Supporting Information

Stabilization of Diborane(4) by transition metal fragments and a novel metal to π Dewar-Chatt-Duncanson model of back donation

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Full References

a) The full reference for Gaussian09 (reference number **17)**

Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, 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, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

Table S1 Comparision of Singlet and Triplet spin state energies for metal complexes 6-9(a-d). In all the cases Singlet spin state is the low energy state.

Metal complex	The relative free energies, obtained after adding Gibbs free energy term to the electronic energy @ BP86/TZVP level of theory /kcal.mol^{-1}	
	Singlet spin state	**Triplet spin state**
6*a*	**0.00**	**25.48**
6*b*	**0.00**	**24.52**
6*c*	**0.00**	**24.94**
6*d*	**0.00**	**2.75**
7*a*	**0.00**	**8.50**
7*b*	**0.00**	**10.30**
7*c*	**0.00**	**10.03**
8*a*	**0.00**	**17.36**
8*b*	**0.00**	**19.44**
8*c*	**0.00**	**12.77**
9*a*	**0.00**	**16.17**
9*b*	**0.00**	**11.62**
9*c*	**0.00**	**--**

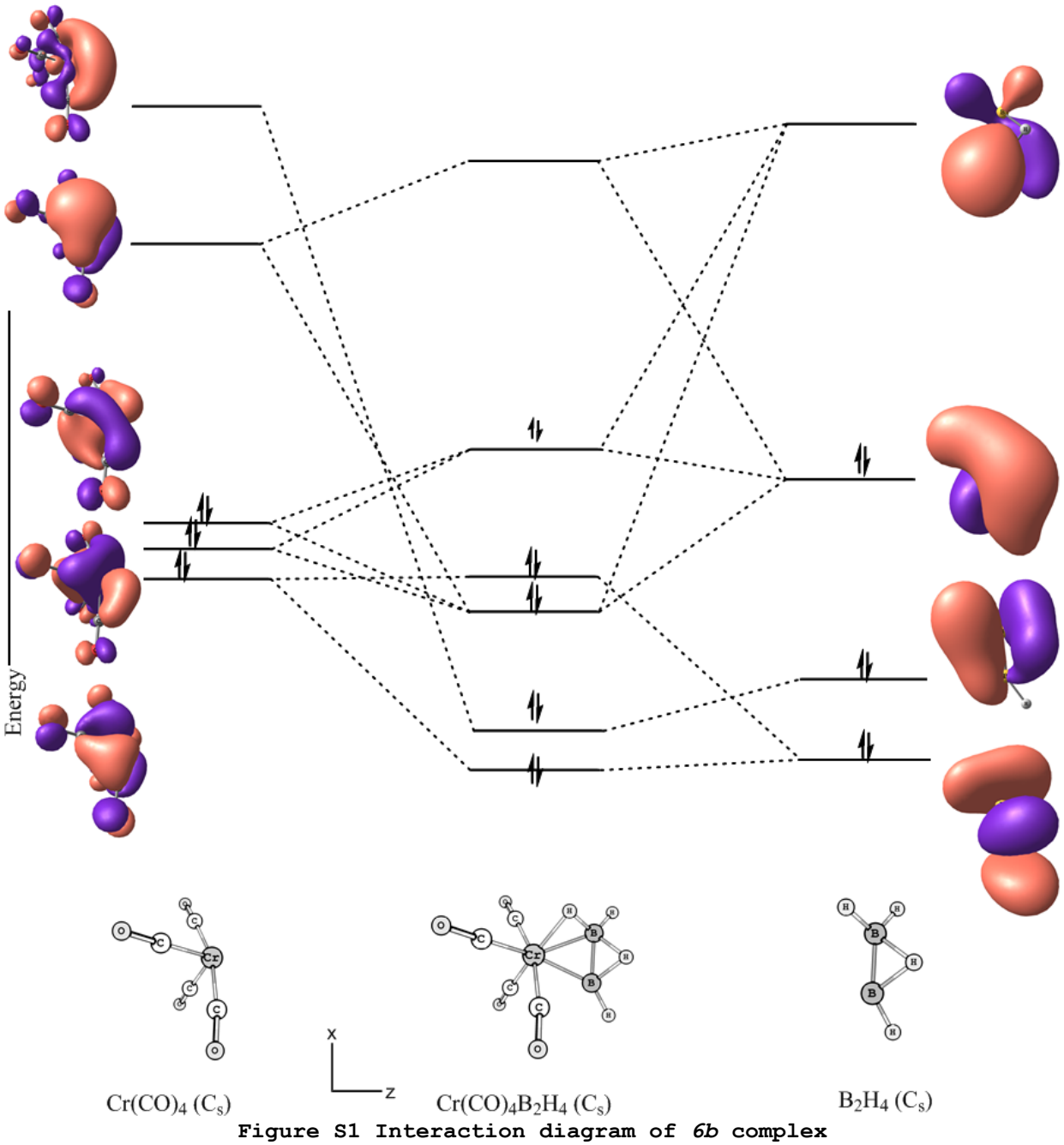

Figure S1 Interaction diagram of *6b* complex

Optimized coordinates of structures (Singlet spin state) 1-5, 6a-d and 7-9a-c at BP86/TZVP level of theory.

