Mononuclear Bis(pentalene) Sandwich Compounds of the First-Row Transition Metals: Variable Hapticity of the Pentalene Rings and Intramolecular Coupling Reactions

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Supporting Information

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Complete Gaussian09 reference (Reference 44).

Table S1. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO-LUMO gaps, and spin expectation values for the $(C_8H_6)_2Ti$ structures.

	Ti-1S (C_1)		**Ti-2S (C_2)**		**Ti-3S (D_2)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
–HOMO(α)	0.17809	0.15818	0.17804	0.15730	0.17273	0.15307
–LUMO(α)	0.03985	0.06716	0.03830	0.06583	0.03932	0.06799
gap/eV	3.76	2.48	3.80	2.49	3.63	2.32
E+1466	-0.47364	-0.60604	-0.47312	-0.60562	-0.47081	-0.60357
ΔE	0.0	0.0	0.3	0.3	1.8	1.5
Nimg	none	none	1(60i)	1(53i)	1(189i)	1(186i)
$\langle S^2 \rangle$	0.00	0.00	0.00	0.00	0.00	0.00

	Ti-4S (D_{2d})		**Ti-5T (C_s)**		**Ti-6T (C_2)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
–HOMO(α)	0.14606	0.13051	0.10862	0.12146	0.13760	0.10688
–LUMO(α)	0.05166	0.08196	0.02606	0.05015	0.04951	0.08759
gap/eV	2.57	1.32	2.25	1.94	2.40	0.52
E+1466	-0.45617	-0.59023	-0.45349	-0.57476	-0.43745	-0.55107
ΔE	11.0	9.9	12.6	19.6	22.7	34.5
Nimg	1(93i)	1(89i)	none	none	none	none
$\langle S^2 \rangle$	0.00	0.00	2.02	2.01	2.01	2.01

Table S2. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO-LUMO gaps, and spin expectation values $\langle S^2 \rangle$ for the $(C_8H_6)_2V$ doublet structures.

	V-1D (C_1)		**V-2D (C_2)**		**V-3D (D_2)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.13791	0.13283	0.18729	0.09629	0.17640	0.11281
-LUMO(α)	0.06815	0.08206	0.06416	0.08906	0.06392	0.08195
gap/eV	1.90	1.38	3.35	0.20	3.06	0.84
E+1560	-0.97471	-1.13522	-0.96083	-1.11743	-0.94888	-1.10449
ΔE	0.0	0.0	8.7	11.2	16.2	19.3
Nimg	none	none	none	none	1(194i)	1(197i)
$\langle S^2 \rangle$	0.79	0.76	0.87	0.78	0.89	0.78

	V-4D (C_2)		**V-5D (C_s)**	
	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.14420	0.12373	0.16717	0.12052
-LUMO(α)	0.07323	0.09156	0.07052	0.09470
gap/eV	1.93	0.88	2.63	0.70
E+1560	-0.93841	-1.10022	-0.92257	-1.08631
ΔE	22.8	22.0	32.7	30.7
Nimg	none	none	none	none
$\langle S^2 \rangle$	0.77	1.64	0.77	1.54

Table S3. Total energies (E in hartree), relative energies (ΔE in kcal/mol), and HOMO-LUMO gaps, and spin expectation values $\langle S^2 \rangle$ for the $(C_8H_6)_2V$ quartet structures.

	V-6Q (C_2)		**V-7Q (C_s)**		**V-8Q (C_1)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
–HOMO(α)	0.16506	0.12567	0.16831	0.12317	0.13268	0.12709
–LUMO(α)	0.02572	0.05441	0.02001	0.05747	0.04074	0.08529
gap/eV	3.79	1.94	4.04	1.79	2.50	1.14
E+1560	-0.98472	-1.11893	-0.96649	-1.10303	-0.95552	-1.09904
ΔE	-6.3	10.2	5.2	20.2	12.0	22.7
Nimg	none	none	none	none	none	none
$\langle S^2 \rangle$	3.77	3.77	3.78	3.78	3.83	3.79

Table S4. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO-LUMO gaps, and spin expectation values $\langle S^2 \rangle$ for the $(C_8H_6)_2Cr$ structures.

	Cr-1S (C_s)		**Cr-2T (C_2)**		**Cr-3T (C_2)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.16826	0.13748	0.17312	0.13816	0.16619	0.15116
-LUMO(α)	0.08835	0.09251	0.02173	0.05915	0.12219	0.13335
gap/eV	2.17	1.22	4.12	2.15	1.20	0.48
E+1661	-0.39837	-0.59555	-0.42815	-0.59538	-0.42215	-0.58929
ΔE	0.0	0.0	–18.7	0.1	-14.9	3.9
Nimg	none	none	none	none	none	none
$\langle S^2 \rangle$	0.00	0.00	2.05	2.04	3.06	2.08

	Cr-4T (C_2)		**Cr-5T (C_s)**		**Cr-6S (C_2)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.16328	0.15281	0.17721	0.13484	0.17327	0.11903
-LUMO(α)	0.11868	0.13628	0.02916	0.05943	0.12494	0.09398
gap/eV	1.21	0.45	4.03	2.05	1.32	0.68
E+1661	-0.41269	-0.58891	-0.41300	-0.58281	-0.37615	-0.56468
ΔE	-9.0	4.2	-9.2	8.0	13.7	19.4
Nimg	none	none	none	none	none	none
$\langle S^2 \rangle$	3.08	2.37	2.05	2.04	0.00	0.00

Table S5. Total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO-LUMO gaps, and spin expectation values $\langle S^2 \rangle$ for the $(C_8H_6)_2Mn$ structures.

	Mn-1D (C_2)		**Mn-2D (C_{2v})**		**Mn-3D (C_s)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.18684	0.13705	0.16829	.0.14958	0.19252	0.14028
-LUMO(α)	0.02388	0.06279	0.11348	0.13968	0.02325	0.05890
gap/eV	4.43	2.02	1.49	0.27	4.60	2.21
E+1767	-0.94620	-1.13414	-0.92480	-1.12439	-0.92950	-1.12120
ΔE	0.0	0.0	13.4	6.1	10.5	6.4
Nimg	none	none	none	none	none	none
$\langle S^2 \rangle$	0.76	0.76	1.93	1.01	0.77	0.76

	Mn-4Q (C_{2v})		**Mn-5Q (C_1)**		**Mn-6Q (C_s)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.17933	0.14324	0.17169	0.12238	0.13908	0.07598
-LUMO(α)	0.05966	0.08441	0.05804	0.09301	0.07598	0.05447
gap/eV	3.27	1.60	3.09	0.80	1.72	0.59
-E	-0.92124	-1.11477	-0.94130	-1.11456	-0.92654	-1.09854
ΔE	15.7	12.2	3.1	12.3	12.3	22.3
Nimg	none	1(56i)	none	none	none	none
$\langle S^2 \rangle$	3.91	3.82	3.84	3.82	3.86	3.82

Table S6. Bond distances (in Å), total energies (E in hartree), relative energies (ΔE in kcal/mol), and HOMO-LUMO gaps for the $(C_8H_6)_2Fe$ singlet structures.

	Fe-1S (C_2)		**Fe-2S (C_s)**		**Fe-3S (C_{2v})**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO	0.15876	0.14795	0.18475	0.14390	0.17185	0.15803
-LUMO	0.05057	0.06314	0.02738	0.06557	0.11482	0.13283
gap/eV	2.94	2.31	4.28	2.13	1.55	0.69
E+1880	-0.68082	-0.90304	-0.66258	-0.88781	-0.63998	-0.87908
ΔE	0.0	0.0	11.4	9.6	25.6	15.0
Nimg	none	none	none	none	1(5i)	none

Table S7. Bond distances (in Å), total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO-LUMO gaps, and spin expectation values $\langle S^2 \rangle$ for the $(C_8H_6)_2Fe$ triplet structures.

	Fe-4T (C_{2h})		**Fe-5T (C_{2v})**		**Fe-6T (C_1)**		**Fe-7T (C_s)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.18151	0.15891	0.17765	0.15031	0.14762	0.11957	0.14910	0.08589
-LUMO(α)	0.05216	0.08326	0.05358	0.04833	0.05155	0.08468	0.04917	0.06439
gap/eV	3.52	2.06	3.38	2.78	2.61	0.95	2.72	0.59
E+1880	-0.65773	-0.87618	-0.65263	-0.87378	-0.66018	-0.85701	-0.64497	-0.84470
ΔE	14.5	16.9	17.7	18.4	13.0	28.9	22.5	36.6
Nimg	none	1(21i)	none	none	none	none	none	none
$\langle S^2 \rangle$	2.08	2.03	2.10	2.03	2.07	2.04	2.09	2.05

Table S8. Bond distances (in Å), total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO-LUMO gaps, and spin expectation values $\langle S^2 \rangle$ for the doublet $(C_8H_6)_2Co$ structures.

	Co-1D (C_2)		**Co-2D (C_{2v})**		**Co-3D (C_2)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.16446	0.14708	0.17650	0.16051	0.15073	0.11268
-LUMO(α)	0.02648	0.09315	0.05967	0.10398	0.07798	0.10924
gap/eV	3.75	1.47	3.18	1.54	1.98	0.09
E+1999	-0.71869	-0.96446	-0.71626	-0.96422	-0.73111	-0.95894
ΔE	0.0	0.0	1.5	0.2	–7.8	3.5
Nimg	none	none	1(27i)	1(19i)	none	none
$\langle S^2 \rangle$	0.86	0.76	0.94	0.76	0.77	0.76

	Co-4D (C_{2h})		**Co-5D (C_s)**	
	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.17789	0.15066	0.12881	0.09324
-LUMO(α)	0.05593	0.09501	0.04164	0.07517
gap/eV	3.32	1.51	2.37	0.49
E+1999	-0.71692	-0.95866	-0.71592	-0.94682
ΔE	1.1	3.6	1.7	11.1
Nimg	1(20i)	1(32i)	none	none
$\langle S^2 \rangle$	0.94	0.77	0.78	0.72

Table S9. Bond distances (in Å), total energies (E in hartree), relative energies (ΔE in kcal/mol), and HOMO-LUMO gaps for the quartet $(C_8H_6)_2Co$ structures.

	Co-6Q (C_2)		**Co-7Q (C_{2h})**		**Co-8Q (C_{2v})**		**Co-9Q (C_s)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.16446	0.12639	0.13970	0.10516	0.14659	0.11246	0.13021	0.09425
-LUMO(α)	0.02648	0.05580	0.07131	0.09819	0.07744	0.09334	0.02690	0.05479
gap/eV	3.75	1.92	1.86	0.19	1.88	0.52	2.81	1.07
E+1999	-0.72800	-0.92939	-0.69953	-0.92430	-0.69238	-0.91985	-0.70767	-0.91073
ΔE	–5.8	22.1	12.0	25.3	16.5	28.0	6.9	33.7
Nimg	none	none	none	none	none	none	none	none
$\langle S^2 \rangle$	3.77	3.77	3.83	3.77	3.87	3.78	3.77	3.77

Table S10. Bond distances (in Å), total energies (E in hartree), relative energies (ΔE in kcal/mol), and HOMO-LUMO gaps for the $(C_8H_6)_2Ni$ singlet structures.

	Ni-1S (C_{2v})		**Ni-2S (C_2)**		**Ni-3S (C_2)**		**Ni-4S (C_1)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO	0.15797	0.13974	0.18624	0.15674	0.16150	0.12701	0.15996	0.12867
-LUMO	0.09604	0.12061	0.06550	0.11701	0.07537	0.11032	0.07006	0.10094
gap/eV	1.69	0.52	3.29	1.08	2.34	0.45	2.45	0.75
E+2125	-0.26123	-0.51787	-0.25532	-0.51443	-0.26034	-0.49859	-0.24596	-0.48998
ΔE	0.0	0.0	3.7	2.2	0.6	12.1	9.6	17.5
Nimg	1(22i)	1(23i)	none	none	none	1(74i)	none	none

Table S11. Bond distances (in Å), total energies (E in hartree), relative energies (ΔE in kcal/mol), HOMO-LUMO gaps, and spin expectation values $\langle S^2 \rangle$ for the triplet $(C_8H_6)_2Ni$ structures.

	Ni-5T (C_2)		**Ni-6T (C_2)**		**Ni-7T (C_{2h})**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.15811	0.13549	0.14888	0.12187	0.15200	0.12137
-LUMO(α)	0.02283	0.05744	0.08308	0.11423	0.07872	0.11247
gap/eV	3.68	2.13	1.79	0.21	1.99	0.24
E+2125	-0.28188	-0.50810	-0.24905	-0.49379	-0.24892	-0.49365
ΔE	-13.0	6.1	7.6	15.1	7.7	15.2
Nimg	none	none	none	none	none	none
$\langle S^2 \rangle$	2.01	2.01	2.16	2.01	2.16	2.01

	Ni-8T (C_2)		**Ni-9T (C_{2v})**		**Ni-10T (C_s)**	
	B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-HOMO(α)	0.13770	0.13015	0.14757	0.11954	0.13620	0.10276
-LUMO(α)	0.06787	0.11231	0.07487	0.10439	0.02580	0.05429
gap/eV	1.90	0.49	1.98	0.41	3.00	1.32
E+2125	-0.24793	-0.49219	-0.24573	-0.49203	-0.26171	-0.49026
ΔE	8.3	16.1	9.7	16.2	–0.3	17.3
Nimg	none	none	2(86i,25i)	1(14i)	none	none
$\langle S^2 \rangle$	2.13	2.01	2.20	2.01	2.01	2.01

Table S12. Optimized coordinates of the **Ti-1S** for the $(C8H6)_2Ti$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-2.395941	1.272890	0.418132	-2.383114	1.271195	0.430154
C	-2.230337	1.536134	-0.933939	-2.221549	1.535874	-0.932845
C	-1.753960	0.347093	-1.625274	-1.752826	0.340385	-1.627629
C	-1.847282	-0.731043	-0.691176	-1.848566	-0.746210	-0.689543
C	-2.057328	-0.127615	0.616974	-2.051149	-0.136343	0.628470
C	-1.145515	-1.977784	-0.487473	-1.133507	-1.993293	-0.488824
C	-0.956005	-2.130602	0.918624	-0.924216	-2.141279	0.922832
C	-1.468554	-0.988534	1.602259	-1.440909	-0.995132	1.614751
H	-2.380871	2.501920	-1.409645	-2.369611	2.510261	-1.410986
H	-1.617218	0.261518	-2.699753	-1.613030	0.253735	-2.710107
H	-0.472031	-2.975754	1.398883	-0.423524	-2.987810	1.402761
H	-1.422632	-0.824680	2.674128	-1.384475	-0.827182	2.693896
H	-2.666885	1.985960	1.189859	-2.646726	1.991061	1.209815
H	-0.838667	-2.687133	-1.248398	-0.820752	-2.703654	-1.258264
C	1.395980	0.918485	1.668760	1.390456	0.931408	1.670649
C	0.858962	2.086237	1.031104	0.841505	2.099008	1.026994
C	1.145608	2.066907	-0.344889	1.128998	2.078344	-0.357832
C	1.928435	0.879785	-0.602164	1.921122	0.888964	-0.614622
C	2.143936	0.197318	0.671888	2.145925	0.207528	0.670194
C	1.847278	-0.121912	-1.637331	1.827703	-0.123158	-1.649128
C	2.038832	-1.384192	-1.015354	2.017797	-1.390623	-1.017338
C	2.173858	-1.220551	0.392743	2.169692	-1.218602	0.396386
H	0.260023	2.842422	1.530761	0.232371	2.857832	1.528853
H	0.789225	2.777313	-1.082535	0.763041	2.788198	-1.103564
H	2.032884	-2.339032	-1.533480	2.000943	-2.355923	-1.533660
H	2.292321	-2.022111	1.113988	2.286930	-2.022541	1.127637
H	1.322551	0.682477	2.725284	1.317291	0.693490	2.735309
H	1.664722	0.046668	-2.693332	1.633522	0.042334	-2.712050
Ti	0.134944	-0.181148	0.006224	0.131811	-0.176736	0.006106

Table S13. Optimized coordinates of the **Ti-2T** for the $(C8H6)_2Ti$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-0.873839	-2.624854	-1.157822	0.798900	2.623859	1.164312
C	-0.572272	-3.377777	0.000000	1.482441	3.070186	0.000000
C	-0.873839	-2.624854	1.157822	0.798900	2.623859	-1.164312
C	-1.404599	-1.344695	0.718675	-0.377202	1.887046	-0.724576
C	-1.404599	-1.344695	-0.718675	-0.377202	1.887046	0.724576
C	-1.986768	-0.118736	1.165797	-1.558072	1.197823	-1.172548
C	-2.346273	0.636782	0.000000	-2.286988	0.771356	0.000000
C	-1.986768	-0.118736	-1.165797	-1.558072	1.197823	1.172548
H	-0.148695	-4.378207	0.000000	2.413836	3.645523	0.000000
H	-0.739158	-2.950535	2.185122	1.099026	2.811814	-2.199907
H	-2.833080	1.606657	0.000000	-3.249164	0.252108	0.000000
H	-2.145770	0.197197	-2.192062	-1.868419	1.023062	2.206770
H	-0.739158	-2.950535	-2.185122	1.099026	2.811814	2.199907
H	-2.145770	0.197197	2.192062	-1.868419	1.023062	-2.206770
C	0.902475	2.219681	-1.307697	-0.546994	-2.311365	1.308300
C	1.219817	1.072144	-2.087415	0.370287	-1.536404	2.089418
C	1.938378	0.123539	-1.306351	1.517031	-1.181453	1.307290
C	2.132626	0.706457	0.000000	1.348680	-1.789555	0.000000
C	1.481229	2.019586	0.000000	0.054557	-2.496038	0.000000
C	1.938378	0.123539	1.306351	1.517031	-1.181453	-1.307290
C	1.219817	1.072144	2.087415	0.370287	-1.536404	-2.089418
C	0.902475	2.219681	1.307697	-0.546994	-2.311365	-1.308300
H	0.920839	0.923765	-3.122002	0.198537	-1.221618	3.124413
H	2.265969	-0.856948	-1.635882	2.350921	-0.554820	1.634457
H	0.920839	0.923765	3.122002	0.198537	-1.221618	-3.124413
H	0.330527	3.079178	1.642129	-1.519752	-2.684240	-1.640297
H	0.330527	3.079178	-1.642129	-1.519752	-2.684240	1.640297
H	2.265969	-0.856948	1.635882	2.350921	-0.554820	-1.634457
Ti	0.000000	0.461450	0.000000	-0.260220	-0.369809	0.000000

Table S14. Optimized coordinates of the **Ti-3T** for the $(C8H6)_2Ti$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	2.135498	0.257579	0.000000	2.107344	0.268690
C	-0.742517	2.236269	1.479491	-0.746678	2.187315	1.502404
C	-1.928441	1.420299	1.382224	-1.925474	1.343916	1.407563
C	-1.906849	0.833719	0.086693	-1.904525	0.759309	0.099505
C	-0.718462	1.246766	-0.587114	-0.716076	1.206138	-0.584367
C	-2.652191	-0.065442	-0.803402	-2.640937	-0.139069	-0.798163
C	-1.942606	-0.237477	-1.947491	-1.941444	-0.270408	-1.968594
C	-0.607219	0.501656	-1.911488	-0.616042	0.492984	-1.932155
H	-0.471020	2.860168	2.326419	-0.469869	2.800348	2.366531
H	-2.706489	1.331182	2.133884	-2.694633	1.225125	2.176489
H	-2.237602	-0.863908	-2.786803	-2.236157	-0.893791	-2.820968
H	-0.507203	1.173040	-2.777183	-0.526674	1.187777	-2.792230
H	0.938310	2.635099	0.043157	0.931764	2.633815	0.048219
H	-3.616270	-0.515359	-0.579284	-3.598660	-0.618555	-0.567141
C	1.928441	-1.420299	1.382224	1.925474	-1.343916	1.407563
C	0.742517	-2.236269	1.479491	0.746678	-2.187315	1.502404
C	0.000000	-2.135498	0.257579	0.000000	-2.107344	0.268690
C	0.718462	-1.246766	-0.587114	0.716076	-1.206138	-0.584367
C	1.906849	-0.833719	0.086693	1.904525	-0.759309	0.099505
C	0.607219	-0.501656	-1.911488	0.616042	-0.492984	-1.932155
C	1.942606	0.237477	-1.947491	1.941444	0.270408	-1.968594
C	2.652191	0.065442	-0.803402	2.640937	0.139069	-0.798163
H	0.471020	-2.860168	2.326419	0.469869	-2.800348	2.366531
H	-0.938310	-2.635099	0.043157	-0.931764	-2.633815	0.048219
H	2.237602	0.863908	-2.786803	2.236157	0.893791	-2.820968
H	3.616270	0.515359	-0.579284	3.598660	0.618555	-0.567141
H	2.706489	-1.331182	2.133884	2.694633	-1.225125	2.176489
H	0.507203	-1.173040	-2.777183	0.526674	-1.187777	-2.792230
Ti	0.000000	0.000000	1.263714	0.000000	0.000000	1.238164

Table S15. Optimized coordinates of the **Ti-3T** for the $(C8H6)_2Ti$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	2.135498	0.257579	0.000000	2.107344	0.268690
C	-0.742517	2.236269	1.479491	-0.746678	2.187315	1.502404
C	-1.928441	1.420299	1.382224	-1.925474	1.343916	1.407563
C	-1.906849	0.833719	0.086693	-1.904525	0.759309	0.099505
C	-0.718462	1.246766	-0.587114	-0.716076	1.206138	-0.584367
C	-2.652191	-0.065442	-0.803402	-2.640937	-0.139069	-0.798163
C	-1.942606	-0.237477	-1.947491	-1.941444	-0.270408	-1.968594
C	-0.607219	0.501656	-1.911488	-0.616042	0.492984	-1.932155
H	-0.471020	2.860168	2.326419	-0.469869	2.800348	2.366531
H	-2.706489	1.331182	2.133884	-2.694633	1.225125	2.176489
H	-2.237602	-0.863908	-2.786803	-2.236157	-0.893791	-2.820968
H	-0.507203	1.173040	-2.777183	-0.526674	1.187777	-2.792230
H	0.938310	2.635099	0.043157	0.931764	2.633815	0.048219
H	-3.616270	-0.515359	-0.579284	-3.598660	-0.618555	-0.567141
C	1.928441	-1.420299	1.382224	1.925474	-1.343916	1.407563
C	0.742517	-2.236269	1.479491	0.746678	-2.187315	1.502404
C	0.000000	-2.135498	0.257579	0.000000	-2.107344	0.268690
C	0.718462	-1.246766	-0.587114	0.716076	-1.206138	-0.584367
C	1.906849	-0.833719	0.086693	1.904525	-0.759309	0.099505
C	0.607219	-0.501656	-1.911488	0.616042	-0.492984	-1.932155
C	1.942606	0.237477	-1.947491	1.941444	0.270408	-1.968594
C	2.652191	0.065442	-0.803402	2.640937	0.139069	-0.798163
H	0.471020	-2.860168	2.326419	0.469869	-2.800348	2.366531
H	-0.938310	-2.635099	0.043157	-0.931764	-2.633815	0.048219
H	2.237602	0.863908	-2.786803	2.236157	0.893791	-2.820968
H	3.616270	0.515359	-0.579284	3.598660	0.618555	-0.567141
H	2.706489	-1.331182	2.133884	2.694633	-1.225125	2.176489
H	0.507203	-1.173040	-2.777183	0.526674	-1.187777	-2.792230
Ti	0.000000	0.000000	1.263714	0.000000	0.000000	1.238164

Table S16. Optimized coordinates of the **Ti-4S** for the $(C8H6)_2Ti$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.712990	1.192700	0.351366	1.717673	1.152540	0.356756
C	1.326901	1.930715	1.532071	1.332200	1.903021	1.541261
C	0.000000	2.435009	1.373185	0.000000	2.415906	1.384585
C	-0.463403	2.022628	0.097905	-0.476761	2.002621	0.104876
C	0.569776	1.231623	-0.528178	0.562241	1.196867	-0.528875
C	-1.575640	2.156733	-0.846720	-1.583120	2.151694	-0.844185
C	-1.271437	1.485609	-1.986392	-1.270359	1.493414	-2.003851
C	0.081247	0.775987	-1.902618	0.083290	0.776522	-1.922497
H	1.948904	2.082668	2.410282	1.954689	2.044015	2.431912
H	-0.546367	3.006154	2.119104	-0.547472	2.986344	2.142914
H	-1.913080	1.405878	-2.861508	-1.911248	1.431138	-2.891330
H	0.739138	1.088617	-2.728690	0.757630	1.099677	-2.744507
H	2.692424	0.771499	0.154267	2.705737	0.733641	0.150983
H	-2.491515	2.713428	-0.663605	-2.505213	2.713413	-0.657338
C	0.000000	-2.435009	1.373185	0.000000	-2.415906	1.384585
C	-1.326901	-1.930715	1.532071	-1.332200	-1.903021	1.541261
C	-1.712990	-1.192700	0.351366	-1.717673	-1.152540	0.356756
C	-0.569776	-1.231623	-0.528178	-0.562241	-1.196867	-0.528875
C	0.463403	-2.022628	0.097905	0.476761	-2.002621	0.104876
C	-0.081247	-0.775987	-1.902618	-0.083290	-0.776522	-1.922497
C	1.271437	-1.485609	-1.986392	1.270359	-1.493414	-2.003851
C	1.575640	-2.156733	-0.846720	1.583120	-2.151694	-0.844185
H	-1.948904	-2.082668	2.410282	-1.954689	-2.044015	2.431912
H	-2.692424	-0.771499	0.154267	-2.705737	-0.733641	0.150983
H	1.913080	-1.405878	-2.861508	1.911248	-1.431138	-2.891330
H	2.491515	-2.713428	-0.663605	2.505213	-2.713413	-0.657338
H	0.546367	-3.006154	2.119104	0.547472	-2.986344	2.142914
H	-0.739138	-1.088617	-2.728690	-0.757630	-1.099677	-2.744507
Ti	0.000000	0.000000	1.184222	0.000000	0.000000	1.185359

Table S17. Optimized coordinates of the **Ti-5T** for the $(C8H6)_2Ti$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.047476	-0.942335	2.397568	-1.076367	-0.953643	2.324181
C	-1.921248	0.174475	2.157713	-1.948543	0.179553	2.090272
C	-1.153778	1.230810	1.560776	-1.163137	1.245728	1.514077
C	0.176908	0.748542	1.409675	0.179487	0.755929	1.377207
C	0.251702	-0.559718	1.973218	0.246148	-0.571980	1.928497
C	1.527813	1.119524	0.807279	1.545362	1.135408	0.805998
C	2.396008	-0.019919	1.358144	2.408278	-0.021015	1.342033
C	1.655248	-0.985590	1.956961	1.646568	-1.005029	1.916709
H	-2.968790	0.233646	2.435584	-3.008871	0.238145	2.351947
H	-1.539643	2.205275	1.281707	-1.542446	2.235341	1.248738
H	3.473102	-0.054031	1.219005	3.495887	-0.052878	1.221022
H	2.039393	-1.913041	2.373413	2.022866	-1.952333	2.317188
H	-1.334104	-1.880571	2.864470	-1.383599	-1.910778	2.759295
H	1.886830	2.098527	1.153580	1.903151	2.119323	1.169709
C	-1.047476	-0.942335	-2.397568	-1.076367	-0.953643	-2.324181
C	-1.921248	0.174475	-2.157713	-1.948543	0.179553	-2.090272
C	-1.153778	1.230810	-1.560776	-1.163137	1.245728	-1.514077
C	0.176908	0.748542	-1.409675	0.179487	0.755929	-1.377207
C	0.251702	-0.559718	-1.973218	0.246148	-0.571980	-1.928497
C	1.527813	1.119524	-0.807279	1.545362	1.135408	-0.805998
C	2.396008	-0.019919	-1.358144	2.408278	-0.021015	-1.342033
C	1.655248	-0.985590	-1.956961	1.646568	-1.005029	-1.916709
H	-2.968790	0.233646	-2.435584	-3.008871	0.238145	-2.351947
H	-1.539643	2.205275	-1.281707	-1.542446	2.235341	-1.248738
H	3.473102	-0.054031	-1.219005	3.495887	-0.052878	-1.221022
H	2.039393	-1.913041	-2.373413	2.022866	-1.952333	-2.317188
H	-1.334104	-1.880571	-2.864470	-1.383599	-1.910778	-2.759295
H	1.886830	2.098527	-1.153580	1.903151	2.119323	-1.169709
Ti	-1.169805	-0.480413	0.000000	-1.137615	-0.478775	0.000000

Table S18. Optimized coordinates of the **Ti-6S** for the $(C8H6)_2Ti$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.012638	-0.987320	2.384367	-1.021106	-0.994103	2.364455
C	-1.917832	0.101530	2.134545	-1.929016	0.101564	2.116704
C	-1.184278	1.196313	1.521124	-1.196795	1.204527	1.492531
C	0.164964	0.714842	1.348355	0.166498	0.715291	1.319195
C	0.267563	-0.585847	1.947482	0.270407	-0.594613	1.928639
C	1.527338	1.131258	0.798532	1.539987	1.144615	0.797140
C	2.404457	-0.002156	1.351250	2.416571	-0.001341	1.337197
C	1.674574	-0.986115	1.937437	1.674862	-0.999211	1.917415
H	-2.960505	0.127888	2.437414	-2.983008	0.121224	2.412528
H	-1.566882	2.195017	1.343836	-1.574840	2.218270	1.341285
H	3.485835	-0.010518	1.240870	3.508286	-0.002261	1.245849
H	2.073003	-1.907540	2.353982	2.073038	-1.933859	2.326579
H	-1.282030	-1.936957	2.838327	-1.298157	-1.955006	2.811104
H	1.860022	2.111872	1.170355	1.870062	2.130453	1.186552
C	-1.012638	-0.987320	-2.384367	-1.021106	-0.994103	-2.364455
C	-1.917832	0.101530	-2.134545	-1.929016	0.101564	-2.116704
C	-1.184278	1.196313	-1.521124	-1.196795	1.204527	-1.492531
C	0.164964	0.714842	-1.348355	0.166498	0.715291	-1.319195
C	0.267563	-0.585847	-1.947482	0.270407	-0.594613	-1.928639
C	1.527338	1.131258	-0.798532	1.539987	1.144615	-0.797140
C	2.404457	-0.002156	-1.351250	2.416571	-0.001341	-1.337197
C	1.674574	-0.986115	-1.937437	1.674862	-0.999211	-1.917415
H	-2.960505	0.127888	-2.437414	-2.983008	0.121224	-2.412528
H	-1.566882	2.195017	-1.343836	-1.574840	2.218270	-1.341285
H	3.485835	-0.010518	-1.240870	3.508286	-0.002261	-1.245849
H	2.073003	-1.907540	-2.353982	2.073038	-1.933859	-2.326579
H	-1.282030	-1.936957	-2.838327	-1.298157	-1.955006	-2.811104
H	1.860022	2.111872	-1.170355	1.870062	2.130453	-1.186552
Ti	-1.195848	-0.370436	0.000000	-1.193076	-0.367200	0.000000

Table S19. Optimized coordinates of the **V-1D** for the $(C8H6)_2V$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	2.790393	0.908322	-0.530199	2.781235	0.909385	-0.490192
C	3.124711	0.849302	0.853807	3.109440	0.824275	0.896569
C	2.449567	-0.207133	1.503536	2.417427	-0.248468	1.527305
C	1.677791	-0.868551	0.496659	1.642226	-0.890773	0.502312
C	1.889751	-0.154816	-0.768600	1.864410	-0.152753	-0.755738
C	0.810428	-1.983582	0.227841	0.763620	-2.001561	0.203542
C	0.481611	-1.960148	-1.176965	0.442013	-1.949041	-1.209496
C	1.060604	-0.799478	-1.767247	1.048819	-0.780403	-1.779416
H	3.812035	1.533938	1.347802	3.801803	1.501245	1.411758
H	2.549786	-0.493708	2.545181	2.503368	-0.550388	2.574694
H	-0.149074	-2.680212	-1.689308	-0.196921	-2.657438	-1.745295
H	0.961489	-0.521649	-2.812252	0.956334	-0.476864	-2.826554
H	3.160656	1.630847	-1.250406	3.164789	1.644048	-1.203814
H	0.498018	-2.753680	0.925890	0.431422	-2.782357	0.893467
C	-1.503364	1.406003	-1.346863	-1.502132	1.382716	-1.371081
C	-0.481652	2.135563	-0.675411	-0.453625	2.114464	-0.721599
C	-0.540317	1.894557	0.721802	-0.500397	1.904262	0.690858
C	-1.674086	1.032817	0.965170	-1.652064	1.062301	0.965658
C	-2.275439	0.718534	-0.337232	-2.278323	0.729083	-0.330878
C	-1.699619	-0.172534	1.758059	-1.644201	-0.144011	1.771997
C	-2.316784	-1.185682	0.974464	-2.262806	-1.178529	0.998984
C	-2.644307	-0.678999	-0.316079	-2.629407	-0.681507	-0.295375
H	0.296955	2.712598	-1.164406	0.340981	2.663479	-1.235757
H	0.186632	2.233003	1.451887	0.248707	2.242160	1.411209
H	-2.462971	-2.213890	1.292698	-2.379022	-2.217100	1.324627
H	-3.085336	-1.246667	-1.128423	-3.081822	-1.262592	-1.102753
H	-1.655954	1.364894	-2.419796	-1.671527	1.318563	-2.448594
H	-1.278428	-0.301042	2.749393	-1.192648	-0.259654	2.760398
V	-0.423024	-0.211717	-0.145422	-0.426212	-0.198250	-0.149308

Table S20. Optimized coordinates of the **V-2D** for the $(C8H6)_2V$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	2.841639	0.484168	-1.392256	2.469214	0.489357
C	0.345877	2.839490	-0.854509	-1.100494	2.643794	-0.861697
C	-0.430178	1.827466	-1.570992	-1.267539	1.372788	-1.575798
C	-1.448929	1.380086	-0.673306	-1.939470	0.472737	-0.673891
C	-1.054173	1.843136	0.650043	-1.811486	1.074497	0.657802
C	-2.176022	0.133726	-0.509379	-1.939470	-0.976231	-0.514137
C	-2.189629	-0.161672	0.872942	-1.784216	-1.246367	0.874254
C	-1.455352	0.845554	1.592389	-1.640103	-0.002501	1.599861
H	1.117486	3.455440	-1.308918	-0.739842	3.569980	-1.321452
H	-0.398677	1.661415	-2.644376	-1.158858	1.240082	-2.657449
H	-2.637955	-1.041537	1.323672	-1.721318	-2.242245	1.322510
H	-1.274056	0.843492	2.662378	-1.468893	0.083636	2.676428
H	0.453166	3.434672	1.272014	-1.289541	3.213764	1.283804
H	-2.607239	-0.476894	-1.294342	-2.006022	-1.723157	-1.308604
C	1.455352	-0.845554	1.592389	1.640103	0.002501	1.599861
C	2.189629	0.161672	0.872942	1.784216	1.246367	0.874254
C	2.176022	-0.133726	-0.509379	1.939470	0.976231	-0.514137
C	1.448929	-1.380086	-0.673306	1.939470	-0.472737	-0.673891
C	1.054173	-1.843136	0.650043	1.811486	-1.074497	0.657802
C	0.430178	-1.827466	-1.570992	1.267539	-1.372788	-1.575798
C	-0.345877	-2.839490	-0.854509	1.100494	-2.643794	-0.861697
C	0.000000	-2.841639	0.484168	1.392256	-2.469214	0.489357
H	2.637955	1.041537	1.323672	1.721318	2.242245	1.322510
H	2.607239	0.476894	-1.294342	2.006022	1.723157	-1.308604
H	-1.117486	-3.455440	-1.308918	0.739842	-3.569980	-1.321452
H	-0.453166	-3.434672	1.272014	1.289541	-3.213764	1.283804
H	1.274056	-0.843492	2.662378	1.468893	-0.083636	2.676428
H	0.398677	-1.661415	-2.644376	1.158858	-1.240082	-2.657449
V	0.000000	0.000000	0.003603	0.000000	0.000000	0.002651

