.67603
C	-3.48816	-3.24828	0.43611
H	-3.42123	-2.62324	1.34508
C	-2.06119	-3.74244	0.13329
H	-2.05186	-4.38583	-0.76564
H	-1.65646	-4.32630	0.97644
H	-1.36631	-2.90493	-0.03975
C	-4.43432	-4.42057	0.75313
H	-5.46225	-4.07086	0.95732
H	-4.07284	-4.97061	1.64031
H	-4.48440	-5.14415	-0.08097
C	3.68042	0.84783	-1.21100
C	4.43113	-0.27498	-1.63255
C	4.82224	-0.32970	-2.98550
H	5.40422	-1.18877	-3.34204
C	4.46924	0.69066	-3.87777
H	4.78757	0.63676	-4.92615
C	3.68477	1.77005	-3.44140
H	3.38750	2.54553	-4.15643
C	3.25665	1.86969	-2.10411
C	4.77034	-1.41593	-0.68100
H	4.34484	-1.18708	0.31122
C	4.07267	-2.71737	-1.11227
H	2.97990	-2.58168	-1.09937
H	4.30538	-3.52705	-0.40093
H	4.38528	-3.04111	-2.12287
C	6.29213	-1.60330	-0.53396
H	6.75749	-1.91267	-1.48843
H	6.51182	-2.38565	0.21455
H	6.79130	-0.67016	-0.21338
C	2.38576	3.03104	-1.63576
H	1.72897	2.65070	-0.83282
C	1.44526	3.57466	-2.72167
H	1.99140	4.09627	-3.52963
H	0.74066	4.28922	-2.26738
H	0.84196	2.76456	-3.16444
C	3.24530	4.15792	-1.02666
H	3.87884	3.78725	-0.20184
H	2.59470	4.95187	-0.62336
H	3.91302	4.60069	-1.78888
C	-0.35691	4.40249	0.88463
C	1.77423	-4.17427	2.01355
C	-1.07400	-2.14694	-3.00083
H	-1.84166	-2.87768	-2.72246
C	-1.47279	-0.89610	-3.50252
H	-2.53977	-0.67406	-3.59962
C	-0.50926	0.05782	-3.87224
H	-0.81846	1.03715	-4.25641
C	0.85458	-0.25964	-3.74755
H	1.62204	0.46468	-4.03716
C	1.24872	-1.51147	-3.24449
H	2.31727	-1.73725	-3.15643
C	0.29209	-2.47824	-2.85809
C	0.71343	-3.81041	-2.28963
H	1.64850	-4.16998	-2.75201
H	-0.06596	-4.57665	-2.44055
H	0.89356	-3.71753	-1.20260

^{H}7·PhMe, **$^{H\text{-}opt}$**

Pb	-0.07357	-0.03231	-0.33057
S	-1.50544	3.37007	0.23891
S	1.19920	-2.39084	2.02412
F	-0.98201	5.41081	1.77612
F	0.24653	3.69265	2.16943
F	0.60748	4.88867	0.42254
F	2.13729	-4.56462	3.09892
F	2.30441	-4.51178	0.95527
F	0.39676	-4.87032	1.87411
O	-0.57275	2.36280	-0.36877
O	-2.07425	4.30018	-0.73317
O	-2.42672	2.79496	1.23065
O	0.65772	-2.16071	0.63550
O	0.20203	-2.22667	3.08172
O	2.51292	-1.76676	2.23407
N	-3.53285	-0.45858	0.64102
N	-2.27593	0.11668	2.29028
N	-0.02957	0.63052	2.21673
N	2.19165	1.16553	1.94847
N	3.33695	1.08757	0.12865
C	-2.27802	-0.27546	1.00748
C	-4.50893	-0.15172	1.69394
H	-5.10197	-1.04032	1.94298
H	-5.18935	0.64164	1.36453
C	-3.61552	0.30153	2.84924
H	-3.75570	1.36127	3.09289
H	-3.75559	-0.30922	3.74839
C	-1.12976	0.51903	2.95139
C	-1.14875	0.79580	4.32164
H	-2.06044	0.70412	4.90251
C	0.05065	1.15407	4.92034
H	0.08385	1.35137	5.99020
C	1.20942	1.26185	4.16223
H	2.15407	1.54173	4.61650
C	1.10687	1.00388	2.79326
C	2.14099	0.86943	0.63986
C	3.54430	1.45766	2.41897
H	3.90567	0.60767	3.01275
H	3.56720	2.36902	3.02557
C	4.30202	1.61644	1.10192
H	4.53292	2.66595	0.87568
H	5.23519	1.04360	1.08548
H	-3.79248	-0.71999	-0.29659
H	3.54121	0.96659	-0.85033
C	-0.33756	4.40871	1.21782
C	1.53229	-4.20537	1.98604
C	-1.00334	-2.24379	-3.05043

