Supporting Information for

Evidence for $\pi_{CHR}\rightarrow d_M$ Bonding in Transition Metal Carbene Compounds (L_nM=CHR) and Its Decisive Role in the α-Agostic Effect

Xuhui Lin[a,*], Weiqin Tian[a], Wei Wu [b,*], Yirong Mo[c,*]

[a] School of Life Science and Engineering, Southwest Jiaotong University, Chengdu, Sichuan 610031, China

[b] The State Key Laboratory of Physical Chemistry of Solid Surfaces, iChEM, Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry and College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, Fujian 361005, China

[c] Department of Nanoscience, Joint School of Nanoscience and Nanoengineering, University of North Carolina at Greensboro, Greensboro, NC 27401, United States

E-mail: xuhui.lin@swjtu.edu.cn (XL); weiwu@xmu.edu.cn (WW); y_mo3@uncg.edu (YM).

Methodology

Block-localized wavefunction (BLW) method. Most popular computational approaches for bonding analyses are MO-based and either project out localized orbitals from delocalized canonical MOs or build a molecular wave function from its fragmental canonical molecular orbitals (MOs), or partition molecular electron densities to atomic or fragmental parts based on certain criteria. These top-down approaches are essentially post-SCF methods as the generated local orbitals are not optimal. Alternatively, valence bond (VB) theory adopts a bottom-up approach and builds wave functions for Lewis (localized or resonance) structures with local such as atomic or fragmental orbitals, which are self-consistently optimized, and the final molecular wave function is composed of a few Lewis structures for a system with the computational algorithm similar to the MCSCF within the MO theory. The resonance energy is estimated with the energy difference between the final molecular wave function and the most stable resonance structure.

To combine the advantages of both MO and VB theories, we proposed the BLW method where a BLW represents a unique electron-localized diabatic state (usually the most stable resonance state). The fundamental assumption is that all electrons and primitive basis functions (χ) can be divided into k subgroups (blocks), and each MO is block-localized and expanded in only one block. Assuming that there are m_i basis functions and n_i electrons for block i, we can express block-localized MOs for this block as

$$\varphi_j^i = \sum_{\mu=1}^{m_i} c_{j\mu}^i \chi_\mu^i \tag{1}$$

Subsequently, the BLW for a closed-shell is defined using a Slater determinant as

$$\begin{aligned}\Psi(\mathrm{BLW}) &= \left|(\varphi_1^1)^2(\varphi_2^1)^2\cdots(\varphi_{n_1^1/2})^2\cdots(\varphi_{n_i^i/2})^2\cdots(\varphi_{n_k^k/2})^2\right\rangle \\ &= \hat{A}[\Phi_1\cdots\Phi_i\cdots\Phi_k]\end{aligned} \tag{2}$$

where Φ_i is the Hartree product of all occupied block-localized MOs in block i. Orbitals in the same subspace are subject to the orthogonality constraint as in MO theory, but

orbitals from different subspaces are nonorthogonal as in VB theory. Since Eq. 6 is self-consistently optimized by minimizing its expectation energy, all local orbitals are naturally optimal. The BLW method is available at the DFT level with the geometry optimization and spectra computation capabilities.

The primary aim of this study is to provide a quantitative assessment of the magnitude of the π electron delocalization from the occupied CHR orbital of π symmetry to the low-lying vacant metal *d* orbital(s). To this end, we built the reference BLW state where the concerned d_M orbital remained vacant (i.e., removed from the expansion space of any occupied orbitals)

$$\Psi_{\mathrm{BLW}}(\pi \rightarrow d_M) = \hat{A}[\varphi_{d_M}^{0}\psi] \tag{3}$$

The $\pi \rightarrow d_M$ charge transfer interaction is thus evaluated as the energy difference between the BLW state and the regular delocalized DFT states. It should be noted that $\pi \rightarrow d_{xz}$ interaction has two origins, one coming from $\pi_{R'} \rightarrow d_{xz}$ between ancillary ligands (R′) and metal center, the other being concerning $\pi_{CHR} \rightarrow d_{xz}$.