Table S21. Optimized coordinates of the **V-3D** for the $(C8H6)_2V$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.775263	1.718654	0.522854	-1.751101	1.728258	0.515324
C	-1.555017	1.969645	-0.832449	-1.530178	1.973909	-0.851160
C	-1.588115	0.726189	-1.572637	-1.557551	0.717723	-1.583022
C	-2.027632	-0.292775	-0.664209	-2.016089	-0.300231	-0.666520
C	-2.027632	0.292775	0.664209	-2.016089	0.300231	0.666520
C	-1.775263	-1.718654	-0.522854	-1.751101	-1.728258	-0.515324
C	-1.555017	-1.969645	0.832449	-1.530178	-1.973909	0.851160
C	-1.588115	-0.726189	1.572637	-1.557551	-0.717723	1.583022
H	-1.312611	2.936722	-1.263579	-1.278874	2.944362	-1.290509
H	-1.458080	0.629388	-2.646277	-1.421742	0.610057	-2.663418
H	-1.312611	-2.936722	1.263579	-1.278874	-2.944362	1.290509
H	-1.458080	-0.629388	2.646277	-1.421742	-0.610057	2.663418
H	-1.725282	2.445600	1.327006	-1.695358	2.463843	1.322668
H	-1.725282	-2.445600	-1.327006	-1.695358	-2.463843	-1.322668
C	1.588115	0.726189	1.572637	1.557551	0.717723	1.583022
C	1.555017	1.969645	0.832449	1.530178	1.973909	0.851160
C	1.775263	1.718654	-0.522854	1.751101	1.728258	-0.515324
C	2.027632	0.292775	-0.664209	2.016089	0.300231	-0.666520
C	2.027632	-0.292775	0.664209	2.016089	-0.300231	0.666520
C	1.588115	-0.726189	-1.572637	1.557551	-0.717723	-1.583022
C	1.555017	-1.969645	-0.832449	1.530178	-1.973909	-0.851160
C	1.775263	-1.718654	0.522854	1.751101	-1.728258	0.515324
H	1.312611	2.936722	1.263579	1.278874	2.944362	1.290509
H	1.725282	2.445600	-1.327006	1.695358	2.463843	-1.322668
H	1.312611	-2.936722	-1.263579	1.278874	-2.944362	-1.290509
H	1.725282	-2.445600	1.327006	1.695358	-2.463843	1.322668
H	1.458080	0.629388	2.646277	1.421742	0.610057	2.663418
H	1.458080	-0.629388	-2.646277	1.421742	-0.610057	-2.663418
V	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Table S22. Optimized coordinates of the **V-4D** for the $(C8H6)_2V$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.721177	1.093976	0.338387	0.000000	2.074222	0.309996
C	1.328606	1.765083	1.551852	-0.737230	2.100438	1.555334
C	0.000000	2.299206	1.407474	-1.905962	1.252757	1.439201
C	-0.444996	1.969202	0.103306	-1.901586	0.718470	0.109438
C	0.588736	1.197874	-0.545593	-0.712867	1.185479	-0.570896
C	-1.548494	2.146791	-0.844141	-2.638131	-0.160612	-0.807578
C	-1.243023	1.508443	-2.001793	-1.942121	-0.263638	-1.982376
C	0.097117	0.774861	-1.928677	-0.614364	0.496313	-1.935436
H	1.935855	1.839893	2.449868	-0.454390	2.670575	2.445503
H	-0.553100	2.826876	2.178870	-2.649793	1.079173	2.221965
H	-1.881940	1.459082	-2.881252	-2.242932	-0.863538	-2.849393
H	0.763164	1.079339	-2.750406	-0.521217	1.200684	-2.787469
H	2.688515	0.648628	0.138023	0.926580	2.614279	0.100978
H	-2.461210	2.703749	-0.647510	-3.594298	-0.647196	-0.585336
C	0.000000	-2.299206	1.407474	1.905962	-1.252757	1.439201
C	-1.328606	-1.765083	1.551852	0.737230	-2.100438	1.555334
C	-1.721177	-1.093976	0.338387	0.000000	-2.074222	0.309996
C	-0.588736	-1.197874	-0.545593	0.712867	-1.185479	-0.570896
C	0.444996	-1.969202	0.103306	1.901586	-0.718470	0.109438
C	-0.097117	-0.774861	-1.928677	0.614364	-0.496313	-1.935436
C	1.243023	-1.508443	-2.001793	1.942121	0.263638	-1.982376
C	1.548494	-2.146791	-0.844141	2.638131	0.160612	-0.807578
H	-1.935855	-1.839893	2.449868	0.454390	-2.670575	2.445503
H	-2.688515	-0.648628	0.138023	-0.926580	-2.614279	0.100978
H	1.881940	-1.459082	-2.881252	2.242932	0.863538	-2.849393
H	2.461210	-2.703749	-0.647510	3.594298	0.647196	-0.585336
H	0.553100	-2.826876	2.178870	2.649793	-1.079173	2.221965
H	-0.763164	-1.079339	-2.750406	0.521217	-1.200684	-2.787469
V	0.000000	0.000000	1.132827	0.000000	0.000000	1.108491

Table S23. Optimized coordinates of the **V-5D** for the $(C8H6)_2V$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.027074	-1.043754	2.239920	-1.070457	-1.011616	2.237405
C	-1.906969	0.080102	2.061275	-1.950053	0.119701	2.028846
C	-1.167968	1.210113	1.539398	-1.174077	1.227004	1.507449
C	0.171445	0.723421	1.327857	0.177565	0.746698	1.352266
C	0.261023	-0.624207	1.832288	0.249326	-0.599785	1.872421
C	1.539944	1.150294	0.799749	1.549876	1.149457	0.804351
C	2.410855	0.000136	1.329567	2.412561	-0.013327	1.329750
C	1.668474	-1.017236	1.837629	1.652181	-1.018021	1.869180
H	-2.968808	0.079990	2.293946	-3.019142	0.145939	2.259289
H	-1.551023	2.215397	1.407549	-1.561488	2.224893	1.289117
H	3.494438	-0.000359	1.244004	3.503271	-0.030116	1.233106
H	2.057990	-1.962266	2.206765	2.031829	-1.973416	2.246406
H	-1.315105	-2.016407	2.625144	-1.373546	-1.988530	2.626075
H	1.870704	2.127594	1.178890	1.901125	2.131243	1.180382
C	-1.027074	-1.043754	-2.239920	-1.070457	-1.011616	-2.237405
C	-1.906969	0.080102	-2.061275	-1.950053	0.119701	-2.028846
C	-1.167968	1.210113	-1.539398	-1.174077	1.227004	-1.507449
C	0.171445	0.723421	-1.327857	0.177565	0.746698	-1.352266
C	0.261023	-0.624207	-1.832288	0.249326	-0.599785	-1.872421
C	1.539944	1.150294	-0.799749	1.549876	1.149457	-0.804351
C	2.410855	0.000136	-1.329567	2.412561	-0.013327	-1.329750
C	1.668474	-1.017236	-1.837629	1.652181	-1.018021	-1.869180
H	-2.968808	0.079990	-2.293946	-3.019142	0.145939	-2.259289
H	-1.551023	2.215397	-1.407549	-1.561488	2.224893	-1.289117
H	3.494438	-0.000359	-1.244004	3.503271	-0.030116	-1.233106
H	2.057990	-1.962266	-2.206765	2.031829	-1.973416	-2.246406
H	-1.315105	-2.016407	-2.625144	-1.373546	-1.988530	-2.626075
H	1.870704	2.127594	-1.178890	1.901125	2.131243	-1.180382
V	-1.155354	-0.288449	0.000000	-1.092485	-0.357451	0.000000

Table S24. Optimized coordinates of the **V-6Q** for the $(C8H6)_2V$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	2.121846	0.290235	0.000000	2.103813	0.295552
C	-0.724655	2.178505	1.530417	-0.716780	2.134314	1.551828
C	-1.902765	1.363289	1.421332	-1.891486	1.297105	1.446174
C	-1.905392	0.823692	0.101765	-1.904398	0.771649	0.110233
C	-0.726942	1.259298	-0.580152	-0.727530	1.234326	-0.583374
C	-2.649614	-0.072934	-0.794532	-2.640805	-0.130087	-0.788671
C	-1.943487	-0.233062	-1.942160	-1.943107	-0.259574	-1.959391
C	-0.608579	0.506719	-1.904384	-0.617297	0.501197	-1.924001
H	-0.442352	2.766927	2.397803	-0.426226	2.713786	2.432833
H	-2.656227	1.228902	2.190593	-2.637417	1.137964	2.229549
H	-2.241015	-0.851218	-2.786593	-2.241097	-0.878714	-2.813684
H	-0.502271	1.170469	-2.774897	-0.518882	1.179358	-2.795704
H	0.938628	2.624247	0.082645	0.939346	2.620885	0.083100
H	-3.611063	-0.528894	-0.571214	-3.596891	-0.612326	-0.556644
C	1.902765	-1.363289	1.421332	1.891486	-1.297105	1.446174
C	0.724655	-2.178505	1.530417	0.716780	-2.134314	1.551828
C	0.000000	-2.121846	0.290235	0.000000	-2.103813	0.295552
C	0.726942	-1.259298	-0.580152	0.727530	-1.234326	-0.583374
C	1.905392	-0.823692	0.101765	1.904398	-0.771649	0.110233
C	0.608579	-0.506719	-1.904384	0.617297	-0.501197	-1.924001
C	1.943487	0.233062	-1.942160	1.943107	0.259574	-1.959391
C	2.649614	0.072934	-0.794532	2.640805	0.130087	-0.788671
H	0.442352	-2.766927	2.397803	0.426226	-2.713786	2.432833
H	-0.938628	-2.624247	0.082645	-0.939346	-2.620885	0.083100
H	2.241015	0.851218	-2.786593	2.241097	0.878714	-2.813684
H	3.611063	0.528894	-0.571214	3.596891	0.612326	-0.556644
H	2.656227	-1.228902	2.190593	2.637417	-1.137964	2.229549
H	0.502271	-1.170469	-2.774897	0.518882	-1.179358	-2.795704
V	0.000000	0.000000	1.106654	0.000000	0.000000	1.089604

Table S25. Optimized coordinates of the **V-7Q** for the $(C8H6)_2V$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.058773	-1.003944	2.307958	-1.078667	-1.019133	2.253066
C	-1.927999	0.122296	2.108996	-1.947730	0.119677	2.057080
C	-1.159258	1.220733	1.590777	-1.166265	1.231059	1.560341
C	0.174914	0.754158	1.424419	0.178706	0.760434	1.404566
C	0.245097	-0.585628	1.917601	0.242840	-0.595395	1.890443
C	1.522303	1.135552	0.813374	1.537734	1.146118	0.813960
C	2.393268	-0.012785	1.341883	2.404597	-0.015753	1.329160
C	1.651883	-1.002841	1.898047	1.647160	-1.019598	1.870529
H	-2.986047	0.154454	2.350396	-3.018626	0.149147	2.278853
H	-1.553305	2.200859	1.343364	-1.557681	2.223323	1.320845
H	3.471845	-0.035820	1.213347	3.493163	-0.037416	1.213865
H	2.036578	-1.944028	2.281726	2.026837	-1.978041	2.239792
H	-1.345752	-1.960670	2.731677	-1.377237	-1.989347	2.658848
H	1.885423	2.113624	1.155778	1.903824	2.129271	1.167949
C	-1.058773	-1.003944	-2.307958	-1.078667	-1.019133	-2.253066
C	-1.927999	0.122296	-2.108996	-1.947730	0.119677	-2.057080
C	-1.159258	1.220733	-1.590777	-1.166265	1.231059	-1.560341
C	0.174914	0.754158	-1.424419	0.178706	0.760434	-1.404566
C	0.245097	-0.585628	-1.917601	0.242840	-0.595395	-1.890443
C	1.522303	1.135552	-0.813374	1.537734	1.146118	-0.813960
C	2.393268	-0.012785	-1.341883	2.404597	-0.015753	-1.329160
C	1.651883	-1.002841	-1.898047	1.647160	-1.019598	-1.870529
H	-2.986047	0.154454	-2.350396	-3.018626	0.149147	-2.278853
H	-1.553305	2.200859	-1.343364	-1.557681	2.223323	-1.320845
H	3.471845	-0.035820	-1.213347	3.493163	-0.037416	-1.213865
H	2.036578	-1.944028	-2.281726	2.026837	-1.978041	-2.239792
H	-1.345752	-1.960670	-2.731677	-1.377237	-1.989347	-2.658848
H	1.885423	2.113624	-1.155778	1.903824	2.129271	-1.167949
V	-1.091944	-0.373362	0.000000	-1.076567	-0.360122	0.000000

Table S26. Optimized coordinates of the **V-8Q** for the $(C8H6)_2V$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-2.520655	1.533960	-0.292134	-2.447878	1.599616	-0.192360
C	-3.159203	0.731283	-1.266490	-3.137340	0.852546	-1.189953
C	-2.881592	-0.634194	-1.032488	-2.908031	-0.537926	-1.009756
C	-2.039033	-0.706866	0.147640	-2.054800	-0.685351	0.156304
C	-1.817674	0.642367	0.610772	-1.776799	0.648126	0.673252
C	-1.402069	-1.599348	1.060555	-1.384923	-1.636001	0.999428
C	-0.782362	-0.797359	2.077035	-0.702214	-0.890774	2.033312
C	-1.048753	0.588675	1.814148	-0.948917	0.520982	1.846154
H	-3.757160	1.111703	-2.090180	-3.734572	1.289384	-1.997219
H	-3.239061	-1.470738	-1.625347	-3.305278	-1.344431	-1.633251
H	-0.214575	-1.180615	2.919217	-0.103602	-1.328719	2.837264
H	-0.712201	1.422630	2.420584	-0.564406	1.324418	2.479816
H	-2.553364	2.617665	-0.233790	-2.432653	2.689283	-0.096268
H	-1.370655	-2.683091	1.008516	-1.374720	-2.724438	0.892324
C	2.526199	1.134498	0.919281	2.570818	1.043163	0.942196
C	1.853166	2.178556	0.286360	1.954608	2.153024	0.340340
C	1.275727	1.710937	-0.957153	1.336529	1.752997	-0.912993
C	1.785713	0.393887	-1.192535	1.762937	0.406024	-1.191496
C	2.437914	-0.023902	0.046372	2.402403	-0.087319	0.036886
C	1.243375	-0.789411	-1.831091	1.168486	-0.727511	-1.882234
C	1.570424	-1.896880	-0.997794	1.437398	-1.887067	-1.080799
C	2.263456	-1.443817	0.169882	2.159237	-1.508104	0.108287
H	1.727997	3.181153	0.686370	1.893072	3.156859	0.773008
H	0.715606	2.320331	-1.660793	0.794774	2.414302	-1.596595
H	1.306088	-2.931331	-1.198043	1.117458	-2.906423	-1.318001
H	2.586002	-2.075711	0.991574	2.452130	-2.189107	0.912547
H	2.999486	1.170030	1.895783	3.058185	1.021396	1.921436
H	0.693362	-0.835997	-2.765406	0.611130	-0.710632	-2.822691
V	0.260465	-0.294798	0.099015	0.217365	-0.295237	0.069053

Table S27. Optimized coordinates of the **Cr-1S** for the $(C8H6)_2Cr$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.501583	0.762721	1.183721	-1.514589	0.664452	1.192647
C	1.452120	1.592667	0.000000	-2.144213	0.110408	0.000000
C	1.501583	0.762721	-1.183721	-1.514589	0.664452	-1.192647
C	1.749504	-0.578834	-0.743177	-0.635440	1.719603	-0.746401
C	1.749504	-0.578834	0.743177	-0.635440	1.719603	0.746401
C	2.011302	-1.899041	-1.179844	0.223003	2.762371	-1.185691
C	2.195121	-2.668566	0.000000	0.704859	3.398985	0.000000
C	2.011302	-1.899041	1.179844	0.223003	2.762371	1.185691
H	1.406673	2.676835	0.000000	-2.970585	-0.605768	0.000000
H	1.511539	1.128493	-2.204988	-1.815482	0.450223	-2.221878
H	2.454536	-3.727070	0.000000	1.360734	4.279742	0.000000
H	2.107600	-2.250150	2.201212	0.435212	3.060617	2.215332
H	1.511539	1.128493	2.204988	-1.815482	0.450223	2.221878
H	2.107600	-2.250150	-2.201212	0.435212	3.060617	-2.215332
C	-1.755812	1.621732	1.170768	-0.168452	-2.369937	1.180227
C	-1.538499	2.404642	0.000000	-0.926437	-2.680562	0.000000
C	-1.755812	1.621732	-1.170768	-0.168452	-2.369937	-1.180227
C	-2.168211	0.308937	-0.735868	1.130907	-1.889233	-0.739281
C	-2.168211	0.308937	0.735868	1.130907	-1.889233	0.739281
C	-1.538499	-0.912641	-1.171622	1.660131	-0.611172	-1.180803
C	-1.168468	-1.635405	0.000000	1.970887	0.146031	0.000000
C	-1.538499	-0.912641	1.171622	1.660131	-0.611172	1.180803
H	-1.183036	3.430991	0.000000	-1.965942	-3.022949	0.000000
H	-1.601595	1.944434	-2.194000	-0.514263	-2.452213	-2.212983
H	-0.572751	-2.542996	0.000000	2.261514	1.202252	0.000000
H	-1.301969	-1.192466	2.191339	1.724620	-0.252897	2.210136
H	-1.601595	1.944434	2.194000	-0.514263	-2.452213	2.212983
H	-1.301969	-1.192466	-2.191339	1.724620	-0.252897	-2.210136
Cr	-0.282360	0.462797	0.000000	-0.180133	-0.526122	0.000000

Table S28. Optimized coordinates of the **Cr-2T** for the $(C8H6)_2Cr$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.722473	1.096387	0.351730	1.730071	1.050152	0.355824
C	1.321707	1.725103	1.588042	1.326999	1.676831	1.604338
C	0.000000	2.258872	1.444448	0.000000	2.222264	1.463927
C	-0.425430	1.978327	0.115328	-0.430587	1.957588	0.121982
C	0.613423	1.238692	-0.553464	0.614615	1.209211	-0.557948
C	-1.541936	2.147725	-0.823077	-1.542079	2.143662	-0.819988
C	-1.244824	1.509492	-1.982813	-1.237515	1.521216	-2.000460
C	0.098101	0.780825	-1.921329	0.103562	0.781923	-1.942445
H	1.924880	1.779612	2.488926	1.929101	1.711293	2.517177
H	-0.565406	2.761230	2.222892	-0.570228	2.716989	2.255415
H	-1.891266	1.457859	-2.856523	-1.885037	1.487115	-2.884669
H	0.745312	1.070899	-2.762655	0.765146	1.076812	-2.783237
H	2.680546	0.628040	0.157549	2.692841	0.573912	0.155803
H	-2.456447	2.698787	-0.618047	-2.463195	2.698250	-0.609195
C	0.000000	-2.258872	1.444448	0.000000	-2.222264	1.463927
C	-1.321707	-1.725103	1.588042	-1.326999	-1.676831	1.604338
C	-1.722473	-1.096387	0.351730	-1.730071	-1.050152	0.355824
C	-0.613423	-1.238692	-0.553464	-0.614615	-1.209211	-0.557948
C	0.425430	-1.978327	0.115328	0.430587	-1.957588	0.121982
C	-0.098101	-0.780825	-1.921329	-0.103562	-0.781923	-1.942445
C	1.244824	-1.509492	-1.982813	1.237515	-1.521216	-2.000460
C	1.541936	-2.147725	-0.823077	1.542079	-2.143662	-0.819988
H	-1.924880	-1.779612	2.488926	-1.929101	-1.711293	2.517177
H	-2.680546	-0.628040	0.157549	-2.692841	-0.573912	0.155803
H	1.891266	-1.457859	-2.856523	1.885037	-1.487115	-2.884669
H	2.456447	-2.698787	-0.618047	2.463195	-2.698250	-0.609195
H	0.565406	-2.761230	2.222892	0.570228	-2.716989	2.255415
H	-0.745312	-1.070899	-2.762655	-0.765146	-1.076812	-2.783237
Cr	0.000000	0.000000	1.004555	0.000000	0.000000	0.999777

Table S29. Optimized coordinates of the **Cr-3T** for the $(C8H6)_2Cr$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-0.088405	2.083197	1.553646	0.131676	1.985357	1.497312
C	-1.312402	1.395098	1.848238	-1.071446	1.341317	1.969064
C	-1.965253	1.043418	0.613700	-1.916248	1.027773	0.841216
C	-1.153185	1.536835	-0.456974	-1.271667	1.542878	-0.346535
C	0.000000	2.218961	0.122792	0.000000	2.160995	0.064381
C	-1.026755	1.611515	-1.894489	-1.353801	1.627625	-1.783000
C	0.150111	2.333351	-2.158804	-0.179627	2.289654	-2.223859
C	0.804110	2.704364	-0.947311	0.670493	2.607431	-1.117727
H	-1.678558	1.157676	2.842457	-1.279718	1.069847	3.008019
H	-2.898359	0.494258	0.532631	-2.869171	0.492839	0.897335
H	0.525227	2.559818	-3.153934	0.059673	2.500885	-3.271877
H	1.735423	3.255638	-0.866188	1.645867	3.098869	-1.173552
H	0.608897	2.461812	2.294673	0.962689	2.308036	2.130975
H	-1.709415	1.196097	-2.627702	-2.157780	1.242798	-2.415861
C	1.965253	-1.043418	0.613700	1.916248	-1.027773	0.841216
C	1.312402	-1.395098	1.848238	1.071446	-1.341317	1.969064
C	0.088405	-2.083197	1.553646	-0.131676	-1.985357	1.497312
C	0.000000	-2.218961	0.122792	0.000000	-2.160995	0.064381
C	1.153185	-1.536835	-0.456974	1.271667	-1.542878	-0.346535
C	-0.804110	-2.704364	-0.947311	-0.670493	-2.607431	-1.117727
C	-0.150111	-2.333351	-2.158804	0.179627	-2.289654	-2.223859
C	1.026755	-1.611515	-1.894489	1.353801	-1.627625	-1.783000
H	1.678558	-1.157676	2.842457	1.279718	-1.069847	3.008019
H	-0.608897	-2.461812	2.294673	-0.962689	-2.308036	2.130975
H	-0.525227	-2.559818	-3.153934	-0.059673	-2.500885	-3.271877
H	1.709415	-1.196097	-2.627702	2.157780	-1.242798	-2.415861
H	2.898359	-0.494258	0.532631	2.869171	-0.492839	0.897335
H	-1.735423	-3.255638	-0.866188	-1.645867	-3.098869	-1.173552
Cr	0.000000	0.000000	0.741107	0.000000	0.000000	0.618321

Table S30. Optimized coordinates of the **Cr-4T** for the $(C8H6)_2Cr$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	3.261361	0.528532	0.000000	3.161941	0.359038
C	-0.175219	3.542379	-0.838143	-0.044473	3.356763	-1.039840
C	0.502852	2.581039	-1.645689	0.717040	2.344669	-1.717828
C	1.151971	1.676471	-0.755124	1.301619	1.516553	-0.709279
C	0.835721	2.088085	0.608875	0.836373	2.003811	0.597250
C	1.956823	0.484322	-0.675659	2.056646	0.295303	-0.480459
C	2.169124	0.195937	0.709140	2.086263	0.063266	0.934329
C	1.465294	1.167713	1.510223	1.296690	1.079481	1.609696
H	-0.761397	4.370256	-1.229799	-0.603470	4.153226	-1.543256
H	0.522745	2.556026	-2.730461	0.827155	2.235964	-2.800447
H	2.737818	-0.644251	1.095556	2.559511	-0.793969	1.422554
H	1.448246	1.190412	2.595454	1.140625	1.143289	2.689777
H	-0.400456	3.831023	1.360776	-0.491604	3.778047	1.117068
H	2.344539	-0.104780	-1.500975	2.509571	-0.354091	-1.235297
C	-1.465294	-1.167713	1.510223	-1.296690	-1.079481	1.609696
C	-2.169124	-0.195937	0.709140	-2.086263	-0.063266	0.934329
C	-1.956823	-0.484322	-0.675659	-2.056646	-0.295303	-0.480459
C	-1.151971	-1.676471	-0.755124	-1.301619	-1.516553	-0.709279
C	-0.835721	-2.088085	0.608875	-0.836373	-2.003811	0.597250
C	-0.502852	-2.581039	-1.645689	-0.717040	-2.344669	-1.717828
C	0.175219	-3.542379	-0.838143	0.044473	-3.356763	-1.039840
C	0.000000	-3.261361	0.528532	0.000000	-3.161941	0.359038
H	-2.737818	0.644251	1.095556	-2.559511	0.793969	1.422554
H	-2.344539	0.104780	-1.500975	-2.509571	0.354091	-1.235297
H	0.761397	-4.370256	-1.229799	0.603470	-4.153226	-1.543256
H	0.400456	-3.831023	1.360776	0.491604	-3.778047	1.117068
H	-1.448246	-1.190412	2.595454	-1.140625	-1.143289	2.689777
H	-0.522745	-2.556026	-2.730461	-0.827155	-2.235964	-2.800447
Cr	0.000000	0.000000	0.313043	0.000000	0.000000	0.252680

Table S31. Optimized coordinates of the **Cr-5T** for the $(C8H6)_2Cr$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.054822	-1.048244	2.202229	1.059140	-1.069896	2.160010
C	-1.942244	0.061735	2.001145	-0.062315	-1.957645	1.965829
C	-1.184798	1.195090	1.512306	-1.206708	-1.192343	1.484927
C	0.171055	0.736506	1.361987	-0.742169	0.175629	1.337292
C	0.248823	-0.612930	1.850205	0.622268	0.249498	1.823683
C	1.536588	1.148902	0.804811	-1.161385	1.553101	0.803554
C	2.401965	-0.005255	1.334813	0.009067	2.414556	1.317190
C	1.656644	-1.014199	1.853725	1.030672	1.653824	1.824799
H	-3.005957	0.061587	2.217243	-0.059787	-3.032235	2.171025
H	-1.579401	2.188934	1.334861	-2.212873	-1.585420	1.321900
H	3.484867	-0.013796	1.242309	0.014705	3.507399	1.243447
H	2.042433	-1.959939	2.224997	1.992938	2.036244	2.181381
H	-1.343641	-2.030127	2.563220	2.052902	-1.368061	2.506100
H	1.884735	2.124129	1.173044	-2.139874	1.903841	1.188645
C	-1.054822	-1.048244	-2.202229	1.059140	-1.069896	-2.160010
C	-1.942244	0.061735	-2.001145	-0.062315	-1.957645	-1.965829
C	-1.184798	1.195090	-1.512306	-1.206708	-1.192343	-1.484927
C	0.171055	0.736506	-1.361987	-0.742169	0.175629	-1.337292
C	0.248823	-0.612930	-1.850205	0.622268	0.249498	-1.823683
C	1.536588	1.148902	-0.804811	-1.161385	1.553101	-0.803554
C	2.401965	-0.005255	-1.334813	0.009067	2.414556	-1.317190
C	1.656644	-1.014199	-1.853725	1.030672	1.653824	-1.824799
H	-3.005957	0.061587	-2.217243	-0.059787	-3.032235	-2.171025
H	-1.579401	2.188934	-1.334861	-2.212873	-1.585420	-1.321900
H	3.484867	-0.013796	-1.242309	0.014705	3.507399	-1.243447
H	2.042433	-1.959939	-2.224997	1.992938	2.036244	-2.181381
H	-1.343641	-2.030127	-2.563220	2.052902	-1.368061	-2.506100
H	1.884735	2.124129	-1.173044	-2.139874	1.903841	-1.188645
Cr	-1.040193	-0.261702	0.000000	0.255048	-1.035176	0.000000

Table S32. Optimized coordinates of the **Cr-6S** for the $(C8H6)_2Cr$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	2.933328	0.474973	0.000000	2.936719	0.485473
C	-0.342619	2.945233	-0.855313	-0.346816	2.956996	-0.852955
C	0.359014	1.853961	-1.557274	0.332226	1.838916	-1.550612
C	1.364588	1.373712	-0.676035	1.365021	1.360631	-0.676883
C	0.965856	1.838747	0.647803	0.948885	1.818273	0.656506
C	2.090022	0.123815	-0.522562	2.077962	0.098896	-0.535428
C	2.087600	-0.189797	0.853459	2.057984	-0.242483	0.845590
C	1.351665	0.826288	1.575790	1.324771	0.778810	1.581205
H	-1.055047	3.617729	-1.325296	-1.050134	3.648437	-1.327833
H	0.300797	1.665265	-2.626396	0.265184	1.643196	-2.627007
H	2.524439	-1.077440	1.299095	2.488484	-1.148035	1.282377
H	1.159015	0.810048	2.643633	1.122806	0.749632	2.655347
H	-0.384076	3.580946	1.256486	-0.366758	3.599549	1.274310
H	2.513579	-0.487895	-1.310737	2.492054	-0.518525	-1.336179
C	-1.351665	-0.826288	1.575790	-1.324771	-0.778810	1.581205
C	-2.087600	0.189797	0.853459	-2.057984	0.242483	0.845590
C	-2.090022	-0.123815	-0.522562	-2.077962	-0.098896	-0.535428
C	-1.364588	-1.373712	-0.676035	-1.365021	-1.360631	-0.676883
C	-0.965856	-1.838747	0.647803	-0.948885	-1.818273	0.656506
C	-0.359014	-1.853961	-1.557274	-0.332226	-1.838916	-1.550612
C	0.342619	-2.945233	-0.855313	0.346816	-2.956996	-0.852955
C	0.000000	-2.933328	0.474973	0.000000	-2.936719	0.485473
H	-2.524439	1.077440	1.299095	-2.488484	1.148035	1.282377
H	-2.513579	0.487895	-1.310737	-2.492054	0.518525	-1.336179
H	1.055047	-3.617729	-1.325296	1.050134	-3.648437	-1.327833
H	0.384076	-3.580946	1.256486	0.366758	-3.599549	1.274310
H	-1.159015	-0.810048	2.643633	-1.122806	-0.749632	2.655347
H	-0.300797	-1.665265	-2.626396	-0.265184	-1.643196	-2.627007
Cr	0.000000	0.000000	0.034847	0.000000	0.000000	0.030134

Table S33. Optimized coordinates of the **Mn-1D** for the $(C8H6)_2Mn$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.7825970	-0.3611090	-1.8653000	0.690322	-0.372740	-1.881259
C	1.4181070	-1.6163160	-1.5468080	1.326598	-1.640837	-1.566448
C	2.1625400	-1.4717850	-0.3332090	2.113143	-1.493907	-0.369623
C	2.0044180	-0.1222250	0.0963020	1.987452	-0.128963	0.055913
C	1.1347660	0.5593310	-0.8212050	1.087106	0.561588	-0.847949
C	2.3597290	0.8149180	1.1722800	2.384737	0.814346	1.112527
C	1.6926830	1.9799930	0.9787890	1.727766	1.999474	0.921946
C	0.7585350	1.9229950	-0.2290020	0.752415	1.943223	-0.256432
H	1.3508780	-2.5242140	-2.1379470	1.229382	-2.561701	-2.149587
H	2.7275790	-2.2555940	0.1606880	2.685018	-2.287313	0.120028
H	1.7497120	2.8531150	1.6256820	1.818250	2.884357	1.563316
H	0.9296380	2.7727830	-0.9054460	0.905055	2.793132	-0.951850
H	0.1570710	-0.1670800	-2.7294160	0.039066	-0.173817	-2.736719
H	3.0450650	0.6036930	1.9894380	3.094290	0.599674	1.919323
C	-2.1625570	-1.4717550	0.3332880	-2.113147	-1.493901	0.369617
C	-1.4181460	-1.6162180	1.5469020	-1.326612	-1.640830	1.566447
C	-0.7826210	-0.3610000	1.8653270	-0.690332	-0.372736	1.881262
C	-1.1347470	0.5593770	0.8211610	-1.087106	0.561592	0.847949
C	-2.0043890	-0.1222300	-0.0963190	-1.987449	-0.128956	-0.055917
C	-0.7585260	1.9230110	0.2288890	-0.752408	1.943227	0.256433
C	-1.6926840	1.9799500	-0.9788970	-1.727756	1.999482	-0.921947
C	-2.3597230	0.8148620	-1.1723320	-2.384728	0.814355	-1.112532
H	-1.3509330	-2.5240780	2.1381070	-1.229400	-2.561696	2.149585
H	-0.1571180	-0.1669070	2.7294450	-0.039083	-0.173814	2.736728
H	-1.7497280	2.8530440	-1.6258270	-1.818236	2.884366	-1.563317
H	-3.0450650	0.6035990	-1.9894750	-3.094280	0.599686	-1.919331
H	-2.7275930	-2.2555800	-0.1605870	-2.685025	-2.287303	-0.120036
H	-0.9296180	2.7728340	0.9052910	-0.905044	2.793136	0.951850
Mn	0.0000090	-0.9214560	0.0000340	0.000000	-0.907809	0.000004

Table S34. Optimized coordinates of the **Mn-2D** for the $(C8H6)_2Mn$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.165491	2.171919	-1.526470	-1.173138	-2.152070	-1.492646
C	0.000000	2.302753	-2.319724	0.000000	-2.294018	-2.289841
C	-1.165491	2.171919	-1.526470	1.173138	-2.152070	-1.492646
C	-0.728923	1.967728	-0.179235	0.734790	-1.946328	-0.144804
C	0.728923	1.967728	-0.179235	-0.734790	-1.946328	-0.144804
C	-1.176438	1.759764	1.166100	1.185385	-1.630754	1.194086
C	0.000000	1.661794	2.005002	0.000000	-1.517879	2.028172
C	1.176438	1.759764	1.166100	-1.185385	-1.630754	1.194086
H	0.000000	2.463470	-3.395120	0.000000	-2.463241	-3.372477
H	-2.190536	2.212602	-1.880180	2.205912	-2.180853	-1.850353
H	0.000000	1.566850	3.085808	0.000000	-1.334216	3.105748
H	2.201604	1.724392	1.520620	-2.217720	-1.570662	1.549040
H	2.190536	2.212602	-1.880180	-2.205912	-2.180853	-1.850353
H	-2.201604	1.724392	1.520620	2.217720	-1.570662	1.549040
C	1.165491	-2.171919	-1.526470	-1.173138	2.152070	-1.492646
C	0.000000	-2.302753	-2.319724	0.000000	2.294018	-2.289841
C	-1.165491	-2.171919	-1.526470	1.173138	2.152070	-1.492646
C	-0.728923	-1.967728	-0.179235	0.734790	1.946328	-0.144804
C	0.728923	-1.967728	-0.179235	-0.734790	1.946328	-0.144804
C	-1.176438	-1.759764	1.166100	1.185385	1.630754	1.194086
C	0.000000	-1.661794	2.005002	0.000000	1.517879	2.028172
C	1.176438	-1.759764	1.166100	-1.185385	1.630754	1.194086
H	0.000000	-2.463470	-3.395120	0.000000	2.463241	-3.372477
H	-2.190536	-2.212602	-1.880180	2.205912	2.180853	-1.850353
H	0.000000	-1.566850	3.085808	0.000000	1.334216	3.105748
H	2.201604	-1.724392	1.520620	-2.217720	1.570662	1.549040
H	2.190536	-2.212602	-1.880180	-2.205912	2.180853	-1.850353
H	-2.201604	-1.724392	1.520620	2.217720	1.570662	1.549040
Mn	0.000000	0.000000	0.751361	0.000000	0.000000	0.620779

Table S35. Optimized coordinates of the **Mn-3D** for the $(C8H6)_2Mn$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.074970	-1.070340	2.116572	1.071073	-1.096270	2.040023
C	-0.038298	-1.955274	1.931654	-0.053910	-1.987315	1.841967
C	-1.185683	-1.182851	1.509658	-1.206427	-1.185854	1.450607
C	-0.741285	0.175089	1.378843	-0.750520	0.183218	1.351290
C	0.622498	0.242110	1.816561	0.629453	0.241281	1.781790
C	-1.151324	1.539021	0.810795	-1.160694	1.561437	0.807297
C	0.008698	2.400921	1.331684	0.014998	2.416499	1.318439
C	1.026032	1.651502	1.825709	1.039932	1.647551	1.803469
H	-0.034025	-3.022505	2.128977	-0.064811	-3.063108	2.038651
H	-2.179677	-1.576377	1.326144	-2.212436	-1.572012	1.265486
H	0.018765	3.483968	1.240594	0.028584	3.508983	1.240599
H	1.979556	2.033243	2.180811	2.009832	2.022062	2.147457
H	2.069300	-1.362189	2.439010	2.083401	-1.405668	2.318550
H	-2.125300	1.896417	1.170832	-2.138060	1.919576	1.185738
C	1.074970	-1.070340	-2.116572	1.071073	-1.096270	-2.040023
C	-0.038298	-1.955274	-1.931654	-0.053910	-1.987315	-1.841967
C	-1.185683	-1.182851	-1.509658	-1.206427	-1.185854	-1.450607
C	-0.741285	0.175089	-1.378843	-0.750520	0.183218	-1.351290
C	0.622498	0.242110	-1.816561	0.629453	0.241281	-1.781790
C	-1.151324	1.539021	-0.810795	-1.160694	1.561437	-0.807297
C	0.008698	2.400921	-1.331684	0.014998	2.416499	-1.318439
C	1.026032	1.651502	-1.825709	1.039932	1.647551	-1.803469
H	-0.034025	-3.022505	-2.128977	-0.064811	-3.063108	-2.038651
H	-2.179677	-1.576377	-1.326144	-2.212436	-1.572012	-1.265486
H	0.018765	3.483968	-1.240594	0.028584	3.508983	-1.240599
H	1.979556	2.033243	-2.180811	2.009832	2.022062	-2.147457
H	2.069300	-1.362189	-2.439010	2.083401	-1.405668	-2.318550
H	-2.125300	1.896417	-1.170832	-2.138060	1.919576	-1.185738
Mn	0.206219	-0.980290	0.000000	0.223205	-0.967449	0.000000

Table S36. Optimized coordinates of the **Mn-4Q** for the $(C8H6)_2Mn$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.165396	1.686443	-1.585047	1.170330	1.704509	-1.583910
C	0.000000	1.664928	-2.385840	0.000000	1.694340	-2.391160
C	-1.165396	1.686443	-1.585047	-1.170330	1.704509	-1.583910
C	-0.727840	1.767498	-0.214993	-0.731668	1.762606	-0.204781
C	0.727840	1.767498	-0.214993	0.731668	1.762606	-0.204781
C	-1.180909	1.775720	1.146663	-1.189290	1.727535	1.166265
C	0.000000	1.803838	1.984606	0.000000	1.735444	2.011231
C	1.180909	1.775720	1.146663	1.189290	1.727535	1.166265
H	0.000000	1.614308	-3.471870	0.000000	1.660301	-3.486094
H	-2.190551	1.673797	-1.938999	-2.204047	1.690765	-1.939372
H	0.000000	1.849778	3.069142	0.000000	1.745476	3.105033
H	2.205808	1.792197	1.500778	2.222271	1.730536	1.522804
H	2.190551	1.673797	-1.938999	2.204047	1.690765	-1.939372
H	-2.205808	1.792197	1.500778	-2.222271	1.730536	1.522804
C	1.165396	-1.686443	-1.585047	1.170330	-1.704509	-1.583910
C	0.000000	-1.664928	-2.385840	0.000000	-1.694340	-2.391160
C	-1.165396	-1.686443	-1.585047	-1.170330	-1.704509	-1.583910
C	-0.727840	-1.767498	-0.214993	-0.731668	-1.762606	-0.204781
C	0.727840	-1.767498	-0.214993	0.731668	-1.762606	-0.204781
C	-1.180909	-1.775720	1.146663	-1.189290	-1.727535	1.166265
C	0.000000	-1.803838	1.984606	0.000000	-1.735444	2.011231
C	1.180909	-1.775720	1.146663	1.189290	-1.727535	1.166265
H	0.000000	-1.614308	-3.471870	0.000000	-1.660301	-3.486094
H	-2.190551	-1.673797	-1.938999	-2.204047	-1.690765	-1.939372
H	0.000000	-1.849778	3.069142	0.000000	-1.745476	3.105033
H	2.205808	-1.792197	1.500778	2.222271	-1.730536	1.522804
H	2.190551	-1.673797	-1.938999	2.204047	-1.690765	-1.939372
H	-2.205808	-1.792197	1.500778	-2.222271	-1.730536	1.522804
Mn	0.000000	0.000000	0.922168	0.000000	0.000000	0.877031

