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Electronic Supplementary information

Manganese(III) acetate-mediated activation of C-H bonds of weak C-H acids; addition of *o*-caboranes, its derivatives and some organic CH-acids to [60]-fullerene

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1. Additional mass spectra

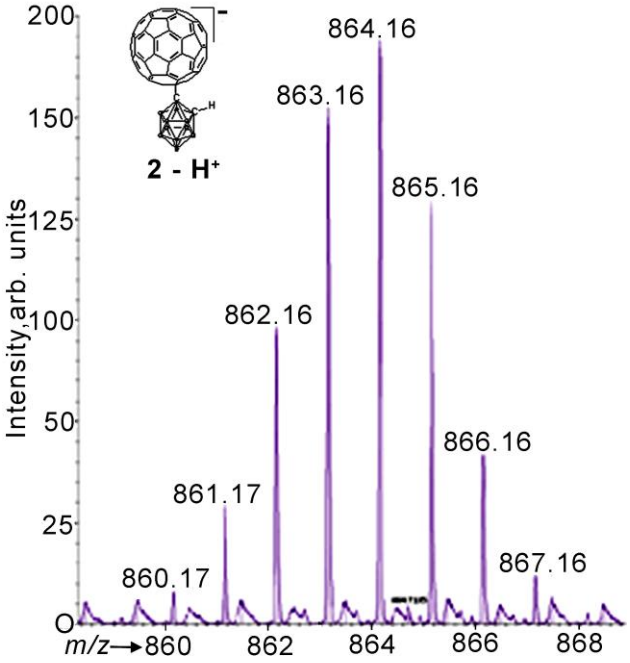

Fig. S1 NI APCI mass spectrum of a benzene solution of product **2** from the reaction of C_{60} with *o*-carborane and $Mn(OAc)_3 \cdot 2H_2O$ taken in the molar ratio of 1:2:2 carried out in chlorobezene at r.t. for 3 h.

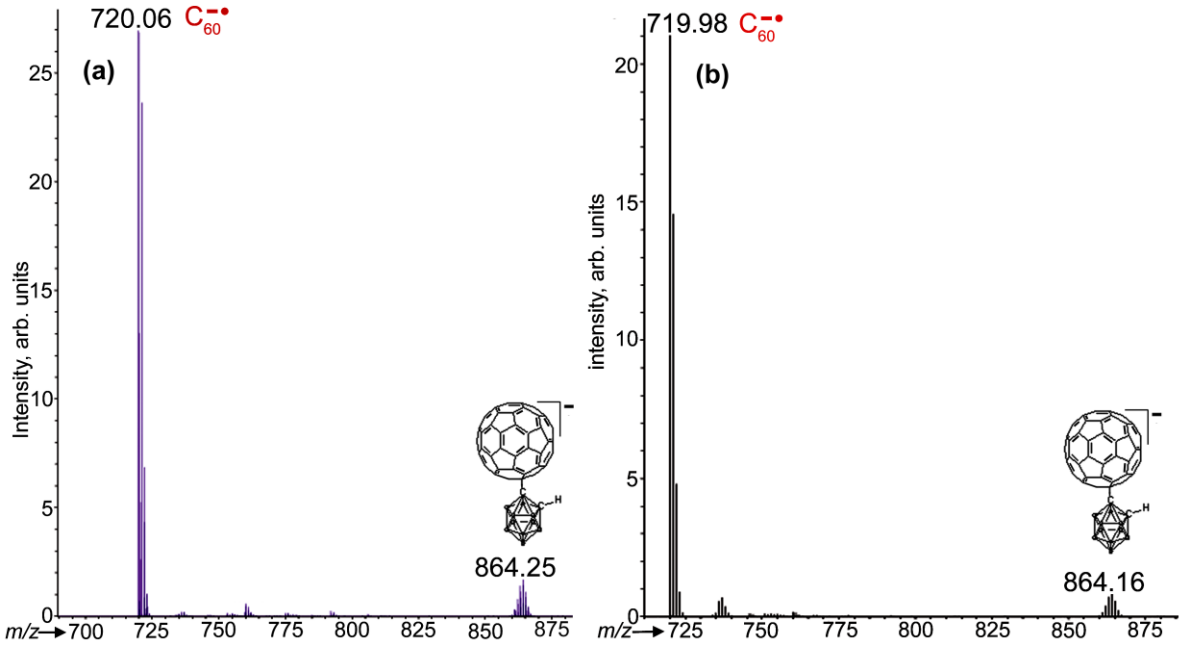

Fig. S2. NI APCI mass spectra in the high mass region of the products from the reaction of C_{60} with *o*-carborane and $Mn(OAc)_3 \cdot 2H_2O$ (molar ratio 1:21:20) carried out in chlorobenzene at 100 °C; the spectra were recorded **(a)** after 1h of heating and **(b)** after 11 h.