The xyz coordinates of all studied structures optimized at PBE0-D3 level

$[VCH_2]^+$ DFT (Cs) E = -110.4673014

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.7116046196	0.0000000000
H	1.1305418716	1.5262344973	0.0000000000
H	-0.3014607466	2.7570359930	0.0000000000

$[VCH_2]^+$ DFT (C2v) E = -110.4649275

V	0.0000056292	0.4527291877	-0.0000000000
C	-0.0000046963	-1.3112978182	0.0000000000
H	0.9300090620	-1.8911734628	-0.0000000000
H	-0.9300099949	-1.8911849067	-0.0000000000

$[VCH_2]^+$ BLW(C2v) E = -110.4563124

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.8067492204	0.0000000000
H	0.9297560805	2.3789089648	0.0000000000
H	-0.9296832406	2.3790179983	0.0000000000

$[Cl_2VCHMe]^-$ DFT E = -1070.41747

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.7206948087	0.0000000000
H	1.1336378877	1.3644545478	0.0000000000
C	-0.1419538813	3.2003396728	-0.0218444255
H	0.2883053920	3.6801421228	0.8700052033
H	0.3375955891	3.6562274247	-0.9009721370
H	-1.2016619998	3.4718761557	-0.0550980498
CL	-0.2405230521	-0.9775227852	2.0288190319
CL	-0.1909603343	-0.9785837436	-2.0331081909

$[Cl_2VCHMe]^-$ BLW E = -1070.394257

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.8326670309	0.0000000000
H	0.9973561133	2.2883256426	0.0000000000
C	-1.1501640387	2.7936085555	0.0050360053
H	-1.1281951421	3.4625580755	0.8812782954
H	-1.1498856047	3.4469214112	-0.8831895063
H	-2.1192678232	2.2847715756	0.0212269046
CL	0.0193927358	-0.8972367596	2.0954194885
CL	-0.0100752637	-0.9074681090	-2.0907582456

$[Cl_2VCHMe]^+$ DFT E = -1070.048281

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.7831001495	0.0000000000
H	1.0669260122	2.0746691030	0.0000000000
C	-0.9786172857	2.8719490659	0.0929446290
H	-0.7751248619	3.4500468428	1.0066701017
H	-0.8092881314	3.5716144295	-0.7384884425
H	-2.0159286971	2.5394874592	0.0915777457
CL	-1.8161450351	-0.5968118546	0.7770217629
CL	1.8097130639	-0.7054227978	0.7388243857

$[Cl_2VCHMe]^+$ BLW E = -1069.988555

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.8282187025	0.0000000000
H	0.9785841082	2.3096729334	0.0000000000
C	-1.1751378598	2.6524290090	0.2708511275
H	-1.0896968069	2.9437238914	1.3355357784
H	-1.1185680296	3.5911752735	-0.2948749028
H	-2.1506048494	2.1837955385	0.1289500201
CL	-0.8858036493	-0.3914295267	1.8729309304
CL	2.1023045903	-0.2324142812	0.0399309959

[CH2CH3Cl2VCHMe] DFT E = -1149.508867

V	0.0657181723	-0.0860465835	0.0426584538
C	-0.2988443205	1.5894028546	0.0109512500
H	0.8416630557	1.5895559231	0.1010424628
CL	0.8752600276	-0.5840036289	2.0277065686
CL	1.1409945575	-0.5881817935	-1.8097450910
C	-0.9724233859	2.8945212722	-0.0482391119
H	-0.7738338964	3.4854179318	0.8538593488
H	-0.6311372583	3.4777107046	-0.9117148003
H	-2.0533368276	2.7568355192	-0.1350823758
C	-1.8371688096	-0.5500511435	-0.0899843536
H	-2.2914529812	-0.1888234689	-1.0120199859
H	-2.3891488537	-0.2074765698	0.7855062350
C	-1.4872189547	-2.0341835507	-0.0838318583
H	-0.3978949483	-2.2434223265	0.0247487934
H	-1.9359294958	-2.5548555015	0.7633827325
H	-1.7571717527	-2.5210649675	-1.0217806569

[CH2CH3Cl2V-CHMe] BLWT E = -1149.468673

V	0.1780651782	-0.0577511910	0.0915729553
C	0.1233177524	1.7542493706	0.0321140283
H	1.1153921925	2.2153325373	0.0216728638
CL	0.9294543827	-0.5055633254	2.1194112616
CL	1.1671384726	-0.5844724152	-1.8063622240
C	-1.0414496098	2.6758677703	-0.0160665913
H	-0.9980592549	3.4054881570	0.8029070470
H	-1.0239025480	3.2581467491	-0.9478853092
H	-2.0055274666	2.1673421265	0.0380047811
C	-1.7645335510	-0.4467932340	-0.0253824482
H	-2.2591588471	0.0104306611	-0.8818332496
H	-2.2017516288	-0.1074481180	0.9188789946
C	-1.5841792969	-1.9573292982	-0.1100418831
H	-0.7550147447	-2.3199112230	0.5212591119
H	-2.4632978208	-2.4915195286	0.2628225745
H	-1.3800781497	-2.2893904384	-1.1292452627