Table S37. Optimized coordinates of the **Mn-5Q** for the $(C8H6)_2Mn$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-0.878841	-0.112616	1.877807	-0.769840	-0.092683	1.903659
C	-1.641863	-1.320887	1.649758	-1.580061	-1.282614	1.688603
C	-2.365331	-1.190990	0.422280	-2.358390	-1.115491	0.486778
C	-1.989752	0.072182	-0.139143	-1.960263	0.149381	-0.086821
C	-1.094770	0.733279	0.776164	-0.998054	0.774228	0.811558
C	-2.229590	0.977398	-1.270582	-2.214467	1.084610	-1.191218
C	-1.452544	2.080825	-1.122496	-1.393620	2.172951	-1.052328
C	-0.575075	2.006669	0.124164	-0.467298	2.047388	0.157338
H	-1.704222	-2.158298	2.337826	-1.633016	-2.136901	2.370000
H	-3.048961	-1.922345	0.003312	-3.083892	-1.829074	0.086679
H	-1.400260	2.913180	-1.821339	-1.339001	3.019150	-1.747457
H	-0.704774	2.900145	0.751297	-0.531426	2.939837	0.811110
H	-0.222736	0.058482	2.723849	-0.065959	0.047341	2.727677
H	-2.909944	0.786956	-2.097004	-2.935082	0.928721	-2.001751
C	2.075588	-1.591152	-0.185962	1.918786	-1.703414	-0.220210
C	1.419233	-1.700884	-1.461463	1.215572	-1.774297	-1.490173
C	0.858681	-0.415836	-1.805612	0.733874	-0.441654	-1.827770
C	1.292057	0.506684	-0.788262	1.270135	0.453355	-0.820686
C	2.050933	-0.198371	0.167367	2.029146	-0.299826	0.115566
C	0.962856	1.885642	-0.242901	1.054589	1.856804	-0.271822
C	1.810643	1.915543	1.025563	1.949994	1.841469	0.967161
C	2.394674	0.712576	1.262882	2.469302	0.591679	1.190330
H	1.348586	-2.602308	-2.062923	1.066984	-2.677436	-2.089886
H	0.319322	-0.178688	-2.716325	0.184685	-0.160835	-2.730546
H	1.885936	2.797420	1.658108	2.106000	2.726143	1.595209
H	3.016221	0.463871	2.119715	3.107478	0.304053	2.033411
H	2.604853	-2.387590	0.326960	2.407811	-2.541239	0.284755
H	1.223409	2.711163	-0.920685	1.331554	2.669948	-0.971653
Mn	-0.169153	-1.181695	-0.081607	-0.240503	-1.154441	-0.101094

Table S38. Optimized coordinates of the **Mn-6Q** for the $(C8H6)_2Mn$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.012568	-1.039671	2.317546	-1.014941	-1.090983	2.213717
C	-1.913739	0.068884	2.083283	-1.924320	0.033447	2.007705
C	-1.159921	1.200696	1.605911	-1.159230	1.193702	1.574023
C	0.169257	0.726547	1.382519	0.186498	0.712863	1.364504
C	0.267767	-0.618029	1.919118	0.288205	-0.649829	1.890645
C	1.523515	1.141124	0.811566	1.549586	1.141734	0.821810
C	2.403431	0.010100	1.352128	2.430678	0.018742	1.367200
C	1.676678	-0.997718	1.904926	1.693076	-1.020744	1.889193
H	-2.968202	0.078557	2.342209	-2.989151	0.032307	2.259422
H	-1.564127	2.182906	1.388465	-1.549056	2.203002	1.421275
H	3.484413	0.005805	1.237591	3.521913	0.023997	1.268704
H	2.083545	-1.928184	2.292548	2.104414	-1.965070	2.261678
H	-1.295755	-2.004046	2.726946	-1.312566	-2.079638	2.575652
H	1.860242	2.126355	1.161046	1.872871	2.143223	1.164748
C	-1.012568	-1.039671	-2.317546	-1.014941	-1.090983	-2.213717
C	-1.913739	0.068884	-2.083283	-1.924320	0.033447	-2.007705
C	-1.159921	1.200696	-1.605911	-1.159230	1.193702	-1.574023
C	0.169257	0.726547	-1.382519	0.186498	0.712863	-1.364504
C	0.267767	-0.618029	-1.919118	0.288205	-0.649829	-1.890645
C	1.523515	1.141124	-0.811566	1.549586	1.141734	-0.821810
C	2.403431	0.010100	-1.352128	2.430678	0.018742	-1.367200
C	1.676678	-0.997718	-1.904926	1.693076	-1.020744	-1.889193
H	-2.968202	0.078557	-2.342209	-2.989151	0.032307	-2.259422
H	-1.564127	2.182906	-1.388465	-1.549056	2.203002	-1.421275
H	3.484413	0.005805	-1.237591	3.521913	0.023997	-1.268704
H	2.083545	-1.928184	-2.292548	2.104414	-1.965070	-2.261678
H	-1.295755	-2.004046	-2.726946	-1.312566	-2.079638	-2.575652
H	1.860242	2.126355	-1.161046	1.872871	2.143223	-1.164748
Mn	-1.066131	-0.273040	0.000000	-1.115659	-0.191313	0.000000

Table S39. Optimized coordinates of the **Fe-1S**for the $(C8H6)_2Fe$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.597225	-0.350533	-1.892746	1.890242	0.561971	0.358815
C	1.164413	-1.639238	-1.573880	1.555046	1.115239	1.662516
C	1.987340	-1.510431	-0.397935	0.370900	1.947040	1.532968
C	1.946243	-0.132407	-0.012877	0.000000	1.932494	0.137334
C	1.061029	0.571234	-0.898454	0.897459	1.041852	-0.574196
C	2.398093	0.808500	1.023989	-1.026282	2.395787	-0.810438
C	1.757608	1.991646	0.854028	-0.841480	1.767401	-2.011766
C	0.742089	1.942244	-0.285279	0.292898	0.743150	-1.960733
H	1.001181	-2.553861	-2.134018	2.111585	0.937562	2.587175
H	2.535174	-2.311812	0.085467	-0.122550	2.491133	2.342476
H	1.879719	2.870444	1.483889	-1.469106	1.901434	-2.900852
H	0.862935	2.791210	-0.972530	0.993712	0.859331	-2.810811
H	-0.098154	-0.146818	-2.698881	2.701697	-0.139881	0.149977
H	3.125362	0.585488	1.800764	-1.811670	3.125990	-0.585657
C	-1.987302	-1.510454	0.397916	-0.370900	-1.947040	1.532968
C	-1.164402	-1.639240	1.573883	-1.555046	-1.115239	1.662516
C	-0.597238	-0.350525	1.892754	-1.890242	-0.561971	0.358815
C	-1.061028	0.571236	0.898453	-0.897459	-1.041852	-0.574196
C	-1.946216	-0.132421	0.012858	0.000000	-1.932494	0.137334
C	-0.742097	1.942242	0.285275	-0.292898	-0.743150	-1.960733
C	-1.757624	1.991642	-0.854031	0.841480	-1.767401	-2.011766
C	-2.398091	0.808486	-1.023997	1.026282	-2.395787	-0.810438
H	-1.001143	-2.553850	2.134033	-2.111585	-0.937562	2.587175
H	0.098150	-0.146809	2.698882	-2.701697	0.139881	0.149977
H	-1.879752	2.870447	-1.483881	1.469106	-1.901434	-2.900852
H	-3.125363	0.585463	-1.800767	1.811670	-3.125990	-0.585657
H	-2.535129	-2.311843	-0.085479	0.122550	-2.491133	2.342476
H	-0.862949	2.791213	0.972521	-0.993712	-0.859331	-2.810811
Fe	-0.000011	-0.870814	0.000010	0.000000	0.000000	0.862360

Table S40. Optimized coordinates of the **Fe-2S**for the $(C8H6)_2Fe$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.105247	-1.102044	1.937211	1.121400	-1.117969	1.879789
C	-0.038949	-1.966697	1.807182	-0.036983	-1.984948	1.762865
C	-1.199637	-1.167210	1.489284	-1.210679	-1.174180	1.470422
C	-0.750022	0.185815	1.365473	-0.755933	0.190205	1.349920
C	0.641284	0.231551	1.718963	0.652051	0.233378	1.694063
C	-1.157807	1.557722	0.812598	-1.168711	1.572721	0.811614
C	0.019610	2.406103	1.317937	0.024051	2.419168	1.298254
C	1.051458	1.638552	1.749968	1.066729	1.637449	1.721912
H	-0.037532	-3.042779	1.946671	-0.037646	-3.070868	1.895837
H	-2.199113	-1.551434	1.317856	-2.223166	-1.555932	1.312897
H	0.031387	3.490818	1.251294	0.034214	3.513189	1.246839
H	2.022776	2.005468	2.070786	2.053380	2.003152	2.025492
H	2.112854	-1.414174	2.188931	2.139734	-1.436297	2.117689
H	-2.126784	1.922827	1.176947	-2.140635	1.942865	1.190349
C	1.105247	-1.102044	-1.937211	1.121400	-1.117969	-1.879789
C	-0.038949	-1.966697	-1.807182	-0.036983	-1.984948	-1.762865
C	-1.199637	-1.167210	-1.489284	-1.210679	-1.174180	-1.470422
C	-0.750022	0.185815	-1.365473	-0.755933	0.190205	-1.349920
C	0.641284	0.231551	-1.718963	0.652051	0.233378	-1.694063
C	-1.157807	1.557722	-0.812598	-1.168711	1.572721	-0.811614
C	0.019610	2.406103	-1.317937	0.024051	2.419168	-1.298254
C	1.051458	1.638552	-1.749968	1.066729	1.637449	-1.721912
H	-0.037532	-3.042779	-1.946671	-0.037646	-3.070868	-1.895837
H	-2.199113	-1.551434	-1.317856	-2.223166	-1.555932	-1.312897
H	0.031387	3.490818	-1.251294	0.034214	3.513189	-1.246839
H	2.022776	2.005468	-2.070786	2.053380	2.003152	-2.025492
H	2.112854	-1.414174	-2.188931	2.139734	-1.436297	-2.117689
H	-2.126784	1.922827	-1.176947	-2.140635	1.942865	-1.190349
Fe	0.166870	-0.931806	0.000000	0.155582	-0.927004	0.000000

Table S41. Optimized coordinates of the **Fe-3S**for the $(C8H6)_2Fe$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.168291	1.639387	1.176412	1.177869	1.621280	1.178428
C	0.000000	1.598162	2.010146	0.000000	1.571595	2.020186
C	-1.168291	1.639387	1.176412	-1.177869	1.621280	1.178428
C	-0.728039	1.836511	-0.182036	-0.732579	1.832119	-0.183960
C	0.728039	1.836511	-0.182036	0.732579	1.832119	-0.183960
C	-1.163533	2.047928	-1.524537	-1.169774	2.058114	-1.531044
C	0.000000	2.181110	-2.320076	0.000000	2.201784	-2.329996
C	1.163533	2.047928	-1.524537	1.169774	2.058114	-1.531044
H	0.000000	1.462934	3.087130	0.000000	1.440839	3.106806
H	-2.192405	1.589351	1.532688	-2.211195	1.574028	1.535098
H	0.000000	2.333681	-3.396515	0.000000	2.366723	-3.413138
H	2.188281	2.075712	-1.881347	2.202636	2.086954	-1.890060
H	2.192405	1.589351	1.532688	2.211195	1.574028	1.535098
H	-2.188281	2.075712	-1.881347	-2.202636	2.086954	-1.890060
C	1.168291	-1.639387	1.176412	1.177869	-1.621280	1.178428
C	0.000000	-1.598162	2.010146	0.000000	-1.571595	2.020186
C	-1.168291	-1.639387	1.176412	-1.177869	-1.621280	1.178428
C	-0.728039	-1.836511	-0.182036	-0.732579	-1.832119	-0.183960
C	0.728039	-1.836511	-0.182036	0.732579	-1.832119	-0.183960
C	-1.163533	-2.047928	-1.524537	-1.169774	-2.058114	-1.531044
C	0.000000	-2.181110	-2.320076	0.000000	-2.201784	-2.329996
C	1.163533	-2.047928	-1.524537	1.169774	-2.058114	-1.531044
H	0.000000	-1.462934	3.087130	0.000000	-1.440839	3.106806
H	-2.192405	-1.589351	1.532688	-2.211195	-1.574028	1.535098
H	0.000000	-2.333681	-3.396515	0.000000	-2.366723	-3.413138
H	2.188281	-2.075712	-1.881347	2.202636	-2.086954	-1.890060
H	2.192405	-1.589351	1.532688	2.211195	-1.574028	1.535098
H	-2.188281	-2.075712	-1.881347	-2.202636	-2.086954	-1.890060
Fe	0.000000	0.000000	0.709862	0.000000	0.000000	0.716463

Table S42. Optimized coordinates of the **Fe-4T** for the $(C8H6)_2Fe$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	3.003033	1.163972	0.000000	2.999398	1.169514
C	-0.448340	3.671699	0.000000	-0.440491	3.679477	0.000000
C	0.000000	3.003033	-1.163972	0.000000	2.999398	-1.169514
C	0.786457	1.879421	-0.726712	0.776373	1.860172	-0.730688
C	0.786457	1.879421	0.726712	0.776373	1.860172	0.730688
C	1.560073	0.754761	-1.171374	1.544383	0.721527	-1.180444
C	2.062447	0.084931	0.000000	2.044658	0.041262	0.000000
C	1.560073	0.754761	1.171374	1.544383	0.721527	1.180444
H	-1.072391	4.562062	0.000000	-1.059592	4.583444	0.000000
H	-0.206382	3.292062	-2.189706	-0.206686	3.290645	-2.203474
H	2.672391	-0.812646	0.000000	2.655692	-0.866394	0.000000
H	1.750161	0.453797	2.196556	1.732533	0.419467	2.214755
H	-0.206382	3.292062	2.189706	-0.206686	3.290645	2.203474
H	1.750161	0.453797	-2.196556	1.732533	0.419467	-2.214755
C	-1.560073	-0.754761	1.171374	-1.544383	-0.721527	1.180444
C	-2.062447	-0.084931	0.000000	-2.044658	-0.041262	0.000000
C	-1.560073	-0.754761	-1.171374	-1.544383	-0.721527	-1.180444
C	-0.786457	-1.879421	-0.726712	-0.776373	-1.860172	-0.730688
C	-0.786457	-1.879421	0.726712	-0.776373	-1.860172	0.730688
C	0.000000	-3.003033	-1.163972	0.000000	-2.999398	-1.169514
C	0.448340	-3.671699	0.000000	0.440491	-3.679477	0.000000
C	0.000000	-3.003033	1.163972	0.000000	-2.999398	1.169514
H	-2.672391	0.812646	0.000000	-2.655692	0.866394	0.000000
H	-1.750161	-0.453797	-2.196556	-1.732533	-0.419467	-2.214755
H	1.072391	-4.562062	0.000000	1.059592	-4.583444	0.000000
H	0.206382	-3.292062	2.189706	0.206686	-3.290645	2.203474
H	-1.750161	-0.453797	2.196556	-1.732533	-0.419467	2.214755
H	0.206382	-3.292062	-2.189706	0.206686	-3.290645	-2.203474
Fe	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Table S43. Optimized coordinates of the **Fe-5T**for the $(C8H6)_2Fe$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.175422	1.699672	1.164312	1.183641	1.660177	1.174407
C	0.000000	1.702909	1.999081	0.000000	1.655572	2.017029
C	-1.175421	1.699680	1.164312	-1.183641	1.660177	1.174407
C	-0.725441	1.738905	-0.199669	-0.729177	1.718156	-0.196920
C	0.725438	1.738905	-0.199669	0.729177	1.718156	-0.196920
C	-1.163384	1.733242	-1.575106	-1.168210	1.735844	-1.580663
C	0.000000	1.748384	-2.377944	0.000000	1.762536	-2.389735
C	1.163383	1.733240	-1.575104	1.168210	1.735844	-1.580663
H	-0.000002	1.687999	3.084526	0.000000	1.631376	3.111105
H	-2.200449	1.691175	1.518796	-2.217683	1.648541	1.529338
H	0.000002	1.739525	-3.465035	0.000000	1.768751	-3.485118
H	2.189000	1.727030	-1.929149	2.202161	1.730766	-1.937096
H	2.200452	1.691184	1.518792	2.217683	1.648541	1.529338
H	-2.189001	1.727034	-1.929149	-2.202161	1.730766	-1.937096
C	1.175421	-1.699680	1.164312	1.183641	-1.660177	1.174407
C	0.000000	-1.702909	1.999081	0.000000	-1.655572	2.017029
C	-1.175422	-1.699672	1.164312	-1.183641	-1.660177	1.174407
C	-0.725438	-1.738905	-0.199669	-0.729177	-1.718156	-0.196920
C	0.725441	-1.738905	-0.199669	0.729177	-1.718156	-0.196920
C	-1.163383	-1.733240	-1.575104	-1.168210	-1.735844	-1.580663
C	0.000000	-1.748384	-2.377944	0.000000	-1.762536	-2.389735
C	1.163384	-1.733242	-1.575106	1.168210	-1.735844	-1.580663
H	0.000002	-1.687999	3.084526	0.000000	-1.631376	3.111105
H	-2.200452	-1.691184	1.518792	-2.217683	-1.648541	1.529338
H	-0.000002	-1.739525	-3.465035	0.000000	-1.768751	-3.485118
H	2.189001	-1.727034	-1.929149	2.202161	-1.730766	-1.937096
H	2.200449	-1.691175	1.518796	2.217683	-1.648541	1.529338
H	-2.189000	-1.727030	-1.929149	-2.202161	-1.730766	-1.937096
Fe	0.000000	0.000000	0.830764	0.000000	0.000000	0.820299

Table S44. Optimized coordinates of the **Fe-6T**for the $(C8H6)_2Fe$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-0.910612	-0.280399	1.871479	-0.776285	-0.297565	1.884428
C	-1.595685	-1.506965	1.547515	-1.492693	-1.521520	1.569918
C	-2.357000	-1.334471	0.340045	-2.326001	-1.313606	0.408049
C	-2.053917	-0.038473	-0.141673	-2.030050	-0.003510	-0.078691
C	-1.136677	0.602823	0.781418	-1.052667	0.618842	0.818888
C	-2.335939	0.907875	-1.227345	-2.362474	0.971637	-1.125986
C	-1.589906	2.027103	-1.046139	-1.597010	2.093557	-0.955283
C	-0.681337	1.935757	0.178521	-0.625157	1.968949	0.220732
H	-1.602907	-2.398465	2.167764	-1.471846	-2.433316	2.174756
H	-2.988297	-2.084544	-0.124278	-2.982339	-2.060523	-0.046825
H	-1.578772	2.889256	-1.710106	-1.614330	2.976225	-1.605861
H	-0.836941	2.795004	0.846837	-0.733593	2.821192	0.921473
H	-0.277422	-0.117708	2.735991	-0.087881	-0.159660	2.721323
H	-3.026854	0.733496	-2.048544	-3.100625	0.818296	-1.921131
C	2.206746	-1.506200	-0.230139	2.086215	-1.576304	-0.245576
C	1.484952	-1.675367	-1.469451	1.333944	-1.728277	-1.478479
C	0.884768	-0.423476	-1.830493	0.778172	-0.444089	-1.853494
C	1.220567	0.505233	-0.779648	1.177674	0.482415	-0.806785
C	2.109542	-0.141348	0.138013	2.091368	-0.188073	0.093373
C	0.844881	1.882475	-0.225181	0.882701	1.888054	-0.258156
C	1.744500	1.955324	1.008683	1.840014	1.947361	0.936167
C	2.428642	0.798783	1.212469	2.488622	0.751547	1.134402
H	1.444146	-2.591729	-2.049675	1.231335	-2.661998	-2.039510
H	0.297009	-0.221964	-2.719128	0.189192	-0.216831	-2.745918
H	1.786435	2.837438	1.643956	1.950204	2.845857	1.554160
H	3.105975	0.602232	2.040142	3.192416	0.537368	1.946541
H	2.752059	-2.289308	0.287414	2.603247	-2.386478	0.276823
H	1.057779	2.710906	-0.916790	1.081580	2.706689	-0.979232
Fe	-0.065899	-0.966025	-0.035463	-0.105984	-0.949358	-0.070679

Table S45. Optimized coordinates of the **Fe-7T**for the $(C8H6)_2Fe$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.047308	-1.038685	2.226824	1.037085	-1.078414	2.112442
C	-1.923900	0.077490	1.985205	-0.099843	-1.947712	1.863088
C	-1.136655	1.222071	1.573454	-1.248591	-1.117472	1.491947
C	0.187687	0.757137	1.405472	-0.780931	0.220563	1.400289
C	0.249152	-0.618819	1.856931	0.621200	0.248319	1.805973
C	1.539825	1.145633	0.818210	-1.150438	1.580514	0.827465
C	2.400797	-0.010629	1.337305	0.032050	2.420635	1.323367
C	1.653566	-1.021857	1.854039	1.054806	1.642005	1.808368
H	-2.987311	0.097419	2.204154	-0.141429	-3.020552	2.074057
H	-1.531819	2.207505	1.353344	-2.253061	-1.494367	1.283756
H	3.482674	-0.027423	1.232951	0.059704	3.512817	1.240294
H	2.039478	-1.972028	2.213795	2.032078	2.007365	2.140595
H	-1.347270	-2.013983	2.595717	2.031813	-1.400647	2.433358
H	1.904632	2.122720	1.159488	-2.129136	1.968151	1.166395
C	-1.047308	-1.038685	-2.226824	1.037085	-1.078414	-2.112442
C	-1.923900	0.077490	-1.985205	-0.099843	-1.947712	-1.863088
C	-1.136655	1.222071	-1.573454	-1.248591	-1.117472	-1.491947
C	0.187687	0.757137	-1.405472	-0.780931	0.220563	-1.400289
C	0.249152	-0.618819	-1.856931	0.621200	0.248319	-1.805973
C	1.539825	1.145633	-0.818210	-1.150438	1.580514	-0.827465
C	2.400797	-0.010629	-1.337305	0.032050	2.420635	-1.323367
C	1.653566	-1.021857	-1.854039	1.054806	1.642005	-1.808368
H	-2.987311	0.097419	-2.204154	-0.141429	-3.020552	-2.074057
H	-1.531819	2.207505	-1.353344	-2.253061	-1.494367	-1.283756
H	3.482674	-0.027423	-1.232951	0.059704	3.512817	-1.240294
H	2.039478	-1.972028	-2.213795	2.032078	2.007365	-2.140595
H	-1.347270	-2.013983	-2.595717	2.031813	-1.400647	-2.433358
H	1.904632	2.122720	-1.159488	-2.129136	1.968151	-1.166395
Fe	-1.007643	-0.268327	0.000000	0.277539	-1.029492	0.000000

Table S46. Optimized coordinates of the **Co-1D**for the $(C8H6)_2Co$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-0.076204	1.931335	1.519620	0.087922	1.940155	1.444455
C	-1.272394	1.179806	1.815597	-1.107193	1.252363	1.912461
C	-1.895312	0.794031	0.568422	-1.883007	0.833694	0.755907
C	-1.107548	1.341250	-0.490705	-1.207365	1.317524	-0.421586
C	0.000000	2.090032	0.094583	0.000000	2.047095	0.006729
C	-0.996676	1.445247	-1.926200	-1.259226	1.363133	-1.860211
C	0.127881	2.252003	-2.182380	-0.130977	2.114790	-2.281573
C	0.760612	2.651607	-0.971106	0.654720	2.537279	-1.164307
H	-1.636344	0.932403	2.807555	-1.367622	1.061129	2.957850
H	-2.790220	0.187495	0.473448	-2.811974	0.257178	0.792523
H	0.478237	2.522500	-3.175954	0.113795	2.330838	-3.328009
H	1.652276	3.264236	-0.886082	1.581472	3.115926	-1.208098
H	0.604795	2.335956	2.261562	0.869110	2.351726	2.090318
H	-1.655534	0.998731	-2.662366	-2.010552	0.901308	-2.505337
C	1.895312	-0.794031	0.568422	1.883007	-0.833694	0.755907
C	1.272394	-1.179806	1.815597	1.107193	-1.252363	1.912461
C	0.076204	-1.931335	1.519620	-0.087922	-1.940155	1.444455
C	0.000000	-2.090032	0.094583	0.000000	-2.047095	0.006729
C	1.107548	-1.341250	-0.490705	1.207365	-1.317524	-0.421586
C	-0.760612	-2.651607	-0.971106	-0.654720	-2.537279	-1.164307
C	-0.127881	-2.252003	-2.182380	0.130977	-2.114790	-2.281573
C	0.996676	-1.445247	-1.926200	1.259226	-1.363133	-1.860211
H	1.636344	-0.932403	2.807555	1.367622	-1.061129	2.957850
H	-0.604795	-2.335956	2.261562	-0.869110	-2.351726	2.090318
H	-0.478237	-2.522500	-3.175954	-0.113795	-2.330838	-3.328009
H	1.655534	-0.998731	-2.662366	2.010552	-0.901308	-2.505337
H	2.790220	-0.187495	0.473448	2.811974	-0.257178	0.792523
H	-1.652276	-3.264236	-0.886082	-1.581472	-3.115926	-1.208098
Co	0.000000	0.000000	0.786285	0.000000	0.000000	0.803667

Table S47. Optimized coordinates of the **Co-2D**for the $(C8H6)_2Co$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.173991	1.684923	1.146453	1.181638	1.650983	1.152752
C	0.000000	1.628947	1.986477	0.000000	1.615910	1.999551
C	-1.173991	1.684923	1.146453	-1.181638	1.650983	1.152752
C	-0.731844	1.823810	-0.205090	-0.738918	1.802148	-0.211018
C	0.731844	1.823810	-0.205090	0.738918	1.802148	-0.211018
C	-1.167736	1.988253	-1.557455	-1.176073	1.954461	-1.564793
C	0.000000	2.088693	-2.352062	0.000000	2.048778	-2.364413
C	1.167736	1.988253	-1.557455	1.176073	1.954461	-1.564793
H	0.000000	1.558779	3.069541	0.000000	1.550563	3.091966
H	-2.198699	1.651338	1.502713	-2.214132	1.618560	1.512796
H	0.000000	2.214284	-3.432485	0.000000	2.166760	-3.454340
H	2.191717	2.015263	-1.914950	2.207446	1.974156	-1.926345
H	2.198699	1.651338	1.502713	2.214132	1.618560	1.512796
H	-2.191717	2.015263	-1.914950	-2.207446	1.974156	-1.926345
C	1.173991	-1.684923	1.146453	1.181638	-1.650983	1.152752
C	0.000000	-1.628947	1.986477	0.000000	-1.615910	1.999551
C	-1.173991	-1.684923	1.146453	-1.181638	-1.650983	1.152752
C	-0.731844	-1.823810	-0.205090	-0.738918	-1.802148	-0.211018
C	0.731844	-1.823810	-0.205090	0.738918	-1.802148	-0.211018
C	-1.167736	-1.988253	-1.557455	-1.176073	-1.954461	-1.564793
C	0.000000	-2.088693	-2.352062	0.000000	-2.048778	-2.364413
C	1.167736	-1.988253	-1.557455	1.176073	-1.954461	-1.564793
H	0.000000	-1.558779	3.069541	0.000000	-1.550563	3.091966
H	-2.198699	-1.651338	1.502713	-2.214132	-1.618560	1.512796
H	0.000000	-2.214284	-3.432485	0.000000	-2.166760	-3.454340
H	2.191717	-2.015263	-1.914950	2.207446	-1.974156	-1.926345
H	2.198699	-1.651338	1.502713	2.214132	-1.618560	1.512796
H	-2.191717	-2.015263	-1.914950	-2.207446	-1.974156	-1.926345
Co	0.000000	0.000000	0.798076	0.000000	0.000000	0.804101

Table S48. Optimized coordinates of the **Co-3D**for the $(C8H6)_2Co$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.748005	1.052597	0.348072	1.760229	0.980551	0.351384
C	1.309524	1.565770	1.611595	1.311008	1.465721	1.637398
C	0.000000	2.179489	1.455130	0.000000	2.100018	1.486752
C	-0.372197	2.014295	0.104444	-0.359673	1.995747	0.111092
C	0.650423	1.231667	-0.554067	0.665918	1.203557	-0.560878
C	-1.466843	2.221821	-0.846796	-1.439951	2.241172	-0.844772
C	-1.187819	1.559351	-1.999105	-1.162879	1.587240	-2.019171
C	0.125161	0.780045	-1.922499	0.138099	0.780485	-1.944108
H	1.889602	1.561628	2.529047	1.886599	1.427226	2.567004
H	-0.565928	2.661972	2.244832	-0.571257	2.570972	2.291081
H	-1.828430	1.527007	-2.878039	-1.800694	1.585722	-2.910900
H	0.787847	1.035366	-2.762013	0.818465	1.028012	-2.783803
H	2.679488	0.532824	0.156718	2.693000	0.448829	0.149876
H	-2.361653	2.809237	-0.655894	-2.332960	2.844993	-0.648666
C	0.000000	-2.179489	1.455130	0.000000	-2.100018	1.486752
C	-1.309524	-1.565770	1.611595	-1.311008	-1.465721	1.637398
C	-1.748005	-1.052597	0.348072	-1.760229	-0.980551	0.351384
C	-0.650423	-1.231667	-0.554067	-0.665918	-1.203557	-0.560878
C	0.372197	-2.014295	0.104444	0.359673	-1.995747	0.111092
C	-0.125161	-0.780045	-1.922499	-0.138099	-0.780485	-1.944108
C	1.187819	-1.559351	-1.999105	1.162879	-1.587240	-2.019171
C	1.466843	-2.221821	-0.846796	1.439951	-2.241172	-0.844772
H	-1.889602	-1.561628	2.529047	-1.886599	-1.427226	2.567004
H	-2.679488	-0.532824	0.156718	-2.693000	-0.448829	0.149876
H	1.828430	-1.527007	-2.878039	1.800694	-1.585722	-2.910900
H	2.361653	-2.809237	-0.655894	2.332960	-2.844993	-0.648666
H	0.565928	-2.661972	2.244832	0.571257	-2.570972	2.291081
H	-0.787847	-1.035366	-2.762013	-0.818465	-1.028012	-2.783803
Co	0.000000	0.000000	0.902571	0.000000	0.000000	0.891054

Table S49. Optimized coordinates of the **Co-4D**for the $(C8H6)_2Co$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	3.051895	1.167267	0.000000	3.052855	1.174614
C	-0.434130	3.725294	0.000000	-0.425482	3.736413	0.000000
C	0.000000	3.051895	-1.167267	0.000000	3.052855	-1.174614
C	0.756129	1.912481	-0.729681	0.742076	1.898866	-0.735213
C	0.756129	1.912481	0.729681	0.742076	1.898866	0.735213
C	1.528067	0.791614	-1.173460	1.504260	0.758154	-1.181208
C	2.022542	0.112565	0.000000	2.008469	0.076765	0.000000
C	1.528067	0.791614	1.173460	1.504260	0.758154	1.181208
H	-1.032371	4.633706	0.000000	-1.013354	4.661673	0.000000
H	-0.191106	3.352556	-2.192195	-0.187645	3.358609	-2.207393
H	2.634765	-0.783444	0.000000	2.621990	-0.829064	0.000000
H	1.722061	0.489770	2.197745	1.695634	0.451821	2.213811
H	-0.191106	3.352556	2.192195	-0.187645	3.358609	2.207393
H	1.722061	0.489770	-2.197745	1.695634	0.451821	-2.213811
C	-1.528067	-0.791614	1.173460	-1.504260	-0.758154	1.181208
C	-2.022542	-0.112565	0.000000	-2.008469	-0.076765	0.000000
C	-1.528067	-0.791614	-1.173460	-1.504260	-0.758154	-1.181208
C	-0.756129	-1.912481	-0.729681	-0.742076	-1.898866	-0.735213
C	-0.756129	-1.912481	0.729681	-0.742076	-1.898866	0.735213
C	0.000000	-3.051895	-1.167267	0.000000	-3.052855	-1.174614
C	0.434130	-3.725294	0.000000	0.425482	-3.736413	0.000000
C	0.000000	-3.051895	1.167267	0.000000	-3.052855	1.174614
H	-2.634765	0.783444	0.000000	-2.621990	0.829064	0.000000
H	-1.722061	-0.489770	-2.197745	-1.695634	-0.451821	-2.213811
H	1.032371	-4.633706	0.000000	1.013354	-4.661673	0.000000
H	0.191106	-3.352556	2.192195	0.187645	-3.358609	2.207393
H	-1.722061	-0.489770	2.197745	-1.695634	-0.451821	2.213811
H	0.191106	-3.352556	-2.192195	0.187645	-3.358609	-2.207393
Co	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Table S50. Optimized coordinates of the **Co-5D**for the $(C8H6)_2Co$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.090631	-1.059920	2.083066	1.115608	-1.082609	1.986818
C	-0.051785	-1.929481	1.892490	-0.045468	-1.949886	1.822896
C	-1.216850	-1.138481	1.577395	-1.224025	-1.141901	1.548339
C	-0.748325	0.186463	1.386066	-0.751527	0.197232	1.374360
C	0.645794	0.246789	1.789433	0.664237	0.248421	1.752861
C	-1.152380	1.546105	0.819632	-1.158251	1.567020	0.828935
C	0.005965	2.404913	1.333049	0.008345	2.419179	1.332030
C	1.037971	1.652592	1.800756	1.061345	1.649144	1.770426
H	-0.053792	-3.001635	2.064740	-0.048213	-3.033197	1.978776
H	-2.210609	-1.528407	1.388408	-2.235367	-1.524066	1.388313
H	0.014943	3.488461	1.246460	0.017175	3.512461	1.261575
H	1.997422	2.037488	2.136243	2.038869	2.030970	2.083554
H	2.081142	-1.372788	2.393931	2.121415	-1.408881	2.262975
H	-2.130637	1.902702	1.165320	-2.145317	1.926467	1.173941
C	1.090631	-1.059920	-2.083066	1.115608	-1.082609	-1.986818
C	-0.051785	-1.929481	-1.892490	-0.045468	-1.949886	-1.822896
C	-1.216850	-1.138481	-1.577395	-1.224025	-1.141901	-1.548339
C	-0.748325	0.186463	-1.386066	-0.751527	0.197232	-1.374360
C	0.645794	0.246789	-1.789433	0.664237	0.248421	-1.752861
C	-1.152380	1.546105	-0.819632	-1.158251	1.567020	-0.828935
C	0.005965	2.404913	-1.333049	0.008345	2.419179	-1.332030
C	1.037971	1.652592	-1.800756	1.061345	1.649144	-1.770426
H	-0.053792	-3.001635	-2.064740	-0.048213	-3.033197	-1.978776
H	-2.210609	-1.528407	-1.388408	-2.235367	-1.524066	-1.388313
H	0.014943	3.488461	-1.246460	0.017175	3.512461	-1.261575
H	1.997422	2.037488	-2.136243	2.038869	2.030970	-2.083554
H	2.081142	-1.372788	-2.393931	2.121415	-1.408881	-2.262975
H	-2.130637	1.902702	-1.165320	-2.145317	1.926467	-1.173941
Co	0.195215	-0.961459	0.000000	0.165174	-0.958768	0.000000

Table S51 Optimized coordinates of the **Co-6Q**for the $(C8H6)_2Co$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.715987	1.151780	0.253917	1.714590	1.051672	0.268477
C	1.333107	1.738076	1.509628	1.323804	1.639768	1.531756
C	0.000000	2.285456	1.383594	0.000000	2.237112	1.391386
C	-0.411380	2.040348	0.043620	-0.395139	2.031246	0.033071
C	0.616665	1.312740	-0.632205	0.630370	1.269102	-0.638007
C	-1.560711	2.155529	-0.858103	-1.520219	2.195264	-0.886927
C	-1.292592	1.471878	-2.001126	-1.249994	1.513730	-2.046531
C	0.072591	0.789040	-1.953846	0.095812	0.787872	-1.981143
H	1.971273	1.822814	2.384088	1.951747	1.685856	2.427196
H	-0.537270	2.831919	2.151640	-0.538325	2.790324	2.165630
H	-1.962817	1.373878	-2.852633	-1.910372	1.449936	-2.919462
H	0.684779	1.072481	-2.822516	0.741758	1.059266	-2.840474
H	2.654534	0.647675	0.051897	2.650778	0.524272	0.070658
H	-2.479480	2.695971	-0.643295	-2.433793	2.763658	-0.679496
C	0.000000	-2.285456	1.383594	0.000000	-2.237112	1.391386
C	-1.333107	-1.738076	1.509628	-1.323804	-1.639768	1.531756
C	-1.715987	-1.151780	0.253917	-1.714590	-1.051672	0.268477
C	-0.616665	-1.312740	-0.632205	-0.630370	-1.269102	-0.638007
C	0.411380	-2.040348	0.043620	0.395139	-2.031246	0.033071
C	-0.072591	-0.789040	-1.953846	-0.095812	-0.787872	-1.981143
C	1.292592	-1.471878	-2.001126	1.249994	-1.513730	-2.046531
C	1.560711	-2.155529	-0.858103	1.520219	-2.195264	-0.886927
H	-1.971273	-1.822814	2.384088	-1.951747	-1.685856	2.427196
H	-2.654534	-0.647675	0.051897	-2.650778	-0.524272	0.070658
H	1.962817	-1.373878	-2.852633	1.910372	-1.449936	-2.919462
H	2.479480	-2.695971	-0.643295	2.433793	-2.763658	-0.679496
H	0.537270	-2.831919	2.151640	0.538325	-2.790324	2.165630
H	-0.684779	-1.072481	-2.822516	-0.741758	-1.059266	-2.840474
Co	0.000000	0.000000	1.130219	0.000000	0.000000	1.166182