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1 – B_2H_4 [D_{2h}] (*ts*)

5	0.000000000	0.000000000	0.876489000
5	0.000000000	0.000000000	-0.876489000
1	0.000000000	1.022165000	1.514541000
1	0.000000000	-1.022165000	1.514541000
1	0.000000000	1.022165000	-1.514541000
1	0.000000000	-1.022165000	-1.514541000

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2 – B_2H_4 [C_s]

5	-0.099870000	0.813501000	0.000000000
5	-0.099870000	-0.721651000	0.000000000
1	-0.066023000	2.000019000	0.000000000
1	-0.003038000	-1.328624000	1.037752000
1	1.070799000	0.197979000	0.000000000
1	-0.003038000	-1.328624000	-1.037752000

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3 – B_2H_4 [D_{2d}]

5	0.000000000	0.000000000	0.811915000
5	0.000000000	0.000000000	-0.811915000
1	-0.721236000	0.721237000	1.460736000
1	0.721236000	-0.721237000	1.460736000
1	-0.721236000	-0.721237000	-1.460736000
1	0.721236000	0.721237000	-1.460736000

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4 - B_2H_4 [C_{2v}]

5	0.000000000	0.735443000	-0.118412000
5	0.000000000	-0.735443000	-0.118412000
1	0.000000000	1.909669000	0.013885000
1	0.905659000	0.000000000	0.578176000
1	-0.905659000	0.000000000	0.578176000
1	0.000000000	-1.909669000	0.013885000

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5 – B_3H_5 [C_{2v}]

5	0.000000000	0.804732000	-0.485626000
5	0.000000000	-0.804732000	-0.485626000
1	0.000000000	1.416342000	0.597142000
1	0.000000000	1.533883000	-1.419208000
1	0.000000000	-1.416342000	0.597142000
1	0.000000000	-1.533883000	-1.419208000
5	0.000000000	0.000000000	0.885015000
1	0.000000000	0.000000000	2.075312000

Optimized coordinates of Metal Complexes of B_2H_4 with $Cr(CO)_4$ (6), Mn(CO)Cp (7), $Fe(CO)_3$ (8), CoCp (9) [type a-d] (Singlet spin state) at BP86/TZVP level of theory.

6a – $Cr(CO)_4B_2H_4$

24	-0.000022000	0.301635000	-0.000007000
5	-0.000884000	2.316269000	-0.819002000
5	-0.000923000	2.316319000	0.818862000
1	-0.001437000	3.218518000	-1.607043000
1	-0.000138000	1.268065000	-1.506373000
1	-0.001483000	3.218616000	1.606848000
1	-0.000290000	1.268157000	1.506298000
6	1.901383000	0.075762000	0.000099000
6	0.000396000	-0.934950000	-1.410352000
6	-1.901296000	0.074818000	-0.000097000
6	0.000168000	-0.934860000	1.410414000
8	-3.039086000	-0.118910000	-0.000230000
8	0.000502000	-1.698163000	-2.283334000
8	3.039265000	-0.117412000	0.000227000
8	0.000446000	-1.698034000	2.283430000

6b – $Cr(CO)_4B_2H_4$

5	1.367728000	-1.748439000	-0.384731000
5	0.071267000	-2.025103000	-1.350972000
1	2.362827000	-2.184815000	0.103965000
1	-0.330512000	-0.929411000	-1.881353000
1	1.349673000	-2.330129000	-1.610979000
1	-0.524414000	-2.970903000	-1.777484000
24	-0.035917000	-0.238133000	-0.228653000
6	1.755333000	0.245343000	-0.059083000

6	-0.061917000	-0.024890000	1.615841000
8	-0.073920000	0.060468000	2.774000000
8	2.828295000	0.673533000	0.111699000
6	-0.285706000	1.554036000	-0.740923000
6	-1.950663000	-0.323147000	-0.068448000
8	-3.094193000	-0.343572000	0.081499000
8	-0.401783000	2.645833000	-1.111232000

6c – $Cr(CO)_4B_2H_4$

24	0.017407000	0.230130000	-0.000241000
5	-1.605243000	1.341134000	-0.001122000
5	-3.133045000	1.998333000	-0.000825000
1	-0.867888000	1.384649000	-1.049612000
1	-0.868106000	1.385574000	1.047574000
1	-4.130333000	1.324112000	-0.000287000
1	-3.291565000	3.193149000	-0.000736000
6	-1.383397000	-1.022480000	-0.000097000
6	1.645296000	1.252775000	-0.000168000
6	0.743079000	-0.759312000	1.407290000
6	0.744031000	-0.760656000	-1.406378000
8	-2.204926000	-1.842798000	0.000129000
8	2.645561000	1.828417000	-0.000038000
8	1.151726000	-1.354414000	-2.316395000
8	1.149829000	-1.352442000	2.318143000

6d – $Cr(CO)_4B_2H_4$

24	-0.000037000	0.000051000	-0.308360000
5	-0.774047000	0.008792000	1.780513000
5	0.773374000	-0.006808000	1.781120000
1	-1.858997000	0.020440000	2.263057000
1	0.009139000	0.911027000	2.416724000
1	-0.009842000	-0.908462000	2.417554000
1	1.858359000	-0.017933000	2.263570000
6	-0.002930000	1.894419000	-0.271350000
6	-1.897977000	-0.004270000	-0.423590000
6	0.003224000	-1.894255000	-0.270554000
6	1.897954000	0.003464000	-0.423462000
8	0.005112000	-3.054456000	-0.202147000
8	-3.055074000	-0.007675000	-0.512056000
8	-0.004587000	3.054621000	-0.203287000
8	3.055046000	0.005963000	-0.511843000