E-[Cl3V-CHMe] DFT E = -1530.480730

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.7296748229	0.0000000000
H	1.1165211111	1.7277293979	0.0000000000
CL	1.0882627465	-0.6230391185	1.7616297472
CL	1.0636721436	-0.6184919042	-1.7785259732
CL	-2.0430509773	-0.5140555849	0.0109148707
C	-0.7280101046	3.0087664617	-0.0006087413
H	-0.4614328383	3.6025398624	0.8819263509
H	-0.4650298620	3.5994856044	-0.8862706293
H	-1.8069207890	2.8419880789	0.0018300299

E-[Cl3V-CHMe] BLW E = -1530.426183

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.7997565191	0.0000000000
H	1.0198488998	2.1932139013	0.0000000000
CL	1.0909933665	-0.4220390520	1.8341302171
CL	1.0849017997	-0.4239451183	-1.8375034051
CL	-2.1403357870	-0.3849891934	0.0041897135
C	-1.1243079357	2.7572670791	-0.0009018382
H	-1.0525183870	3.4089422674	0.8800663407
H	-1.0502035473	3.4111633383	-0.8799762077
H	-2.1018769051	2.2794144575	-0.0025449873

Z-[Cl3V-CHMe] DFT E = -1530.480552

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.7537688409	0.0000000000
H	1.0473060236	2.0883357271	0.0000000000
C	-1.0810981451	2.7640326031	0.0251735196
H	-0.9942613602	3.3779493193	0.9304636052
H	-0.9863930348	3.4353896969	-0.8372289133
H	-2.0723754149	2.3094006214	0.0070456924
CL	1.9956695853	-0.7244684383	-0.0910509803
CL	-1.0814786776	-0.4796198427	1.7959851463
CL	-1.2741648215	-0.4962778334	-1.6531825586

Z-[Cl3V-CHMe] BLW E = -1530.430432

V	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	1.7952021769	0.0000000000
H	0.9807603919	2.2669404962	0.0000000000
C	-1.2109900431	2.6306042087	0.0051381322
H	-1.1757918608	3.3151600212	0.8630179013
H	-1.2206726666	3.2523399122	-0.9007877041
H	-2.1434065180	2.0660855192	0.0464892414
CL	2.1547013441	-0.2733560527	-0.0865083429
CL	-0.9762484620	-0.4394886185	1.8904511119
CL	-1.1246749977	-0.4248433625	-1.8104135054

[C5H5Cl2V-CHMe] DFT E = -1263.760631 a.u.

V	-0.0173708256	0.0263880393	0.0066729662
C	-0.0018131041	1.7814898861	0.0005546667
H	1.1131701358	1.7353992425	0.0197187888
C	-2.1263513630	0.3426477097	0.6818712849
C	-1.7233178500	-0.9353228537	1.1240804178
C	-1.4359256251	-1.7255372813	-0.0101302221
C	-1.6841331997	-0.9446379443	-1.1599133168
C	-2.1018790242	0.3368688883	-0.7422569128
H	-1.0223451302	-2.7237816903	0.0010143876
H	-1.5802515967	-1.2313756685	2.1519201215
H	-2.4028843529	1.1730700174	1.3135812469
H	-1.5058958241	-1.2489553705	-2.1798273689
H	-2.3563007978	1.1620268428	-1.3899615574
CL	1.2259019220	-0.5073192509	1.7804018128
CL	1.2865398051	-0.5209442101	-1.7184529653
C	-0.6039346492	3.1256902744	-0.0142711609
H	-0.2984325261	3.6965032687	0.8715784084

H	-0.2659591863	3.6917950047	-0.8912800021
H	-1.6968391871	3.0906708853	-0.0343424150

[C5H5Cl2V-CHMe] BLW E = -1263.699816 a.u.