Table S52 Optimized coordinates of the **Co-7Q**for the $(C8H6)_2Co$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	3.095759	1.158334	0.000000	3.094141	1.164783
C	-0.466010	3.764290	0.000000	-0.457792	3.775121	0.000000
C	0.000000	3.095759	-1.158334	0.000000	3.094141	-1.164783
C	0.800322	1.981662	-0.717846	0.787419	1.964278	-0.722581
C	0.800322	1.981662	0.717846	0.787419	1.964278	0.722581
C	1.578075	0.849853	-1.161442	1.546076	0.808238	-1.169830
C	2.129665	0.211061	0.000000	2.094078	0.156401	0.000000
C	1.578075	0.849853	1.161442	1.546076	0.808238	1.169830
H	-1.093679	4.650925	0.000000	-1.075881	4.678552	0.000000
H	-0.207331	3.380260	-2.185982	-0.207127	3.380395	-2.200798
H	2.767387	-0.666068	0.000000	2.729060	-0.733396	0.000000
H	1.780753	0.561685	2.188673	1.742539	0.515002	2.205704
H	-0.207331	3.380260	2.185982	-0.207127	3.380395	2.200798
H	1.780753	0.561685	-2.188673	1.742539	0.515002	-2.205704
C	-1.578075	-0.849853	1.161442	-1.546076	-0.808238	1.169830
C	-2.129665	-0.211061	0.000000	-2.094078	-0.156401	0.000000
C	-1.578075	-0.849853	-1.161442	-1.546076	-0.808238	-1.169830
C	-0.800322	-1.981662	-0.717846	-0.787419	-1.964278	-0.722581
C	-0.800322	-1.981662	0.717846	-0.787419	-1.964278	0.722581
C	0.000000	-3.095759	-1.158334	0.000000	-3.094141	-1.164783
C	0.466010	-3.764290	0.000000	0.457792	-3.775121	0.000000
C	0.000000	-3.095759	1.158334	0.000000	-3.094141	1.164783
H	-2.767387	0.666068	0.000000	-2.729060	0.733396	0.000000
H	-1.780753	-0.561685	-2.188673	-1.742539	-0.515002	-2.205704
H	1.093679	-4.650925	0.000000	1.075881	-4.678552	0.000000
H	0.207331	-3.380260	2.185982	0.207127	-3.380395	2.200798
H	-1.780753	-0.561685	2.188673	-1.742539	-0.515002	2.205704
H	0.207331	-3.380260	-2.185982	0.207127	-3.380395	-2.200798
Co	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Table S53 Optimized coordinates of the **Co-8Q**for the $(C8H6)_2Co$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.163523	1.762461	1.171450	1.170603	1.707441	1.173016
C	0.000000	1.811123	2.009036	0.000000	1.759699	2.019842
C	-1.163523	1.762461	1.171450	-1.170603	1.707441	1.173016
C	-0.716590	1.825574	-0.202314	-0.721054	1.792792	-0.208551
C	0.716590	1.825574	-0.202314	0.721054	1.792792	-0.208551
C	-1.156959	1.865463	-1.578940	-1.163348	1.847192	-1.591134
C	0.000000	1.908253	-2.390978	0.000000	1.899829	-2.408373
C	1.156959	1.865463	-1.578940	1.163348	1.847192	-1.591134
H	0.000000	1.782475	3.093428	0.000000	1.733734	3.112820
H	-2.190349	1.758166	1.523551	-2.206193	1.696522	1.525481
H	0.000000	1.933971	-3.476811	0.000000	1.940094	-3.502052
H	2.184621	1.870979	-1.930242	2.199424	1.852824	-1.943716
H	2.190349	1.758166	1.523551	2.206193	1.696522	1.525481
H	-2.184621	1.870979	-1.930242	-2.199424	1.852824	-1.943716
C	1.163523	-1.762461	1.171450	1.170603	-1.707441	1.173016
C	0.000000	-1.811123	2.009036	0.000000	-1.759699	2.019842
C	-1.163523	-1.762461	1.171450	-1.170603	-1.707441	1.173016
C	-0.716590	-1.825574	-0.202314	-0.721054	-1.792792	-0.208551
C	0.716590	-1.825574	-0.202314	0.721054	-1.792792	-0.208551
C	-1.156959	-1.865463	-1.578940	-1.163348	-1.847192	-1.591134
C	0.000000	-1.908253	-2.390978	0.000000	-1.899829	-2.408373
C	1.156959	-1.865463	-1.578940	1.163348	-1.847192	-1.591134
H	0.000000	-1.782475	3.093428	0.000000	-1.733734	3.112820
H	-2.190349	-1.758166	1.523551	-2.206193	-1.696522	1.525481
H	0.000000	-1.933971	-3.476811	0.000000	-1.940094	-3.502052
H	2.184621	-1.870979	-1.930242	2.199424	-1.852824	-1.943716
H	2.190349	-1.758166	1.523551	2.206193	-1.696522	1.525481
H	-2.184621	-1.870979	-1.930242	-2.199424	-1.852824	-1.943716
Co	0.000000	0.000000	0.800449	0.000000	0.000000	0.820512

Table S54 Optimized coordinates of the **Co-9Q**for the $(C8H6)_2Co$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.021749	-1.007747	2.251046	1.02346	-1.03183	2.15480
C	-1.890206	0.128422	2.046081	-0.14120	-1.89075	1.97143
C	-1.095152	1.231178	1.571147	-1.25082	-1.07323	1.52833
C	0.238107	0.759420	1.435072	-0.76239	0.26559	1.40784
C	0.292126	-0.585305	1.916980	0.60439	0.30222	1.86669
C	1.583017	1.123292	0.820478	-1.12517	1.62367	0.82580
C	2.443994	-0.027778	1.353747	0.03610	2.47344	1.35522
C	1.691566	-1.015449	1.902679	1.04290	1.69531	1.86914
H	-2.945364	0.172313	2.296638	-0.19505	-2.95650	2.21290
H	-1.474490	2.217426	1.325981	-2.25823	-1.43825	1.31271
H	3.522822	-0.060041	1.227355	0.07096	3.56304	1.24945
H	2.068201	-1.960027	2.286369	2.00733	2.06178	2.23667
H	-1.321885	-1.967567	2.659354	1.99693	-1.35324	2.53617
H	1.958854	2.101398	1.147355	-2.11162	2.00106	1.15459
C	-1.021749	-1.007747	-2.251046	1.02346	-1.03183	-2.15480
C	-1.890206	0.128422	-2.046081	-0.14120	-1.89075	-1.97143
C	-1.095152	1.231178	-1.571147	-1.25082	-1.07323	-1.52833
C	0.238107	0.759420	-1.435072	-0.76239	0.26559	-1.40784
C	0.292126	-0.585305	-1.916980	0.60439	0.30222	-1.86669
C	1.583017	1.123292	-0.820478	-1.12517	1.62367	-0.82580
C	2.443994	-0.027778	-1.353747	0.03610	2.47344	-1.35522
C	1.691566	-1.015449	-1.902679	1.04290	1.69531	-1.86914
H	-2.945364	0.172313	-2.296638	-0.19505	-2.95650	-2.21290
H	-1.474490	2.217426	-1.325981	-2.25823	-1.43825	-1.31271
H	3.522822	-0.060041	-1.227355	0.07096	3.56304	-1.24945
H	2.068201	-1.960027	-2.286369	2.00733	2.06178	-2.23667
H	-1.321885	-1.967567	-2.659354	1.99693	-1.35324	-2.53617
H	1.958854	2.101398	-1.147355	-2.11162	2.00106	-1.15459
Co	-1.130248	-0.306645	0.000000	0.29082	-1.18996	0.00000

Table S55 Optimized coordinates of the **Ni-1S** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.178685	1.731284	1.094959	1.186495	1.719051	1.100003
C	0.000000	1.764181	1.936508	0.000000	1.762160	1.946522
C	-1.178685	1.731284	1.094959	-1.186495	1.719051	1.100003
C	-0.744466	1.741297	-0.266361	-0.749129	1.720108	-0.269346
C	0.744466	1.741297	-0.266361	0.749129	1.720108	-0.269346
C	-1.177407	1.669397	-1.607851	-1.184142	1.634591	-1.616765
C	0.000000	1.628482	-2.404195	0.000000	1.584326	-2.417892
C	1.177407	1.669397	-1.607851	1.184142	1.634591	-1.616765
H	0.000000	1.846282	3.019048	0.000000	1.852943	3.037140
H	-2.201300	1.743436	1.458022	-2.217305	1.733292	1.465188
H	0.000000	1.588406	-3.492056	0.000000	1.540136	-3.514082
H	2.197889	1.650826	-1.972784	2.212491	1.615368	-1.984414
H	2.201300	1.743436	1.458022	2.217305	1.733292	1.465188
H	-2.197889	1.650826	-1.972784	-2.212491	1.615368	-1.984414
C	1.178685	-1.731284	1.094959	1.186495	-1.719051	1.100003
C	0.000000	-1.764181	1.936508	0.000000	-1.762160	1.946522
C	-1.178685	-1.731284	1.094959	-1.186495	-1.719051	1.100003
C	-0.744466	-1.741297	-0.266361	-0.749129	-1.720108	-0.269346
C	0.744466	-1.741297	-0.266361	0.749129	-1.720108	-0.269346
C	-1.177407	-1.669397	-1.607851	-1.184142	-1.634591	-1.616765
C	0.000000	-1.628482	-2.404195	0.000000	-1.584326	-2.417892
C	1.177407	-1.669397	-1.607851	1.184142	-1.634591	-1.616765
H	0.000000	-1.846282	3.019048	0.000000	-1.852943	3.037140
H	-2.201300	-1.743436	1.458022	-2.217305	-1.733292	1.465188
H	0.000000	-1.588406	-3.492056	0.000000	-1.540136	-3.514082
H	2.197889	-1.650826	-1.972784	2.212491	-1.615368	-1.984414
H	2.201300	-1.743436	1.458022	2.217305	-1.733292	1.465188
H	-2.197889	-1.650826	-1.972784	-2.212491	-1.615368	-1.984414
Ni	0.000000	0.000000	0.975692	0.000000	0.000000	0.984065

Table S56 Optimized coordinates of the **Ni-2S** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	2.465433	-1.851680	-0.207936	2.329413	-1.919833
C	0.945106	3.354587	-1.302948	0.805313	3.238792	-1.506252
C	0.957684	3.282473	0.129019	0.956229	3.236029	-0.079324
C	-0.019087	2.341052	0.487872	0.000000	2.318876	0.423703
C	-0.629360	1.819593	-0.747497	-0.736076	1.746920	-0.728770
C	-0.643519	1.648077	1.589629	-0.532425	1.705596	1.620514
C	-1.725007	0.847557	1.068246	-1.670350	0.878700	1.240160
C	-1.653356	0.891249	-0.377570	-1.728254	0.838549	-0.213560
H	1.582695	4.014744	-1.887580	1.394441	3.863398	-2.188417
H	1.600785	3.853478	0.790618	1.668935	3.834094	0.494930
H	-2.441379	0.280405	1.652820	-2.343324	0.354875	1.924544
H	-2.303493	0.335481	-1.046711	-2.444814	0.248899	-0.793714
H	-0.220940	2.326912	-2.904545	-0.527736	2.137007	-2.947120
H	-0.429690	1.781243	2.646137	-0.223713	1.901829	2.652104
C	1.653356	-0.891249	-0.377570	1.728254	-0.838549	-0.213560
C	1.725007	-0.847557	1.068246	1.670350	-0.878700	1.240160
C	0.643519	-1.648077	1.589629	0.532425	-1.705596	1.620514
C	0.019087	-2.341052	0.487872	0.000000	-2.318876	0.423703
C	0.629360	-1.819593	-0.747497	0.736076	-1.746920	-0.728770
C	-0.957684	-3.282473	0.129019	-0.956229	-3.236029	-0.079324
C	-0.945106	-3.354587	-1.302948	-0.805313	-3.238792	-1.506252
C	0.000000	-2.465433	-1.851680	0.207936	-2.329413	-1.919833
H	2.441379	-0.280405	1.652820	2.343324	-0.354875	1.924544
H	0.429690	-1.781243	2.646137	0.223713	-1.901829	2.652104
H	-1.582695	-4.014744	-1.887580	-1.394441	-3.863398	-2.188417
H	0.220940	-2.326912	-2.904545	0.527736	-2.137007	-2.947120
H	2.303493	-0.335481	-1.046711	2.444814	-0.248899	-0.793714
H	-1.600785	-3.853478	0.790618	-1.668935	-3.834094	0.494930
Ni	0.000000	0.000000	0.484202	0.000000	0.000000	0.559846

Table S57 Optimized coordinates of the **Ni-3S** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.970922	0.009722	0.483158	1.656668	1.018119	0.489311
C	-1.939677	-0.810729	1.658275	1.173577	1.685121	1.678293
C	-1.384011	-2.125527	1.323054	0.000000	2.512234	1.342242
C	-0.951055	-2.057061	0.006846	-0.319610	2.246147	0.007566
C	-1.189365	-0.702271	-0.487018	0.615407	1.222769	-0.492569
C	-0.227975	-2.785582	-1.027349	-1.310983	2.483979	-1.031572
C	0.000000	-1.961951	-2.085883	-1.058433	1.662727	-2.104104
C	-0.555764	-0.552930	-1.875691	0.168243	0.767823	-1.892835
H	-2.420031	-0.565644	2.601254	1.705172	1.723249	2.634752
H	-1.286674	-2.954595	2.016625	-0.535646	3.153753	2.047640
H	0.523664	-2.241812	-2.998114	-1.647725	1.629843	-3.028637
H	-1.290884	-0.319754	-2.661649	0.926965	0.970931	-2.678211
H	-2.418435	0.993403	0.391377	2.572844	0.430715	0.388494
H	0.087856	-3.824066	-0.961039	-2.140382	3.197344	-0.965939
C	1.384011	2.125527	1.323054	0.000000	-2.512234	1.342242
C	1.939677	0.810729	1.658275	-1.173577	-1.685121	1.678293
C	1.970922	-0.009722	0.483158	-1.656668	-1.018119	0.489311
C	1.189365	0.702271	-0.487018	-0.615407	-1.222769	-0.492569
C	0.951055	2.057061	0.006846	0.319610	-2.246147	0.007566
C	0.555764	0.552930	-1.875691	-0.168243	-0.767823	-1.892835
C	0.000000	1.961951	-2.085883	1.058433	-1.662727	-2.104104
C	0.227975	2.785582	-1.027349	1.310983	-2.483979	-1.031572
H	2.420031	0.565644	2.601254	-1.705172	-1.723249	2.634752
H	2.418435	-0.993403	0.391377	-2.572844	-0.430715	0.388494
H	-0.523664	2.241812	-2.998114	1.647725	-1.629843	-3.028637
H	-0.087856	3.824066	-0.961039	2.140382	-3.197344	-0.965939
H	1.286674	2.954595	2.016625	0.535646	-3.153753	2.047640
H	1.290884	0.319754	-2.661649	-0.926965	-0.970931	-2.678211
Ni	0.000000	0.000000	0.974240	0.000000	0.000000	0.973136

Table S58 Optimized coordinates of the **Ni-4S** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	2.398772	0.016039	-1.158193	2.322677	0.205067	-1.188845
C	2.830492	-0.598574	0.092235	2.835133	-0.354548	0.065938
C	2.174489	0.026219	1.190271	2.143300	0.237265	1.183087
C	1.213744	0.916290	0.614350	1.108203	1.057550	0.614126
C	1.452952	1.000420	-0.818714	1.302729	1.126507	-0.842890
C	0.034076	1.824682	0.963650	-0.152117	1.849903	0.966647
C	-0.091289	2.626327	-0.329937	-0.371468	2.624652	-0.327882
C	0.652071	2.102003	-1.340217	0.394412	2.138635	-1.361432
H	3.574705	-1.385624	0.169847	3.656106	-1.074324	0.139946
H	2.284581	-0.242554	2.235107	2.307231	0.005074	2.238287
H	-0.778751	3.461494	-0.433048	-1.135157	3.403840	-0.425310
H	0.659250	2.453707	-2.368573	0.336885	2.467450	-2.404531
H	2.792571	-0.219138	-2.141241	2.708108	-0.023503	-2.185930
H	0.213890	2.467966	1.834825	-0.049036	2.504464	1.851929
C	-1.810415	-1.871025	-1.036438	-1.556666	-2.025157	-1.082382
C	-0.876942	-2.557224	-0.128414	-0.556743	-2.604981	-0.161375
C	-0.701820	-1.770909	1.062198	-0.503876	-1.825641	1.066399
C	-1.179815	-0.467136	0.692083	-1.125415	-0.571719	0.689902
C	-2.020882	-0.614212	-0.509095	-1.929636	-0.800673	-0.542706
C	-1.312137	0.956541	1.231331	-1.418957	0.826887	1.232675
C	-2.473975	1.459306	0.381070	-2.619359	1.204638	0.376004
C	-2.806116	0.596512	-0.625133	-2.838846	0.313152	-0.659493
H	-0.588392	-3.600944	-0.222950	-0.142145	-3.614141	-0.265771
H	-0.249438	-2.094148	1.994588	-0.085169	-2.132332	2.030244
H	-2.933993	2.433043	0.538116	-3.202376	2.118656	0.543307
H	-3.568065	0.785548	-1.377965	-3.612112	0.429220	-1.427889
H	-2.228167	-2.302263	-1.940531	-1.903105	-2.495588	-2.006901
H	-1.530445	0.998751	2.306878	-1.634458	0.854409	2.317983
Ni	0.623322	-0.879550	-0.081476	0.734107	-0.816159	-0.020429

Table S59 Optimized coordinates of the **Ni-5T** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.711189	1.113968	0.302320	1.715901	1.053051	0.318212
C	1.312125	1.703377	1.557341	1.306514	1.633033	1.587541
C	0.000000	2.268740	1.410434	0.000000	2.230812	1.432046
C	-0.398683	2.037164	0.060286	-0.387710	2.033625	0.062117
C	0.632462	1.304643	-0.609685	0.645861	1.280754	-0.610295
C	-1.532814	2.178317	-0.856659	-1.507620	2.204971	-0.864917
C	-1.260396	1.498360	-2.000738	-1.234106	1.525844	-2.024889
C	0.090521	0.788788	-1.939149	0.105666	0.790232	-1.954699
H	1.925630	1.753722	2.451277	1.914092	1.658918	2.496675
H	-0.555959	2.790372	2.182306	-0.560953	2.752160	2.212117
H	-1.920072	1.417826	-2.862174	-1.890561	1.467293	-2.901035
H	0.716106	1.056396	-2.802938	0.751489	1.048973	-2.817695
H	2.647780	0.601211	0.113937	2.653060	0.523246	0.130209
H	-2.445379	2.732309	-0.650264	-2.420560	2.775418	-0.660298
C	0.000000	-2.268740	1.410434	0.000000	-2.230812	1.432046
C	-1.312125	-1.703377	1.557341	-1.306514	-1.633033	1.587541
C	-1.711189	-1.113968	0.302320	-1.715901	-1.053051	0.318212
C	-0.632462	-1.304643	-0.609685	-0.645861	-1.280754	-0.610295
C	0.398683	-2.037164	0.060286	0.387710	-2.033625	0.062117
C	-0.090521	-0.788788	-1.939149	-0.105666	-0.790232	-1.954699
C	1.260396	-1.498360	-2.000738	1.234106	-1.525844	-2.024889
C	1.532814	-2.178317	-0.856659	1.507620	-2.204971	-0.864917
H	-1.925630	-1.753722	2.451277	-1.914092	-1.658918	2.496675
H	-2.647780	-0.601211	0.113937	-2.653060	-0.523246	0.130209
H	1.920072	-1.417826	-2.862174	1.890561	-1.467293	-2.901035
H	2.445379	-2.732309	-0.650264	2.420560	-2.775418	-0.660298
H	0.555959	-2.790372	2.182306	0.560953	-2.752160	2.212117
H	-0.716106	-1.056396	-2.802938	-0.751489	-1.048973	-2.817695
Ni	0.000000	0.000000	1.001640	0.000000	0.000000	0.990667

Table S60 Optimized coordinates of the **Ni-6T** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	2.999420	-1.461675	0.000000	3.039808	-1.452086
C	0.651620	3.815736	-0.483608	0.635233	3.857100	-0.455826
C	0.345770	3.358691	0.809415	0.335321	3.368363	0.841030
C	-0.536686	2.226404	0.658262	-0.523582	2.221620	0.669451
C	-0.744139	2.012807	-0.756014	-0.727447	2.024223	-0.759838
C	-1.280319	1.238019	1.369962	-1.245782	1.188860	1.366620
C	-2.011362	0.444941	0.400347	-1.985323	0.408262	0.378129
C	-1.621357	0.875434	-0.908356	-1.585872	0.864728	-0.932175
H	1.288082	4.666557	-0.712083	1.256546	4.733293	-0.670056
H	0.696698	3.789199	1.742374	0.679315	3.794269	1.788232
H	-2.701843	-0.359838	0.628741	-2.679640	-0.408538	0.592907
H	-1.988149	0.451947	-1.838558	-1.948282	0.449558	-1.877683
H	0.063448	3.124932	-2.538608	0.064932	3.181771	-2.535176
H	-1.359535	1.126492	2.447516	-1.326152	1.058564	2.450545
C	1.621357	-0.875434	-0.908356	1.585872	-0.864728	-0.932175
C	2.011362	-0.444941	0.400347	1.985323	-0.408262	0.378129
C	1.280319	-1.238019	1.369962	1.245782	-1.188860	1.366620
C	0.536686	-2.226404	0.658262	0.523582	-2.221620	0.669451
C	0.744139	-2.012807	-0.756014	0.727447	-2.024223	-0.759838
C	-0.345770	-3.358691	0.809415	-0.335321	-3.368363	0.841030
C	-0.651620	-3.815736	-0.483608	-0.635233	-3.857100	-0.455826
C	0.000000	-2.999420	-1.461675	0.000000	-3.039808	-1.452086
H	2.701843	0.359838	0.628741	2.679640	0.408538	0.592907
H	1.359535	-1.126492	2.447516	1.326152	-1.058564	2.450545
H	-1.288082	-4.666557	-0.712083	-1.256546	-4.733293	-0.670056
H	-0.063448	-3.124932	-2.538608	-0.064932	-3.181771	-2.535176
H	1.988149	-0.451947	-1.838558	1.948282	-0.449558	-1.877683
H	-0.696698	-3.789199	1.742374	-0.679315	-3.794269	1.788232
Ni	0.000000	0.000000	0.178616	0. 000000	0. 000000	0. 165672

Table S61 Optimized coordinates of the **Ni-7T** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	0.000000	3.225930	1.161807	0.000000	3.250815	1.169753
C	-0.447286	3.904015	0.000000	-0.436147	3.942350	0.000000
C	0.000000	3.225930	-1.161807	0.000000	3.250815	-1.169753
C	0.762950	2.094858	-0.721694	0.742337	2.104004	-0.727737
C	0.762950	2.094858	0.721694	0.742337	2.104004	0.727737
C	1.517716	0.956016	-1.165149	1.475852	0.938435	-1.172197
C	2.050233	0.296706	0.000000	2.018099	0.274887	0.000000
C	1.517716	0.956016	1.165149	1.475852	0.938435	1.172197
H	-1.044220	4.812143	0.000000	-1.016363	4.871243	0.000000
H	-0.194145	3.521692	-2.188529	-0.190984	3.551407	-2.204376
H	2.697472	-0.573658	0.000000	2.670511	-0.602328	0.000000
H	1.727273	0.669146	2.191504	1.683296	0.647592	2.206864
H	-0.194145	3.521692	2.188529	-0.190984	3.551407	2.204376
H	1.727273	0.669146	-2.191504	1.683296	0.647592	-2.206864
C	-1.517716	-0.956016	1.165149	-1.475852	-0.938435	1.172197
C	-2.050233	-0.296706	0.000000	-2.018099	-0.274887	0.000000
C	-1.517716	-0.956016	-1.165149	-1.475852	-0.938435	-1.172197
C	-0.762950	-2.094858	-0.721694	-0.742337	-2.104004	-0.727737
C	-0.762950	-2.094858	0.721694	-0.742337	-2.104004	0.727737
C	0.000000	-3.225930	-1.161807	0.000000	-3.250815	-1.169753
C	0.447286	-3.904015	0.000000	0.436147	-3.942350	0.000000
C	0.000000	-3.225930	1.161807	0.000000	-3.250815	1.169753
H	-2.697472	0.573658	0.000000	-2.670511	0.602328	0.000000
H	-1.727273	-0.669146	-2.191504	-1.683296	-0.647592	-2.206864
H	1.044220	-4.812143	0.000000	1.016363	-4.871243	0.000000
H	0.194145	-3.521692	2.188529	0.190984	-3.551407	2.204376
H	-1.727273	-0.669146	2.191504	-1.683296	-0.647592	2.206864
H	0.194145	-3.521692	-2.188529	0.190984	-3.551407	-2.204376
Ni	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Table S62 Optimized coordinates of the **Ni-8T** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-0.145763	2.056005	1.541926	0.066825	2.053905	1.438212
C	-1.331869	1.306394	1.770530	-1.127381	1.390839	1.892189
C	-1.881700	0.907820	0.477603	-1.869375	0.937477	0.714495
C	-1.073134	1.489473	-0.532249	-1.196741	1.435956	-0.451121
C	0.000000	2.225338	0.107620	0.000000	2.150472	-0.012807
C	-0.917467	1.642450	-1.970528	-1.245752	1.501389	-1.897950
C	0.196152	2.457071	-2.169996	-0.124290	2.252582	-2.310925
C	0.782106	2.825086	-0.903896	0.657145	2.655231	-1.167139
H	-1.748339	1.047945	2.738454	-1.415261	1.219284	2.932955
H	-2.779950	0.313387	0.339642	-2.809549	0.377824	0.743499
H	0.577550	2.770355	-3.138495	0.123070	2.493717	-3.350347
H	1.663974	3.444937	-0.771036	1.585065	3.234537	-1.198186
H	0.491332	2.473481	2.315485	0.832944	2.485952	2.089131
H	-1.552191	1.212390	-2.738131	-2.005264	1.057045	-2.546953
C	1.881700	-0.907820	0.477603	1.869375	-0.937477	0.714495
C	1.331869	-1.306394	1.770530	1.127381	-1.390839	1.892189
C	0.145763	-2.056005	1.541926	-0.066825	-2.053905	1.438212
C	0.000000	-2.225338	0.107620	0.000000	-2.150472	-0.012807
C	1.073134	-1.489473	-0.532249	1.196741	-1.435956	-0.451121
C	-0.782106	-2.825086	-0.903896	-0.657145	-2.655231	-1.167139
C	-0.196152	-2.457071	-2.169996	0.124290	-2.252582	-2.310925
C	0.917467	-1.642450	-1.970528	1.245752	-1.501389	-1.897950
H	1.748339	-1.047945	2.738454	1.415261	-1.219284	2.932955
H	-0.491332	-2.473481	2.315485	-0.832944	-2.485952	2.089131
H	-0.577550	-2.770355	-3.138495	-0.123070	-2.493717	-3.350347
H	1.552191	-1.212390	-2.738131	2.005264	-1.057045	-2.546953
H	2.779950	-0.313387	0.339642	2.809549	-0.377824	0.743499
H	-1.663974	-3.444937	-0.771036	-1.585065	-3.234537	-1.198186
Ni	0.000000	0.000000	0.809144	0.000000	0.000000	0.864298

Table S63 Optimized coordinates of the **Ni-9T** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	1.165548	1.790201	1.128277	1.172356	1.741182	1.132486
C	0.000000	1.770263	1.974637	0.000000	1.735875	1.986571
C	-1.165548	1.790201	1.128277	-1.172356	1.741182	1.132486
C	-0.722439	1.936055	-0.227127	-0.729479	1.907962	-0.233431
C	0.722439	1.936055	-0.227127	0.729479	1.907962	-0.233431
C	-1.161316	2.103745	-1.581676	-1.169807	2.085243	-1.586465
C	0.000000	2.211147	-2.386035	0.000000	2.200064	-2.394843
C	1.161316	2.103745	-1.581676	1.169807	2.085243	-1.586465
H	0.000000	1.716135	3.058004	0.000000	1.682202	3.078600
H	-2.192170	1.770690	1.482385	-2.206813	1.719528	1.489718
H	0.000000	2.346073	-3.464282	0.000000	2.346869	-3.480123
H	2.187670	2.141372	-1.934176	2.203819	2.121875	-1.941921
H	2.192170	1.770690	1.482385	2.206813	1.719528	1.489718
H	-2.187670	2.141372	-1.934176	-2.203819	2.121875	-1.941921
C	1.165548	-1.790201	1.128277	1.172356	-1.741182	1.132486
C	0.000000	-1.770263	1.974637	0.000000	-1.735875	1.986571
C	-1.165548	-1.790201	1.128277	-1.172356	-1.741182	1.132486
C	-0.722439	-1.936055	-0.227127	-0.729479	-1.907962	-0.233431
C	0.722439	-1.936055	-0.227127	0.729479	-1.907962	-0.233431
C	-1.161316	-2.103745	-1.581676	-1.169807	-2.085243	-1.586465
C	0.000000	-2.211147	-2.386035	0.000000	-2.200064	-2.394843
C	1.161316	-2.103745	-1.581676	1.169807	-2.085243	-1.586465
H	0.000000	-1.716135	3.058004	0.000000	-1.682202	3.078600
H	-2.192170	-1.770690	1.482385	-2.206813	-1.719528	1.489718
H	0.000000	-2.346073	-3.464282	0.000000	-2.346869	-3.480123
H	2.187670	-2.141372	-1.934176	2.203819	-2.121875	-1.941921
H	2.192170	-1.770690	1.482385	2.206813	-1.719528	1.489718
H	-2.187670	-2.141372	-1.934176	-2.203819	-2.121875	-1.941921
Ni	0.000000	0.000000	0.853183	0.000000	0.000000	0.857463

Table 64 Optimized coordinates of the **Ni-10T** for the $(C8H6)_2Ni$ structures

	B3LYP			BP86		
	x	y	z	x	y	z
C	-1.031761	-1.041880	2.201570	1.068021	-1.046229	2.133420
C	-1.898524	0.089305	2.028569	-0.074548	-1.915439	1.975391
C	-1.114651	1.212492	1.573809	-1.214536	-1.119842	1.549450
C	0.224300	0.756093	1.430736	-0.757738	0.233382	1.420971
C	0.284091	-0.604813	1.874077	0.621632	0.288285	1.845407
C	1.568047	1.136847	0.821349	-1.143653	1.585003	0.827662
C	2.435418	-0.016096	1.340897	0.016405	2.451544	1.336249
C	1.685214	-1.021755	1.862591	1.040833	1.686710	1.837248
H	-2.961256	0.111559	2.247974	-0.093792	-2.988317	2.186851
H	-1.504496	2.200602	1.354532	-2.218657	-1.506330	1.355899
H	3.515663	-0.035958	1.225435	0.032916	3.541689	1.233826
H	2.066246	-1.972384	2.226420	2.007408	2.066572	2.185092
H	-1.329786	-2.017160	2.571843	2.059425	-1.354110	2.476444
H	1.938225	2.115447	1.152361	-2.130725	1.957011	1.160349
C	-1.031761	-1.041880	-2.201570	1.068021	-1.046229	-2.133420
C	-1.898524	0.089305	-2.028569	-0.074548	-1.915439	-1.975391
C	-1.114651	1.212492	-1.573809	-1.214536	-1.119842	-1.549450
C	0.224300	0.756093	-1.430736	-0.757738	0.233382	-1.420971
C	0.284091	-0.604813	-1.874077	0.621632	0.288285	-1.845407
C	1.568047	1.136847	-0.821349	-1.143653	1.585003	-0.827662
C	2.435418	-0.016096	-1.340897	0.016405	2.451544	-1.336249
C	1.685214	-1.021755	-1.862591	1.040833	1.686710	-1.837248
H	-2.961256	0.111559	-2.247974	-0.093792	-2.988317	-2.186851
H	-1.504496	2.200602	-1.354532	-2.218657	-1.506330	-1.355899
H	3.515663	-0.035958	-1.225435	0.032916	3.541689	-1.233826
H	2.066246	-1.972384	-2.226420	2.007408	2.066572	-2.185092
H	-1.329786	-2.017160	-2.571843	2.059425	-1.354110	-2.476444
H	1.938225	2.115447	-1.152361	-2.130725	1.957011	-1.160349
Ni	-1.045528	-0.247376	0.000000	0.214638	-1.049785	0.000000

Table S65. Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ti-1S** of $(C_8H_6)_2Ti$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
76(1)	74(1)	785(82)	752(56)	1288(2)	1251(5)
79(4)	76(2)	788(8)	755(22)	1303(7)	1262(4)
124(1)	121(1)	795(7)	767(44)	1310(5)	1269(4)
137(0)	137(0)	801(59)	769(26)	1327(1)	1287(1)
186(1)	187(1)	807(1)	773(0)	1332(5)	1292(3)
210(0)	205(0)	811(5)	775(6)	1402(7)	1360(3)
279(3)	276(3)	867(1)	836(1)	1415(2)	1377(1)
302(1)	297(1)	871(0)	839(0)	1424(2)	1383(1)
323(4)	320(4)	887(5)	843(3)	1435(1)	1392(1)
340(2)	335(4)	891(1)	851(1)	1457(3)	1415(2)
360(2)	356(2)	900(6)	859(2)	1465(4)	1424(4)
413(2)	402(2)	901(10)	862(2)	1471(3)	1430(2)
454(2)	441(2)	905(5)	873(5)	1490(12)	1448(6)
463(1)	449(1)	913(9)	883(20)	1495(3)	1456(1)
528(30)	511(20)	1017(8)	989(8)	1519(8)	1478(6)
561(4)	539(3)	1031(6)	998(5)	3212(2)	3138(3)
571(2)	550(2)	1038(4)	1009(5)	3226(2)	3149(3)
612(0)	592(0)	1050(4)	1021(7)	3226(1)	3150(1)
644(3)	626(2)	1054(13)	1024(10)	3227(1)	3152(1)
690(4)	673(2)	1067(1)	1036(1)	3228(6)	3153(8)
711(53)	684(58)	1075(3)	1043(2)	3241(2)	3167(3)
715(7)	693(0)	1081(1)	1049(0)	3243(6)	3168(7)
720(1)	698(0)	1130(10)	1101(7)	3245(1)	3171(2)
737(7)	720(4)	1137(2)	1108(1)	3247(2)	3173(3)
765(11)	736(13)	1186(1)	1146(1)	3251(2)	3176(2)
769(13)	740(8)	1188(0)	1147(0)	3253(2)	3179(3)
773(18)	744(20)	1277(9)	1238(9)	3256(1)	3181(1)

Table S66 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ti-2T** of $(C_8H_6)_2Ti$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
36(0)	44(0)	767(47)	740(0)	1285(0)	1246(0)
67(0)	66(0)	776(0)	744(1)	1290(21)	1255(21)
101(0)	103(0)	783(71)	755(2)	1299(10)	1257(5)
132(1)	128(1)	790(32)	761(67)	1318(1)	1283(0)
182(0)	180(0)	806(6)	778(6)	1326(16)	1292(13)
222(1)	225(1)	824(1)	786(2)	1361(1)	1318(1)
272(8)	278(10)	857(7)	811(13)	1400(7)	1360(8)
302(1)	307(2)	869(1)	834(3)	1409(1)	1370(1)
334(6)	335(2)	872(2)	836(1)	1437(1)	1387(1)
344(8)	348(0)	878(3)	837(0)	1447(2)	1401(1)
347(0)	352(11)	901(17)	858(0)	1449(6)	1404(0)
379(2)	373(4)	905(1)	860(6)	1454(0)	1407(3)
438(3)	429(2)	906(0)	876(0)	1485(63)	1444(0)
461(1)	450(0)	915(2)	882(12)	1489(0)	1450(64)
505(3)	487(1)	1013(2)	986(3)	1504(0)	1465(0)
549(16)	532(8)	1020(3)	997(5)	3219(4)	3144(0)
561(3)	539(2)	1031(5)	999(1)	3219(0)	3145(5)
584(6)	559(8)	1038(31)	1007(28)	3220(0)	3146(0)
644(1)	624(0)	1048(11)	1015(15)	3230(0)	3155(6)
666(0)	651(0)	1066(0)	1035(0)	3231(5)	3156(1)
677(2)	659(1)	1068(9)	1038(10)	3237(2)	3162(4)
690(0)	664(1)	1072(0)	1041(2)	3242(1)	3168(12)
705(72)	677(75)	1128(1)	1103(1)	3243(7)	3171(1)
717(0)	695(0)	1133(5)	1104(3)	3244(5)	3172(3)
746(1)	724(18)	1180(2)	1140(1)	3249(3)	3177(3)
757(14)	729(12)	1184(0)	1143(0)	3250(0)	3177(2)
766(0)	735(12)	1278(0)	1240(1)	3251(1)	3178(0)