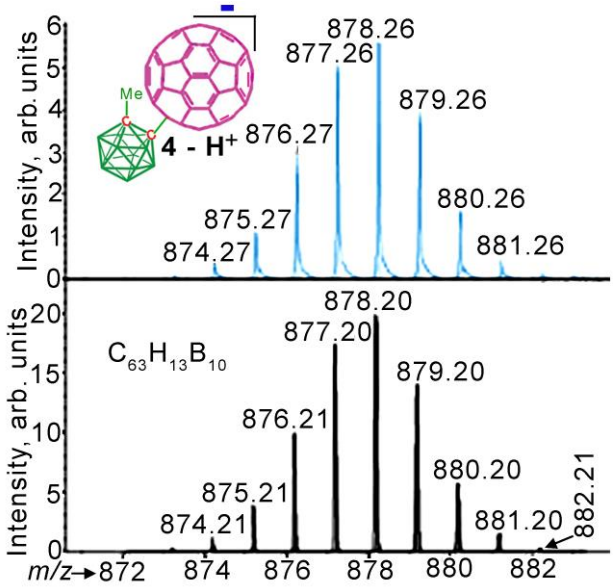

Fig. S3. NI APCI mass spectrum of product **4** from the reaction of C_{60} with 1-Me-*o*-carborane and $Mn(OAc)_3 \cdot 2H_2O$ taken in the molar ratio of 1:20:20 conducted in chlorobenzene at r.t. for 168 h.

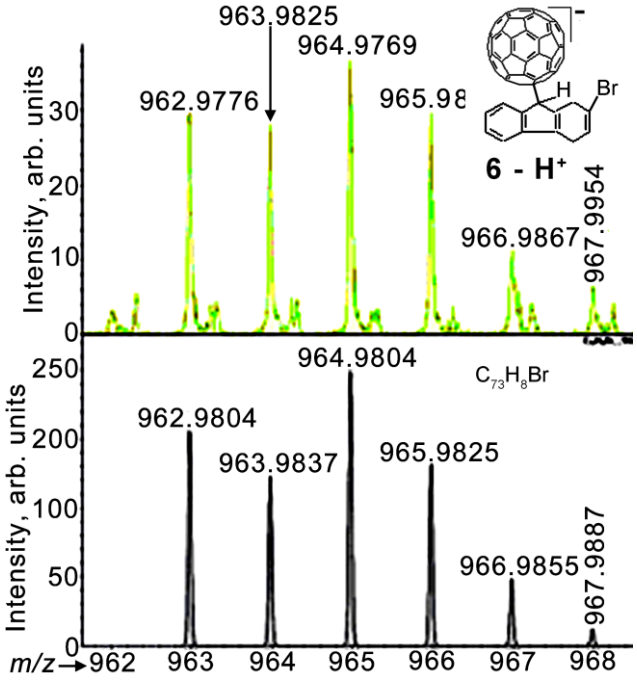

Fig. S4. (a) NI APCI mass spectrum of product **6** obtained *via* the reaction of C_{60} with 2-Br-9H-fluorene and $Mn(OAc)_3{\cdot}2H_2O$ (molar ratio 1:20:20) carried out in chlorobenzene at r.t. for 144 h, **(b)** Simulated spectrum of deprotonated **6**.

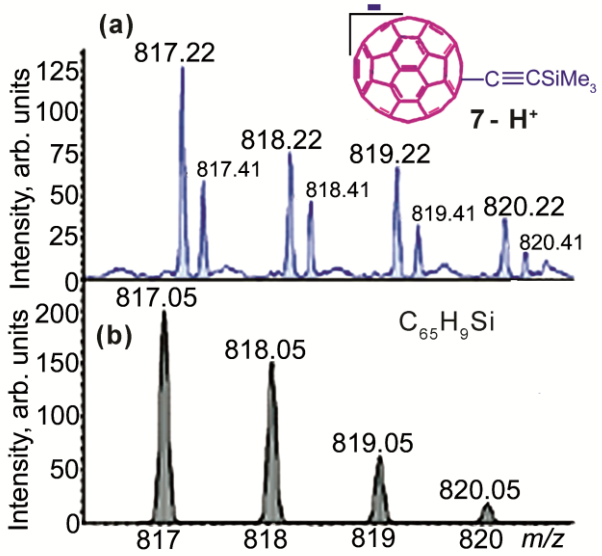

Fig. S5. (a) NI ACPI mass spectrum of $HC_{60}C_2SiMe_3$ (**7**) obtained from the reaction of C_{60} with trimethylsilylacetylene and $Mn(OAc)_3{\cdot}2H_2O$ (molar ratio 1:20:20) conducted in chlorobenzene at r.t. for 144 h, **(b)** Simulated spectrum of deprotonated **7**.