6e – $Cr(CO)_5B_2H_4$

24	0.000074000	0.000057000	-0.062773000
5	0.770756000	-0.000196000	-2.212100000
5	-0.769972000	-0.000158000	-2.212057000
1	1.865991000	-0.000375000	-2.665136000
1	0.000854000	0.911825000	-2.840020000
1	-1.864891000	-0.000162000	-2.665896000
1	0.000520000	-0.911934000	-2.840082000
6	-1.896277000	0.000101000	0.036140000
6	0.000426000	1.902988000	-0.097174000
6	1.896418000	-0.000496000	0.037325000
8	3.049679000	-0.001006000	0.147685000
8	0.000681000	3.061136000	-0.106995000
8	-3.049586000	-0.000007000	0.146093000
6	-0.000674000	0.000518000	1.817589000
8	-0.001272000	0.000799000	2.976149000
6	-0.000139000	-1.902841000	-0.096585000
8	-0.000338000	-3.060993000	-0.106093000

7a – $Mn(CO)CpB_2H_4$

25	0.169270000	0.281370000	0.026599000
5	1.714214000	1.414126000	0.747674000
5	1.150357000	2.047921000	-0.626022000
1	0.804589000	0.746812000	1.448338000
1	2.642112000	1.483699000	1.504017000
1	0.386412000	1.300623000	-1.317660000
1	1.274106000	3.047344000	-1.278560000
6	-1.618588000	0.006919000	-1.137714000
6	-1.118700000	-1.268133000	0.740486000
6	-1.597344000	0.002695000	1.181225000
6	-1.918248000	0.789364000	0.028310000
6	-1.129121000	-1.258362000	-0.702674000
1	-0.814754000	-2.094304000	1.377406000
1	-1.693553000	0.321072000	2.216240000
1	-2.293621000	1.809124000	0.034857000
1	-1.744291000	0.323631000	-2.169872000
1	-0.817264000	-2.075133000	-1.348322000
6	1.522584000	-0.881815000	-0.121169000
8	2.357268000	-1.693922000	-0.208809000

7b – $Mn(CO)CpB_2H_4$

25	-0.156658000	0.279946000	-0.127553000
5	-0.787335000	2.129323000	-0.399918000
5	-1.638197000	1.154980000	0.698794000
1	-0.500751000	1.320768000	-1.420314000
1	-2.047244000	2.284360000	-0.103828000
1	-0.353717000	3.237876000	-0.552311000
1	-2.567162000	1.131812000	1.452367000
6	1.393719000	-0.010960000	1.285897000
6	1.199643000	-1.362750000	-0.589218000
6	1.808968000	-0.143395000	-0.992155000
6	1.932438000	0.699652000	0.154246000
6	0.949835000	-1.286717000	0.828815000
1	0.955380000	-2.200541000	-1.236626000
1	2.088054000	0.121212000	-2.009361000
1	2.346540000	1.704183000	0.167651000
1	1.341087000	0.355774000	2.307088000
1	0.499540000	-2.063936000	1.440495000
6	-1.587329000	-0.759095000	-0.182492000
8	-2.487657000	-1.516510000	-0.172659000

7c – $Mn(CO)CpB_2H_4$

25	-0.083325000	-0.250057000	-0.003033000
5	-3.405706000	-1.320591000	0.015787000
5	-1.778946000	-0.968316000	0.018942000
1	-3.889937000	-2.089747000	-0.776008000
1	-4.160452000	-0.809133000	0.803802000
1	-0.967710000	-1.186745000	-1.024409000
1	-1.018597000	-0.987824000	1.131487000
6	1.706125000	-0.454324000	-1.147939000
6	1.564439000	0.925029000	0.713084000
6	1.690124000	-0.416933000	1.172874000
6	1.797800000	-1.272022000	0.026651000
6	1.570880000	0.901836000	-0.731305000
1	1.465724000	1.808306000	1.337934000
1	1.695131000	-0.735368000	2.212055000
1	1.877663000	-2.356061000	0.045174000
1	1.726848000	-0.805051000	-2.176415000
1	1.480820000	1.765547000	-1.384280000
6	-1.106409000	1.205573000	-0.026013000
8	-1.692605000	2.219637000	-0.038909000

7e – $Mn(CO)_2CpB_2H_4$

25	0.067591000	-0.000178000	0.055677000
6	-1.617513000	1.154688000	-0.639755000
6	-1.617972000	-1.155000000	-0.638939000
6	-1.879568000	-0.715916000	0.694586000
6	-1.879324000	0.716670000	0.694098000
6	-1.455117000	-0.000481000	-1.469997000
1	-1.549697000	-2.189975000	-0.964439000
1	-2.060239000	-1.358382000	1.552932000
1	-2.059578000	1.359868000	1.551980000
1	-1.549061000	2.189369000	-0.966157000
1	-1.244781000	-0.000865000	-2.535843000
6	1.192137000	1.253184000	-0.508647000
8	1.913080000	2.088278000	-0.899134000
1	1.011757000	-1.867044000	2.346188000
5	0.836735000	-0.779163000	1.895796000
1	1.915606000	-0.001092000	2.155130000
5	0.837353000	0.778180000	1.894906000
1	0.232420000	-0.000476000	2.833811000
1	1.012985000	1.865412000	2.346757000
6	1.192726000	-1.252684000	-0.509462000
8	1.914188000	-2.087055000	-0.900502000

8a – $Fe(CO)_3B_2H_4$

26	-0.166660000	-0.010384000	-0.273879000
5	-1.662876000	0.757628000	-1.486670000
5	-1.691039000	-0.843617000	-1.404320000
1	-0.549938000	1.352099000	-1.190963000
1	-2.356921000	1.659916000	-1.856395000
1	-0.597160000	-1.443155000	-1.049813000
1	-2.416197000	-1.755358000	-1.678880000
6	-0.177761000	-1.215485000	1.031724000
6	-0.120458000	1.323361000	0.899419000
6	1.589753000	-0.069688000	-0.731238000
8	2.705742000	-0.108890000	-1.022232000
8	-0.101101000	2.192722000	1.661691000
8	-0.195421000	-2.001670000	1.879594000