Table S67 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ti-3T** of $(C_8H_6)_2Ti$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
94(4)	89(3)	781(31)	736(5)	1257(0)	1213(1)
127(0)	124(0)	792(4)	745(5)	1289(5)	1244(3)
201(0)	197(1)	803(57)	766(43)	1317(5)	1268(8)
216(0)	229(1)	832(16)	786(18)	1336(0)	1291(4)
228(0)	237(0)	842(29)	799(1)	1339(0)	1293(0)
254(0)	262(1)	853(0)	806(13)	1387(0)	1343(0)
286(9)	289(6)	869(13)	835(14)	1388(4)	1346(2)
314(1)	304(0)	892(5)	860(1)	1419(0)	1367(1)
321(26)	339(9)	913(8)	878(1)	1423(4)	1373(4)
392(17)	395(1)	938(4)	887(1)	1468(7)	1418(6)
402(2)	399(1)	938(0)	889(6)	1469(3)	1420(2)
404(6)	401(6)	962(3)	938(3)	1512(2)	1468(1)
453(2)	438(2)	973(2)	942(2)	1512(5)	1469(7)
459(2)	446(1)	1005(2)	974(4)	1602(1)	1540(17)
480(0)	466(0)	1013(13)	978(10)	1603(5)	1540(4)
569(21)	546(13)	1022(25)	989(24)	3044(9)	2963(12)
596(0)	564(0)	1027(20)	994(27)	3049(45)	2967(53)
619(5)	601(4)	1032(1)	997(3)	3202(1)	3128(3)
642(0)	624(0)	1079(2)	1044(3)	3202(1)	3128(1)
665(4)	640(5)	1081(0)	1046(2)	3217(14)	3141(9)
673(13)	642(17)	1126(4)	1090(5)	3221(0)	3145(1)
679(9)	650(11)	1139(1)	1103(0)	3226(18)	3151(19)
708(2)	681(0)	1175(5)	1129(4)	3226(6)	3151(6)
717(75)	686(77)	1185(2)	1138(1)	3237(1)	3161(1)
754(17)	716(17)	1198(3)	1150(2)	3237(0)	3161(3)
759(48)	720(17)	1220(4)	1172(3)	3251(1)	3178(0)
773(14)	731(48)	1256(1)	1209(0)	3251(0)	3178(0)

Table S68 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ti-4S** of $(C_8H_6)_2Ti$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
61(18)	-22(24)	791(12)	752(55)	1266(0)	1216(0)
112(1)	107(1)	793(40)	758(7)	1283(1)	1241(0)
120(3)	119(3)	797(15)	760(13)	1308(5)	1259(5)
218(7)	211(6)	834(13)	805(9)	1336(0)	1291(1)
232(0)	233(0)	858(10)	819(11)	1338(8)	1292(12)
245(1)	244(2)	861(1)	822(3)	1377(3)	1327(2)
280(1)	276(1)	873(7)	839(5)	1380(8)	1328(9)
295(0)	286(0)	882(6)	848(4)	1396(1)	1355(0)
303(0)	299(0)	895(0)	859(3)	1402(8)	1361(8)
382(0)	367(0)	933(4)	881(0)	1433(11)	1381(15)
393(1)	398(0)	933(0)	882(4)	1439(7)	1388(5)
397(2)	402(0)	957(3)	930(4)	1515(12)	1476(13)
450(3)	434(2)	979(0)	949(0)	1522(5)	1484(6)
465(0)	453(0)	998(6)	964(32)	1601(18)	1538(31)
494(0)	481(0)	999(31)	966(10)	1604(10)	1544(16)
572(0)	544(0)	1025(2)	995(5)	3028(17)	2938(22)
581(0)	555(0)	1030(12)	1000(13)	3032(56)	2943(72)
613(7)	596(6)	1032(23)	1001(19)	3201(3)	3126(4)
634(0)	611(1)	1076(3)	1042(3)	3201(1)	3126(1)
639(1)	615(0)	1079(1)	1046(1)	3214(0)	3135(0)
674(11)	646(10)	1124(12)	1087(18)	3214(1)	3135(1)
681(33)	652(39)	1133(0)	1097(0)	3225(20)	3149(15)
703(0)	676(3)	1177(0)	1132(0)	3225(6)	3149(8)
715(65)	684(66)	1178(9)	1132(12)	3228(1)	3150(0)
742(25)	704(17)	1209(0)	1164(0)	3228(3)	3150(10)
752(24)	713(3)	1215(4)	1167(4)	3248(1)	3172(1)
760(6)	716(12)	1256(2)	1213(1)	3249(1)	3172(2)

Table S69 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ti-5T** of $(C_8H_6)_2Ti$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
84(0)	88(0)	782(14)	755(33)	1255(0)	1204(0)
134(1)	131(1)	792(34)	756(11)	1289(7)	1247(4)
186(3)	199(2)	812(3)	766(4)	1307(1)	1259(5)
221(1)	238(0)	822(4)	775(5)	1337(3)	1290(11)
245(0)	242(2)	851(22)	801(24)	1340(3)	1294(3)
248(0)	252(2)	857(13)	805(13)	1387(1)	1343(1)
263(1)	265(1)	874(5)	841(4)	1387(1)	1346(0)
323(2)	324(2)	891(2)	856(4)	1418(2)	1372(1)
331(3)	338(0)	912(5)	866(4)	1420(1)	1375(1)
393(15)	384(1)	920(5)	868(1)	1466(0)	1414(1)
398(1)	402(0)	929(8)	880(5)	1469(0)	1422(0)
398(2)	416(4)	931(2)	892(6)	1518(0)	1469(1)
437(5)	425(3)	976(14)	944(1)	1518(1)	1472(1)
477(12)	465(9)	977(4)	951(18)	1601(6)	1531(22)
483(0)	466(2)	1015(0)	979(0)	1604(6)	1532(14)
584(4)	554(3)	1018(9)	984(11)	3054(6)	2969(8)
593(1)	563(0)	1032(6)	1000(11)	3069(57)	2982(68)
637(1)	619(1)	1035(15)	1005(8)	3207(2)	3134(3)
644(4)	622(4)	1077(0)	1041(0)	3212(3)	3138(4)
667(0)	635(3)	1083(1)	1050(3)	3220(0)	3141(6)
673(2)	647(16)	1129(1)	1093(4)	3221(1)	3141(1)
688(11)	655(2)	1138(6)	1103(10)	3231(1)	3157(1)
699(0)	671(1)	1176(2)	1127(3)	3233(1)	3160(0)
719(48)	687(62)	1190(0)	1141(0)	3236(1)	3162(13)
755(34)	707(25)	1192(4)	1143(5)	3236(17)	3163(4)
755(47)	708(14)	1239(3)	1190(5)	3247(0)	3174(0)
767(1)	726(1)	1248(1)	1200(1)	3249(2)	3177(3)

Table S70 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ti-6S** of $(C_8H_6)_2Ti$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
83(0)	82(0)	775(1)	733(15)	1255(0)	1206(0)
130(0)	125(0)	777(5)	745(2)	1278(2)	1237(4)
214(1)	206(5)	791(19)	755(16)	1298(6)	1251(8)
230(19)	226(20)	792(9)	755(2)	1339(5)	1296(11)
258(3)	254(0)	845(10)	806(8)	1345(2)	1301(2)
261(1)	258(5)	846(16)	807(16)	1373(0)	1333(0)
262(1)	261(1)	875(5)	842(4)	1377(25)	1338(25)
317(1)	304(11)	881(12)	848(15)	1391(14)	1343(12)
317(12)	310(0)	906(1)	869(3)	1396(2)	1349(3)
398(2)	400(1)	913(5)	871(3)	1431(1)	1376(3)
415(2)	410(1)	929(0)	876(7)	1435(7)	1381(6)
423(8)	414(5)	930(9)	888(5)	1530(11)	1490(11)
438(0)	440(1)	976(3)	943(2)	1533(2)	1493(2)
481(6)	467(4)	985(36)	957(52)	1596(9)	1528(19)
486(1)	468(6)	1000(17)	968(16)	1597(9)	1533(15)
572(11)	547(13)	1016(15)	985(21)	3036(11)	2947(14)
582(2)	559(4)	1018(28)	989(4)	3049(79)	2958(103)
631(3)	612(2)	1019(4)	992(17)	3205(1)	3130(1)
645(6)	625(8)	1074(0)	1041(0)	3210(3)	3134(3)
673(0)	645(0)	1080(5)	1046(5)	3219(1)	3140(2)
676(4)	652(10)	1127(4)	1092(9)	3219(1)	3140(1)
688(12)	659(3)	1137(3)	1102(4)	3228(2)	3153(2)
696(0)	668(0)	1176(4)	1130(6)	3231(1)	3153(3)
720(68)	689(67)	1177(3)	1131(4)	3231(2)	3153(3)
732(85)	693(80)	1187(3)	1140(2)	3233(17)	3157(17)
738(7)	706(0)	1235(4)	1187(4)	3244(0)	3167(0)
768(1)	730(4)	1245(2)	1199(1)	3246(3)	3168(5)

Table S71 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **V-1D** of $(C_8H_6)_2V$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
29(1)	24(0)	790(43)	754(15)	1284(1)	1244(0)
89(1)	90(0)	793(4)	756(8)	1302(9)	1257(8)
123(0)	126(0)	802(50)	763(29)	1308(2)	1266(4)
136(1)	142(1)	807(5)	768(27)	1319(10)	1282(6)
177(2)	183(1)	816(5)	778(2)	1321(25)	1286(10)
238(1)	240(3)	819(4)	786(5)	1385(4)	1355(2)
302(13)	307(14)	855(3)	817(6)	1405(0)	1371(1)
328(12)	333(11)	868(1)	835(1)	1417(1)	1377(1)
339(0)	346(1)	876(0)	838(1)	1435(1)	1386(2)
352(8)	353(10)	883(1)	842(0)	1438(1)	1390(1)
362(4)	359(6)	884(0)	858(2)	1451(1)	1405(3)
399(8)	391(10)	906(13)	863(4)	1453(3)	1407(0)
446(5)	435(3)	914(1)	865(4)	1477(0)	1433(0)
469(0)	458(1)	925(4)	891(10)	1504(2)	1461(7)
528(2)	513(1)	1019(6)	987(4)	1532(7)	1494(2)
555(2)	531(2)	1035(6)	1001(6)	3198(14)	3126(13)
577(3)	558(3)	1039(16)	1010(18)	3223(0)	3148(0)
613(2)	588(2)	1049(6)	1017(12)	3230(7)	3154(1)
644(0)	626(1)	1052(7)	1024(6)	3231(2)	3156(5)
664(3)	644(1)	1063(7)	1031(6)	3232(5)	3158(10)
669(2)	651(7)	1070(0)	1039(1)	3237(11)	3161(1)
695(69)	667(73)	1077(2)	1043(5)	3239(0)	3164(12)
712(12)	687(6)	1123(11)	1095(9)	3245(2)	3169(2)
717(0)	694(3)	1138(1)	1108(0)	3249(0)	3177(0)
726(10)	697(0)	1185(0)	1142(0)	3254(0)	3180(0)
757(3)	736(16)	1186(0)	1145(0)	3256(0)	3183(0)
776(19)	741(7)	1283(13)	1241(13)	3262(0)	3186(0)

Table S72 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **V-2D** of $(C_8H_6)_2V$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
66(0)	71(0)	777(0)	750(0)	1268(8)	1229(4)
106(0)	112(0)	779(36)	753(51)	1318(11)	1272(9)
118(0)	119(0)	786(13)	767(8)	1319(1)	1274(1)
139(0)	143(0)	802(2)	776(11)	1327(0)	1286(0)
140(3)	155(3)	813(15)	781(4)	1331(5)	1290(2)
186(1)	178(1)	828(4)	786(2)	1388(13)	1344(2)
220(2)	228(1)	865(0)	830(0)	1394(0)	1350(0)
268(3)	277(3)	866(0)	831(0)	1430(2)	1391(2)
331(3)	328(2)	884(3)	837(1)	1431(6)	1391(3)
343(3)	344(5)	886(0)	839(2)	1467(7)	1424(2)
358(3)	354(4)	892(4)	842(5)	1471(1)	1427(1)
420(6)	411(8)	892(0)	844(0)	1494(38)	1451(15)
448(1)	437(1)	901(0)	873(0)	1499(0)	1456(0)
455(1)	447(0)	902(25)	875(24)	1512(2)	1465(4)
503(14)	489(11)	1008(11)	982(12)	1514(1)	1469(1)
566(0)	542(0)	1008(3)	983(1)	3216(4)	3141(3)
569(1)	550(1)	1035(8)	1006(5)	3216(0)	3141(0)
606(0)	581(0)	1035(1)	1006(0)	3229(0)	3153(1)
628(5)	608(5)	1051(1)	1019(1)	3229(9)	3154(12)
686(5)	668(7)	1053(16)	1022(15)	3233(0)	3157(0)
689(0)	672(0)	1082(5)	1048(3)	3233(0)	3158(0)
712(0)	681(0)	1085(0)	1052(0)	3244(1)	3168(0)
713(117)	682(105)	1126(2)	1096(1)	3244(1)	3170(3)
717(3)	692(1)	1128(13)	1099(8)	3245(11)	3170(14)
720(1)	696(0)	1185(1)	1143(0)	3246(3)	3171(3)
766(7)	735(8)	1186(0)	1145(0)	3257(0)	3180(3)
769(27)	744(17)	1268(2)	1229(6)	3257(2)	3180(0)

Table S73 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **V-3D** of $(C_8H_6)_2V$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-194(5)	-197(5)	769(0)	738(0)	1271(2)	1233(1)
88(0)	92(0)	778(1)	751(0)	1317(10)	1273(8)
111(5)	97(6)	797(5)	770(0)	1319(0)	1275(0)
119(1)	124(0)	801(0)	773(12)	1335(0)	1296(0)
120(1)	143(1)	815(0)	791(0)	1342(0)	1302(0)
152(0)	156(0)	821(1)	791(2)	1384(9)	1344(1)
191(0)	200(0)	865(0)	833(0)	1396(0)	1354(0)
243(6)	238(4)	866(1)	834(2)	1433(3)	1393(2)
249(0)	244(0)	889(0)	840(0)	1438(0)	1399(0)
307(1)	303(1)	891(7)	841(8)	1464(4)	1419(1)
332(0)	325(0)	893(0)	846(0)	1478(0)	1432(0)
401(0)	391(0)	894(0)	846(2)	1483(0)	1441(1)
443(1)	430(1)	904(0)	878(0)	1486(0)	1442(1)
444(3)	432(3)	906(34)	880(28)	1498(8)	1456(3)
484(13)	472(9)	1017(14)	987(13)	1502(0)	1462(0)
551(2)	515(5)	1018(3)	988(1)	3221(2)	3147(2)
552(2)	520(1)	1037(2)	1012(0)	3222(0)	3147(0)
605(0)	579(0)	1041(0)	1015(0)	3223(0)	3148(0)
628(5)	609(5)	1049(1)	1018(2)	3223(1)	3148(0)
688(15)	671(21)	1052(17)	1021(19)	3235(0)	3160(0)
701(0)	683(0)	1086(3)	1053(2)	3235(0)	3160(0)
716(16)	694(22)	1090(0)	1057(0)	3235(0)	3160(0)
718(0)	694(0)	1125(1)	1096(1)	3237(12)	3162(17)
741(0)	710(1)	1131(5)	1103(2)	3246(0)	3171(0)
751(182)	718(166)	1186(0)	1144(0)	3246(1)	3171(1)
752(31)	726(30)	1187(0)	1146(0)	3248(12)	3173(16)
763(11)	736(10)	1270(2)	1231(5)	3248(0)	3173(0)

Table S74 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **V-4D** of $(C_8H_6)_2V$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
119(13)	95(3)	793(31)	749(0)	1265(0)	1214(1)
120(1)	123(0)	794(20)	751(1)	1283(0)	1243(2)
172(1)	146(9)	799(11)	763(28)	1313(7)	1265(6)
239(0)	229(0)	831(7)	791(11)	1336(0)	1292(9)
249(3)	232(7)	843(6)	794(3)	1343(27)	1293(0)
257(0)	238(0)	859(9)	806(9)	1380(3)	1346(1)
300(1)	273(0)	880(4)	837(6)	1385(3)	1347(5)
304(0)	300(3)	886(10)	853(5)	1393(17)	1358(2)
315(8)	305(0)	924(39)	872(0)	1398(1)	1359(0)
388(1)	381(0)	935(1)	887(0)	1435(4)	1402(9)
413(1)	407(0)	936(5)	888(4)	1439(3)	1407(4)
415(0)	418(11)	958(1)	935(2)	1522(1)	1459(5)
451(2)	439(1)	978(1)	937(2)	1524(0)	1468(0)
464(0)	448(2)	998(5)	972(4)	1603(16)	1540(15)
489(1)	475(0)	1007(7)	972(13)	1605(7)	1542(5)
574(0)	549(0)	1020(17)	989(16)	3035(17)	2962(14)
578(5)	553(0)	1021(22)	993(16)	3039(56)	2966(60)
617(8)	601(4)	1025(4)	999(8)	3201(1)	3128(3)
631(0)	619(0)	1072(0)	1044(1)	3201(2)	3128(1)
643(6)	623(3)	1081(5)	1044(1)	3217(0)	3151(0)
671(7)	640(13)	1124(13)	1088(8)	3223(24)	3151(20)
678(25)	649(17)	1132(1)	1098(2)	3226(25)	3151(4)
699(0)	674(0)	1178(8)	1129(9)	3226(6)	3152(1)
727(41)	690(62)	1181(3)	1137(0)	3233(1)	3165(0)
745(18)	715(17)	1205(0)	1151(2)	3233(4)	3165(1)
764(44)	731(47)	1219(2)	1171(2)	3254(0)	3177(1)
764(4)	741(9)	1257(8)	1210(0)	3254(4)	3177(1)

Table S75 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **V-5D** of $(C_8H_6)_2V$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
87(0)	88(0)	779(24)	748(3)	1256(0)	1206(0)
147(1)	141(0)	782(13)	755(26)	1282(1)	1244(5)
223(1)	212(2)	790(23)	761(2)	1300(6)	1257(6)
245(18)	247(1)	794(4)	768(6)	1334(3)	1291(8)
259(2)	249(5)	833(1)	793(15)	1344(11)	1294(2)
276(1)	256(5)	836(3)	796(12)	1377(1)	1342(1)
301(9)	269(0)	873(5)	840(4)	1388(11)	1345(9)
311(17)	306(15)	879(14)	851(8)	1390(11)	1361(2)
314(1)	325(2)	900(1)	869(0)	1397(0)	1365(3)
402(0)	388(0)	910(5)	869(3)	1431(2)	1400(3)
424(2)	408(22)	926(0)	876(7)	1437(3)	1408(2)
427(7)	419(1)	928(7)	888(3)	1524(0)	1471(6)
460(6)	430(1)	972(2)	942(2)	1525(5)	1474(0)
477(5)	462(3)	976(29)	946(32)	1594(7)	1532(14)
489(0)	467(6)	1004(7)	976(1)	1598(14)	1535(16)
560(5)	544(3)	1015(10)	982(16)	3048(10)	2968(10)
568(6)	556(0)	1018(9)	997(10)	3061(69)	2980(84)
631(2)	614(3)	1020(30)	1001(23)	3206(2)	3133(2)
642(2)	620(3)	1072(0)	1040(0)	3211(3)	3137(4)
669(1)	640(2)	1081(9)	1047(1)	3216(0)	3150(0)
673(4)	640(16)	1126(3)	1092(3)	3216(2)	3151(0)
688(1)	654(1)	1137(8)	1100(9)	3229(2)	3156(2)
692(0)	666(0)	1177(2)	1129(2)	3234(16)	3160(13)
725(58)	691(58)	1177(1)	1140(1)	3240(0)	3161(1)
747(60)	710(23)	1182(4)	1140(6)	3241(6)	3162(3)
754(23)	722(26)	1237(3)	1191(5)	3246(0)	3173(0)
775(6)	731(3)	1245(2)	1201(0)	3248(3)	3174(3)

Table S76 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **V-6Q** of $(C_8H_6)_2V$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
119(0)	113(0)	802(45)	762(1)	1259(1)	1217(1)
127(0)	124(0)	806(0)	768(40)	1286(5)	1244(4)
208(0)	202(0)	815(0)	772(0)	1315(1)	1266(3)
213(0)	217(1)	831(18)	802(12)	1338(8)	1293(12)
233(2)	236(1)	860(1)	813(5)	1338(1)	1295(0)
271(3)	270(4)	862(15)	813(12)	1389(2)	1347(3)
290(3)	290(5)	872(8)	840(6)	1390(3)	1349(2)
315(0)	309(0)	890(1)	857(1)	1411(0)	1366(0)
342(4)	346(5)	914(1)	880(0)	1415(2)	1370(1)
392(17)	393(5)	938(4)	890(0)	1462(2)	1415(3)
415(2)	414(2)	938(0)	892(4)	1462(2)	1416(1)
417(2)	418(3)	961(2)	929(2)	1505(2)	1461(1)
455(2)	442(1)	962(2)	938(2)	1505(0)	1462(0)
461(1)	449(1)	1003(2)	974(3)	1602(3)	1543(4)
489(1)	479(0)	1014(5)	981(5)	1603(7)	1544(9)
587(0)	560(0)	1024(7)	991(6)	3048(9)	2971(10)
592(1)	563(1)	1034(14)	1003(17)	3053(37)	2975(41)
622(7)	607(6)	1035(13)	1003(11)	3203(1)	3129(2)
638(0)	622(0)	1078(1)	1045(1)	3203(2)	3129(1)
668(8)	642(12)	1079(4)	1046(4)	3227(18)	3152(20)
675(10)	645(12)	1125(7)	1089(8)	3227(6)	3152(6)
687(20)	657(14)	1138(0)	1102(0)	3229(0)	3156(0)
709(0)	682(0)	1171(2)	1121(2)	3229(1)	3156(1)
723(35)	695(41)	1185(2)	1140(1)	3241(2)	3167(2)
755(13)	721(11)	1196(2)	1151(2)	3241(1)	3167(1)
770(73)	732(49)	1219(2)	1172(1)	3251(1)	3176(1)
778(9)	741(3)	1256(0)	1209(0)	3251(1)	3176(2)

Table S77 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **V-7Q** of $(C_8H_6)_2V$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
85(0)	85(0)	785(18)	758(19)	1254(0)	1206(1)
140(0)	139(1)	794(38)	759(11)	1288(4)	1247(4)
201(0)	207(1)	803(0)	761(13)	1304(0)	1258(2)
241(3)	236(0)	813(0)	773(0)	1334(2)	1290(5)
243(0)	245(4)	855(10)	807(7)	1339(6)	1294(6)
266(0)	267(0)	857(11)	811(10)	1388(0)	1347(0)
274(3)	273(2)	872(4)	839(5)	1393(5)	1352(3)
322(1)	326(3)	889(2)	857(2)	1413(1)	1370(1)
351(8)	353(8)	908(1)	872(2)	1417(1)	1373(1)
389(11)	382(2)	915(2)	875(0)	1464(1)	1416(2)
413(4)	415(0)	928(8)	879(7)	1467(1)	1423(0)
426(2)	422(6)	931(2)	889(2)	1509(0)	1465(0)
437(3)	434(1)	959(12)	933(16)	1510(2)	1467(1)
475(12)	464(9)	974(4)	943(3)	1602(6)	1539(10)
493(2)	479(1)	1014(0)	980(0)	1604(5)	1540(5)
578(1)	551(1)	1018(6)	985(5)	3063(6)	2984(6)
596(0)	569(0)	1032(7)	1001(9)	3078(48)	2997(54)
642(2)	621(3)	1037(22)	1007(18)	3208(2)	3135(2)
643(3)	625(2)	1074(0)	1040(0)	3213(4)	3139(4)
670(0)	643(1)	1083(5)	1050(5)	3226(0)	3153(0)
674(4)	650(8)	1128(1)	1093(1)	3228(0)	3154(0)
692(4)	659(1)	1137(3)	1100(3)	3232(1)	3158(2)
699(0)	671(0)	1171(3)	1123(4)	3237(1)	3163(17)
718(46)	689(50)	1189(0)	1144(0)	3238(16)	3164(0)
762(17)	725(19)	1191(4)	1145(3)	3240(4)	3166(5)
765(65)	729(44)	1240(3)	1194(3)	3248(1)	3174(1)
774(14)	739(3)	1247(1)	1199(0)	3249(2)	3174(3)

Table S78 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **V-8Q** of $(C_8H_6)_2V$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
31(0)	42(0)	773(2)	738(3)	1282(0)	1244(2)
66(0)	65(0)	775(5)	739(2)	1290(24)	1258(18)
90(0)	84(0)	782(68)	748(43)	1309(5)	1267(5)
122(1)	111(1)	796(11)	761(1)	1319(1)	1284(2)
133(0)	134(0)	807(5)	775(10)	1329(15)	1302(10)
183(2)	190(2)	823(3)	786(5)	1356(0)	1311(1)
230(2)	235(4)	858(3)	814(2)	1390(3)	1346(2)
264(2)	276(2)	865(0)	829(0)	1404(8)	1366(6)
321(1)	328(2)	872(0)	834(1)	1425(1)	1378(0)
350(3)	354(1)	881(4)	837(2)	1447(2)	1396(3)
354(8)	360(11)	883(2)	841(1)	1455(5)	1410(8)
377(2)	381(4)	886(4)	842(4)	1476(18)	1438(23)
438(3)	431(2)	899(12)	870(1)	1481(69)	1447(63)
455(2)	442(2)	901(2)	871(13)	1506(2)	1467(2)
478(6)	459(1)	1019(2)	989(2)	1510(5)	1475(6)
552(9)	538(2)	1019(2)	989(6)	3218(2)	3144(2)
564(2)	540(2)	1022(6)	1004(28)	3220(1)	3145(1)
576(10)	558(11)	1035(29)	1007(1)	3225(1)	3153(1)
614(5)	589(7)	1038(6)	1009(9)	3230(0)	3156(1)
665(0)	649(0)	1050(11)	1018(7)	3232(3)	3159(3)
682(2)	659(2)	1067(9)	1037(12)	3234(4)	3160(5)
685(1)	668(2)	1077(2)	1043(2)	3239(2)	3166(1)
695(5)	674(8)	1125(5)	1098(5)	3242(1)	3167(3)
707(30)	682(48)	1131(4)	1104(1)	3243(8)	3170(14)
709(47)	684(48)	1182(1)	1142(1)	3244(10)	3170(7)
723(43)	691(16)	1184(0)	1144(0)	3247(1)	3174(2)
769(13)	735(10)	1277(8)	1239(10)	3253(1)	3177(2)

Table S79 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Cr-1S** of $(C_8H_6)_2Cr$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
41(0)	52(0)	791(5)	758(19)	1280(0)	1235(0)
129(0)	129(0)	801(2)	761(1)	1300(4)	1255(1)
138(0)	131(0)	812(0)	774(25)	1305(9)	1258(7)
154(2)	153(1)	813(67)	780(1)	1327(98)	1291(69)
155(1)	157(1)	827(7)	784(6)	1333(4)	1302(2)
261(2)	267(4)	833(2)	790(2)	1336(2)	1314(3)
312(7)	320(11)	856(7)	801(6)	1397(0)	1362(0)
351(9)	345(4)	862(0)	827(1)	1416(1)	1366(1)
360(0)	366(21)	874(4)	848(6)	1422(8)	1377(1)
365(13)	367(0)	885(5)	849(1)	1433(0)	1383(7)
418(31)	417(41)	911(9)	863(3)	1446(7)	1395(4)
426(9)	420(3)	913(5)	871(6)	1448(0)	1399(0)
447(12)	434(11)	929(3)	879(8)	1474(0)	1423(0)
482(2)	473(7)	941(5)	901(7)	1517(117)	1483(82)
535(0)	515(1)	1013(2)	982(0)	1535(3)	1500(1)
549(2)	522(2)	1018(7)	985(9)	3190(14)	3117(15)
574(0)	554(0)	1037(20)	1002(3)	3228(0)	3148(1)
629(1)	603(1)	1041(19)	1009(9)	3231(1)	3149(0)
642(5)	631(2)	1046(6)	1017(19)	3236(3)	3154(1)
663(9)	641(11)	1055(2)	1024(5)	3240(7)	3156(6)
679(19)	663(11)	1069(0)	1036(0)	3241(0)	3165(8)
703(0)	683(97)	1074(2)	1039(3)	3244(9)	3168(14)
704(102)	684(1)	1106(18)	1078(15)	3248(4)	3170(2)
711(2)	687(0)	1143(1)	1109(0)	3258(0)	3182(1)
723(0)	702(0)	1182(0)	1137(0)	3262(0)	3186(1)
778(2)	742(12)	1184(0)	1140(0)	3263(0)	3188(0)
787(16)	752(5)	1269(28)	1231(21)	3266(0)	3191(0)

Table S80 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Cr-2T** of $(C_8H_6)_2Cr$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
123(1)	120(1)	794(8)	755(1)	1261(0)	1215(1)
131(0)	126(0)	802(2)	758(1)	1281(3)	1239(2)
216(6)	210(9)	808(10)	763(18)	1310(5)	1261(6)
219(0)	221(0)	833(14)	793(2)	1337(1)	1292(12)
255(22)	246(26)	850(1)	803(6)	1337(9)	1293(1)
261(0)	259(0)	854(7)	811(12)	1386(3)	1341(2)
302(2)	296(1)	873(7)	839(6)	1389(1)	1345(3)
313(1)	310(3)	882(2)	849(1)	1396(5)	1348(1)
317(3)	313(3)	901(0)	866(0)	1400(2)	1355(2)
392(2)	384(2)	936(0)	887(0)	1438(7)	1386(9)
416(1)	421(2)	936(3)	888(4)	1442(3)	1392(2)
424(3)	429(4)	956(1)	931(2)	1504(6)	1460(7)
456(0)	443(0)	965(2)	935(2)	1511(1)	1470(1)
464(0)	452(0)	998(3)	967(5)	1603(13)	1543(19)
499(0)	489(0)	1004(14)	969(14)	1604(6)	1545(8)
577(0)	548(0)	1021(4)	988(5)	3041(14)	2958(17)
586(0)	558(0)	1030(14)	999(15)	3045(50)	2962(58)
617(7)	603(6)	1032(17)	1000(14)	3202(2)	3127(2)
629(0)	613(0)	1070(3)	1039(4)	3202(1)	3127(2)
646(2)	618(2)	1074(0)	1041(0)	3226(19)	3151(21)
672(6)	644(6)	1122(6)	1086(8)	3226(6)	3151(6)
683(20)	655(24)	1132(0)	1097(0)	3229(0)	3152(0)
705(0)	677(1)	1179(7)	1132(7)	3229(0)	3153(0)
722(53)	693(59)	1181(0)	1137(0)	3241(1)	3165(1)
747(16)	712(14)	1200(0)	1154(1)	3242(2)	3165(3)
774(72)	740(50)	1217(3)	1170(3)	3253(1)	3175(1)
783(8)	745(5)	1258(2)	1213(0)	3253(1)	3175(2)

Table S81 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Cr-3T** of $(C_8H_6)_2Cr$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
27(0)	42(0)	761(1)	731(1)	1281(82)	1247(1)
58(0)	76(0)	762(5)	735(1)	1287(5)	1264(60)
67(1)	78(0)	787(21)	765(62)	1305(2)	1271(0)
106(1)	94(2)	798(0)	771(1)	1325(7)	1281(3)
132(0)	145(0)	810(0)	781(4)	1327(15)	1285(13)
193(0)	188(0)	818(4)	783(1)	1345(7)	1323(10)
208(0)	217(1)	848(205)	821(32)	1382(3)	1355(0)
265(0)	295(1)	857(0)	824(0)	1408(0)	1376(1)
329(125)	348(23)	867(25)	838(12)	1410(7)	1377(0)
357(2)	353(0)	874(0)	844(1)	1429(143)	1389(1)
364(3)	365(16)	888(9)	846(0)	1439(0)	1391(1)
367(8)	392(11)	890(1)	847(1)	1460(326)	1456(100)
414(50)	436(0)	891(0)	860(11)	1494(2)	1464(0)
443(2)	439(7)	893(1)	863(0)	1520(17)	1490(10)
445(10)	455(1)	1020(12)	992(8)	1538(0)	1499(0)
557(53)	546(10)	1022(1)	993(0)	3215(21)	3142(9)
565(1)	550(1)	1025(63)	1006(8)	3215(7)	3142(7)
589(0)	570(0)	1035(2)	1009(35)	3227(0)	3153(0)
595(26)	579(16)	1036(35)	1012(3)	3227(0)	3153(0)
650(40)	638(1)	1049(0)	1025(0)	3234(0)	3160(0)
668(3)	647(0)	1067(23)	1035(13)	3234(0)	3160(2)
668(1)	655(1)	1070(4)	1037(4)	3239(0)	3164(0)
683(2)	660(0)	1117(14)	1093(6)	3239(15)	3165(13)
700(23)	683(108)	1128(5)	1102(0)	3247(1)	3172(1)
703(1)	685(0)	1185(2)	1147(1)	3247(2)	3173(12)
707(65)	690(3)	1185(0)	1147(0)	3249(7)	3173(4)
717(1)	692(1)	1262(478)	1237(10)	3250(6)	3173(0)

Table S82 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Cr-4T** of $(C_8H_6)_2Cr$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
26(0)	44(0)	757(1)	731(2)	1279(126)	1241(9)
51(1)	60(1)	759(0)	736(0)	1285(8)	1270(41)
64(0)	76(0)	791(66)	761(0)	1308(3)	1274(4)
95(0)	104(0)	792(0)	765(55)	1325(4)	1284(2)
137(2)	110(8)	807(0)	772(5)	1327(5)	1287(4)
187(1)	188(0)	813(0)	785(1)	1339(15)	1330(1)
208(0)	200(1)	847(284)	822(29)	1382(1)	1348(1)
254(0)	280(0)	861(0)	826(0)	1408(25)	1376(0)
343(174)	357(2)	868(31)	840(12)	1413(4)	1382(2)
349(0)	358(1)	876(1)	842(0)	1427(273)	1391(8)
365(3)	369(33)	887(14)	843(3)	1440(0)	1398(1)
368(6)	380(10)	889(1)	845(1)	1460(485)	1450(131)
408(150)	436(1)	889(0)	863(14)	1490(0)	1458(0)
443(1)	443(3)	892(0)	864(0)	1515(22)	1484(13)
446(7)	463(1)	1020(2)	990(12)	1535(0)	1497(1)
557(121)	542(0)	1021(74)	990(7)	3214(50)	3141(23)
568(0)	548(18)	1022(14)	1009(3)	3215(1)	3141(2)
591(0)	573(0)	1036(1)	1010(38)	3230(1)	3155(0)
594(31)	585(14)	1036(79)	1013(1)	3230(0)	3155(0)
651(81)	642(11)	1048(0)	1020(1)	3237(0)	3164(3)
658(1)	648(3)	1066(47)	1039(24)	3237(0)	3164(6)
669(1)	652(1)	1070(0)	1042(0)	3238(1)	3165(0)
683(0)	665(0)	1114(54)	1087(29)	3238(9)	3166(2)
697(25)	681(63)	1128(4)	1099(3)	3245(26)	3171(15)
706(1)	687(72)	1185(4)	1146(0)	3245(1)	3171(3)
710(114)	688(1)	1185(1)	1147(0)	3250(4)	3175(2)
711(0)	693(1)	1261(708)	1233(36)	3250(0)	3176(1)

Table S83 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Cr-5T** of $(C_8H_6)_2Cr$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
89(0)	89(0)	781(7)	757(17)	1255(0)	1205(0)
154(0)	151(0)	791(14)	758(5)	1281(2)	1240(3)
213(0)	215(0)	804(8)	762(5)	1299(5)	1253(6)
257(12)	249(13)	819(2)	780(1)	1335(5)	1292(9)
263(2)	256(2)	842(12)	797(12)	1342(4)	1298(4)
281(1)	282(1)	846(5)	797(4)	1380(0)	1340(0)
284(9)	287(6)	874(6)	840(5)	1389(10)	1349(4)
321(19)	313(28)	884(5)	852(8)	1395(7)	1349(8)
328(1)	330(1)	902(1)	867(1)	1402(2)	1355(3)
402(3)	394(0)	909(3)	868(0)	1438(2)	1384(4)
423(6)	413(6)	927(0)	876(8)	1442(3)	1392(1)
428(0)	436(3)	928(8)	885(3)	1516(6)	1473(6)
465(2)	452(3)	968(22)	939(2)	1518(0)	1475(0)
479(6)	467(4)	972(3)	943(30)	1597(6)	1530(10)
495(1)	490(1)	1007(4)	973(4)	1599(9)	1535(13)
566(5)	541(4)	1016(8)	985(7)	3051(9)	2968(11)
588(0)	562(0)	1025(7)	995(7)	3065(68)	2980(80)
628(3)	611(3)	1027(27)	998(23)	3206(1)	3131(1)
640(2)	620(2)	1070(0)	1037(0)	3211(3)	3136(3)
671(0)	645(1)	1075(5)	1044(5)	3229(0)	3152(0)
674(2)	649(5)	1125(2)	1089(3)	3230(0)	3153(0)
693(3)	662(1)	1135(3)	1100(4)	3230(2)	3155(3)
696(0)	669(1)	1178(1)	1132(3)	3234(15)	3158(15)
723(52)	694(57)	1181(1)	1136(2)	3240(1)	3163(1)
756(31)	717(25)	1183(5)	1137(4)	3241(4)	3165(7)
769(51)	736(35)	1238(3)	1190(4)	3249(0)	3172(1)
780(11)	745(8)	1247(1)	1201(0)	3250(3)	3173(4)

Table S84 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Cr-6S** of $(C_8H_6)_2Cr$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
65(0)	60(0)	785(0)	758(0)	1265(1)	1223(1)
87(5)	99(2)	795(45)	770(46)	1318(13)	1270(12)
110(0)	117(0)	803(3)	779(3)	1320(3)	1272(0)
117(0)	119(0)	817(1)	789(1)	1327(1)	1282(0)
167(0)	173(0)	843(9)	800(7)	1330(8)	1285(3)
249(1)	248(1)	859(5)	817(8)	1380(15)	1332(1)
272(10)	268(12)	863(3)	824(1)	1386(0)	1336(0)
289(4)	299(3)	863(1)	828(0)	1431(5)	1385(4)
326(6)	318(2)	883(2)	832(2)	1431(15)	1386(6)
361(4)	360(5)	884(2)	835(6)	1481(11)	1434(0)
406(15)	413(19)	888(2)	841(0)	1483(0)	1434(0)
429(10)	416(9)	891(1)	844(0)	1499(110)	1458(52)
456(1)	447(4)	902(17)	874(15)	1512(3)	1469(2)
472(1)	470(2)	903(0)	874(0)	1533(8)	1485(14)
507(3)	491(3)	992(5)	965(1)	1535(0)	1486(0)
569(0)	543(0)	994(6)	965(7)	3214(2)	3136(1)
574(2)	554(1)	1026(3)	994(2)	3215(2)	3137(7)
596(0)	567(0)	1027(14)	995(4)	3226(1)	3151(1)
618(7)	592(6)	1050(1)	1016(1)	3226(10)	3151(8)
675(5)	652(85)	1052(14)	1020(14)	3234(0)	3157(0)
677(0)	653(4)	1083(7)	1048(4)	3235(1)	3158(0)
690(3)	657(29)	1086(0)	1050(0)	3244(0)	3166(0)
691(129)	657(0)	1124(0)	1092(0)	3245(4)	3169(8)
708(3)	681(2)	1129(29)	1099(23)	3246(16)	3172(18)
715(1)	688(1)	1184(1)	1141(0)	3246(0)	3172(0)
753(4)	722(5)	1186(0)	1144(0)	3258(0)	3178(6)
765(8)	741(1)	1264(14)	1221(11)	3258(3)	3178(0)