2. Notes.

Note 1. It was shown that $Mn(OAc)_3{\cdot}2H_2O$ appeared in the NI APCI mass spectrum as anion $^{-}Mn(OAc)_3$ (an ion peak at *m/z* 231. 95, calculated 231.978), i.e., water was lost in the course of

mass spectral analysis. Thus, basing on the MS analysis, we cannot tell whether water retained or not in the products of the reactions of the change an acetyl group for carboranyl one or for other groups. Since it is of no significance for understanding the reaction mechanism, we decided on not to reflect water in the schemes of the reactions.

Note 2. Since mass spectrometer is a chemical reactor, there was a possibility that C_{60} and o-carborane could react in the APCI ion source of it under corona discharge as it was observed in the electron ionization (EI) source of a mass spectrometer.[S1] The reaction could also proceed in the mass spectrometer between all three reagents, especially so since the vaporizer of it was heated at 350 °C. In this connection a test experiment was performed under the same conditions with the same amounts of C_{60}, *o*-carborane, and the solvent. The NI APCI mass spectrum displayed virtually no fullerene derivatives. An 1 ml sample was taken, chlorobenzene was replaced by benzene, and 10 mg (0.04 mmol; *ca.* one tenth of the amount that was used in the run which the test one was compared with) of $Mn(OAc)_3 \cdot 2H_2O$ were added. The solution was then subjected to NI APCI mass spectrometry. Very small intensity ion peaks of monoadduct **2** were found in the spectrum (the relative abundance of the 854 Da ion in respect to that of the 720 Da ion [$C_{60}^{+\bullet}$] was 4%). At the same time, this abundance proved to be 25% after 68 h of the reaction in the experiment the test one was compared with. The abundance achieved 65%, and pronounced polyaddition was observed after 168 h(Fig. 4). Thus, all indicates that the reactions investigated occurred mainly outside of the mass spectrometer. This conclusion finds support in the facts that in several experiments, signals of paramagnetic fullerene derivatives, though weak, were registered when samples of the reaction mixtures were irradiated by visible light indicating the presence the corresponding dimers.

Note 3. These values are not the actual yields of the adducts because they don't take into account the difference in volatilities and cross-sections of ionization between the adducts and C_{60}. Moreover, some fractionation could occur when the reaction mixtures (after the removal of chlorobenzene) were extracted by benzene for the MS analyses. Nevertheless, in spite of all of this, these values provide a certain picture of the efficiency of the processes.

3. Details of the quantum-chemical calculations

The PBE/3ζ density functional theory method (Priroda 11 program) was used for calculations as it accurately describes thermodynamic and kinetic parameters of fullerene reactions, and spectral and physicochemical parameters of fullerene compounds.

The structures obtained by the standard DFT-optimizations were proved to correspond to the minima of the potential energy surfaces *via* the vibration modes solving (their hessians contain

no imaginary frequencies). Then the heat effects (enthalpy changes) in chemical reactions were calculated as the differences between the total energies E_{tot} of the resulting fullerene adduct and reactants taking into account the zero-point vibrational energy corrections ε_{ZPV} and the temperature corrections H_{corr} (T = 298 K):

$$\Delta H_r^\circ = \sum_{products} \left(E_{tot,i} + \varepsilon_{ZPV,i} + H_{corr,i}\right) - \sum_{reactants} \left(E_{tot,i} + \varepsilon_{ZPV,i} + H_{corr,i}\right)$$

The Gibbs energy changes were calculated similarly using the corrections G_{corr} (T = 298 K):

$$\Delta G_r^\circ = \sum_{products} \left(E_{tot,i} + \varepsilon_{ZPV,i} + G_{corr,i}\right) - \sum_{reactants} \left(E_{tot,i} + \varepsilon_{ZPV,i} + G_{corr,i}\right)$$

The spin densities and atomic charges were estimated within the Mulliken population analysis. The most stable structures of two *o*-carborane–fullerene radical adducts differ in spin density distribution due to different symmetry point groups (C_1 *versus* C_S) (Table S1).