8b – $Fe(CO)_3B_2H_4$

26	-0.000850000	-0.195985000	-0.232899000
5	-0.054181000	-1.797023000	-1.382564000
5	-1.504217000	-1.311686000	-0.740241000
1	0.537709000	-2.701431000	-1.899635000

1	0.712602000	-0.713837000	-1.587114000
1	-1.301977000	-2.109510000	-1.781755000
1	-2.642525000	-1.541742000	-0.476283000
6	1.525768000	-0.418572000	0.705374000
6	-1.194429000	0.222934000	1.008746000
6	0.245901000	1.505969000	-0.724397000
8	0.382459000	2.588189000	-1.110837000
8	-1.970917000	0.501109000	1.823077000
8	2.469065000	-0.608836000	1.347241000

8c – $Fe(CO)_3B_2H_4$

26	0.052410000	0.173896000	-0.159982000
5	3.466115000	0.590249000	-0.763853000
5	1.816113000	0.543873000	-0.618744000
1	4.170863000	0.967959000	0.136810000
1	4.017346000	0.193593000	-1.758977000
1	1.132586000	1.323317000	0.244760000
1	0.917617000	0.323950000	-1.564930000
6	0.323633000	-0.743628000	1.334746000
6	-0.970247000	-1.081870000	-0.905730000
6	-1.339468000	1.279003000	0.165568000
8	-2.178530000	2.032196000	0.423099000
8	-1.592567000	-1.906407000	-1.425834000
8	0.509132000	-1.341011000	2.308655000

8e – $Fe(CO)_4B_2H_4$

26	0.000053000	-0.001090000	0.040689000
5	0.000468000	0.758025000	2.037944000
5	0.001988000	-0.809612000	2.019487000
1	-0.000502000	1.840856000	2.526990000
1	0.905604000	-0.032439000	2.660944000
1	0.003864000	-1.903802000	2.482500000
1	-0.902596000	-0.034562000	2.661665000
6	0.001372000	-1.479448000	-0.988913000
6	1.795366000	0.003224000	0.157645000
6	-0.002293000	1.496419000	-0.960582000
8	-0.004413000	2.462544000	-1.598567000
8	2.948546000	0.006825000	0.253113000
8	0.002250000	-2.433194000	-1.645208000
6	-1.795205000	-0.000416000	0.159207000
8	-2.948316000	0.001017000	0.255498000

9a – $CoCpB_2H_4$

27	0.428691000	-0.000070000	-0.060157000
5	2.292419000	0.800088000	-0.005523000
5	2.292488000	-0.799995000	-0.005496000
1	1.190370000	1.424815000	-0.200050000
1	3.083638000	1.697496000	0.098919000
1	1.190457000	-1.424817000	-0.200144000
1	3.083724000	-1.697379000	0.099020000
6	-1.190095000	-1.153228000	0.430071000
6	-1.189505000	1.150971000	0.437384000
6	-1.321311000	0.711707000	-0.937786000
6	-1.321903000	-0.705525000	-0.942257000
6	-1.143008000	-0.003731000	1.282826000
1	-1.135890000	2.185369000	0.768599000
1	-1.368203000	1.359099000	-1.809627000
1	-1.369380000	-1.347420000	-1.818112000
1	-1.137100000	-2.189685000	0.754907000
1	-1.041858000	-0.007207000	2.364395000

9b – $CoCpB_2H_4$

27	0.441884000	-0.141502000	-0.095225000
5	1.981552000	0.910990000	0.006678000
5	2.237271000	-0.734300000	0.069277000
1	2.292101000	2.058687000	0.130665000
1	1.276016000	-1.315617000	-0.693574000
1	3.124431000	0.276106000	-0.189021000
1	3.032511000	-1.598324000	0.323645000
6	-1.118678000	1.150954000	-0.554351000
6	-1.384231000	-0.145203000	-1.101380000
6	-1.461784000	-1.093386000	-0.017573000
6	-1.190589000	-0.400669000	1.188900000
6	-0.965929000	0.993680000	0.860324000
1	-1.015574000	2.076028000	-1.114374000
1	-1.504079000	-0.377302000	-2.156980000
1	-1.638507000	-2.161202000	-0.118372000
1	-0.730125000	1.782007000	1.570379000
1	-1.134506000	-0.835538000	2.183397000

9c – $CoCpB_2H_4$

27	-0.275907000	-0.000016000	-0.173616000

5	-2.085446000	-0.000046000	-0.165996000
5	-3.707127000	0.000018000	0.106530000
1	-1.366204000	1.078334000	-0.544538000
1	-1.366184000	-1.078410000	-0.544518000
1	-4.332784000	-1.024421000	0.239392000
1	-4.332683000	1.024531000	0.239308000
6	1.268880000	1.151442000	0.527990000
6	1.268958000	-1.151457000	0.527860000
6	1.607050000	-0.707904000	-0.807139000
6	1.606997000	0.708055000	-0.807061000
6	1.100518000	-0.000059000	1.363523000
1	1.150400000	-2.186547000	0.838916000
1	1.775051000	-1.351703000	-1.666624000
1	1.774950000	1.351960000	-1.666475000
1	1.150257000	2.186491000	0.839158000
1	0.845126000	-0.000127000	2.419312000

9e – $Co(CO)CpB_2H_4$

27	-0.180186000	0.066154000	-0.000041000
6	1.431706000	-0.670861000	1.170699000
6	1.431926000	-0.670186000	-1.170858000
6	1.718880000	0.648927000	-0.722403000
6	1.718747000	0.648515000	0.723109000
6	1.218928000	-1.478288000	-0.000335000
1	1.360772000	-1.001229000	-2.203013000
1	1.913425000	1.511131000	-1.355963000
1	1.913265000	1.510345000	1.357182000
1	1.360214000	-1.002453000	2.202656000
1	0.956402000	-2.533756000	-0.000680000
6	-1.641782000	-0.843071000	-0.000106000
8	-2.643072000	-1.443757000	-0.000071000
1	-1.351055000	2.094396000	-1.879402000
5	-1.121370000	1.679629000	-0.786288000
1	-2.220077000	1.810009000	-0.000145000
5	-1.121847000	1.679155000	0.786399000
1	-0.625968000	2.677557000	0.000311000
1	-1.351738000	2.093760000	1.879537000

Optimized coordinates of Transition states and intermediates involved in type *a* to *b* transformations (Singlet spin state) at BP86/TZVP level of theory.