Table S85 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Mn-1D** of $(C_8H_6)_2Mn$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
128(0)	111(1)	800(27)	769(4)	1260(0)	1215(0)
145(0)	123(1)	828(3)	769(5)	1283(5)	1241(4)
216(0)	212(2)	829(2)	786(1)	1310(3)	1258(7)
231(1)	220(1)	837(14)	800(11)	1338(7)	1290(5)
272(0)	267(21)	855(11)	803(9)	1340(2)	1296(2)
285(22)	268(0)	867(0)	819(6)	1393(2)	1348(1)
313(1)	305(1)	876(13)	839(6)	1393(2)	1348(2)
323(3)	315(2)	887(1)	852(0)	1403(1)	1354(3)
332(7)	334(8)	904(0)	868(1)	1403(3)	1357(2)
396(3)	387(1)	939(1)	890(1)	1447(5)	1391(8)
440(10)	437(1)	939(3)	891(3)	1450(1)	1394(0)
441(2)	440(10)	954(2)	921(2)	1504(2)	1460(2)
463(0)	455(0)	958(1)	933(1)	1510(0)	1468(0)
466(0)	460(1)	999(2)	969(3)	1606(3)	1546(10)
508(1)	501(3)	1008(8)	971(8)	1606(8)	1547(3)
580(0)	549(3)	1021(2)	986(2)	3052(12)	2972(14)
593(1)	567(1)	1037(10)	1002(9)	3057(41)	2976(46)
619(6)	576(11)	1039(12)	1005(10)	3202(1)	3126(1)
635(2)	617(14)	1071(0)	1035(1)	3202(2)	3126(3)
654(6)	617(3)	1076(7)	1043(7)	3226(19)	3145(2)
678(8)	648(16)	1121(4)	1084(4)	3226(6)	3148(1)
687(17)	651(9)	1133(0)	1096(0)	3229(0)	3150(21)
710(0)	681(0)	1175(3)	1126(3)	3230(0)	3150(7)
723(42)	686(60)	1184(0)	1137(0)	3242(3)	3158(4)
757(8)	715(23)	1198(1)	1151(2)	3242(1)	3159(0)
787(64)	722(7)	1219(3)	1169(4)	3251(3)	3168(5)
800(5)	756(64)	1259(1)	1210(0)	3251(4)	3168(7)

Table S86 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Mn-2D** of $(C_8H_6)_2Mn$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
30(0)	37(0)	760(0)	726(0)	1268(3)	1241(0)
59(0)	68(0)	765(2)	736(1)	1290(0)	1255(38)
94(0)	95(1)	789(36)	771(54)	1293(2)	1259(5)
112(1)	112(0)	810(3)	781(0)	1330(11)	1298(0)
164(0)	167(0)	816(0)	784(6)	1334(5)	1310(17)
169(2)	173(0)	833(0)	792(0)	1350(16)	1312(6)
197(0)	217(1)	837(0)	811(5)	1356(0)	1317(0)
268(1)	303(0)	838(121)	816(2)	1397(9)	1368(4)
337(124)	359(40)	859(31)	839(17)	1404(0)	1370(0)
368(4)	388(0)	874(1)	846(2)	1422(149)	1380(4)
380(0)	402(11)	890(1)	846(1)	1432(1)	1382(0)
389(7)	425(6)	890(0)	847(0)	1460(320)	1453(115)
401(25)	434(0)	892(0)	863(2)	1493(10)	1468(0)
441(8)	439(2)	896(1)	868(0)	1520(0)	1488(0)
442(0)	449(1)	1001(1)	987(0)	1538(0)	1493(0)
555(76)	547(17)	1011(31)	989(2)	3215(8)	3140(6)
559(5)	550(1)	1015(40)	990(3)	3216(7)	3141(7)
583(0)	571(1)	1018(0)	993(27)	3232(0)	3156(0)
588(39)	579(13)	1027(7)	1011(4)	3232(1)	3159(0)
638(0)	626(1)	1048(0)	1017(0)	3238(0)	3162(0)
655(4)	645(3)	1061(30)	1030(16)	3239(0)	3164(3)
668(3)	646(0)	1063(12)	1032(7)	3239(0)	3166(0)
672(0)	660(5)	1109(3)	1085(6)	3239(12)	3166(14)
704(0)	684(103)	1130(0)	1089(0)	3245(13)	3171(7)
707(2)	687(0)	1179(0)	1141(0)	3246(10)	3172(12)
710(89)	692(2)	1181(0)	1143(0)	3251(1)	3175(2)
718(1)	699(4)	1261(330)	1233(13)	3252(2)	3178(8)

Table S87 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Mn-3D** of $(C_8H_6)_2Mn$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
90(0)	98(0)	795(31)	756(38)	1255(0)	1204(0)
161(0)	171(2)	798(7)	769(6)	1284(4)	1239(5)
208(0)	186(4)	824(0)	789(6)	1300(2)	1253(5)
265(2)	235(3)	836(1)	795(4)	1336(4)	1289(9)
271(6)	261(2)	858(3)	812(10)	1341(4)	1292(3)
287(0)	280(8)	866(14)	830(12)	1385(0)	1331(1)
307(11)	283(0)	875(11)	841(10)	1393(8)	1338(6)
333(1)	337(40)	889(1)	858(1)	1403(3)	1359(1)
338(29)	349(5)	903(0)	868(0)	1410(2)	1367(2)
407(3)	391(0)	908(2)	869(0)	1447(2)	1393(2)
422(7)	407(6)	929(1)	878(8)	1450(0)	1402(1)
448(0)	438(2)	929(8)	883(3)	1515(1)	1471(0)
467(2)	446(5)	957(15)	939(19)	1516(0)	1471(0)
481(7)	479(1)	972(3)	940(2)	1601(3)	1534(5)
497(1)	487(1)	1012(2)	976(1)	1602(7)	1539(11)
569(2)	543(4)	1019(5)	984(5)	3063(7)	2981(8)
595(1)	563(1)	1031(5)	997(7)	3077(58)	2992(68)
631(6)	610(8)	1035(18)	1003(13)	3206(1)	3132(2)
638(2)	617(1)	1068(0)	1033(0)	3211(2)	3136(3)
675(1)	644(2)	1076(6)	1040(2)	3226(0)	3146(0)
676(0)	645(3)	1123(1)	1086(1)	3228(1)	3146(1)
699(3)	659(3)	1134(1)	1097(3)	3230(2)	3151(1)
701(0)	670(0)	1172(4)	1128(4)	3234(18)	3153(13)
723(44)	694(46)	1186(4)	1140(5)	3235(0)	3155(3)
765(8)	724(13)	1186(0)	1140(1)	3237(7)	3159(19)
783(45)	736(12)	1240(3)	1190(3)	3248(3)	3165(16)
784(19)	755(5)	1246(1)	1200(0)	3248(5)	3165(5)

Table S88 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Mn-4Q** of $(C_8H_6)_2Mn$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
39(0)	-56(0)	744(2)	717(0)	1275(0)	1236(12)
84(0)	68(0)	751(0)	717(2)	1281(11)	1240(65)
86(0)	78(0)	780(48)	741(0)	1288(0)	1248(1)
135(0)	129(1)	782(0)	742(56)	1320(0)	1291(0)
187(0)	172(0)	795(0)	760(0)	1331(15)	1297(6)
193(0)	186(0)	803(0)	761(0)	1347(8)	1310(2)
229(0)	220(0)	811(1)	767(0)	1360(5)	1323(2)
281(1)	288(1)	836(121)	794(2)	1399(276)	1355(0)
344(135)	331(0)	847(47)	826(19)	1403(7)	1364(9)
364(0)	362(21)	873(0)	839(1)	1404(0)	1373(48)
392(4)	400(3)	883(1)	839(0)	1434(0)	1387(0)
407(6)	405(8)	886(8)	845(3)	1450(114)	1421(127)
412(47)	429(0)	887(3)	862(4)	1490(10)	1451(3)
444(0)	436(18)	893(0)	867(0)	1502(0)	1459(0)
448(5)	441(2)	1006(27)	978(0)	1521(1)	1481(1)
545(36)	534(5)	1010(0)	981(0)	3213(11)	3140(3)
561(0)	543(0)	1016(8)	983(7)	3217(7)	3143(7)
591(0)	564(0)	1019(21)	989(22)	3233(0)	3158(1)
597(26)	573(15)	1034(0)	1009(0)	3234(1)	3158(0)
649(13)	637(1)	1049(0)	1024(0)	3242(0)	3165(0)
652(1)	640(0)	1063(30)	1036(12)	3243(6)	3167(8)
666(0)	643(1)	1066(7)	1037(9)	3246(0)	3171(0)
672(1)	644(0)	1108(0)	1073(0)	3247(2)	3172(3)
691(0)	669(0)	1111(7)	1082(4)	3248(12)	3172(7)
699(63)	671(101)	1177(1)	1135(0)	3250(7)	3174(9)
705(3)	677(1)	1178(0)	1136(1)	3254(1)	3178(1)
709(3)	687(2)	1247(425)	1227(0)	3254(1)	3178(2)

Table S89 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Mn-5Q** of $(C_8H_6)_2Mn$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
124(0)	118(1)	798(52)	761(2)	1260(0)	1214(0)
129(0)	125(0)	806(3)	762(45)	1283(2)	1238(2)
189(0)	185(0)	814(2)	771(4)	1313(0)	1262(2)
200(2)	198(4)	835(18)	790(2)	1331(2)	1283(5)
218(1)	221(2)	850(1)	808(13)	1340(10)	1292(12)
242(1)	236(1)	861(16)	817(13)	1378(3)	1325(6)
264(2)	265(3)	868(3)	836(4)	1384(10)	1342(8)
304(3)	298(4)	885(10)	850(7)	1401(1)	1351(1)
323(7)	326(6)	917(0)	880(3)	1410(2)	1371(0)
359(8)	354(1)	936(2)	887(0)	1466(3)	1410(4)
370(4)	356(1)	938(2)	890(4)	1477(3)	1436(4)
400(0)	396(1)	958(2)	923(2)	1490(3)	1444(4)
450(5)	435(5)	963(2)	939(2)	1516(5)	1474(4)
459(1)	448(1)	1000(2)	969(2)	1596(3)	1530(7)
479(4)	461(5)	1008(6)	973(6)	1599(4)	1538(6)
557(5)	523(4)	1019(7)	983(10)	3055(10)	2978(18)
592(2)	565(2)	1027(23)	991(22)	3060(36)	2986(30)
625(3)	607(1)	1034(14)	1002(14)	3202(2)	3127(2)
637(2)	616(10)	1070(1)	1035(1)	3203(2)	3129(3)
661(4)	623(3)	1074(3)	1040(1)	3224(0)	3148(0)
667(6)	635(6)	1125(10)	1087(11)	3226(14)	3150(14)
678(18)	645(14)	1133(1)	1093(2)	3226(11)	3152(11)
695(3)	665(5)	1162(3)	1108(4)	3228(0)	3154(1)
720(38)	689(42)	1181(1)	1134(1)	3239(2)	3160(3)
748(12)	713(11)	1194(4)	1147(5)	3242(1)	3167(1)
761(53)	721(32)	1220(1)	1170(1)	3246(2)	3168(2)
771(14)	734(6)	1252(1)	1205(1)	3254(1)	3178(2)

Table S90 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Mn-6Q** of $(C_8H_6)_2Mn$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
56(0)	54(0)	777(5)	749(0)	1257(0)	1210(0)
109(0)	117(0)	777(0)	751(2)	1279(4)	1234(4)
161(0)	168(1)	791(9)	761(30)	1296(0)	1246(7)
183(2)	172(2)	798(33)	761(7)	1329(4)	1284(0)
194(1)	195(2)	836(16)	786(12)	1335(8)	1296(7)
236(3)	232(2)	841(14)	792(11)	1365(0)	1314(4)
255(0)	250(0)	873(1)	839(0)	1368(13)	1321(20)
284(0)	304(3)	874(0)	839(1)	1390(23)	1339(14)
299(7)	313(9)	897(10)	864(0)	1396(0)	1343(1)
368(21)	361(8)	908(2)	865(2)	1447(4)	1391(4)
375(3)	384(4)	933(9)	875(2)	1449(0)	1396(0)
391(0)	398(0)	933(2)	875(13)	1536(1)	1498(1)
434(4)	420(4)	958(9)	919(6)	1539(2)	1498(5)
465(1)	430(1)	978(4)	953(2)	1590(8)	1507(19)
478(8)	463(7)	1012(0)	977(4)	1592(7)	1516(32)
538(1)	494(15)	1015(17)	979(47)	3060(7)	2987(6)
568(11)	546(11)	1019(2)	982(2)	3074(52)	3000(53)
634(0)	609(0)	1020(28)	983(13)	3205(2)	3129(2)
641(0)	613(4)	1063(7)	1038(5)	3210(3)	3134(3)
656(2)	633(5)	1072(5)	1038(6)	3227(1)	3151(1)
664(2)	636(0)	1126(0)	1087(0)	3228(0)	3151(0)
672(4)	649(7)	1127(6)	1089(5)	3228(2)	3152(2)
697(2)	674(5)	1171(4)	1117(8)	3233(16)	3155(16)
726(44)	696(57)	1186(4)	1138(5)	3240(1)	3162(1)
755(56)	720(32)	1186(1)	1138(3)	3241(2)	3162(5)
760(30)	722(25)	1239(3)	1191(0)	3249(1)	3171(2)
771(25)	745(17)	1245(0)	1193(4)	3251(2)	3172(2)

Table S91 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe-1S** of $(C_8H_6)_2Fe$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
137(0)	133(0)	810(0)	769(1)	1258(2)	1215(1)
171(0)	168(1)	818(3)	785(1)	1281(3)	1237(2)
229(1)	235(3)	839(14)	804(4)	1310(6)	1260(8)
244(2)	238(2)	841(4)	808(10)	1336(10)	1290(13)
276(0)	269(0)	866(0)	816(13)	1337(1)	1292(1)
326(1)	320(0)	867(8)	819(4)	1381(2)	1334(2)
332(10)	324(12)	875(13)	840(8)	1388(1)	1340(0)
348(13)	351(15)	888(1)	853(0)	1404(0)	1356(1)
370(6)	375(7)	910(0)	875(0)	1414(2)	1364(1)
432(11)	423(10)	936(2)	888(1)	1448(2)	1396(1)
457(1)	449(5)	937(2)	890(2)	1449(2)	1397(2)
460(6)	459(8)	944(2)	909(2)	1496(1)	1449(1)
470(5)	463(4)	958(1)	935(1)	1500(0)	1453(1)
491(6)	494(11)	998(1)	969(1)	1606(3)	1546(3)
521(5)	516(10)	1009(4)	974(4)	1608(10)	1548(11)
576(0)	544(0)	1018(3)	984(3)	3060(13)	2982(14)
589(0)	561(0)	1031(13)	997(14)	3064(42)	2986(45)
628(5)	615(4)	1034(12)	1000(10)	3202(1)	3126(1)
639(3)	621(4)	1069(2)	1037(2)	3202(2)	3126(3)
666(7)	638(7)	1074(2)	1040(2)	3227(19)	3150(22)
679(10)	653(14)	1121(4)	1084(5)	3227(6)	3150(6)
692(12)	668(12)	1132(0)	1095(0)	3237(0)	3154(2)
708(0)	680(0)	1173(3)	1123(3)	3237(1)	3155(1)
727(41)	701(48)	1185(1)	1140(0)	3248(3)	3166(8)
757(3)	724(2)	1194(1)	1148(2)	3248(2)	3166(1)
789(39)	754(23)	1219(2)	1172(2)	3256(4)	3173(6)
802(36)	767(27)	1257(0)	1208(0)	3256(3)	3173(8)

Table S92 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe-2S** of $(C_8H_6)_2Fe$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
99(0)	101(0)	796(40)	761(7)	1253(0)	1203(0)
178(1)	181(1)	806(4)	773(2)	1284(3)	1241(3)
228(1)	236(3)	823(7)	782(12)	1299(4)	1252(5)
265(2)	259(3)	848(1)	816(1)	1330(4)	1285(6)
292(2)	282(2)	865(0)	821(2)	1338(6)	1291(6)
295(0)	294(0)	875(11)	835(10)	1381(0)	1335(0)
330(7)	326(6)	878(12)	842(10)	1392(2)	1346(1)
353(5)	361(10)	891(2)	857(2)	1405(3)	1358(2)
402(1)	391(0)	902(0)	867(0)	1415(2)	1365(2)
405(22)	404(13)	905(1)	868(0)	1450(1)	1398(2)
438(17)	428(24)	925(1)	876(7)	1457(0)	1408(1)
463(3)	456(6)	926(7)	880(1)	1502(0)	1454(0)
488(7)	481(9)	951(14)	927(15)	1504(2)	1457(2)
493(1)	498(2)	969(2)	936(2)	1599(2)	1532(2)
524(3)	524(4)	1010(0)	974(0)	1602(9)	1538(10)
567(1)	542(1)	1017(5)	983(4)	3069(7)	2990(8)
592(1)	562(0)	1027(9)	994(10)	3083(58)	3002(63)
637(1)	615(0)	1035(13)	1003(10)	3207(1)	3131(1)
640(7)	624(8)	1065(0)	1030(0)	3211(3)	3136(3)
676(1)	653(4)	1077(4)	1044(3)	3230(1)	3148(0)
680(4)	653(7)	1122(1)	1084(1)	3231(1)	3150(2)
697(2)	669(2)	1133(2)	1096(3)	3233(1)	3155(3)
699(0)	670(1)	1169(4)	1123(4)	3235(18)	3159(0)
724(49)	696(52)	1185(0)	1139(0)	3241(0)	3159(20)
767(5)	730(6)	1185(3)	1140(3)	3243(8)	3160(16)
785(13)	746(20)	1240(2)	1191(3)	3252(2)	3170(4)
785(25)	759(18)	1245(1)	1197(0)	3253(6)	3170(10)

Table S93 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe-3S** of $(C_8H_6)_2Fe$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-5(0)	23(0)	782(0)	746(0)	1296(0)	1250(0)
73(0)	64(0)	791(3)	754(3)	1308(41)	1266(29)
114(2)	114(1)	833(58)	795(47)	1311(5)	1270(1)
115(0)	115(0)	845(13)	810(11)	1332(26)	1305(0)
174(0)	173(0)	854(0)	813(0)	1343(0)	1313(13)
237(3)	232(3)	854(15)	815(9)	1349(15)	1317(18)
260(1)	244(1)	864(0)	827(0)	1374(0)	1351(0)
306(1)	301(0)	870(0)	833(1)	1418(0)	1375(6)
362(56)	360(44)	888(9)	846(1)	1422(4)	1378(0)
378(0)	381(0)	892(1)	849(1)	1440(1)	1390(0)
386(13)	398(14)	893(1)	850(1)	1441(0)	1391(0)
446(0)	434(0)	896(1)	852(0)	1512(28)	1475(9)
447(25)	440(1)	899(0)	865(1)	1516(84)	1475(62)
450(4)	447(26)	904(0)	872(0)	1517(0)	1482(0)
473(0)	471(3)	1009(0)	991(2)	1526(0)	1496(0)
570(8)	549(4)	1027(0)	993(0)	3215(9)	3140(5)
575(1)	550(1)	1032(4)	1002(1)	3216(5)	3140(6)
587(3)	561(1)	1037(4)	1007(32)	3225(0)	3142(0)
596(39)	573(24)	1041(43)	1009(1)	3227(0)	3144(1)
600(1)	600(0)	1049(0)	1024(0)	3233(0)	3152(0)
661(1)	643(0)	1065(22)	1034(17)	3235(3)	3154(12)
671(0)	646(0)	1068(6)	1037(8)	3236(0)	3160(0)
678(5)	662(5)	1122(5)	1091(4)	3236(14)	3161(3)
704(0)	687(0)	1134(0)	1103(0)	3243(4)	3161(14)
719(6)	695(106)	1188(0)	1144(0)	3243(13)	3163(19)
724(97)	697(6)	1190(0)	1146(0)	3245(3)	3168(6)
733(4)	702(4)	1269(1)	1235(7)	3247(9)	3168(12)

Table 94 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe-4T** of $(C_8H_6)_2Fe$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
24(0)	-21(0)	762(0)	730(0)	1286(8)	1239(9)
71(0)	71(0)	764(0)	730(0)	1290(153)	1258(0)
113(0)	105(0)	823(0)	789(0)	1294(0)	1258(38)
114(0)	115(0)	832(60)	794(0)	1333(0)	1308(0)
192(0)	196(0)	834(0)	798(45)	1347(0)	1311(0)
251(24)	243(1)	854(1)	802(1)	1348(5)	1312(1)
264(2)	248(18)	855(28)	819(4)	1358(8)	1323(4)
291(0)	297(0)	858(0)	820(0)	1409(0)	1363(11)
367(0)	368(0)	884(0)	838(7)	1410(9)	1366(0)
386(12)	382(14)	886(12)	843(0)	1434(78)	1387(18)
395(0)	394(0)	889(0)	848(0)	1441(0)	1394(0)
423(20)	417(27)	890(0)	848(2)	1472(336)	1442(180)
438(47)	433(0)	893(2)	864(3)	1487(0)	1452(0)
443(0)	435(2)	900(0)	873(0)	1506(0)	1472(0)
448(3)	447(25)	1014(0)	988(0)	1519(0)	1477(0)
551(44)	528(24)	1026(0)	994(4)	3214(13)	3140(10)
574(0)	552(0)	1027(4)	1002(0)	3214(0)	3140(0)
589(0)	563(0)	1033(81)	1002(45)	3232(1)	3150(0)
594(37)	571(21)	1033(0)	1006(0)	3232(0)	3151(0)
642(0)	629(0)	1043(0)	1017(0)	3235(0)	3159(2)
664(1)	638(0)	1065(23)	1036(25)	3235(10)	3160(0)
667(0)	647(11)	1065(0)	1037(0)	3239(0)	3161(0)
673(0)	651(0)	1114(0)	1083(2)	3239(6)	3161(19)
702(0)	680(0)	1120(3)	1087(0)	3243(31)	3168(0)
705(3)	682(3)	1182(0)	1141(0)	3243(0)	3168(22)
712(0)	684(0)	1184(0)	1142(0)	3250(0)	3168(14)
715(137)	688(135)	1275(0)	1236(0)	3251(2)	3169(0)

Table S95 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe-5T** of $(C_8H_6)_2Fe$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
48(0)	36(0)	756(0)	726(0)	1275(0)	1239(10)
90(0)	87(0)	758(2)	731(2)	1283(10)	1252(36)
120(0)	119(0)	813(0)	774(0)	1295(5)	1259(2)
138(3)	137(3)	816(44)	783(42)	1329(0)	1301(0)
206(0)	200(0)	830(1)	801(3)	1340(15)	1308(5)
225(0)	237(3)	843(49)	809(1)	1352(4)	1318(2)
272(1)	265(1)	844(1)	814(2)	1366(14)	1332(10)
302(6)	305(3)	863(0)	829(0)	1409(5)	1364(0)
367(46)	375(9)	875(19)	836(5)	1411(0)	1365(8)
391(0)	378(0)	884(0)	840(0)	1417(175)	1384(20)
411(5)	408(12)	887(2)	843(1)	1442(0)	1393(0)
413(12)	429(15)	890(1)	849(2)	1457(102)	1428(93)
441(53)	432(0)	892(3)	866(1)	1491(0)	1452(0)
445(0)	455(0)	901(1)	874(0)	1498(0)	1459(0)
459(1)	460(26)	1017(0)	986(0)	1518(0)	1477(0)
548(12)	535(0)	1020(20)	991(4)	3214(4)	3140(1)
564(0)	542(0)	1024(5)	993(0)	3216(8)	3142(5)
592(2)	564(2)	1029(0)	1004(18)	3231(0)	3149(0)
596(23)	572(13)	1035(17)	1007(0)	3232(1)	3150(3)
651(5)	634(0)	1046(0)	1021(0)	3239(0)	3161(0)
660(0)	639(0)	1067(12)	1038(7)	3240(7)	3162(0)
663(0)	642(0)	1068(11)	1040(10)	3243(0)	3163(1)
666(0)	651(2)	1105(0)	1071(0)	3244(5)	3164(19)
692(0)	671(0)	1116(7)	1088(5)	3246(10)	3168(0)
703(94)	677(118)	1182(1)	1140(0)	3247(8)	3169(9)
709(0)	684(0)	1183(0)	1140(1)	3251(2)	3170(21)
713(5)	691(5)	1269(236)	1230(0)	3252(6)	3171(3)

Table S96 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe-6T** of $(C_8H_6)_2Fe$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
99(0)	104(0)	796(41)	759(19)	1261(0)	1216(1)
124(0)	120(0)	801(13)	762(15)	1282(5)	1240(4)
176(0)	183(0)	823(1)	785(1)	1311(1)	1260(4)
189(0)	198(0)	833(16)	804(13)	1321(2)	1275(4)
223(1)	222(1)	856(6)	807(13)	1332(5)	1286(6)
246(2)	241(3)	862(14)	817(1)	1373(1)	1328(6)
270(3)	275(4)	864(1)	831(3)	1380(21)	1333(14)
286(2)	285(3)	880(0)	847(0)	1390(6)	1342(7)
301(2)	298(5)	903(5)	867(2)	1395(5)	1346(5)
369(18)	360(4)	933(2)	875(5)	1441(0)	1384(1)
390(3)	381(3)	941(2)	893(2)	1464(7)	1417(6)
399(7)	413(2)	960(2)	932(1)	1513(9)	1469(15)
455(3)	439(2)	965(2)	935(4)	1519(1)	1473(2)
458(2)	449(2)	1002(5)	970(7)	1590(13)	1513(25)
476(1)	475(0)	1013(4)	977(7)	1604(5)	1546(7)
499(1)	506(1)	1022(10)	988(6)	3050(13)	2972(13)
585(3)	550(3)	1024(22)	993(23)	3054(34)	2976(39)
615(8)	597(3)	1032(11)	1003(9)	3201(1)	3126(2)
633(2)	613(6)	1059(4)	1030(4)	3203(2)	3129(3)
651(9)	621(11)	1076(7)	1041(7)	3226(14)	3150(14)
666(3)	641(8)	1119(6)	1082(9)	3226(10)	3151(0)
676(11)	648(11)	1126(3)	1089(2)	3229(2)	3151(9)
690(6)	669(7)	1176(4)	1126(6)	3230(0)	3153(2)
721(42)	684(40)	1184(1)	1138(1)	3241(2)	3162(3)
747(8)	716(12)	1199(1)	1152(2)	3247(1)	3168(2)
770(48)	733(22)	1219(2)	1170(2)	3252(2)	3171(4)
779(26)	746(41)	1256(1)	1207(0)	3256(2)	3178(2)

Table S97 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Fe-7T** of $(C_8H_6)_2Fe$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
79(0)	90(0)	783(17)	755(19)	1258(0)	1212(1)
132(0)	125(2)	789(76)	756(79)	1279(7)	1236(10)
166(0)	160(1)	803(9)	769(4)	1297(0)	1247(1)
197(0)	179(0)	816(6)	789(1)	1327(5)	1282(4)
199(1)	214(6)	853(12)	803(14)	1329(1)	1286(0)
214(10)	231(4)	858(14)	811(19)	1374(2)	1319(0)
253(0)	244(0)	874(0)	839(1)	1377(3)	1324(1)
296(1)	280(1)	882(0)	840(1)	1395(15)	1350(5)
302(0)	325(9)	900(7)	860(2)	1398(2)	1350(8)
378(0)	365(1)	901(1)	869(0)	1476(13)	1442(9)
383(22)	372(2)	932(8)	871(0)	1479(1)	1442(0)
392(0)	386(0)	932(2)	876(9)	1528(2)	1487(6)
433(5)	423(6)	947(7)	913(5)	1529(0)	1487(0)
472(4)	439(9)	976(3)	944(3)	1592(4)	1523(10)
474(10)	459(7)	1013(0)	976(0)	1592(2)	1525(2)
568(12)	523(7)	1014(7)	978(9)	3071(6)	2998(6)
579(4)	547(11)	1026(1)	991(3)	3086(47)	3012(52)
616(2)	605(3)	1027(18)	991(19)	3206(1)	3131(1)
637(1)	620(2)	1051(9)	1031(3)	3211(2)	3136(3)
644(0)	623(0)	1069(0)	1036(0)	3227(0)	3149(0)
666(1)	633(0)	1123(3)	1083(2)	3228(3)	3149(5)
672(1)	650(1)	1126(1)	1091(2)	3229(2)	3155(2)
698(0)	666(0)	1164(4)	1109(8)	3234(18)	3159(18)
725(35)	698(27)	1191(4)	1145(0)	3240(0)	3161(1)
761(3)	723(4)	1191(0)	1146(6)	3242(3)	3163(5)
770(29)	740(15)	1243(3)	1190(0)	3249(3)	3168(5)
778(24)	741(6)	1245(0)	1198(4)	3250(4)	3170(8)

Table S98 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Co-1D** of $(C_8H_6)_2Co$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
32(0)	29(0)	750(1)	719(1)	1279(44)	1245(3)
71(0)	71(0)	753(9)	722(8)	1286(7)	1247(55)
100(1)	107(1)	823(35)	794(52)	1301(0)	1263(0)
143(5)	135(1)	836(1)	805(0)	1335(5)	1290(0)
178(1)	177(0)	844(94)	812(21)	1338(15)	1297(19)
237(2)	234(5)	851(2)	817(4)	1338(2)	1317(1)
242(3)	235(1)	858(0)	826(0)	1366(5)	1327(1)
293(0)	300(0)	862(5)	828(2)	1407(5)	1368(4)
340(87)	341(41)	885(10)	846(5)	1410(1)	1374(0)
381(10)	385(8)	886(0)	851(0)	1434(18)	1385(1)
395(8)	388(1)	891(0)	854(0)	1436(0)	1386(0)
395(8)	396(26)	894(1)	854(1)	1477(218)	1454(92)
443(1)	434(0)	897(0)	860(1)	1493(1)	1459(0)
446(3)	436(5)	899(1)	863(0)	1520(5)	1491(2)
455(18)	462(7)	1018(1)	989(4)	1536(0)	1500(0)
555(33)	543(10)	1022(2)	991(0)	3212(13)	3137(8)
561(4)	547(1)	1022(40)	995(8)	3213(9)	3137(11)
587(1)	566(0)	1031(22)	1000(20)	3232(0)	3150(1)
591(22)	571(11)	1034(1)	1014(5)	3232(1)	3150(0)
644(14)	634(4)	1042(0)	1017(0)	3239(1)	3159(2)
657(6)	639(0)	1065(13)	1032(11)	3239(2)	3159(5)
668(3)	641(2)	1067(6)	1035(6)	3240(1)	3166(2)
669(6)	655(6)	1111(8)	1087(8)	3240(16)	3166(15)
703(9)	680(92)	1124(7)	1098(1)	3250(2)	3168(3)
705(79)	685(2)	1183(0)	1142(0)	3251(6)	3169(11)
706(2)	689(7)	1184(0)	1143(0)	3253(5)	3176(4)
716(0)	692(0)	1263(223)	1235(13)	3253(5)	3176(7)

Table S99 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Co-2D** of $(C_8H_6)_2Co$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-27(0)	-19(0)	752(0)	719(0)	1272(6)	1246(0)
71(0)	69(0)	757(3)	724(4)	1288(0)	1249(42)
117(0)	117(2)	828(1)	800(56)	1299(5)	1265(1)
117(13)	118(0)	836(188)	807(0)	1334(1)	1288(1)
156(0)	155(0)	845(0)	812(15)	1334(0)	1302(22)
226(8)	230(1)	845(7)	815(4)	1343(9)	1309(0)
230(1)	232(5)	856(3)	831(1)	1348(19)	1331(2)
286(1)	295(0)	867(1)	831(0)	1406(0)	1369(5)
320(159)	333(50)	881(8)	846(5)	1409(7)	1373(0)
365(8)	373(9)	888(3)	853(0)	1433(42)	1383(1)
379(0)	384(0)	891(0)	853(0)	1433(3)	1384(0)
387(10)	412(22)	895(0)	856(0)	1465(368)	1455(105)
433(47)	433(0)	895(0)	856(0)	1489(23)	1467(0)
443(0)	435(6)	898(2)	868(0)	1525(0)	1490(0)
444(7)	460(7)	1010(0)	992(0)	1527(0)	1499(0)
546(18)	545(9)	1020(33)	992(3)	3212(13)	3136(7)
550(72)	547(2)	1023(0)	995(2)	3213(9)	3137(12)
581(0)	567(0)	1027(42)	1001(23)	3229(1)	3148(0)
585(40)	573(14)	1032(8)	1013(0)	3230(0)	3150(1)
639(0)	625(1)	1032(0)	1017(5)	3236(0)	3157(0)
646(6)	639(0)	1062(21)	1031(13)	3238(4)	3159(8)
663(0)	639(1)	1065(7)	1033(6)	3240(0)	3166(3)
681(7)	665(8)	1110(6)	1086(9)	3240(11)	3167(0)
689(0)	674(0)	1127(0)	1099(0)	3245(11)	3167(11)
706(74)	683(100)	1183(0)	1143(0)	3246(11)	3168(15)
711(4)	693(1)	1185(0)	1145(0)	3248(4)	3172(7)
717(0)	694(4)	1260(320)	1236(15)	3250(6)	3173(8)

Table S100 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, inkm/mol) for the structure **Co-3D** of $(C_8H_6)_2Co$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
115(0)	119(0)	793(17)	761(25)	1260(0)	1212(3)
141(0)	145(0)	797(2)	766(3)	1285(5)	1241(4)
185(0)	174(5)	806(9)	769(1)	1310(3)	1261(5)
206(0)	193(1)	836(15)	806(11)	1330(9)	1281(15)
230(0)	231(1)	848(3)	808(5)	1331(1)	1286(0)
253(1)	246(2)	861(0)	818(1)	1357(6)	1310(8)
287(2)	284(19)	863(11)	823(7)	1371(6)	1322(8)
302(2)	284(0)	884(0)	851(0)	1397(25)	1348(18)
302(3)	298(4)	902(12)	870(3)	1403(0)	1354(0)
383(22)	372(8)	936(0)	880(0)	1440(2)	1389(5)
383(11)	396(22)	937(4)	881(9)	1447(0)	1399(1)
418(2)	409(2)	957(1)	932(3)	1524(9)	1470(15)
443(3)	426(5)	964(2)	932(2)	1527(1)	1475(2)
457(2)	444(0)	1002(5)	970(13)	1596(19)	1520(41)
461(1)	446(1)	1010(3)	976(2)	1599(9)	1529(17)
493(0)	486(1)	1016(26)	984(22)	3052(11)	2973(12)
587(2)	554(3)	1020(8)	988(12)	3056(40)	2976(45)
618(12)	601(11)	1029(2)	997(3)	3202(2)	3128(4)
639(0)	610(2)	1064(15)	1029(10)	3202(1)	3128(1)
644(3)	621(0)	1078(2)	1041(3)	3226(18)	3151(15)
672(3)	648(1)	1116(11)	1075(19)	3226(5)	3151(4)
677(9)	649(11)	1133(0)	1097(0)	3233(3)	3155(5)
707(1)	679(0)	1179(5)	1130(8)	3234(1)	3155(2)
724(54)	689(67)	1186(0)	1140(0)	3247(1)	3170(3)
751(4)	714(3)	1201(1)	1154(1)	3248(2)	3170(3)
778(86)	746(51)	1221(2)	1174(2)	3257(1)	3179(4)
788(3)	751(1)	1254(2)	1211(0)	3258(2)	3179(2)

Table S101 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, inkm/mol) for the structure **Co-4D** of $(C_8H_6)_2Co$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-20(0)	-32(0)	747(0)	711(0)	1270(0)	1235(293)
66(0)	65(1)	751(0)	711(1)	1290(14)	1245(18)
110(0)	107(0)	827(0)	799(0)	1298(0)	1262(0)
115(0)	116(0)	837(65)	801(121)	1332(0)	1293(9)
155(0)	142(184)	840(0)	808(0)	1338(7)	1304(0)
237(17)	172(0)	841(188)	814(67)	1344(0)	1310(0)
244(1)	235(1)	857(0)	825(1)	1362(0)	1321(1)
277(0)	285(82)	860(1)	825(0)	1407(0)	1368(0)
324(132)	300(0)	885(0)	847(10)	1413(7)	1376(3)
358(0)	362(0)	886(4)	851(0)	1432(60)	1384(14)
377(9)	373(11)	893(4)	851(1)	1438(0)	1389(0)
380(0)	390(0)	894(0)	852(0)	1471(474)	1442(242)
435(42)	431(0)	896(0)	858(3)	1492(0)	1464(0)
441(0)	432(5)	896(0)	869(0)	1516(0)	1482(0)
443(6)	447(23)	1005(0)	987(0)	1529(0)	1485(0)
551(83)	531(41)	1027(0)	995(4)	3212(38)	3136(48)
560(0)	553(0)	1028(122)	998(74)	3212(0)	3137(0)
585(0)	566(0)	1028(5)	999(0)	3233(1)	3153(2)
593(36)	573(21)	1028(0)	1009(0)	3233(0)	3153(0)
622(0)	619(0)	1045(1)	1017(3)	3239(5)	3160(0)
644(44)	623(38)	1063(35)	1033(38)	3239(0)	3160(5)
675(0)	643(0)	1064(0)	1034(0)	3239(0)	3166(0)
677(0)	659(0)	1099(0)	1078(0)	3240(8)	3166(13)
697(0)	679(0)	1127(6)	1094(7)	3245(27)	3170(5)
705(2)	680(0)	1182(0)	1141(0)	3245(0)	3170(0)
709(0)	681(141)	1184(0)	1142(0)	3252(0)	3171(22)
711(142)	681(2)	1264(514)	1233(0)	3252(3)	3172(0)