Table S1. Heat effects ($\Delta H°_r$), Gibbs free energies ($\Delta G°_r$) of formation, and spin density parameters of *o*-carboranylfullerenyl radicals

Fullerenyl radical (symmetry)	Highest spin densities on the reaction sites in the positions relative to the carboranyl addend			$\Delta H°_r$, kJ mol^{-1}	$\Delta G°_r$, kJ mol^{-1}
	2	**4**	**16**		
$^{\bullet}C_{60}$(*o*-$C_2HB_{10}H_{10}$) (C_1) (C–C bond between the *o*-carboranyl moiety and C_{60})	0.440	0.220[a]	0.060[a]	-359.8[b] –102.2[c]	-350.6[b] -55.0[c]
$^{\bullet}C_{60}$(9-*o*-$C_2H_2B_{10}H_9$) (C_S) (9-B–C bond between the *o*-carboranyl moiety and and C_{60})	0.420	0.203	0.088	–154.0[d]	-110.6[d]

[a] Average for two positions (a slight split of the spin density due to the unsymmetrical structure). [b] For the reaction $C_{60}^{\bullet+}$ + $[Mn(OAc)_2$(*o*-$C_2HB_{10}H_{10})]^{\bullet-}$ → $^{\bullet}C_{60}$(*o*-$C_2HB_{10}H_{10}$) + $^{\bullet}Mn(OAc)_2$, [c] for the reaction C_{60} + (*o*-$C_2HB_{10}H_{10})^{\bullet}$ → $^{\bullet}C_{60}$(*o*-$C_2HB_{10}H_{10}$) and [d] C_{60} + (9-*o*-$C_2H_2B_{10}H_9)^{\bullet}$ → $^{\bullet}C_{60}$ (9-*o*-$C_2H_2B_{10}H_9$).

Table S2. Heat effects ($\Delta H°_r$) of dimerization and characteristics of *o*-carboranylfullerenyl radicals

2 $^{\bullet}C_{60}$(*o*-carboranyl) → [1,4,1',4'-C_{60}(*o*-carboranyl)]$_2$

Type of the bond between the *o*-carboranyl moiety and C_{60}	$\Delta H°_r$, kJ mol^{-1}	Characteristics of o-carboranylfullerenyl radicals		
		Spin density at the carbon atom of the fullerene core in position 4 toward the attachment site of *o*-carboranyl moiety [a]	Positive charge at the 4-C atom of the fullerene core[a]	$-E_{SOMO}$, a.e.
C–C	+0.3	0.220	0.150	0.201
9-B-C	–5.6	0.203	0.077	0.177

[a] The averaged value for two atoms in positions 4. Note that the spin densities are twice larger at the 2-C atoms of the fullerene cage (~0.4 for both radicals). However, we consider only the dimerization 1,4-1',4' as the only probable mode due to steric hindrances making two other modes, 1,2-1',2' and 1',2-1',4', impossible.

Table S3. Heat effects ($\Delta H°_r$) of formation of the regioisomeric $^{\bullet}C_{70}$(*o*-$C_2HB_{10}H_{10}$) radicals *via* reaction $C_{70}^{\bullet+}$ + [$Mn(OAc)_2$(*o*-$C_2HB_{10}H_{10}$)]$^{\bullet-}$ → $^{\bullet}C_{70}$(*o*-$C_2HB_{10}H_{10}$) + $^{\bullet}Mn(OAc)_2$ against the curvature indices of the reaction sites of the C_{70} molecule

Reaction site of the C_{70} molecule	Curvature index of the reaction site, Å^{-1} (from Ref. 21)	$\Delta H°_r$, kJ mol^{-1}
a	0.3028	–340.9
b	0.2972	–340.0
c	0.2852	–335.2
d	0.2522	–333.0
e	0.2116	–288.7

*The above product-forming step seems to be irreversible, so that is kinetically controlled rather than thermodynamically. However, in the frameworks of the Bell-Evans-Polyanyi (BEP) porinciple[S2] the conclusion based on the heat effects that the additions to the carbons in positions ***a*** are more favorable appears to be valid. With that, the ratio of the regioisomers obtained could be affected by the point that the amount of the ***a*** sites is 10, while those of the ***c*** and ***d*** are 20 and 20.