V	-0.0545981525	0.0585701497	0.0089051932
C	0.0571017202	1.8625070123	0.0025006851
H	1.1511608268	1.9689302873	0.0057120591
C	-2.1514989732	0.2521396372	0.6866726238
C	-1.8205203352	-1.0586644641	1.1234239240
C	-1.6180572041	-1.8702070262	-0.0051008441
C	-1.7839700083	-1.0701012682	-1.1480971211
C	-2.1288600800	0.2450443659	-0.7359332608
H	-1.3133817383	-2.9062118506	0.0051259775
H	-1.7144845434	-1.3621617864	2.1541233596
H	-2.4025640982	1.0876290180	1.3230900858
H	-1.6448814800	-1.3842748572	-2.1716247722
H	-2.3600238571	1.0738681641	-1.3883646214
CL	1.1619771713	-0.3394389809	1.8573526413
CL	1.2139764574	-0.3480384756	-1.8043516378
C	-0.6806720713	3.1341141105	-0.0077442367
H	-0.3901997856	3.7286496598	0.8691530751
H	-0.3774527116	3.7225222993	-0.8844207321
H	-1.7662118960	3.0278463591	-0.0146757297

[OCH3Cl2V-CHMe] DFT E = -1185.449308

V	0.6020267661	-0.0037298729	-0.0250561881
C	0.0627326598	1.6649731484	0.0224513446
H	1.0312759884	2.1949839226	0.0656192773
CL	1.7738985370	-0.3192115095	1.7888505798
CL	1.8825955628	-0.1852309492	-1.7832506813
C	-1.1769409691	2.4710741056	0.0206630565
H	-1.2363489290	3.0873865362	0.9264592786
H	-1.1883929150	3.1577533950	-0.8350220633
H	-2.0682575914	1.8426627529	-0.0286455516
O	-0.8076751346	-0.9142606780	-0.0948336906
C	-1.8280289658	-1.8717953080	-0.1108538472
H	-1.7376737033	-2.5126175043	0.7700877691
H	-2.7961254336	-1.3645207516	-0.0970673466
H	-1.7435504805	-2.4752892537	-1.0181192327

[OCH3Cl2V-CHMe] BLW E = -1185.392505

V	0.2386825215	-0.1041286336	0.0761185474
C	0.1847737007	1.7015979085	0.0146906588
H	1.1509219262	2.2108680529	0.0162106842
CL	1.0300229502	-0.5581826236	2.0792311685
CL	1.4927517162	-0.5935975252	-1.6719049259
C	-1.0511420895	2.5123888526	-0.0610037798
H	-1.1121743879	3.2031320918	0.7900551603
H	-1.0315117850	3.1352059489	-0.9657974699
H	-1.9526488032	1.8984799360	-0.0812330139
O	-1.5038756511	-0.3662692837	-0.1205587276
C	-1.6471506126	-1.7781635026	-0.1202194552
H	-0.6796964932	-2.2990117471	0.0295938798
H	-2.3039772921	-2.0812118523	0.6981115090
H	-2.0454403085	-2.1089295890	-1.0820115312

[COCl2V-CHMe] DFT E = -1183.331687

V	0.0569860640	-0.1393407956	0.0231759965
C	-0.2827202718	1.6107827837	0.2058773847
H	0.4550434345	2.1207766406	-0.4411093927
CL	-0.8880060378	-1.1855806674	1.5398847902
CL	1.9085951542	-0.4866664300	-0.8658549261
C	-1.1971997478	2.4707315186	0.9689539274
H	-0.5934957954	3.1080965128	1.6317392852
H	-1.7079669879	3.1622692506	0.2847798125
H	-1.9283989995	1.9226242400	1.5619255501
C	-1.2648108817	-0.1983286152	-1.5076400666
O	-2.0010644598	-0.2299795557	-2.3491070708

[COCl2V-CHMe] BLW E = -1183.259501

V	-0.0707953122	-0.1864824348	0.0404061198
C	-0.0895153776	1.6183889363	0.2376794050
H	0.8740831791	2.1236955865	0.1480023927
CL	-0.1765891201	-0.8716166965	2.0441598554
CL	1.7223256919	-0.4196803345	-1.0836491218
C	-1.2578217965	2.3480161650	0.7384249772
H	-0.9732996956	2.7965026366	1.7027745754
H	-1.4988957032	3.1856747900	0.0688212054
H	-2.1580379501	1.7457231739	0.8932423456
C	-1.5248888419	-0.1162538677	-1.4630038086
O	-2.2896036029	-0.0685830724	-2.2742326558