Table S102 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, inkm/mol) for the structure **Co-5D** of $(C_8H_6)_2Co$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
83(0)	83(0)	783(20)	750(6)	1257(0)	1210(0)
154(0)	155(0)	790(84)	758(61)	1279(8)	1236(12)
178(0)	194(0)	800(12)	766(13)	1295(0)	1247(1)
198(0)	195(0)	815(10)	788(11)	1327(3)	1280(0)
213(2)	207(8)	858(5)	811(1)	1331(11)	1287(12)
254(1)	244(0)	866(9)	823(5)	1365(3)	1317(0)
292(3)	281(3)	876(0)	841(1)	1373(4)	1328(6)
310(1)	325(7)	885(1)	843(1)	1396(16)	1346(7)
326(11)	334(6)	897(1)	857(3)	1401(1)	1350(1)
382(7)	366(4)	898(6)	863(0)	1467(9)	1420(6)
406(2)	404(10)	930(3)	870(2)	1471(2)	1423(0)
412(4)	417(0)	930(7)	873(9)	1528(1)	1482(1)
435(4)	423(4)	943(6)	913(3)	1532(3)	1485(1)
466(1)	441(0)	975(3)	947(3)	1590(8)	1511(16)
474(7)	460(4)	1015(0)	981(0)	1590(3)	1515(12)
561(4)	515(21)	1015(4)	981(4)	3075(6)	3002(5)
566(8)	542(5)	1019(1)	987(3)	3089(47)	3015(48)
617(0)	578(1)	1022(20)	989(28)	3206(1)	3131(1)
639(0)	612(0)	1053(12)	1027(9)	3211(2)	3135(3)
648(1)	630(1)	1066(3)	1032(4)	3229(0)	3150(0)
668(1)	641(0)	1122(4)	1081(5)	3229(2)	3151(7)
673(2)	648(4)	1123(0)	1086(0)	3230(5)	3154(2)
697(2)	670(1)	1161(5)	1108(10)	3234(17)	3157(17)
728(37)	697(45)	1189(4)	1143(5)	3244(0)	3165(0)
763(1)	725(5)	1190(0)	1143(0)	3247(4)	3167(8)
766(21)	733(18)	1242(3)	1186(0)	3254(2)	3174(4)
778(13)	744(16)	1243(0)	1196(4)	3254(2)	3175(3)

Table S103 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, inkm/mol) for the structure **Co-6Q** of $(C_8H_6)_2Co$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
104(0)	98(0)	785(12)	743(6)	1256(1)	1212(3)
121(0)	118(0)	792(1)	757(4)	1287(3)	1246(3)
166(1)	157(1)	804(39)	764(34)	1315(0)	1268(1)
179(0)	179(0)	832(18)	797(18)	1331(4)	1287(6)
187(0)	197(1)	847(31)	804(12)	1333(0)	1290(0)
205(0)	199(1)	851(0)	807(2)	1372(2)	1326(2)
233(0)	243(0)	867(5)	835(4)	1373(3)	1327(8)
275(4)	281(11)	887(1)	856(0)	1408(0)	1364(1)
298(1)	286(1)	913(4)	880(0)	1413(5)	1367(5)
334(37)	330(3)	937(0)	887(0)	1465(1)	1422(0)
372(0)	352(0)	937(4)	889(8)	1466(2)	1425(1)
387(1)	371(1)	960(2)	932(1)	1504(1)	1468(1)
454(3)	439(4)	961(2)	936(2)	1508(2)	1470(3)
456(0)	440(0)	1001(3)	972(6)	1594(2)	1528(10)
474(2)	457(2)	1014(4)	982(3)	1594(7)	1529(3)
591(0)	563(0)	1019(20)	985(22)	3050(8)	2973(9)
594(1)	567(1)	1025(8)	991(10)	3055(37)	2977(38)
626(10)	608(6)	1031(9)	999(5)	3202(1)	3127(1)
637(0)	624(0)	1074(1)	1042(3)	3202(2)	3127(3)
658(4)	628(6)	1076(2)	1042(1)	3226(19)	3149(0)
672(7)	642(5)	1125(8)	1090(10)	3226(6)	3150(0)
680(12)	644(9)	1136(0)	1104(0)	3228(0)	3150(21)
705(0)	674(0)	1167(3)	1116(4)	3229(0)	3151(6)
718(44)	689(46)	1183(1)	1139(1)	3244(2)	3168(3)
751(8)	716(9)	1195(3)	1150(3)	3244(1)	3169(2)
765(77)	736(60)	1218(2)	1172(1)	3253(1)	3179(0)
776(15)	742(2)	1255(0)	1210(0)	3253(3)	3179(4)

Table S1104 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, inkm/mol) for the structure **Co-7Q** of $(C_8H_6)_2Co$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
22(0)	22(0)	785(0)	749(0)	1285(0)	1240(3)
58(0)	57(0)	788(0)	753(0)	1289(1)	1246(0)
88(0)	87(0)	791(0)	760(0)	1292(0)	1262(0)
97(0)	94(0)	794(55)	768(44)	1294(76)	1262(29)
171(0)	180(0)	850(0)	811(0)	1337(31)	1308(0)
196(13)	196(15)	854(1)	821(0)	1346(0)	1313(8)
233(1)	225(1)	855(0)	821(0)	1351(13)	1317(23)
249(0)	260(0)	868(0)	824(0)	1399(0)	1356(26)
273(0)	275(0)	873(0)	825(0)	1403(26)	1359(0)
318(0)	305(8)	873(0)	825(0)	1452(33)	1402(14)
321(9)	353(4)	886(0)	843(0)	1452(0)	1406(0)
351(3)	356(0)	887(2)	846(0)	1474(0)	1442(214)
379(0)	391(4)	902(12)	874(7)	1479(268)	1443(0)
431(0)	421(0)	908(0)	880(0)	1486(0)	1455(0)
435(7)	423(6)	940(0)	970(0)	1502(0)	1466(0)
457(0)	532(0)	1022(0)	990(0)	3218(0)	3144(0)
555(0)	533(7)	1022(0)	991(1)	3218(0)	3144(0)
557(16)	544(20)	1034(5)	1005(80)	3229(0)	3153(3)
571(18)	555(0)	1036(101)	1007(0)	3229(13)	3153(0)
587(0)	561(0)	1037(0)	1014(2)	3230(4)	3155(12)
657(0)	641(0)	1065(31)	1035(33)	3230(0)	3155(0)
662(0)	642(2)	1066(0)	1036(0)	3233(0)	3156(0)
679(0)	643(1)	1112(0)	1086(0)	3234(7)	3157(14)
684(3)	654(0)	1129(0)	1089(0)	3242(28)	3168(29)
690(4)	676(5)	1173(0)	1137(0)	3242(0)	3168(0)
713(0)	680(0)	1181(2)	1140(1)	3256(0)	3177(3)
714(152)	681(147)	1233(0)	1240(0)	3256(1)	3177(0)

Table S105 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Co-8Q** of $(C_8H_6)_2Co$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
33(0)	22(0)	770(41)	738(29)	1265(125)	1234(2)
62(0)	69(0)	788(7)	750(0)	1268(0)	1258(29)
88(0)	100(2)	790(3)	751(4)	1284(1)	1266(3)
100(4)	103(0)	790(0)	758(7)	1293(34)	1275(0)
118(0)	176(0)	838(0)	802(0)	1311(0)	1299(0)
179(0)	195(2)	840(9)	815(2)	1341(40)	1308(22)
189(0)	244(1)	853(0)	820(0)	1352(4)	1318(4)
230(6)	262(2)	859(0)	825(0)	1389(49)	1352(45)
251(1)	270(1)	869(0)	827(5)	1405(0)	1359(0)
261(10)	289(1)	874(6)	830(0)	1429(66)	1400(20)
328(1)	322(2)	874(0)	837(1)	1454(19)	1409(1)
336(20)	364(0)	884(0)	846(2)	1464(8)	1428(45)
364(0)	386(9)	901(14)	873(6)	1470(4)	1436(3)
433(0)	421(0)	903(6)	880(1)	1480(0)	1447(0)
436(6)	424(5)	967(0)	978(1)	1486(101)	1450(42)
490(1)	523(5)	1000(0)	985(0)	3219(1)	3145(0)
545(0)	529(1)	1021(0)	994(2)	3220(1)	3146(0)
549(2)	543(12)	1022(2)	1002(0)	3231(0)	3153(0)
562(33)	551(0)	1027(7)	1002(0)	3231(0)	3154(2)
574(0)	555(0)	1042(58)	1010(54)	3232(11)	3156(0)
650(3)	633(0)	1067(11)	1037(10)	3232(4)	3157(10)
655(0)	642(0)	1069(19)	1040(12)	3237(0)	3159(0)
656(1)	647(0)	1093(1)	1071(0)	3237(6)	3159(12)
685(0)	662(0)	1110(0)	1072(0)	3244(7)	3169(6)
691(0)	663(0)	1176(1)	1137(1)	3245(11)	3170(12)
703(135)	670(139)	1182(0)	1139(0)	3254(2)	3175(2)
712(0)	681(0)	1256(0)	1230(0)	3255(4)	3176(6)

Table S106 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Co-9Q** of $(C_8H_6)_2Co$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
52(0)	39(0)	784(22)	750(2)	1255(0)	1209(0)
132(0)	127(0)	789(22)	756(10)	1285(3)	1244(5)
153(0)	159(0)	803(12)	764(13)	1301(0)	1256(1)
171(0)	162(0)	808(6)	767(20)	1330(0)	1284(0)
175(1)	186(1)	852(19)	809(21)	1333(4)	1291(5)
203(1)	187(1)	858(21)	810(11)	1366(6)	1322(1)
237(0)	241(0)	871(1)	836(3)	1370(0)	1324(9)
277(0)	278(7)	883(1)	846(0)	1409(2)	1366(2)
316(2)	303(2)	909(3)	875(1)	1412(2)	1372(1)
339(41)	332(6)	911(2)	875(2)	1465(0)	1421(0)
366(0)	357(0)	930(8)	881(2)	1466(1)	1421(0)
386(0)	367(1)	933(3)	882(8)	1512(4)	1475(0)
435(4)	422(5)	949(8)	919(8)	1513(1)	1475(4)
470(9)	452(6)	973(4)	945(3)	1593(2)	1521(4)
482(3)	456(4)	1012(7)	981(7)	1596(5)	1524(7)
580(5)	557(2)	1013(0)	981(0)	3068(5)	2996(5)
600(1)	565(0)	1025(1)	991(2)	3084(46)	3011(46)
636(0)	617(1)	1029(31)	995(32)	3207(1)	3132(2)
641(2)	620(0)	1073(1)	1039(3)	3212(4)	3136(4)
659(0)	629(2)	1073(1)	1047(2)	3228(0)	3150(0)
671(3)	649(6)	1130(0)	1094(2)	3229(0)	3150(0)
690(6)	653(3)	1130(3)	1096(0)	3230(2)	3155(3)
700(0)	667(0)	1169(4)	1124(6)	3236(17)	3159(18)
715(51)	690(44)	1189(0)	1144(0)	3237(1)	3161(1)
757(12)	723(20)	1190(4)	1145(4)	3239(3)	3163(5)
762(73)	735(60)	1241(3)	1192(0)	3249(3)	3171(4)
775(20)	744(13)	1244(0)	1197(3)	3250(3)	3172(4)

Table S107 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-1S** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-22(0)	-23(0)	742(5)	705(5)	1283(23)	1239(25)
91(2)	98(2)	749(0)	711(0)	1297(0)	1255(0)
108(0)	112(0)	818(71)	782(0)	1303(9)	1262(9)
146(1)	145(1)	820(0)	783(65)	1305(1)	1263(0)
151(0)	154(0)	831(0)	798(0)	1315(44)	1273(31)
190(0)	197(0)	842(0)	806(0)	1329(24)	1285(14)
212(7)	209(7)	851(0)	815(0)	1381(1)	1341(2)
287(0)	288(1)	856(0)	825(0)	1414(0)	1371(6)
348(4)	342(3)	860(0)	834(0)	1420(6)	1373(0)
357(10)	347(11)	875(0)	843(0)	1421(0)	1374(0)
363(6)	360(6)	883(1)	846(0)	1423(0)	1390(0)
366(0)	363(0)	885(2)	850(1)	1493(8)	1466(10)
448(0)	436(13)	902(0)	858(0)	1533(0)	1498(0)
448(13)	436(0)	906(0)	859(0)	1537(1)	1499(0)
459(0)	451(1)	949(0)	967(0)	1571(0)	1537(0)
532(11)	525(8)	1021(17)	992(17)	3204(2)	3128(2)
574(0)	555(0)	1024(4)	992(9)	3207(15)	3132(17)
590(0)	567(0)	1024(8)	994(3)	3231(0)	3152(0)
602(0)	581(1)	1029(0)	999(0)	3232(0)	3153(1)
603(3)	630(0)	1055(2)	1024(2)	3240(0)	3163(0)
664(3)	646(3)	1057(1)	1026(1)	3241(3)	3163(5)
669(14)	655(10)	1061(10)	1034(4)	3246(0)	3171(1)
685(0)	663(0)	1108(18)	1082(18)	3248(5)	3172(8)
690(10)	672(8)	1125(0)	1097(0)	3250(0)	3172(0)
715(1)	691(0)	1184(0)	1144(0)	3251(6)	3174(7)
727(116)	697(111)	1189(0)	1147(0)	3251(4)	3176(4)
730(9)	700(9)	1229(0)	1226(0)	3253(5)	3178(7)

Table S108 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-2S** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
11(1)	-9(0)	765(0)	725(2)	1286(11)	1243(11)
64(0)	67(0)	765(10)	726(0)	1293(2)	1254(4)
73(0)	70(0)	810(0)	774(42)	1310(2)	1264(0)
123(2)	130(0)	811(46)	777(1)	1311(4)	1266(2)
127(0)	130(1)	854(3)	822(0)	1328(22)	1289(17)
201(5)	194(3)	856(0)	824(3)	1330(151)	1292(107)
204(1)	195(2)	868(0)	832(2)	1375(2)	1339(3)
272(1)	270(1)	870(2)	836(0)	1408(10)	1364(3)
321(17)	309(14)	877(0)	843(0)	1409(0)	1373(0)
347(8)	352(6)	885(5)	848(4)	1427(1)	1380(1)
369(0)	363(0)	889(12)	851(0)	1439(1)	1392(1)
370(0)	366(1)	896(0)	852(2)	1505(17)	1473(11)
439(3)	428(4)	897(3)	857(0)	1522(0)	1484(0)
442(8)	428(6)	903(0)	864(4)	1530(0)	1485(0)
460(7)	451(6)	962(5)	962(1)	1563(3)	1530(1)
557(50)	548(13)	1022(0)	990(1)	3209(5)	3134(7)
579(1)	559(0)	1023(19)	996(13)	3209(12)	3134(11)
591(0)	571(0)	1031(13)	998(14)	3231(3)	3153(2)
594(7)	572(3)	1032(12)	999(15)	3231(0)	3154(0)
605(6)	619(1)	1048(0)	1024(1)	3236(1)	3158(1)
662(2)	649(1)	1062(9)	1029(7)	3236(0)	3158(3)
675(2)	650(2)	1063(5)	1031(4)	3240(8)	3166(11)
678(52)	661(16)	1123(14)	1094(7)	3240(3)	3166(2)
690(16)	666(33)	1123(11)	1094(3)	3246(13)	3173(12)
714(1)	694(1)	1186(1)	1144(0)	3247(5)	3173(7)
731(141)	700(147)	1188(2)	1145(1)	3255(0)	3175(2)
732(1)	701(1)	1232(22)	1218(3)	3255(1)	3175(2)

Table S109 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-3S** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
71(1)	-74(3)	790(18)	746(1)	1266(0)	1215(1)
93(0)	85(1)	796(0)	755(11)	1281(3)	1238(3)
119(1)	103(1)	806(23)	764(9)	1306(1)	1258(1)
142(0)	140(0)	836(9)	801(27)	1331(24)	1284(19)
205(2)	198(1)	847(33)	806(9)	1338(0)	1295(0)
230(0)	226(1)	858(2)	815(3)	1354(5)	1302(5)
260(3)	260(2)	865(8)	829(1)	1356(1)	1304(1)
287(2)	287(3)	881(3)	848(3)	1388(46)	1341(37)
297(0)	292(0)	890(36)	860(20)	1394(0)	1347(0)
363(33)	354(17)	944(0)	891(1)	1441(1)	1391(3)
404(0)	401(1)	944(4)	892(8)	1441(1)	1391(2)
412(8)	414(4)	965(1)	940(1)	1567(7)	1513(3)
459(4)	441(5)	979(1)	946(1)	1569(0)	1515(2)
459(1)	444(1)	998(2)	969(3)	1595(26)	1535(34)
476(0)	465(0)	1000(27)	969(31)	1600(8)	1541(9)
562(14)	541(11)	1011(5)	981(2)	3031(12)	2948(13)
589(7)	564(7)	1018(7)	981(5)	3034(37)	2951(41)
612(22)	596(21)	1037(1)	1005(2)	3200(2)	3125(3)
640(0)	614(7)	1072(24)	1036(17)	3200(1)	3125(1)
646(9)	624(0)	1080(0)	1044(0)	3224(19)	3148(20)
678(2)	653(10)	1118(15)	1079(16)	3224(7)	3148(7)
679(8)	656(1)	1134(2)	1098(2)	3226(4)	3148(5)
704(6)	675(5)	1183(6)	1137(9)	3227(2)	3149(3)
732(35)	701(41)	1185(0)	1138(0)	3241(2)	3166(3)
752(2)	717(2)	1212(0)	1166(0)	3242(1)	3166(0)
774(65)	739(55)	1219(2)	1170(2)	3249(2)	3172(9)
783(1)	742(24)	1250(8)	1208(8)	3249(6)	3172(3)

Table S110 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-4S** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
71(0)	68(0)	780(26)	752(18)	1261(0)	1213(1)
98(0)	106(1)	792(4)	759(11)	1276(7)	1231(10)
140(1)	153(2)	797(19)	764(10)	1296(2)	1247(1)
171(0)	174(0)	810(46)	772(43)	1331(21)	1283(12)
204(1)	212(0)	843(13)	797(8)	1339(11)	1291(7)
240(1)	242(1)	863(6)	817(4)	1344(7)	1295(16)
252(3)	252(2)	869(3)	836(3)	1359(4)	1312(3)
271(0)	282(2)	878(1)	844(1)	1385(25)	1335(13)
301(6)	296(7)	891(22)	850(8)	1411(11)	1358(7)
368(20)	359(10)	905(2)	860(6)	1434(3)	1382(10)
398(10)	392(8)	935(6)	884(6)	1448(3)	1405(2)
418(1)	411(4)	944(5)	893(5)	1541(3)	1488(4)
437(4)	425(3)	960(4)	922(2)	1562(2)	1498(1)
476(1)	447(1)	983(11)	952(13)	1593(8)	1525(9)
484(12)	467(11)	985(4)	957(4)	1600(7)	1557(6)
552(5)	532(6)	1012(11)	983(6)	3061(11)	2988(15)
600(11)	589(8)	1021(1)	985(6)	3079(41)	3011(37)
638(1)	615(0)	1027(9)	991(9)	3198(2)	3121(2)
639(0)	620(1)	1071(16)	1033(6)	3213(3)	3132(3)
659(5)	635(4)	1078(7)	1040(8)	3216(3)	3136(3)
666(3)	644(1)	1123(7)	1085(3)	3221(12)	3143(15)
694(9)	664(10)	1133(6)	1092(5)	3230(5)	3145(8)
698(16)	678(15)	1168(4)	1118(7)	3230(0)	3155(2)
734(30)	704(40)	1181(3)	1135(4)	3235(8)	3158(9)
757(21)	716(4)	1191(1)	1145(1)	3242(5)	3166(6)
761(30)	735(24)	1235(2)	1185(2)	3245(1)	3169(2)
776(10)	739(16)	1246(4)	1201(3)	3252(3)	3176(4)

Table 111 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-5T** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
108(0)	104(0)	796(68)	760(58)	1259(2)	1216(3)
130(0)	130(0)	798(1)	761(2)	1286(4)	1243(4)
181(0)	172(0)	812(0)	774(1)	1312(0)	1264(0)
182(0)	176(0)	833(19)	803(14)	1332(8)	1287(13)
199(1)	187(0)	853(0)	809(1)	1334(0)	1292(0)
201(0)	197(2)	856(17)	810(11)	1373(5)	1328(3)
230(0)	227(0)	870(7)	836(7)	1373(3)	1330(7)
292(2)	284(4)	887(0)	854(0)	1401(0)	1358(0)
296(0)	285(0)	913(1)	879(0)	1404(3)	1359(2)
344(30)	331(11)	936(0)	886(0)	1460(2)	1412(1)
373(0)	361(0)	937(4)	888(6)	1461(1)	1416(1)
394(0)	382(0)	956(2)	922(1)	1498(0)	1454(4)
454(3)	439(4)	959(2)	936(2)	1499(3)	1456(0)
457(0)	440(0)	1000(3)	970(5)	1594(3)	1528(8)
477(2)	460(2)	1013(5)	979(5)	1594(7)	1529(4)
589(0)	560(0)	1020(6)	987(6)	3054(9)	2978(9)
593(1)	562(1)	1033(9)	1003(10)	3058(36)	2981(36)
624(9)	608(7)	1035(20)	1004(17)	3203(1)	3128(1)
636(0)	621(0)	1070(0)	1037(0)	3203(2)	3128(3)
656(7)	626(7)	1073(4)	1041(5)	3226(19)	3151(20)
673(7)	639(6)	1123(7)	1087(9)	3226(6)	3151(6)
679(20)	650(18)	1137(0)	1102(0)	3234(0)	3158(1)
707(0)	674(1)	1167(3)	1116(3)	3234(1)	3159(1)
720(32)	691(37)	1184(1)	1140(1)	3246(2)	3171(3)
750(7)	714(7)	1195(3)	1150(3)	3246(1)	3171(1)
761(60)	725(41)	1219(1)	1172(1)	3255(1)	3179(2)
774(8)	737(4)	1257(0)	1210(0)	3255(3)	3179(5)

Table S112 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-6T** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
15(0)	17(0)	784(0)	746(1)	1270(165)	1235(94)
56(0)	57(0)	785(0)	747(0)	1283(1)	1245(6)
80(0)	80(0)	790(0)	761(0)	1300(33)	1259(31)
99(0)	100(0)	799(49)	769(38)	1309(6)	1269(6)
136(3)	120(12)	840(57)	808(43)	1332(9)	1291(2)
170(2)	164(2)	852(0)	823(0)	1338(3)	1298(2)
203(1)	208(1)	861(1)	828(0)	1363(0)	1329(1)
240(0)	248(0)	874(0)	833(0)	1400(10)	1359(3)
273(26)	262(24)	876(1)	834(0)	1403(23)	1371(16)
282(0)	301(0)	881(0)	843(0)	1437(15)	1390(7)
345(2)	349(3)	882(0)	852(9)	1446(0)	1398(1)
351(1)	365(0)	888(0)	854(0)	1481(331)	1444(223)
387(13)	404(20)	889(9)	863(3)	1491(46)	1461(34)
417(5)	422(0)	903(0)	876(0)	1497(8)	1470(2)
435(8)	424(8)	912(3)	953(2)	1523(0)	1491(0)
444(5)	543(20)	1016(42)	988(24)	3217(6)	3142(10)
562(39)	545(0)	1017(6)	988(6)	3217(0)	3143(0)
564(0)	548(20)	1029(1)	1002(67)	3229(0)	3151(1)
566(20)	561(0)	1034(66)	1004(0)	3230(1)	3152(2)
575(0)	595(10)	1037(0)	1012(0)	3232(0)	3156(0)
653(9)	635(4)	1065(30)	1032(28)	3232(12)	3157(2)
664(1)	649(1)	1069(0)	1036(0)	3234(0)	3158(0)
677(7)	654(5)	1114(17)	1088(8)	3234(4)	3159(18)
687(3)	658(1)	1139(0)	1110(1)	3242(35)	3168(37)
699(1)	681(2)	1175(5)	1140(1)	3242(0)	3168(0)
721(147)	691(144)	1182(1)	1142(0)	3255(0)	3176(0)
722(0)	691(0)	1212(19)	1218(8)	3255(1)	3176(2)

Table S113 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-7T** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
9(0)	16(0)	783(0)	745(0)	1272(257)	1242(153)
54(0)	52(0)	785(0)	746(0)	1292(0)	1249(0)
84(0)	83(0)	792(0)	764(0)	1295(6)	1250(11)
91(0)	88(0)	801(53)	771(40)	1297(0)	1264(0)
141(0)	107(16)	840(59)	807(47)	1337(3)	1289(2)
163(4)	156(0)	851(0)	821(0)	1345(0)	1305(0)
200(1)	203(1)	853(0)	822(0)	1347(7)	1322(0)
238(0)	246(0)	871(0)	829(0)	1400(0)	1358(0)
265(0)	257(23)	872(0)	829(0)	1403(30)	1370(21)
273(25)	303(0)	877(0)	837(0)	1444(22)	1393(10)
279(0)	341(3)	877(0)	848(7)	1447(0)	1397(0)
343(2)	364(0)	885(0)	851(0)	1482(0)	1448(266)
364(0)	401(24)	887(5)	867(2)	1483(402)	1457(0)
388(12)	422(0)	897(2)	878(0)	1492(0)	1470(0)
435(8)	423(9)	904(0)	947(0)	1520(0)	1486(0)
436(0)	544(0)	1023(0)	991(0)	3217(6)	3143(9)
564(0)	545(7)	1024(2)	992(3)	3217(0)	3143(0)
565(11)	555(40)	1029(128)	999(99)	3229(1)	3152(1)
573(0)	560(0)	1030(0)	1001(0)	3230(0)	3153(0)
575(48)	586(0)	1036(1)	1015(0)	3232(0)	3155(0)
651(13)	631(8)	1063(38)	1030(33)	3232(11)	3156(5)
665(0)	651(0)	1064(0)	1032(0)	3233(0)	3158(0)
673(0)	652(0)	1110(0)	1086(0)	3234(7)	3158(18)
685(5)	656(2)	1142(0)	1111(1)	3242(37)	3168(39)
699(1)	680(2)	1172(0)	1139(0)	3242(0)	3168(0)
718(0)	687(0)	1182(1)	1142(0)	3255(0)	3177(0)
718(153)	687(148)	1208(0)	1214(0)	3255(1)	3177(2)

Table S114 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-8T** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
25(0)	31(0)	771(20)	744(12)	1268(23)	1232(18)
58(0)	47(0)	779(0)	746(0)	1273(16)	1241(5)
65(2)	50(3)	782(32)	749(32)	1313(1)	1265(30)
85(0)	93(0)	794(2)	765(3)	1318(44)	1273(0)
141(0)	149(1)	841(11)	808(15)	1328(0)	1292(10)
183(2)	177(3)	849(0)	813(0)	1349(14)	1295(4)
189(0)	203(0)	854(0)	821(0)	1378(9)	1339(1)
246(0)	243(20)	860(4)	826(1)	1400(7)	1361(10)
252(19)	257(0)	867(3)	835(0)	1408(4)	1371(2)
299(2)	305(3)	875(1)	836(0)	1427(5)	1387(1)
328(3)	327(2)	879(5)	840(2)	1446(8)	1400(1)
357(0)	358(0)	885(0)	844(0)	1488(116)	1449(62)
387(0)	395(5)	887(1)	855(6)	1505(7)	1469(21)
435(2)	424(1)	896(0)	871(0)	1510(44)	1470(15)
435(9)	426(8)	963(9)	960(0)	1530(0)	1502(1)
503(13)	507(10)	1003(24)	983(13)	3216(2)	3142(3)
564(0)	544(4)	1006(18)	983(16)	3217(5)	3143(4)
564(9)	545(0)	1018(2)	1001(1)	3230(0)	3152(0)
573(1)	550(0)	1036(2)	1004(13)	3231(0)	3153(1)
596(5)	609(1)	1041(31)	1009(24)	3233(17)	3158(1)
661(0)	641(2)	1072(8)	1035(9)	3233(1)	3158(3)
662(2)	649(0)	1076(1)	1040(3)	3236(1)	3160(1)
674(17)	652(13)	1120(6)	1092(3)	3236(4)	3160(21)
684(3)	654(3)	1130(25)	1107(5)	3248(4)	3172(5)
697(1)	680(0)	1177(0)	1139(0)	3248(9)	3172(12)
718(125)	687(113)	1181(0)	1142(0)	3253(1)	3175(3)
727(0)	696(0)	1238(14)	1227(3)	3253(3)	3175(4)

Table S115 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-9T** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
-86(0)	-14(0)	777(43)	746(0)	1271(76)	1245(45)
-25(0)	52(0)	784(0)	747(34)	1294(5)	1248(7)
53(0)	69(2)	786(2)	748(3)	1295(0)	1250(0)
81(2)	96(0)	796(7)	768(6)	1297(25)	1267(4)
131(0)	140(0)	839(27)	808(25)	1338(2)	1289(0)
132(0)	169(3)	851(2)	821(0)	1341(0)	1307(18)
167(2)	202(1)	854(0)	824(0)	1349(12)	1323(0)
197(0)	239(22)	864(0)	829(0)	1399(30)	1359(22)
244(20)	253(1)	875(0)	829(0)	1401(0)	1371(0)
245(2)	311(2)	876(0)	841(0)	1445(3)	1393(0)
292(0)	321(1)	876(0)	845(0)	1447(2)	1395(0)
330(1)	357(0)	881(1)	854(0)	1480(104)	1453(84)
351(0)	393(7)	888(2)	865(3)	1486(3)	1459(2)
370(1)	423(0)	896(2)	876(0)	1493(140)	1469(44)
434(0)	424(9)	903(1)	941(0)	1523(0)	1490(0)
435(9)	539(6)	1021(0)	989(0)	3218(1)	3143(3)
558(0)	544(0)	1023(3)	992(4)	3219(1)	3144(2)
561(1)	545(26)	1025(7)	997(5)	3227(0)	3150(1)
565(41)	548(0)	1031(88)	1002(60)	3228(1)	3151(2)
567(5)	568(0)	1033(0)	1015(0)	3232(0)	3154(0)
652(0)	635(1)	1063(13)	1030(13)	3232(1)	3155(7)
669(0)	652(0)	1065(11)	1033(8)	3233(0)	3160(0)
675(0)	656(2)	1118(0)	1093(1)	3233(17)	3160(16)
683(0)	656(0)	1141(0)	1111(0)	3243(9)	3169(10)
694(0)	674(0)	1170(0)	1139(0)	3243(15)	3169(15)
710(137)	682(127)	1182(0)	1142(0)	3253(1)	3174(2)
717(0)	688(0)	1206(0)	1207(0)	3254(2)	3176(5)

Table S116 Harmonic vibrational frequencies (in cm^{-1}) and infrared intensities (in parentheses, in km/mol) for the structure **Ni-10T** of $(C_8H_6)_2Ni$

B3LYP	BP86	B3LYP	BP86	B3LYP	BP86
51(0)	42(0)	785(28)	752(22)	1255(0)	1208(0)
140(0)	137(0)	789(45)	755(39)	1285(5)	1244(6)
162(0)	158(0)	804(2)	767(0)	1301(0)	1254(0)
170(1)	160(0)	816(1)	781(0)	1327(0)	1283(1)
194(1)	186(0)	854(15)	814(11)	1334(7)	1294(8)
200(0)	192(2)	860(15)	819(13)	1371(6)	1327(1)
229(0)	223(0)	870(2)	834(4)	1372(3)	1332(11)
274(0)	271(2)	883(1)	845(1)	1404(3)	1358(1)
314(2)	303(2)	906(2)	872(1)	1408(2)	1367(1)
346(27)	334(11)	909(1)	874(1)	1466(0)	1416(1)
378(1)	369(1)	928(7)	878(1)	1466(1)	1417(0)
390(0)	381(0)	931(3)	879(7)	1503(3)	1460(2)
434(4)	420(4)	946(8)	917(7)	1505(2)	1460(3)
468(9)	452(7)	971(3)	942(3)	1587(1)	1519(1)
484(4)	459(6)	1013(0)	979(0)	1588(3)	1520(5)
577(2)	553(2)	1015(6)	981(5)	3072(5)	2999(5)
599(0)	563(1)	1031(3)	1000(4)	3087(46)	3013(46)
637(0)	614(0)	1035(28)	1004(28)	3208(2)	3133(2)
638(0)	624(0)	1067(0)	1033(0)	3212(4)	3137(4)
659(1)	630(3)	1077(6)	1046(7)	3230(0)	3154(0)
671(3)	648(6)	1127(1)	1092(1)	3231(2)	3156(3)
695(4)	655(1)	1132(2)	1092(1)	3232(0)	3156(1)
695(0)	664(1)	1167(4)	1122(6)	3237(16)	3160(18)
715(49)	686(49)	1189(0)	1143(0)	3240(0)	3165(0)
758(7)	723(12)	1190(4)	1145(4)	3243(4)	3166(7)
759(57)	725(39)	1243(3)	1191(0)	3252(2)	3177(4)
772(14)	739(8)	1244(0)	1198(4)	3253(3)	3177(4)

Table S117. The Ti-C bond distances for the optimized $(C_8H_6)_2T_i$ Structures

	Ti-1S(C_1)			Ti-2S (C_2)			Ti-3S(D_2)	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
TiC1	**2.402**	**2.394**	TiC1	**2.388**	**2.382**	TiC1	**2.385**	**2.385**
TiC2	**2.413**	**2.411**	TiC2	**2.453**	**2.449**	TiC2	**2.603**	**2.599**
TiC3	**2.261**	**2.268**	TiC3	**2.298**	**2.304**	TiC3	**2.475**	**2.472**
TiC4	**2.172**	**2.175**	TiC4	**2.160**	**2.165**	TiC4	**2.183**	**2.186**
TiC5	**2.276**	**2.270**	TiC5	**2.218**	**2.216**	TiC5	**2.183**	**2.186**
TiC6	**2.551**	**2.547**	TiC6	**2.419**	**2.412**	TiC6	**2.385**	**2.385**
TiC7	3.070	3.058	TiC7	2.797	2.790	TiC7	**2.603**	**2.599**
TiC8	2.948	2.933	TiC8	2.697	2.688	TiC8	**2.475**	**2.472**
TiC9	**2.321**	**2.311**	TiC9	**2.298**	**2.304**	TiC9	**2.475**	**2.472**
TiC10	**2.473**	**2.465**	TiC10	**2.453**	**2.449**	TiC10	**2.603**	**2.599**
TiC11	**2.374**	**2.370**	TiC11	**2.388**	**2.382**	TiC11	**2.385**	**2.385**
TiC12	**2.171**	**2.173**	TiC12	**2.218**	**2.216**	TiC12	**2.183**	**2.186**
TiC13	**2.150**	**2.155**	TiC13	**2.160**	**2.165**	TiC13	**2.183**	**2.183**
TiC14	**2.490**	**2.492**	TiC14	2.697	2.688	TiC14	**2.475**	**2.472**
TiC15	**2.591**	**2.593**	TiC15	2.797	2.790	TiC15	**2.603**	**2.599**
TiC16	**2.359**	**2.363**	TiC16	**2.419**	**2.422**	TiC16	**2.385**	**2.385**

	Ti-4S(D_{2d})			Ti-5T(C_s)			Ti-6T(C_2)	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
TiC1	**2.453**	**2.453**	TiC1	**2.375**	**2.349**	TiC1	**2.361**	**2.320**
TiC2	**2.570**	**2.563**	TiC2	**2.353**	**2.326**	TiC2	**2.366**	**2.326**
TiC3	**2.453**	**2.453**	TiC3	**2.375**	**2.349**	TiC3	**2.398**	**2.354**
TiC4	**2.172**	**2.174**	TiC4	**2.398**	**2.373**	TiC4	**2.391**	**2.345**
TiC5	**2.172**	**2.174**	TiC5	**2.398**	**2.373**	TiC5	**2.344**	**2.300**
TiC6	**2.453**	**2.453**	TiC6	3.410	3.382	TiC6	3.363	3.338
TiC7	**2.570**	**2.563**	TiC7	3.882	3.856	TiC7	3.761	3.758
TiC8	**2.453**	**2.453**	TiC8	3.410	3.382	TiC8	3.271	3.267
TiC9	**2.453**	**2.453**	TiC9	**2.370**	**2.359**	TiC9	**2.398**	**2.345**
TiC10	**2.570**	**2.563**	TiC10	**2.494**	**2.475**	TiC10	**2.366**	**2.326**
TiC11	**2.453**	**2.453**	TiC11	**2.362**	**2.351**	TiC11	**2.361**	**2.320**
TiC12	**2.172**	**2.174**	TiC12	**2.147**	**2.146**	TiC12	**2.344**	**2.300**
TiC13	**2.172**	**2.174**	TiC13	**2.150**	**2.149**	TiC13	**2.391**	**2.345**
TiC14	**2.453**	**2.453**	TiC14	**2.362**	**2.351**	TiC14	3.271	3.267
TiC15	**2.570**	**2.563**	TiC15	**2.494**	**2.475**	TiC15	3.761	3.758
TiC16	**2.453**	**2.453**	TiC16	**2.370**	**2.359**	TiC16	3.363	3.338

Table S118. The V-C bond distances for the optimized **$(C_8H_6)_2V$ Doublet** Structures