H	-1.75667	-2.97132	-2.74773
C	-1.39775	-1.02028	-3.59177
H	-2.45684	-0.79472	-3.71200
C	-0.44086	-0.08336	-3.98182
H	-0.74695	0.87685	-4.39285
C	0.91232	-0.38861	-3.83499
H	1.66732	0.33280	-4.14531
C	1.30117	-1.61428	-3.29479
H	2.36084	-1.84573	-3.18278
C	0.35190	-2.56313	-2.88850
C	0.77216	-3.86888	-2.27992
H	1.62648	-4.30056	-2.81435
H	-0.04540	-4.59697	-2.29458
H	1.07049	-3.72189	-1.23406

PhMe^{opt}

C	-1.01640	-2.35429	-3.26267
H	-1.77141	-3.06526	-2.92598
C	-1.41287	-1.16065	-3.86298
H	-2.47312	-0.94629	-3.99161
C	-0.45675	-0.24553	-4.30195
H	-0.76431	0.68639	-4.77396
C	0.89651	-0.53675	-4.13608
H	1.65272	0.16812	-4.47939
C	1.28727	-1.73217	-3.53498
H	2.34809	-1.95267	-3.41288
C	0.33888	-2.65912	-3.08632
C	0.76186	-3.93226	-2.40944
H	1.75110	-4.25804	-2.74965
H	0.05127	-4.74408	-2.60142
H	0.81763	-3.79695	-1.32045

PhMe*

C	-1.00630	-2.23553	-3.03864
H	-1.76934	-2.95411	-2.74454
C	-1.39917	-1.01124	-3.57933
H	-2.45882	-0.79468	-3.69247
C	-0.44110	-0.07544	-3.96916
H	-0.74622	0.88141	-4.39045
C	0.91169	-0.38259	-3.82276
H	1.67468	0.32997	-4.12754
C	1.29900	-1.60903	-3.28320
H	2.35958	-1.83262	-3.18436
C	0.34854	-2.55678	-2.87715
C	0.76716	-3.86338	-2.26926
H	1.71868	-4.21171	-2.68564
H	0.01314	-4.64027	-2.43602
H	0.89910	-3.75287	-1.18569

PhMe$^{H\text{-}opt}$

C	-1.00674	-2.23414	-3.03858
H	-1.76521	-2.95766	-2.73836
C	-1.39961	-1.00995	-3.57952
H	-2.45945	-0.78683	-3.69581
C	-0.44152	-0.07445	-3.97004
H	-0.74621	0.88160	-4.39297
C	0.91127	-0.38180	-3.82407
H	1.67053	0.33560	-4.13294
C	1.29858	-1.60813	-3.28426
H	2.35919	-1.83788	-3.17782
C	0.34811	-2.55557	-2.87752
C	0.76674	-3.86205	-2.26936
H	1.71949	-4.21080	-2.68366
H	0.01622	-4.64217	-2.43840
H	0.89925	-3.76462	-1.18292

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