[CNCl2V-CHMe] DFT E = -1163.124431

V	-0.0184631102	-0.0943481419	0.0765955237
C	-0.2674324060	1.6356382439	0.1571525943
H	0.5579088689	1.9694415464	-0.5000349736
CL	-1.0245522607	-0.9666911566	1.7078749673
CL	1.9813729982	-0.5922319144	-0.4657139218
C	-1.2029269248	2.6470358462	0.6850723697
H	-0.6551520250	3.4455886184	1.1983675101
H	-1.7421453184	3.1082535274	-0.1522877420
H	-1.9309052002	2.2114163312	1.3703557078
C	-1.1977167396	-0.2329448017	-1.4920659743
N	-1.8952002687	-0.3612278081	-2.4116845379

[CNCl2V-CHMe] BLW E = -1163.072936

V	-0.0172437202	-0.1102602503	-0.0903453261
C	-0.0256546090	1.6334431006	0.3146334573
H	0.9563351574	2.1027188546	0.3908210465
CL	-0.2537474102	-1.0118628140	1.8690077966
CL	1.8711670883	-0.3166119919	-1.1421501054
C	-1.2378600617	2.3886120596	0.6817362482
H	-1.1256862223	2.7829709327	1.7001220683
H	-1.3506070930	3.2497782647	0.0099221491
H	-2.1549683355	1.7992754707	0.6294745458
C	-1.5949318593	-0.1535583966	-1.3000834650
N	-2.5098414637	-0.2091203478	-2.0105131250

4-Ta DFT E = -885.92295

TA	-0.2975150006	-0.0574720859	0.1028575819
C	-0.2436929231	1.8469079495	0.0964288904
H	0.8790691630	1.7513380890	0.0909728383
C	-0.7605758349	3.2426744313	0.0789558171
H	-0.4250096553	3.8187165711	0.9500308792
H	-0.4376446145	3.7892318093	-0.8156836224
H	-1.8540381775	3.2462774420	0.0864454776
C	0.9339123005	-0.6413182149	1.8007136858
H	1.8658707127	-0.0707119369	1.8859329360
H	0.3258275382	-0.3225097510	2.6636125505
C	0.8182683111	-0.6175787394	-1.6817736429
H	1.8595217255	-0.2805313118	-1.5651542037
H	0.4266976476	-0.0383393475	-2.5284247950
C	0.7659675690	-2.1197488076	-1.9844713979
H	-0.2586102909	-2.4570476850	-2.1729515304

H	1.3553478076	-2.3794097200	-2.8716726455
H	1.1572343473	-2.7246146818	-1.1592536345
C	1.2058505540	-2.1483031483	1.8714469057
H	1.9041482133	-2.4692773540	1.0919484278
H	1.6488469791	-2.4383227251	2.8315989311
H	0.2925815693	-2.7439528114	1.7545694107
O	-2.0810496562	-0.7586071480	0.1783702336
SI	-3.6535827709	-1.1145485915	-0.0633622447
O	-3.8114758408	-2.6860817727	0.3591739949
H	-4.6245798375	-3.1167554290	0.0956858241
O	-4.1365733074	-0.9451502249	-1.6192021199
H	-4.4698695021	-0.0819205653	-1.8648189265
O	-4.5926938759	-0.0763060348	0.8008307998
H	-4.3049098406	0.1198303648	1.6925478490