6t

5	1.180521000	-2.043004000	-0.039490000
5	0.009020000	-1.821998000	-1.258212000
1	1.723078000	-2.071131000	1.021000000
1	0.068857000	-0.692256000	-1.880187000
1	1.604936000	-2.920827000	-0.779062000
1	-0.476977000	-2.704374000	-1.900544000
24	0.078620000	-0.153278000	-0.198675000
6	1.861141000	0.516505000	-0.131079000
6	0.041019000	0.152404000	1.644868000
8	0.026427000	0.292842000	2.796480000
8	2.928155000	0.955257000	-0.051945000
6	-0.400488000	1.561390000	-0.807880000
6	-1.788507000	-0.475381000	-0.066284000
8	-2.928127000	-0.639154000	0.044470000
8	-0.703984000	2.589559000	-1.248770000

7t

5	1.778085000	1.242265000	0.612063000
5	1.087771000	2.105618000	-0.613576000
1	0.819006000	0.780082000	1.488830000
1	2.830556000	1.249203000	1.180957000
1	0.101643000	1.774491000	-1.239282000
1	1.484222000	3.177723000	-0.980601000
25	0.170765000	0.292196000	0.096949000
6	-1.566387000	-0.029192000	-1.169155000
6	-1.130795000	-1.253772000	0.759066000
6	-1.662142000	0.014592000	1.147935000
6	-1.940578000	0.765122000	-0.035754000
6	-1.067902000	-1.271194000	-0.682329000
1	-0.839328000	-2.059782000	1.426778000
1	-1.814885000	0.354116000	2.169190000
1	-2.328009000	1.780353000	-0.067958000
1	-1.639183000	0.265793000	-2.212501000
1	-0.702275000	-2.092772000	-1.292757000
6	1.528589000	-0.847737000	-0.050077000
8	2.354497000	-1.671850000	-0.141269000

7 (a to b) intermediate

5	-1.634798000	1.245110000	-0.689088000
5	-0.803608000	2.058596000	0.616779000
1	-0.768431000	0.673832000	-1.629949000
1	-2.717956000	1.496929000	-1.116406000
1	0.135760000	2.451346000	1.245611000
1	-1.736091000	2.837870000	0.692079000
25	-0.172943000	0.258121000	-0.193705000
6	1.459108000	0.051883000	1.222327000
6	1.176890000	-1.373399000	-0.594529000
6	1.746046000	-0.154258000	-1.067911000
6	1.934142000	0.717502000	0.051744000
6	0.991155000	-1.236929000	0.825277000
1	0.915081000	-2.239144000	-1.196224000
1	1.984786000	0.078495000	-2.102547000
1	2.326180000	1.730138000	0.008771000
1	1.443928000	0.455046000	2.230306000
1	0.563325000	-1.987491000	1.485005000
6	-1.595589000	-0.761209000	0.093275000
8	-2.487688000	-1.491265000	0.300802000

7t2

25	-0.219544000	0.230961000	-0.149947000
6	1.863982000	0.762926000	0.056958000
6	1.001450000	-1.220424000	0.859883000
6	1.179810000	-1.361687000	-0.562019000
6	1.692958000	-0.127632000	-1.054197000
6	1.427204000	0.087324000	1.239252000
1	0.610345000	-1.980929000	1.530744000
1	0.941009000	-2.239849000	-1.155318000
1	1.912629000	0.102340000	-2.093566000
1	2.242264000	1.779876000	0.003136000
1	1.413447000	0.496924000	2.244687000
6	-1.607289000	-0.875770000	-0.009447000
8	-2.486531000	-1.640500000	0.093838000
1	-0.815955000	0.705213000	-1.561846000
5	-1.693707000	1.280535000	-0.584695000
1	-1.677513000	2.783541000	0.275232000

5	-0.740278000	2.028653000	0.591699000
1	-2.791504000	1.454034000	-1.018988000
1	0.010919000	2.614904000	1.310420000

8t

5	-1.715044000	-0.130482000	1.623699000
5	-2.224663000	-0.527541000	0.112008000
1	-0.743495000	0.283143000	2.203212000
1	-2.592506000	-0.305088000	2.431655000
1	-1.575269000	-0.211572000	-0.990310000
1	-3.265215000	-0.967469000	-0.282097000
26	-0.334892000	-0.021119000	0.013783000
6	0.379620000	-1.355610000	-0.915280000
6	1.130976000	0.150050000	1.033499000
6	0.037317000	1.470679000	-0.905727000
8	0.254583000	2.412816000	-1.539648000
8	2.088993000	0.246839000	1.672519000
8	0.821264000	-2.213900000	-1.553397000