	V-1D(C_1)			V-2D(C_2)			V-3D(D_2)	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
VC1	**2.275**	**2.274**	VC1	**2.315**	**2.289**	VC1	2.350	2.334
VC2	**2.222**	**2.223**	VC2	**2.361**	**2.344**	VC2	2.644	2.639
VC3	**2.191**	**2.189**	VC3	**2.240**	**2.232**	VC3	2.526	2.514
VC4	**1.293**	**2.277**	VC4	**2.112**	**2.108**	VC4	2.154	2.145
VC5	**2.239**	**2.230**	VC5	**2.220**	**2..206**	VC5	2.154	2.145
VC6	3.312	3.301	VC6	**2.450**	**2.446**	VC6	2.350	2.334
VC7	3.385	3.826	VC7	2.986	2.991	VC7	2.644	2.639
VC8	3.425	3.410	VC8	2.882	2.876	VC8	2.526	2.514
VC9	**2.276**	**2.260**	VC9	**2.315**	**2.289**	VC9	2.526	2.514
VC10	**2.406**	**2.378**	VC10	**2.361**	**2.344**	VC10	2.644	2.639
VC11	**2.292**	**2.275**	VC11	**2.240**	**2.232**	VC11	2.350	2.334
VC12	**2.085**	**2.082**	VC12	**2.112**	**2.108**	VC12	2.154	2.145
VC13	**2.082**	**2.079**	VC13	**2.220**	**2..206**	VC13	2.154	2.145
VC14	**2.281**	**2.265**	VC14	**2.450**	**2.446**	VC14	2.526	2.514
VC15	**2.407**	**2.383**	VC15	2.882	2.876	VC15	2.644	2.639
VC16	**2.286**	**2.269**	VC16	2.986	2.991	VC16	2.350	2.334

	V-4D(C_2)			V-5D(C_s)	
	B3LYP	BP86		B3LYP	BP86
VC1	**2.189**	**2.223**	VC1	**2.148**	**2.189**
VC2	**2.249**	**2.270**	VC2	**2.225**	**2.254**
VC3	**2.316**	**2.305**	VC3	**2.367**	**2.331**
VC4	**2.266**	**2.265**	VC4	**2.340**	**2.316**
VC5	**2.144**	**2.176**	VC5	**2.132**	**2.159**
VC6	3.304	3.264	VC6	3.447	2.386
VC7	3.694	3.660	VC7	3.817	3.765
VC8	3.160	3.145	VC8	3.158	3.146
VC9	**2.316**	**2.305**	VC9	**2.148**	**2.189**
VC10	**2.249**	**2.270**	VC10	**2.225**	**2.254**
VC11	**2.189**	**2.223**	VC11	**2.367**	**2.331**
VC12	**2.144**	**2.176**	VC12	**2.340**	**2.316**
VC13	**2.266**	**2.265**	VC13	**2.132**	**2.159**
VC14	3.160	3.145	VC14	3.447	2.386
VC15	3.694	3.660	VC15	3.817	3.765
VC16	3.304	3.264	VC16	3.158	3.146

Table S119. The V-C bond distances for the optimized **$(C_8H_6)_2V$ Quartet** Structures

	V-6Q(C_2)			V-7Q(C_s)			V-8Q(C_1)	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
VC1	**2.249**	**2.273**	VC1	**2.253**	**2.230**	VC1	**2.332**	**2.332**
VC2	**2.298**	**2.335**	VC2	**2.322**	**2.285**	VC2	**2.292**	**2.292**
VC3	**2.321**	**2.362**	VC3	**2.393**	**2.347**	VC3	**2.322**	**2.322**
VC4	**2.276**	**2.306**	VC4	**2.347**	**2.317**	VC4	**2.337**	**2.337**
VC5	**2.203**	**2.227**	VC5	**2.215**	**2.192**	VC5	**2.336**	**2.336**
VC6	3.262	3.243	VC6	3.395	3.369	VC6	3.357	3.315
VC7	3.623	3.625	VC7	3.752	3.742	VC7	3.823	3.763
VC8	3.113	3.117	VC8	3.126	3.125	VC8	3.351	3.281
VC9	**2.321**	**2.362**	VC9	**2.253**	**2.230**	VC9	**2.310**	**2.290**
VC10	**2.298**	**2.335**	VC10	**2.322**	**2.285**	VC10	**2.342**	**2.312**
VC11	**2.249**	**2.273**	VC11	**2.393**	**2.347**	VC11	**2.222**	**2.213**
VC12	**2.203**	**2.227**	VC12	**2.347**	**2.317**	VC12	**2.114**	**2.114**
VC13	**2.276**	**2.306**	VC13	**2.215**	**2.192**	VC13	**2.195**	**2.195**
VC14	3.113	3.243	VC14	3.395	3.369	VC14	**2.484**	**2.532**
VC15	3.623	3.625	VC15	3.752	3.742	VC15	2.948	3.014
VC16	3.262	3.117	VC16	3.126	3.125	VC16	2.802	2.845

Table S120. The Cr-C bond distances for the optimized **$(C_8H_6)_2Cr$** Structures

	Cr-1S(C_s)			**Cr-2T(C_2)**			**Cr-3T(C_2)**	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
CrC1	**2.162**	**2.150**	CrC1	**2.144**	**2.124**	CrC1	**2.238**	**2.175**
CrC2	**2.070**	**2.065**	CrC2	**2.250**	**2.222**	CrC2	**2.212**	**2.184**
CrC3	**2.162**	**2.150**	CrC3	**2.301**	**2.270**	CrC3	**2.229**	**2.186**
CrC4	**2.401**	**2.410**	CrC4	**2.210**	**2.188**	CrC4	**2.264**	**2.220**
CrC5	**2.401**	**2.410**	CrC5	**2.083**	**2.066**	CrC5	**2.303**	**2.231**
CrC6	3.497	3.519	CrC6	3.214	3.207	CrC6	3.255	3.201
CrC7	3.993	4.024	CrC7	3.571	3.584	CrC7	3.725	3.654
CrC8	3.497	3.519	CrC8	3.030	3.046	CrC8	3.288	3.203
CrC9	**2.210**	**2.189**	CrC9	**2.301**	**2.270**	CrC9	**2.229**	**2.186**
CrC10	**2.313**	**2.280**	CrC10	**2.250**	**2.222**	CrC10	**2.212**	**2.184**
CrC11	**2.210**	**2.189**	CrC11	**2.144**	**2.124**	CrC11	**2.238**	**2.175**
CrC12	**2.030**	**2.031**	CrC12	**2.083**	**2.066**	CrC12	**2.308**	**2.231**
CrC13	**2.030**	**2.031**	CrC13	**2.210**	**2.188**	CrC13	**2.264**	**2.220**
CrC14	**2.201**	**2.188**	CrC14	3.030	3.046	CrC14	3.288	3.203
CrC15	**2.278**	**2.254**	CrC15	3.571	3.584	CrC15	3.725	3.654
CrC16	**2.201**	**2.188**	CrC16	3.214	3.207	CrC16	3.255	3.201

	Cr-4T(C_2)			**Cr-5T(C_s)**			**Cr-6S(C_2)**	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
CrC1	**2.245**	**2.203**	CrC1	**2.105**	**2.090**	CrC1	**2.167**	**2.156**
CrC2	**2.214**	**2.196**	CrC2	**2.219**	**2.195**	CrC2	**2.250**	**2.227**
CrC3	**2.223**	**2.165**	CrC3	**2.339**	**2.305**	CrC3	**2.210**	**2.183**
CrC4	**2.268**	**2.199**	CrC4	**2.282**	**2.261**	CrC4	**2.166**	**2.144**
CrC5	**2.298**	**2.218**	CrC5	**2.078**	**2.061**	CrC5	**2.063**	**2.053**
CrC6	3.268	3.164	CrC6	3.358	3.341	CrC6	2.966	2.972
CrC7	3.729	3.597	CrC7	3.701	3.701	CrC7	3.096	3.105
CrC8	3.279	3.146	CrC8	3.046	3.058	CrC8	**2.470**	**2.448**
CrC9	**2.223**	**2.165**	CrC9	**2.105**	**2.090**	CrC9	**2.210**	**2.183**
CrC10	**2.214**	**2.196**	CrC10	**2.219**	**2.195**	CrC10	**2.250**	**2.227**
CrC11	**2.245**	**2.203**	CrC11	**2.339**	**2.305**	CrC11	**2.167**	**2.156**
CrC12	**2.298**	**2.218**	CrC12	**2.282**	**2.261**	CrC12	**2.063**	**2.053**
CrC13	**2.268**	**2.198**	CrC13	**2.078**	**2.061**	CrC13	**2.166**	**2.144**
CrC14	3.279	3.146	CrC14	3.358	3.341	CrC14	**2.470**	**2.448**
CrC15	3.729	3.597	CrC15	3.701	3.701	CrC15	3.096	3.105
CrC16	3.268	3.164	CrC16	3.046	3.058	CrC16	2.966	2.972

Table 121. The Cr-C bond distances for the optimized **$(C_8H_6)_2Mn$** Structures

	Mn-1D(C_2)			**Mn-2D(C_{2v})**			**Mn-3D(C_s)**	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
MnC1	**2.099**	**2.074**	MnC1	**2.157**	**2.096**	MnC1	**2.063**	**2.048**
MnC2	**2.211**	**2.180**	MnC2	**2.082**	**2.070**	MnC2	**2.178**	**2.124**
MnC3	**2.256**	**2.224**	MnC3	**2.157**	**2.096**	MnC3	**2.290**	**2.213**
MnC4	**2.160**	**2.135**	MnC4	**2.295**	**2.217**	MnC4	**2.229**	**2.191**
MnC5	**2.038**	**2.015**	MnC5	**2.295**	**2.217**	MnC5	**2.033**	**2.024**
MnC6	3.156	3.145	MnC6	3.356	3.236	MnC6	3.306	3.280
MnC7	3.499	3.505	MnC7	3.839	3.706	MnC7	3.639	3.638
MnC8	2.953	2.960	MnC8	3.356	3.236	MnC8	2.974	2.994
MnC9	**2.256**	**2.224**	MnC9	**2.157**	**2.096**	MnC9	**2.063**	**2.048**
MnC10	**2.211**	**2.180**	MnC10	**2.082**	**2.070**	MnC10	**2.178**	**2.124**
MnC11	**2.099**	**2.074**	MnC11	**2.157**	**2.096**	MnC11	**2.290**	**2.213**
MnC12	**2.038**	**2.015**	MnC12	**2.295**	**2.217**	MnC12	**2.229**	**2.191**
MnC13	**2.160**	**2.135**	MnC13	**2.295**	**2.217**	MnC13	**2.033**	**2.024**
MnC14	2.953	2.960	MnC14	3.356	3.236	MnC14	3.306	3.280
MnC15	3.499	3.505	MnC15	3.839	3.706	MnC15	3.639	3.638
MnC16	3.156	3.145	MnC16	3.356	3.236	MnC16	2.974	2.994

	Mn-4Q(C_{2v})			**Mn-5Q(C_1)**			**Mn-6Q(C_s)**	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
MnC1	**2.144**	**2.117**	MnC1	**2.148**	**2.107**	MnC1	**2.182**	**2.097**
MnC2	**2.093**	**2.073**	MnC2	**2.167**	**2.106**	MnC2	**2.275**	**2.176**
MnC3	**2.144**	**2.117**	MnC3	**2.284**	**2.231**	MnC3	**2.422**	**2.392**
MnC4	**2.224**	**2.194**	MnC4	**2.441**	**2.435**	MnC4	**2.362**	**2.399**
MnC5	**2.224**	**2.194**	MnC5	**2.342**	**2.321**	MnC5	**2.106**	**2.092**
MnC6	3.239	3.214	MnC6	3.460	3.473	MnC6	3.417	3.485
MnC7	3.703	3.681	MnC7	3.839	3.862	MnC7	3.734	3.807
MnC8	3.239	3.214	MnC8	3.274	3.282	MnC8	3.060	3.091
MnC9	**2.144**	**2.117**	MnC9	**2.253**	**2.198**	MnC9	**2.182**	**2.097**
MnC10	**2.093**	**2.073**	MnC10	**2.277**	**2.239**	MnC10	**2.275**	**2.176**
MnC11	**2.144**	**2.117**	MnC11	**2.342**	**2.329**	MnC11	**2.422**	**2.392**
MnC12	**2.224**	**2.194**	MnC12	**2.293**	**2.264**	MnC12	**2.362**	**2.399**
MnC13	**2.224**	**2.194**	MnC13	**2.211**	**2.158**	MnC13	**2.106**	**2.092**
MnC14	3.239	3.214	MnC14	3.227	3.220	MnC14	3.417	3.485
MnC15	3.703	3.681	MnC15	3.657	3.648	MnC15	3.734	3.807
MnC16	3.239	3.214	MnC16	3.213	3.178	MnC16	3.060	3.091

Table S122. The Fe-C bond distances for the optimized **$(C_8H_6)_2Fe$ Singlet** Structures

	Fe-1S(C_2)			Fe-2S(C_s)			Fe-3S(C_{2v})	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
FeC1	**2.052**	**2.035**	FeC1	**2.159**	**2.122**	FeC1	**2.066**	**2.057**
FeC2	**2.103**	**2.074**	FeC2	**2.093**	**2.065**	FeC2	**2.060**	**2.042**
FeC3	**2.125**	**2.092**	FeC3	**2.035**	**2.022**	FeC3	**2.066**	**2.057**
FeC4	**2.082**	**2.064**	FeC4	**1.989**	**1.975**	FeC4	**2.168**	**2.168**
FeC5	**2.003**	**1.989**	FeC5	**2.129**	**2.113**	FeC5	**2.168**	**2.168**
FeC6	2.923	2.934	FeC6	2.935	2.943	FeC6	3.247	3.264
FeC7	3.466	3.477	FeC7	3.592	3.592	FeC7	3.733	3.759
FeC8	3.102	3.097	FeC8	3.233	3.200	FeC8	3.247	3.264
FeC9	**2.125**	**2.092**	FeC9	**2.159**	**2.122**	FeC9	**2.066**	**2.057**
FeC10	**2.103**	**2.074**	FeC10	**2.093**	**2.065**	FeC10	**2.060**	**2.042**
FeC11	**2.052**	**2.035**	FeC11	**2.035**	**2.022**	FeC11	**2.066**	**2.057**
FeC12	**2.003**	**1.989**	FeC12	**1.989**	**1.975**	FeC12	**2.168**	**2.169**
FeC13	**2.082**	**2.064**	FeC13	**2.129**	**2.113**	FeC13	**2.168**	**2.169**
FeC14	3.102	3.097	FeC14	2.935	2.943	FeC14	3.247	3.264
FeC15	3.466	3.477	FeC15	3.592	3.592	FeC15	3.733	3.759
FeC16	2.923	2.934	FeC16	3.233	3.200	FeC16	3.247	3.264

Table S123. The Fe-C bond distances for the optimized **$(C_8H_6)_2Fe$ Triplet** Structures

	Fe-4T(C_{2h})			Fe-5T(C_{2v})			Fe-6T(C_1)			Fe-7T(C_s)	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
FeC1	3.221	3.219	FeC1	**2.093**	**2.069**	FeC1	**2.102**	**2.053**	FeC1	**2.171**	**2.136**
FeC2	3.699	3.684	FeC2	**2.065**	**2.043**	FeC2	**2.228**	**2.159**	FeC2	**2.214**	**2.111**
FeC3	3.221	3.219	FeC3	**2.093**	**2.069**	FeC3	**2.344**	**2.287**	FeC3	**2.357**	**2.245**
FeC4	**2.163**	**2.144**	FeC4	**2.148**	**2.126**	FeC4	**2.333**	**2.331**	FeC4	**2.269**	**2.139**
FeC5	**2.163**	**2.144**	FeC5	**2.148**	**2.126**	FeC5	**2.091**	**2.059**	FeC5	**2.119**	**2.155**
FeC6	**2.092**	**2.073**	FeC6	3.185	3.185	FeC6	3.301	3.328	FeC6	3.330	3.318
FeC7	**2.064**	**2.045**	FeC7	3.654	3.662	FeC7	3.592	3.362	FeC7	3.670	3.703
FeC8	**2.092**	**2.073**	FeC8	3.185	3.185	FeC8	2.977	3.011	FeC8	3.026	3.088
FeC9	**2.092**	**2.073**	FeC9	**2.093**	**2.069**	FeC9	**2.351**	**2.300**	FeC9	**2.171**	**2.136**
FeC10	**2.064**	**2.045**	FeC10	**2.065**	**2.043**	FeC10	**2.267**	**2.223**	FeC10	**2.214**	**2.111**
FeC11	**2.092**	**2.073**	FeC11	**2.093**	**2.069**	FeC11	**2.195**	**2.167**	FeC11	**2.357**	**2.245**
FeC12	**2.163**	**2.144**	FeC12	**2.148**	**2.126**	FeC12	**2.068**	**2.036**	FeC12	**2.269**	**2.139**
FeC13	**2.163**	**2.144**	FeC13	**2.148**	**2.126**	FeC13	**2.196**	**2.144**	FeC13	**2.119**	**2.155**
FeC14	3.221	3.219	FeC14	3.185	3.185	FeC14	2.974	2.978	FeC14	3.330	3.318
FeC15	3.699	3.684	FeC15	3.654	3.662	FeC15	3.508	3.502	FeC15	3.670	3.703
FeC16	3.221	3.219	FeC16	3.185	3.185	FeC16	3.176	3.164	FeC16	3.026	3.088

Table S124. The Co-C bond distances for the optimized **$(C_8H_6)_2Co$ Doublet** Structures

	Co-1D(C_2)			Co-2D(C_{2v})			Co-3D(C_2)	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
CoC1	**2.067**	**2.045**	CoC1	**2.083**	**2.060**	CoC1	**2.114**	**2.086**
CoC2	**2.018**	**2.006**	CoC2	**2.016**	**2.010**	CoC2	**2.161**	**2.103**
CoC3	**2.066**	**2.060**	CoC3	**2.083**	**2.060**	CoC3	**2.248**	**2.183**
CoC4	**2.158**	**2.167**	CoC4	**2.206**	**2.196**	CoC4	**2.198**	**2.173**
CoC5	**2.202**	**2.197**	CoC5	**2.206**	**2.196**	CoC5	**2.015**	**2.000**
CoC6	3.321	3.247	CoC6	3.296	3.289	CoC6	3.186	3.180
CoC7	3.728	3.743	CoC7	3.780	3.773	CoC7	3.502	3.513
CoC8	3.171	3.277	CoC8	3.296	3.289	CoC8	2.933	2.944
CoC9	**2.066**	**2.060**	CoC9	**2.083**	**2.060**	CoC9	**2.148**	**2.183**
CoC10	**2.018**	**2.006**	CoC10	**2.016**	**2.010**	CoC10	**2.161**	**2.103**
CoC11	**2.067**	**2.045**	CoC11	**2.083**	**2.060**	CoC11	**2.114**	**2.086**
CoC12	**2.202**	**2.197**	CoC12	**2.206**	**2.196**	CoC12	**2.015**	**2.000**
CoC13	**2.158**	**2.167**	CoC13	**2.206**	**2.196**	CoC13	**2.198**	**2.173**
CoC14	3.271	3.277	CoC14	3.296	3.289	CoC14	2.933	2.944
CoC15	3.728	3.743	CoC15	3.780	3.773	CoC15	3.502	3.153
CoC16	3.321	3.247	CoC16	3.296	3.289	CoC16	3.186	3.180

	Co-4D(C_{2h})			Co-5D(C_s)	
	B3LYP	BP86		B3LYP	BP86
CoC1	**2.083**	**2.057**	CoC1	**2.124**	**2.088**
CoC2	**2.026**	**2.010**	CoC2	**2.140**	**2.086**
CoC3	**2.083**	**2.057**	CoC3	**2.269**	**2.206**
CoC4	**2.182**	**2.167**	CoC4	**2.206**	**2.186**
CoC5	**2.182**	**2.167**	CoC5	**2.032**	**2.016**
CoC6	3.268	3.271	CoC6	3.284	3.277
CoC7	3.751	3.761	CoC7	3.626	3.634
CoC8	3.268	3.271	CoC8	2.962	2.970
CoC9	**2.083**	**2.057**	CoC9	**2.124**	**2.088**
CoC10	**2.026**	**2.010**	CoC10	**2.140**	**2.086**
CoC11	**2.083**	**2.057**	CoC11	**2.269**	**2.206**
CoC12	**2.182**	**2.167**	CoC12	**2.206**	**2.186**
CoC13	**2.182**	**2.167**	CoC13	**2.032**	**2.016**
CoC14	3.268	3.271	CoC14	3.284	3.277
CoC15	3.751	3.761	CoC15	3.626	3.634
CoC16	3.268	3.271	CoC16	2.962	2.970

Table S125. The Co-C bond distances for the optimized **$(C_8H_6)_2$Co Quartet** Structures

	Co-6Q(C_2)			Co-7Q(C_{2h})			Co-8Q(C_{2v})			Co-9Q(C_s)	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
CoC1	**2.245**	**2.203**	CoC1	**2.136**	**2.101**	CoC1	**2.144**	**2.100**	CoC1	**2.199**	**2.174**
CoC2	**2.223**	**2.139**	CoC2	**2.140**	**2.100**	CoC2	**2.177**	**2.130**	CoC2	**2.226**	**2.136**
CoC3	**2.299**	**2.248**	CoC3	**2.136**	**2.101**	CoC3	**2.144**	**2.100**	CoC3	**2.360**	**2.281**
CoC4	**2.348**	**2.359**	CoC4	**2.255**	**2.236**	CoC4	**2.203**	**2.189**	CoC4	**2.403**	**2.410**
CoC5	**2.282**	**2.294**	CoC5	**2.255**	**2.236**	CoC5	**2.203**	**2.189**	CoC5	**2.251**	**2.283**
CoC6	3.322	3.368	CoC6	3.305	3.306	CoC6	3.237	3.253	CoC6	3.467	3.519
CoC7	3.694	3.765	CoC7	3.793	3.803	CoC7	3.718	3.746	CoC7	3.832	3.914
CoC8	3.184	3.246	CoC8	3.305	3.306	CoC8	3.237	3.253	CoC8	3.175	3.256
CoC9	**2.299**	**2.248**	CoC9	**2.136**	**2.101**	CoC9	**2.144**	**2.100**	CoC9	**2.199**	**2.174**
CoC10	**2.223**	**2.139**	CoC10	**2.140**	**2.100**	CoC10	**2.177**	**2.130**	CoC10	**2.226**	**2.136**
CoC11	**2.245**	**2.203**	CoC11	**2.136**	**2.101**	CoC11	**2.144**	**2.100**	CoC11	**2.360**	**2.281**
CoC12	**2.282**	**2.294**	CoC12	**2.255**	**2.236**	CoC12	**2.203**	**2.189**	CoC12	**2.403**	**2.410**
CoC13	**2.348**	**2.359**	CoC13	**2.255**	**2.236**	CoC13	**2.203**	**2.189**	CoC13	**2.251**	**2.283**
CoC14	3.184	3.246	CoC14	3.305	3.306	CoC14	3.237	3.253	CoC14	3.467	3.519
CoC15	3.694	3.765	CoC15	3.793	3.803	CoC15	3.718	3.746	CoC15	3.832	3.914
CoC16	3.322	3.368	CoC16	3.305	3.306	CoC16	3.237	3.253	CoC16	3.175	3.256

Table S126. The Ni-C bond distances for the optimized **$(C_8H_6)_2$Ni Singlet** Structures

	Ni-S(C_{2v})			Ni-2S(C_2)			Ni-3S(C_2)			Ni-4S(C_1)	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
NiC1	**2.098**	**2.092**	NiC1	**2.086**	**2.078**	NiC1	**2.031**	**2.004**	NiC1	**1.964**	**1.932**
NiC2	**2.009**	**2.008**	NiC2	**2.009**	**2.006**	NiC2	**2.211**	**2.171**	NiC2	**2.251**	**2.210**
NiC3	**2.098**	**2.092**	NiC3	**2.067**	**2.071**	NiC3	**2.560**	**2.539**	NiC3	**2.796**	**2.799**
NiC4	**2.265**	**2.256**	NiC4	**2.286**	**2.292**	NiC4	**2.464**	**2.466**	NiC4	**2.692**	**2.715**
NiC5	**2.265**	**2.256**	NiC5	**2.341**	**2.323**	NiC5	**2.001**	**2.006**	NiC5	**2.005**	**2.006**
NiC6	3.294	3.292	NiC6	3.396	3.409	NiC6	3.438	3.451	NiC6	3.737	3.801
NiC7	3.752	3.753	NiC7	3.917	3.925	NiC7	3.635	3.654	NiC7	3.909	3.935
NiC8	3.294	3.292	NiC8	3.438	3.434	NiC8	2.956	2.972	NiC8	2.973	2.984
NiC9	**2.098**	**2.092**	NiC9	**2.067**	**2.071**	NiC9	**2.560**	**2.539**	NiC9	**2.201**	**2.132**
NiC10	**2.009**	**2.008**	NiC10	**2.009**	**2.006**	NiC10	**2.211**	**2.171**	NiC10	**2.232**	**2.153**
NiC11	**2.098**	**2.092**	NiC11	**2.086**	**2.078**	NiC11	**2.031**	**2.004**	NiC11	**2.261**	**2.221**
NiC12	**2.265**	**2.256**	NiC12	**2.341**	**2.323**	NiC12	**2.011**	**2.006**	NiC12	**2.183**	**2.185**
NiC13	**2.265**	**2.256**	NiC13	**2.286**	**2.292**	NiC13	**2.464**	**2.466**	NiC13	**2.014**	**2.013**
NiC14	3.294	3.292	NiC14	3.438	3.434	NiC14	2.956	2.972	NiC14	3.236	3.263
NiC15	3.752	3.753	NiC15	3.917	3.925	NiC15	3.635	3.654	NiC15	3.587	3.627
NiC16	3.294	3.292	NiC16	3.396	3.409	NiC16	3.438	3.451	NiC16	2.958	2.978

Table S127. The Ni-C bond distances for the optimized **$(C_8H_6)_2$Ni Singlet** Structures

	Ni-5T(C_2)			Ni-6T(C_2)			Ni-7T(C_{2h})	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
NiC1	**2.158**	**2.123**	NiC1	**2.143**	**2.099**	NiC1	**2.139**	**2.105**
NiC2	**2.221**	**2.175**	NiC2	**2.072**	**2.038**	NiC2	**2.072**	**2.037**
NiC3	**2.305**	**2.274**	NiC3	**2.139**	**2.114**	NiC3	**2.139**	**2.105**
NiC4	**2.279**	**2.269**	NiC4	**2.341**	**2.342**	NiC4	**2.343**	**2.347**
NiC5	**2.168**	**2.150**	NiC5	**2.340**	**2.337**	NiC5	**2.343**	**2.347**
NiC6	3.248	3.252	NiC6	3.419	3.443	NiC6	3.429	3.455
NiC7	3.584	3.598	NiC7	3.927	3.958	NiC7	3.930	3.966
NiC8	3.046	3.051	NiC8	3.435	3.452	NiC8	3.429	3.347
NiC9	**2.305**	**2.274**	NiC9	**2.143**	**2.099**	NiC9	**2.139**	**2.105**
NiC10	**2.221**	**2.175**	NiC10	**2.072**	**2.038**	NiC10	**2.072**	**2.037**
NiC11	**2.158**	**2.123**	NiC11	**2.139**	**2.114**	NiC11	**2.139**	**2.105**
NiC12	**2.168**	**2.156**	NiC12	**2.341**	**2.342**	NiC12	**2.343**	**2.347**
NiC13	**2.279**	**2.269**	NiC13	**2.340**	**2.337**	NiC13	**2.343**	**2.347**
NiC14	3.046	3.051	NiC14	3.435	3.452	NiC14	3.429	3.455
NiC15	3.584	3.598	NiC15	3.927	3.958	NiC15	3.930	3.966
NiC16	3.248	3.252	NiC16	3.419	3.443	NiC16	3.429	3.347

	Ni-8T(C_2)			Ni-9T(C_{2v})			Ni-10T(C_s)	
	B3LYP	BP86		B3LYP	BP86		B3LYP	BP86
NiC1	**2.115**	**2.097**	NiC1	**2.154**	**2.117**	NiC1	**2.148**	**2.109**
NiC2	**2.099**	**2.064**	NiC2	**2.096**	**2.071**	NiC2	**2.226**	**2.176**
NiC3	**2.188**	**2.134**	NiC3	**2.154**	**2.117**	NiC3	**2.341**	**2.298**
NiC4	**2.333**	**2.322**	NiC4	**2.332**	**2.316**	NiC4	**2.325**	**2.316**
NiC5	**2.274**	**2.286**	NiC5	**2.332**	**2.316**	NiC5	**2.160**	**2.147**
NiC6	3.395	3.407	NiC6	3.421	3.419	NiC6	3.395	3.398
NiC7	3.867	3.895	NiC7	3.922	3.927	NiC7	3.737	3.753
NiC8	3.356	3.382	NiC8	3.421	3.419	NiC8	3.069	3.078
NiC9	**2.188**	**2.134**	NiC9	**2.154**	**2.117**	NiC9	**2.148**	**2.109**
NiC10	**2.199**	**2.064**	NiC10	**2.096**	**2.071**	NiC10	**2.226**	**2.176**
NiC11	**2.115**	**2.097**	NiC11	**2.154**	**2.117**	NiC11	**2.341**	**2.298**
NiC12	**2.274**	**2.286**	NiC12	**2.332**	**2.316**	NiC12	**2.325**	**2.316**
NiC13	**2.333**	**2.322**	NiC13	**2.332**	**2.316**	NiC13	**2.160**	**2.147**
NiC14	3.356	3.382	NiC14	3.421	3.419	NiC14	3.395	3.398
NiC15	3.867	3.895	NiC15	3.922	3.927	NiC15	3.737	3.753
NiC16	3.395	3.407	NiC16	3.421	3.419	NiC16	3.069	3.078

Table S128. The Wiberg bond index (WBI) values for all the M-C distances of the global minima of (pentalene)$_2$M (M = Ti - Ni).

	Ti-1S(C_1)					V-1D(C_1)			
	Bond distances		WBI values			Bond distances		WBI values	
	B3LYP	BP86	B3LYP	BP86		B3LYP	BP86	B3LYP	BP86
TiC1	**2.402**	**2.394**	**0.3490**	**0.3563**	VC1	**2.275**	**2.274**	**0.4195**	**0.4146**
TiC2	**2.413**	**2.411**	**0.2901**	**0.2973**	VC2	**2.222**	**2.223**	**0.3771**	**0.3869**
TiC3	**2.261**	**2.268**	**0.4291**	**0.4287**	VC3	**2.191**	**2.189**	**0.4820**	**0.4910**
TiC4	**2.172**	**2.175**	**0.2665**	**0.2759**	VC4	**1.293**	**2.277**	**0.3199**	**0.3339**
TiC5	**2.276**	**2.270**	**0.3225**	**0.3319**	VC5	**2.239**	**2.230**	**0.2486**	**0.2806**
TiC6	**2.551**	**2.547**	**0.4325**	**0.4328**	VC6	3.312	3.301	0.0848	0.0934
TiC7	3.070	3.058	0.0955	0.1018	VC7	3.385	3.826	0.0532	0.0546
TiC8	2.948	2.933	0.1577	0.1693	VC8	3.425	3.410	0.0882	0.0849
TiC9	**2.321**	**2.311**	**0.4154**	**0.4187**	VC9	**2.276**	**2.260**	**0.4252**	**0.4444**
TiC10	**2.473**	**2.465**	**0.2704**	**0.2817**	VC10	**2.406**	**2.378**	**0.2918**	**0.3188**
TiC11	**2.374**	**2.370**	**0.3687**	**0.3735**	VC11	**2.292**	**2.275**	**0.3982**	**0.4145**
TiC12	**2.171**	**2.173**	**0.3228**	**0.3329**	VC12	**2.085**	**2.082**	**0.3494**	**0.3682**
TiC13	**2.150**	**2.155**	**0.2886**	**0.2962**	VC13	**2.082**	**2.079**	**0.3625**	**0.3820**
TiC14	**2.490**	**2.492**	**0.2908**	**0.2946**	VC14	**2.281**	**2.265**	**0.4005**	**0.4177**
TiC15	**2.591**	**2.593**	**0.2163**	**0.2211**	VC15	**2.407**	**2.383**	**0.2786**	**0.3004**
TiC16	**2.359**	**2.363**	**0.4235**	**0.4249**	VC16	**2.286**	**2.269**	**0.4134**	**0.4355**

	Cr-1S(C_s)					Mn-1D(C_2)			
	Bond distances		WBI values			Bond distances		WBI values	
	B3LYP	BP86	B3LYP	BP86		B3LYP	BP86	B3LYP	BP86
CrC1	**2.162**	**2.150**	**0.4642**	**0.4903**	MnC1	**2.099**	**2.074**	**0.3419**	**0.4127**
CrC2	**2.070**	**2.065**	**0.5268**	**0.5400**	MnC2	**2.211**	**2.180**	**0.3075**	**0.3245**
CrC3	**2.162**	**2.150**	**0.4642**	**0.4903**	MnC3	**2.256**	**2.224**	**0.3076**	**0.2961**
CrC4	**2.401**	**2.410**	**0.2815**	**0.2788**	MnC4	**2.160**	**2.135**	**0.2993**	**0.3405**
CrC5	**2.401**	**2.410**	**0.2815**	**0.2788**	MnC5	**2.038**	**2.015**	**0.3609**	**0.4314**
CrC6	3.497	3.519	0.0481	0.0536	MnC6	3.156	3.145	0.0234	0.0267
CrC7	3.993	4.024	0.0936	0.1030	MnC7	3.499	3.505	0.0288	0.0387
CrC8	3.497	3.519	0.0481	0.0536	MnC8	2.953	2.960	0.0227	0.0278
CrC9	**2.210**	**2.189**	**0.4513**	**0.4737**	MnC9	**2.256**	**2.224**	**0.3076**	**0.2916**
CrC10	**2.313**	**2.280**	**0.3284**	**0.3954**	MnC10	**2.211**	**2.180**	**0.3075**	**0.3245**
CrC11	**2.210**	**2.189**	**0.4513**	**0.4737**	MnC11	**2.099**	**2.074**	**0.3419**	**0.4127**
CrC12	**2.030**	**2.031**	**0.4023**	**0.4159**	MnC12	**2.038**	**2.015**	**0.3609**	**0.4314**
CrC13	**2.030**	**2.031**	**0.4023**	**0.4159**	MnC13	**2.160**	**2.135**	**0.2993**	**0.4505**
CrC14	**2.201**	**2.188**	**0.4338**	**0.4527**	MnC14	2.953	2.960	0.0227	0.0278
CrC15	**2.278**	**2.254**	**0.3426**	**0.3651**	MnC15	3.499	3.505	0.0288	0.0387
CrC16	**2.201**	**2.188**	**0.4338**	**0.4527**	MnC16	3.156	3.145	0.0234	0.0267

	Fe-1S(C_2)					Co-1D(C_2)			
	Bond distances		WBI values			Bond distances		WBI values	
	B3LYP	BP86	B3LYP	BP86		B3LYP	BP86	B3LYP	BP86
FeC1	**2.052**	**2.035**	**0.3838**	**0.4078**	CoC1	**2.067**	**2.045**	**0.3609**	**0.3895**
FeC2	**2.103**	**2.074**	**0.3559**	**0.3883**	CoC2	**2.018**	**2.006**	**0.3664**	**0.3799**
FeC3	**2.125**	**2.092**	**0.3491**	**0.3872**	CoC3	**2.066**	**2.060**	**0.3314**	**0.3467**
FeC4	**2.082**	**2.064**	**0.3402**	**0.3603**	CoC4	**2.158**	**2.167**	**0.2635**	**0.2513**
FeC5	**2.003**	**1.989**	**0.3908**	**0.4179**	CoC5	**2.202**	**2.197**	**0.2155**	**0.2279**
FeC6	2.923	2.934	0.0238	0.0259	CoC6	3.321	3.247	0.0376	0.0518
FeC7	3.466	3.477	0.0334	0.0458	CoC7	3.728	3.743	0.0513	0.0568
FeC8	3.102	3.097	0.0210	0.0246	CoC8	3.171	3.277	0.0481	0.0606
FeC9	**2.125**	**2.092**	**0.3491**	**0.3872**	CoC9	**2.066**	**2.060**	**0.3314**	**0.3467**
FeC10	**2.103**	**2.074**	**0.3559**	**0.3883**	CoC10	**2.018**	**2.006**	**0.3664**	**0.3799**
FeC11	**2.052**	**2.035**	**0.3838**	**0.4078**	CoC11	**2.067**	**2.045**	**0.3609**	**0.3895**
FeC12	**2.003**	**1.989**	**0.3908**	**0.4179**	CoC12	**2.202**	**2.197**	**0.2155**	**0.2279**
FeC13	**2.082**	**2.064**	**0.3402**	**0.3603**	CoC13	**2.158**	**2.167**	**0.2635**	**0.2513**
FeC14	3.102	3.097	0.0210	0.0246	CoC14	3.271	3.277	0.0481	0.0606
FeC15	3.466	3.477	0.0334	0.0458	CoC15	3.728	3.743	0.0531	0.0568
FeC16	2.923	2.934	0.0238	0.0259	CoC16	3.321	3.247	0.0376	0.0518

	Ni-S(C_{2v})			
	Bond distances		WBI values	
	B3LYP	BP86	B3LYP	BP86
NiC1	**2.098**	**2.092**	**0.2615**	**0.2722**
NiC2	**2.009**	**2.008**	**0.3273**	**0.3319**
NiC3	**2.098**	**2.092**	**0.2615**	**0.2722**
NiC4	**2.265**	**2.256**	**0.1762**	**0.1794**
NiC5	**2.265**	**2.256**	**0.1762**	**0.1794**
NiC6	3.294	3.292	0.0616	0.0656
NiC7	3.752	3.753	0.0605	0.0615
NiC8	3.294	3.292	0.0616	0.0656
NiC9	**2.098**	**2.092**	**0.2615**	**0.2722**
NiC10	**2.009**	**2.008**	**0.3273**	**0.3319**
NiC11	**2.098**	**2.092**	**0.2615**	**0.2722**
NiC12	**2.265**	**2.256**	**0.1762**	**0.1794**
NiC13	**2.265**	**2.256**	**0.1762**	**0.1794**
NiC14	3.294	3.292	0.0616	0.0656
NiC15	3.752	3.753	0.0605	0.0615
NiC16	3.294	3.292	0.0616	0.0656

Complete Gaussian 09 reference (Reference 44)

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