4-Ta BLW E = -885.8779238

TA	-0.1953978058	-0.2664552162	0.0604778963
C	-0.1152026317	1.6741500420	0.1488286213
H	0.9236077182	2.0247032042	0.1574033735
C	-1.1701699652	2.7334412488	0.2042276179
H	-1.0611198079	3.3635963735	1.0965409887
H	-1.1096335455	3.4038749632	-0.6626279249
H	-2.1804724030	2.3142589274	0.2213466130
C	0.9834968648	-0.7717158702	1.8306029042
H	1.9331720155	-0.2179828630	1.7819910383
H	0.4776442414	-0.3862724754	2.7241469653
C	0.8974022286	-0.6206269295	-1.7945414049
H	1.8196163024	-0.0250995357	-1.8291266927
H	0.2629672111	-0.2028020799	-2.5891318384
C	1.2000668396	-2.0992460297	-2.0622029406
H	0.2938593228	-2.7162662358	-2.0732736080
H	1.6859575957	-2.2443167020	-3.0343533530
H	1.8753768993	-2.5265532528	-1.3125309047
C	1.2496351276	-2.2771252375	1.9540129633
H	1.7732379721	-2.6836349046	1.0802357734
H	1.8773869903	-2.5104322523	2.8221243601
H	0.3233403380	-2.8502210120	2.0707605929
O	-2.1159159083	-0.6848381760	0.0778056909
SI	-3.7221978727	-0.7831013184	-0.0941335168
O	-4.1445516757	-2.2393363846	0.5253522128
H	-5.0309902463	-2.5394895204	0.3249056867
O	-4.2410026385	-0.7312024300	-1.6498580022
H	-4.4359364634	0.1387155134	-1.9980823670

O	-4.4629913980	0.4995019642	0.6368128155
H	-4.1038619955	0.7509447592	1.4876407089

5-W DFT E = -1103.034148

W	0.0321612073	-0.0646191070	0.0752926860
C	-0.0894289939	1.8188338353	0.0666864626
H	0.9414411525	2.1509851108	-0.1696796704
C	-5.0827214182	-1.2325130153	1.3510122266
C	-3.7737663389	-0.7759475901	1.3588987234
C	-2.9270605897	-1.0412807514	0.2734874528
C	-3.4226360773	-1.7741873801	-0.8135988582
C	-4.7347098662	-2.2219380926	-0.8130755581
C	-5.5705487787	-1.9546327460	0.2666706996
N	-1.6363747172	-0.5728995813	0.2895887506
O	1.2853382345	-0.7465704156	-1.2396783338
SI	2.6731096677	-0.4980908485	-2.0565391119
O	2.4574117847	-0.8179043070	-3.6527454297
O	3.9081501666	-1.4526371518	-1.5587055934
O	3.0988607101	1.0512232549	-1.7176996549
C	0.8728201400	-0.3529214084	2.0188589301
C	2.1769919646	0.4082642786	2.2478080591
C	-1.1010904005	2.9047933739	0.2045594666
H	4.0015425553	1.3065579312	-1.9080252319
H	1.6299221905	-0.5359123641	-4.0425078653
H	3.9533664935	-2.3188071547	-1.9633866042
H	0.1431452515	-0.1119499307	2.7960021892
H	1.0454489704	-1.4406138163	2.0825356792
H	-5.1083711764	-2.7849886369	-1.6622873943
H	-6.5962271697	-2.3073744881	0.2628947199
H	-5.7281790785	-1.0203760350	2.1973164648
H	-3.3815273578	-0.2086354820	2.1955995109
H	-2.7643022395	-1.9802218120	-1.6509111507
H	-2.0940373348	2.4965614952	0.4032233430
H	-0.8406363421	3.5819180433	1.0278963597
H	-1.1546780918	3.5171366860	-0.7039135810
H	2.6729276808	0.0855933452	3.1714143986
H	2.8975775830	0.2613290316	1.4356606252
H	1.9886804203	1.4827698028	2.3248124967

5-W BLW E = -1102.925524

W	0.2077865667	-0.2664093331	0.2281145790
C	0.0791469056	1.6477603450	0.0947850617

H	1.0510502507	2.1428529546	0.0364429067
C	-5.0286224751	-0.4413482804	1.2212924047
C	-3.6597121349	-0.2287868531	1.1410949228
C	-2.8456470000	-1.1020223623	0.4008784137
C	-3.4564003057	-2.1826141494	-0.2629337412
C	-4.8229142526	-2.3852601143	-0.1806409228
C	-5.6169512193	-1.5175213456	0.5644367143
N	-1.4830351378	-1.0098427949	0.3638519146
O	1.6519158481	-0.7667570996	-1.0201156706
SI	2.8049312471	-0.0311017582	-1.9111557464
O	2.3076213311	0.1320841658	-3.4684982751
O	4.2297852950	-0.8317393811	-1.9577618781
O	3.0815853313	1.3965393077	-1.1373159484
C	0.9437879881	-0.3479601066	2.2301990996
C	2.0283151643	0.6735605728	2.5623732487
C	-1.1266011455	2.5230550455	0.0050608377
H	3.8409602416	1.9000296487	-1.4309002517
H	1.3744708960	0.2915561133	-3.6097814193
H	4.3093061763	-1.5142231662	-2.6239922302
H	0.1089190201	-0.2752915106	2.9321443258
H	1.3351029899	-1.3753146423	2.3249634500
H	-5.2715209495	-3.2340542595	-0.6873876417
H	-6.6859228193	-1.6858731552	0.6400160877
H	-5.6422771892	0.2322146882	1.8109562340
H	-3.1933056748	0.5930857131	1.6739704725
H	-2.8190095943	-2.8625522947	-0.8178546087
H	-2.0669270159	1.9679441109	-0.0154274997
H	-1.1627341865	3.2177169309	0.8542284873
H	-1.0797386739	3.1412390094	-0.9003338730
H	2.5075450718	0.4461015026	3.5218561340
H	2.8203215595	0.7069011188	1.8063725704
H	1.6019409326	1.6785135688	2.6289251412