9t

5	2.166732000	0.864662000	0.124993000
5	2.156339000	-0.777538000	0.012879000
1	1.338689000	1.744203000	0.143907000
1	1.055766000	-1.472926000	-0.235982000
1	3.274584000	1.326628000	0.223598000
1	3.045340000	-1.581773000	0.026238000
27	0.375165000	-0.099488000	-0.010991000
6	-1.167666000	1.132211000	-0.716505000
1	-1.027722000	1.998426000	-1.358220000
6	-1.357184000	-0.208841000	-1.148685000
1	-1.410519000	-0.556553000	-2.176727000
6	-1.428794000	-1.038071000	0.035273000
1	-1.546850000	-2.119410000	0.043627000
6	-1.311720000	-0.199323000	1.193487000
6	-1.127711000	1.138689000	0.725618000
1	-0.956374000	2.012569000	1.349342000
1	-1.326751000	-0.526268000	2.229282000

Optimized coordinates of Metal Complexes of B_2H_4 with $Cr(CO)_4$ (6), Mn(CO)Cp (7), $Fe(CO)_3$ (8), CoCp (9) [type a-d] (Triplet spin state) at BP86/TZVP level of theory.

6a [S3] – $Cr(CO)_4B_2H_4$

5	0.503387000	2.212471000	-0.816454000
5	0.503211000	2.212583000	0.816262000
1	0.937668000	3.063017000	-1.536499000
1	0.035194000	1.232097000	-1.492480000
1	0.937235000	3.063277000	1.536289000
1	0.034948000	1.232275000	1.492346000
24	-0.004336000	0.225565000	0.000001000
6	1.890740000	-0.017230000	0.000235000
6	-0.179008000	-1.097968000	-1.367239000
6	-1.914744000	0.547821000	-0.000221000
8	-3.057355000	0.700857000	-0.000286000
8	-0.275527000	-1.900613000	-2.191113000
8	3.036340000	-0.166982000	0.000357000
6	-0.179292000	-1.097848000	1.367315000
8	-0.275976000	-1.900532000	2.191134000

6b [S3] – $Cr(CO)_4B_2H_4$

5	-1.559935000	-0.477028000	1.440786000
5	-0.300345000	-0.146668000	2.359876000
1	-2.618280000	-1.016117000	1.536624000
1	0.602677000	0.571425000	1.835375000
1	-1.490683000	0.510768000	2.389510000
1	-0.013709000	-0.425991000	3.487349000
24	0.112194000	0.002813000	0.150206000
6	-1.683389000	0.039206000	-0.401689000
6	0.199643000	-1.787487000	-0.578003000
8	0.239665000	-2.827563000	-1.077570000
8	-2.686379000	0.133782000	-1.006804000
6	0.077017000	1.852218000	-0.388906000
6	2.038706000	0.049546000	0.017138000
8	3.188791000	0.078498000	-0.068021000
8	0.050030000	2.926533000	-0.816150000

6c [S3] – $Cr(CO)_4B_2H_4$

1	-0.737893000	1.042909000	1.333847000

5	-1.363864000	-0.003940000	1.578764000
1	-0.737384000	-1.049370000	1.328910000
5	-2.646259000	-0.006945000	2.569446000
1	-3.783734000	-0.006287000	2.166772000
1	-2.499486000	-0.009996000	3.768156000
24	0.097762000	-0.000029000	0.013101000
8	-2.443040000	0.005525000	-1.693664000
6	-1.490162000	0.003415000	-1.033816000
6	1.748803000	-0.003246000	0.986996000
8	2.748069000	-0.005175000	1.568873000
6	0.580245000	-1.716054000	-0.731104000
6	0.581430000	1.719837000	-0.721369000
8	0.907278000	2.710741000	-1.220971000
8	0.905307000	-2.704322000	-1.236414000

6d [S3] – $Cr(CO)_4B_2H_4$

24	0.000001000	-0.000003000	0.031665000
6	-0.009046000	1.761573000	-0.755812000
6	-1.887694000	-0.008274000	-0.062582000
6	0.009106000	-1.761466000	-0.756042000
8	0.014878000	-2.800571000	-1.266528000
8	-3.046935000	-0.013045000	-0.153118000
8	-0.014782000	2.800744000	-1.266165000
6	1.887706000	0.008161000	-0.062424000
8	3.046940000	0.013331000	-0.153037000
5	-0.779950000	-0.002251000	2.107869000
5	0.779785000	0.001778000	2.107913000
1	-1.852895000	-0.004436000	2.617758000
1	-0.002173000	0.909518000	2.728798000
1	0.001950000	-0.910136000	2.728585000
1	1.852671000	0.003845000	2.617929000

7a [S3] – $Mn(CO)CpB_2H_4$

5	1.548519000	1.521107000	0.875555000
5	1.237801000	1.904748000	-0.720377000
1	0.659205000	1.131845000	1.636954000
1	2.594503000	1.801229000	1.394487000
1	0.764205000	1.065796000	-1.528781000
1	1.646102000	2.861030000	-1.316183000
25	0.226089000	0.241945000	-0.036035000
6	-1.713607000	0.084441000	-1.107757000
6	-1.188621000	-1.263561000	0.686761000

6	-1.691467000	-0.027793000	1.202482000
6	-1.966972000	0.821967000	0.105298000
6	-1.257916000	-1.210498000	-0.756332000
1	-0.889865000	-2.127952000	1.274488000
1	-1.755932000	0.241664000	2.253927000
1	-2.321212000	1.848462000	0.159117000
1	-1.845051000	0.466058000	-2.117644000
1	-0.996245000	-2.014356000	-1.438645000
6	1.609046000	-0.903106000	-0.058407000
8	2.477211000	-1.682546000	-0.078124000

7b [S3] – $Mn(CO)CpB_2H_4$

25	-0.153391000	0.252962000	-0.220350000
6	1.544630000	0.077427000	1.301873000
6	1.323920000	-1.270302000	-0.578541000
6	1.856105000	-0.019612000	-0.999231000
6	1.961074000	0.821783000	0.164629000
6	1.103493000	-1.195655000	0.849322000
1	1.118751000	-2.133931000	-1.205718000
1	2.130291000	0.260460000	-2.013474000
1	2.304097000	1.854029000	0.168744000
1	1.472647000	0.453630000	2.319371000
1	0.704709000	-1.994926000	1.468933000
6	-1.579688000	-0.818934000	-0.124806000
8	-2.352799000	-1.713045000	-0.087188000
1	-0.398131000	1.758588000	-1.097459000
5	-1.158289000	2.168288000	-0.141779000
1	-2.424877000	1.844178000	-0.414428000
5	-1.952765000	0.968964000	0.555033000
1	-1.079086000	3.358326000	-0.038606000
1	-2.873175000	0.725458000	1.273149000

7c [S3] – $Mn(CO)CpB_2H_4$

25	-0.073122000	-0.191323000	-0.136859000
6	1.899092000	-0.405469000	-1.075935000
6	1.566082000	0.902231000	0.805281000
6	1.721517000	-0.445098000	1.237255000
6	1.878767000	-1.257906000	0.080184000
6	1.709147000	0.934090000	-0.635719000
1	1.418641000	1.768147000	1.445466000
1	1.642372000	-0.800509000	2.262089000
1	1.973817000	-2.341521000	0.068813000

1	2.018889000	-0.735532000	-2.105222000
1	1.688305000	1.825950000	-1.256066000
6	-1.218968000	1.179731000	-0.045283000
8	-1.897989000	2.131114000	0.024712000
1	-3.870984000	-2.441253000	-0.291175000
5	-3.458400000	-1.358490000	0.052490000
1	-4.281442000	-0.582478000	0.473314000
5	-1.862878000	-1.013892000	0.023425000
1	-1.092590000	-1.274942000	-0.998932000
1	-1.212474000	-1.267257000	1.051217000

8a [S3] – $Fe(CO)_3B_2H_4$

5	-1.405621000	0.809411000	-1.633210000
5	-2.070525000	-0.443909000	-0.677269000
1	-0.179150000	1.045445000	-1.873048000
1	-2.135069000	1.448013000	-2.336013000
1	-2.256674000	-1.438101000	-1.359574000
1	-2.916478000	-0.226892000	0.151889000
26	-0.009058000	0.071199000	-0.413531000
6	-0.590142000	-1.209633000	0.725163000
6	0.070664000	1.416808000	0.802664000
6	1.770439000	-0.383447000	-0.465906000
8	2.889606000	-0.667506000	-0.473295000
8	0.117403000	2.247778000	1.605101000
8	-0.807278000	-2.011463000	1.536870000

8b [S3] – $Fe(CO)_3B_2H_4$

26	0.063472000	-0.024424000	-0.405265000
6	0.010247000	1.725860000	0.166026000
6	0.319985000	-0.759583000	1.201511000
6	-1.722470000	-0.481389000	-0.490763000
8	-2.839685000	-0.772837000	-0.454191000
8	0.343057000	-1.194437000	2.282024000
8	-0.022532000	2.811477000	0.560935000
5	1.727850000	-0.558995000	-1.679282000
5	2.033499000	-0.574792000	-0.109016000
1	2.474433000	-0.309007000	-2.581827000
1	0.527937000	-0.735797000	-2.030375000
1	2.194367000	-1.631152000	-1.026382000
1	2.852957000	-0.683040000	0.746188000

8c [S3] – $Fe(CO)_3B_2H_4$

26	-0.001902000	0.000000000	-0.369191000
6	0.340152000	-0.000309000	1.398011000
6	-1.181368000	-1.413139000	-0.360864000
6	-1.180743000	1.413533000	-0.360428000
8	-1.944154000	2.279642000	-0.297377000
8	-1.945129000	-2.278931000	-0.297996000
8	0.500685000	-0.000546000	2.545382000
1	4.251883000	-0.000544000	0.353741000
1	4.263258000	-0.000009000	-1.696076000
5	3.619433000	-0.000179000	-0.673949000
5	1.999888000	-0.000057000	-0.712459000
1	1.339073000	1.059186000	-0.893270000
1	1.339185000	-1.059290000	-0.893773000

9a [S3] – $CoCpB_2H_4$

5	-2.225229000	-0.849829000	0.027743000
5	-2.138246000	0.882485000	0.057280000
1	-1.361756000	-1.488674000	-0.675518000
1	-3.180408000	-1.494807000	0.352579000
1	-1.509223000	1.360588000	-0.924484000
1	-2.858989000	1.607806000	0.682294000
27	-0.494897000	-0.077028000	-0.234253000
6	0.928654000	1.008098000	0.870367000
6	1.417393000	-1.149788000	0.186013000
6	1.613906000	-0.268292000	-0.930149000
6	1.370083000	1.063578000	-0.490972000
6	0.974847000	-0.376477000	1.290876000
1	1.507955000	-2.233386000	0.162458000
1	1.931271000	-0.563632000	-1.927338000
1	1.423883000	1.958425000	-1.106522000
1	0.672337000	1.856595000	1.498849000
1	0.725233000	-0.749149000	2.280584000

9b [S3] – $CoCpB_2H_4$

5	-1.915460000	0.960804000	-0.054722000
5	-2.462116000	-0.555610000	0.039529000
1	-2.058753000	2.144715000	-0.031217000
1	-1.642499000	-1.284899000	0.702890000
1	-2.923209000	0.408703000	0.793709000
1	-3.370839000	-1.152633000	-0.466981000

27	-0.445149000	-0.309211000	-0.142738000
6	0.885174000	1.122735000	0.755076000
1	0.589871000	1.979886000	1.354430000
6	1.239513000	-0.170260000	1.254036000
1	1.196591000	-0.486461000	2.293409000
6	1.589690000	-0.988869000	0.140413000
1	1.887898000	-2.034001000	0.187431000
6	1.494352000	-0.189929000	-1.053442000
6	1.063459000	1.113130000	-0.677714000
1	0.893457000	1.952424000	-1.346901000
1	1.701267000	-0.525838000	-2.067095000

Optimized coordinates of C_4H_6 complexes used in estimation of heats of reactions at BP86/TZVP level of theory.