6-Re DFT E = -905.9722463

RE	0.1074748662	0.1375920971	-0.1314443860
C	0.0685269392	1.9935899755	0.1002252650
H	-0.9468400210	2.3288150499	-0.1942981771
C	-0.8214773786	-0.4878028178	1.6556914149
C	-2.2644355525	0.0072528173	1.7246972128
C	1.7569202172	-0.1540025495	0.2846530396
C	3.1755639748	-0.4305183643	0.5115635955
O	-0.6081177834	-0.5810153057	-1.7995824088
SI	-0.2804901388	-1.4737332002	-3.1166400397

O	-1.1039300381	-2.8797175623	-2.9323220504
C	1.0003924799	3.1022966864	0.4442138831
O	-0.6937699950	-0.6379845914	-4.4782529786
O	1.3068363882	-1.8511024954	-3.3243283301
H	-2.8072139752	-0.1448401676	0.7833807410
H	-2.3008237838	1.0754005066	1.9580028594
H	-2.8315089755	-0.5251754975	2.4979298059
H	1.9939193213	2.7221462998	0.6886825854
H	1.0908800887	3.8249149130	-0.3766690525
H	0.6279334609	3.6591573633	1.3137118352
H	-0.8552613710	-3.5838410466	-3.5314272139
H	-1.5189516657	-0.1553947184	-4.4258834235
H	1.8191686875	-1.1997600569	-3.8040874630
H	-0.2774887266	-0.2311102723	2.5649865544
H	-0.7962034650	-1.5874693510	1.5732599365
H	3.5544206767	-1.1716107558	-0.1995087296
H	3.3344149555	-0.8072628643	1.5277034034
H	3.7638503390	0.4867080536	0.3974442560

6-Re BLW E = -905.803857

RE	-0.1370776040	-0.3964495975	0.1318329254
C	-0.1422743845	1.5068531934	-0.0013424894
H	-1.1764066624	1.8629843073	-0.0671246876
C	-1.2431410565	-0.5103923259	1.9641902039
C	-2.6174647839	0.1408127959	1.9096839652
C	1.3549003591	-0.9034367414	1.0827419486
C	2.4633416663	-0.3068836871	1.8403993363
O	-0.6579959632	-1.4496750110	-1.4636838087
SI	-0.4176020276	-1.7641967548	-3.0325409684
O	-0.8328625996	-3.3342882635	-3.2545575927
C	0.9023534721	2.5641521119	0.0370946455
O	-1.2990899409	-0.7241404110	-3.9729642379
O	1.1297432400	-1.5500905941	-3.5494896754
H	-3.1816984712	-0.1484518144	1.0159025809
H	-2.5501022027	1.2325258083	1.9283892487
H	-3.2189217848	-0.1656859995	2.7739124086
H	1.9150417235	2.1612155187	0.0982791592
H	0.8420581670	3.1827810811	-0.8663250485
H	0.7465084060	3.2353665046	0.8910309513
H	-0.5558608781	-3.7177966418	-4.0866344383
H	-2.2059280092	-0.5929817054	-3.6960183133
H	1.2914249021	-0.6960295177	-3.9509186654
H	-0.6863765886	-0.1688062502	2.8365574229

H	-1.3393927870	-1.6020765724	2.0640378723
H	3.4182383716	-0.7660448260	1.5591665064
H	2.2993957517	-0.5715227707	2.8950366296
H	2.5549795701	0.7857622275	1.7823744452