C_4H_6

6	1.549696000	-0.493432000	0.077768000
6	0.726444000	0.553133000	-0.104999000
6	-1.549696000	-0.493432000	-0.077768000
6	-0.726444000	0.553133000	0.104999000
1	-1.161037000	1.511357000	0.413584000
1	1.161037000	1.511357000	-0.413584000
1	2.620287000	-0.413693000	-0.118503000
1	-2.620287000	-0.413693000	0.118503000
1	1.183380000	-1.455870000	0.443860000
1	-1.183380000	-1.455870000	-0.443860000

$Cr(CO)_4C_4H_6$

6	-1.151900000	1.444845000	-1.440616000
6	-0.151618000	2.102296000	-0.721693000
6	-1.151807000	1.445092000	1.440423000
6	-0.151569000	2.102424000	0.721337000
24	0.007213000	0.025162000	-0.000010000
6	1.870810000	0.328216000	-0.000095000
6	0.430975000	-1.097513000	-1.424750000
6	-1.664281000	-0.880340000	0.000182000
8	-2.646589000	-1.495120000	0.000231000

8	0.686067000	-1.780073000	-2.330493000
8	3.029791000	0.414365000	-0.000242000
6	0.431096000	-1.097239000	1.424902000
8	0.686434000	-1.779417000	2.330866000
1	0.717158000	2.511580000	1.240071000
1	0.717079000	2.511357000	-1.240551000
1	-1.037641000	1.316315000	-2.517271000
1	-1.037488000	1.316725000	2.517091000
1	-2.174070000	1.387588000	-1.068439000
1	-2.174006000	1.387810000	1.068320000

$Mn(CO)CpC_4H_6$

25	-0.032665000	-0.013500000	-0.000003000
6	1.774677000	-0.215419000	-1.161720000
6	1.610596000	1.129196000	0.722833000
6	1.774724000	-0.216089000	1.161491000
6	1.882738000	-1.042794000	-0.000360000
6	1.610563000	1.129606000	-0.722270000
1	1.509739000	2.002391000	1.362339000
1	1.810613000	-0.553742000	2.194597000
1	1.998744000	-2.124597000	-0.000675000
1	1.810520000	-0.552469000	-2.195024000
1	1.509660000	2.003165000	-1.361272000
6	-1.041958000	1.444476000	0.000081000
8	-1.686049000	2.423093000	0.000192000
6	-1.547073000	-0.570215000	1.454082000
1	-1.319963000	-0.536756000	2.522345000
1	-2.494144000	-0.094967000	1.190065000
6	-1.069203000	-1.681120000	0.714800000
6	-1.069183000	-1.681071000	-0.714946000
1	-2.494091000	-0.094868000	-1.190162000
6	-1.547013000	-0.570107000	-1.454171000
1	-1.319870000	-0.536594000	-2.522426000
1	-0.489680000	-2.458748000	-1.219575000
1	-0.489712000	-2.458827000	1.219398000

$Fe(CO)_3C_4H_6$

26	0.008278000	-0.000013000	-0.008076000
6	0.222764000	0.000462000	1.762490000
6	1.155256000	1.276580000	-0.501079000

6	1.155236000	-1.276865000	-0.500460000
8	1.902264000	-2.111091000	-0.803551000
8	1.902268000	2.110746000	-0.804377000
8	0.335332000	0.000615000	2.915961000
6	-1.620348000	-1.370264000	0.105981000
1	-2.298077000	-1.018247000	0.885203000
1	-1.424285000	-2.443371000	0.132491000
1	-1.392913000	-1.256933000	-2.090067000
6	-1.571618000	-0.710914000	-1.161694000
6	-1.571597000	0.710453000	-1.161967000
1	-1.392878000	1.256122000	-2.090544000
6	-1.620312000	1.370306000	0.105448000
1	-1.424203000	2.443415000	0.131530000
1	-2.298073000	1.018637000	0.884801000

$CoCpC_4H_6$

27	0.125199000	-0.000013000	-0.043318000
6	-1.556093000	0.712570000	1.032772000
6	-1.584471000	-0.000509000	-1.192971000
6	-1.555022000	-1.152905000	-0.335843000
6	-1.556085000	-0.711765000	1.033366000
6	-1.555071000	1.152581000	-0.336817000
1	-1.615028000	-0.000965000	-2.278821000
1	-1.534001000	-2.188508000	-0.666897000
1	-1.536814000	-1.355526000	1.909629000
1	-1.536835000	1.357058000	1.908499000
1	-1.534087000	2.187910000	-0.668725000
6	1.547324000	-1.355612000	-0.591651000
1	1.307102000	-2.421603000	-0.566050000
1	2.023174000	-1.029715000	-1.520963000
6	1.848432000	-0.716270000	0.653593000
6	1.848403000	0.716316000	0.653590000
1	2.023148000	1.029749000	-1.520962000
6	1.547275000	1.355639000	-0.591659000
1	1.307026000	2.421624000	-0.566069000
1	1.903876000	1.265722000	1.596826000
1	1.903935000	-1.265669000	1.596831000