The optimized geometries of the compounds studied (with total energies, zero-point vibration energies and thermal corrections, T = 298 K)

Fullerene C_{60} (I_h)

$\mathbf{E_{tot}}$ = -2284.295425 a.u.; $\boldsymbol{\varepsilon_{ZPV}}$ = 967.18 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 1025.28 kJ mol^{-1}; $\mathbf{G_{corr}}$ = 861.77 kJ mol^{-1}

6	2.87130356	2.08615446	-0.16169021	6	1.30052412	-2.86379266	-1.65224087
6	1.84913206	3.03343964	-0.03901726	6	0.39846745	-3.48541141	0.56187332
6	3.19661760	1.21900547	0.95824325	6	0.27647027	-3.42965698	-0.88520515
6	1.11262274	3.15032315	1.20834792	6	-0.91522723	-3.24053574	1.13307416
6	2.48761201	1.33152390	2.15902758	6	-1.11262286	-3.15032339	-1.20834792
6	1.42578840	2.31555629	2.28645945	6	-1.84913230	-3.03344011	0.03901730
6	2.99922228	1.30921817	-1.38317883	6	-2.10019231	-1.50858009	2.43637991
6	0.91522717	3.24053574	-1.13307416	6	-1.03836882	-2.49261260	2.30894828
6	2.10019231	1.50858033	-2.43637991	6	-1.57065940	-0.36835387	3.16542482
6	1.03836870	2.49261260	-2.30894828	6	0.14740735	-1.96055162	2.95923591
6	-0.27647024	3.42965698	0.88520521	6	-0.18156636	-0.64768749	3.48856759
6	-0.39846745	3.48541141	-0.56187332	6	0.76638174	0.38041869	3.44826221
6	-1.30052412	2.86379290	1.65224111	6	2.08007646	0.13554311	2.87706161
6	-1.53996265	2.97321963	-1.18787730	6	2.39676499	-1.12829435	2.36749673
6	-2.48630023	2.33173180	1.00195313	6	-1.95993078	0.92865485	2.81404352
6	-2.60374165	2.38540435	-0.39108640	6	0.36200961	1.72774112	3.08325028
6	-2.89383602	1.13575089	1.71998668	6	-0.97521001	1.99664366	2.77217460
6	-3.13327456	1.24517775	-1.12013137	6	1.41204417	-2.19628286	2.40936589
6	-3.40359426	0.03810429	1.01816690	6	-1.42578852	-2.31555629	-2.28645921
6	-3.52559161	0.09385878	-0.42891160	6	-2.48761201	-1.33152378	-2.15902758
6	-2.99922228	-1.30921793	1.38317871	6	-0.36200950	-1.72774076	-3.08324981
6	-3.19661784	-1.21900535	-0.95824319	6	-2.08007622	-0.13554296	-2.87706113
6	-2.87130380	-2.08615470	0.16169026	6	-0.76638162	-0.38041854	-3.44826198
6	3.52559137	-0.09385867	0.42891172	6	0.18156651	0.64768767	-3.48856783
6	3.40359426	-0.03810422	-1.01816678	6	1.57065952	0.36835402	-3.16542506
6	3.13327479	-1.24517751	1.12013149	6	1.95993102	-0.92865485	-2.81404376
6	2.89383602	-1.13575065	-1.71998692	6	0.97521007	-1.99664330	-2.77217460
6	2.60374165	-2.38540411	0.39108658	6	-0.14740723	1.96055210	-2.95923638

6	2.48630023	-2.33173180	-1.00195324	6	-1.41204405	2.19628286	-2.40936589
6	1.53996265	-2.97321939	1.18787706	6	-2.39676476	1.12829447	-2.36749649

Radical cation $C_{60}^{+\bullet}$

$\mathbf{E_{tot}}$ = –2284.020825 a.u.; $\boldsymbol{\varepsilon_{ZPV}}$ = 961.19 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 1020.25 kJ mol^{-1};

$\mathbf{G_{corr}}$ = 846.49 kJ mol^{-1}

6	2.89017892	2.09161854	-0.16276550	6	1.30036199	-2.84192419	-1.64479792
6	1.86878574	3.03904891	-0.04046793	6	0.38735884	-3.46634436	0.55620688
6	3.21815181	1.22462559	0.95721167	6	0.26650301	-3.41116667	-0.87625271
6	1.12906945	3.14753342	1.20417678	6	-0.93218744	-3.23773289	1.13182139
6	2.50638008	1.33594000	2.15551209	6	-1.12924969	-3.14770198	-1.20436919
6	1.44095635	2.31541276	2.27842283	6	-1.86907744	-3.03885674	0.04023211
6	3.02015996	1.31474411	-1.38478553	6	-2.11881471	-1.51231349	2.43508959
6	0.93200010	3.23794246	-1.13211489	6	-1.05390882	-2.49161720	2.30309510
6	2.11861444	1.51249540	-2.43516040	6	-1.58478951	-0.37121004	3.15876675
6	1.05359685	2.49167705	-2.30330563	6	0.13849413	-1.94837880	2.94348073
6	-0.26660836	3.41109180	0.87594020	6	-0.18699639	-0.64885521	3.46818900
6	-0.38748032	3.46670818	-0.55652589	6	0.76935250	0.38300863	3.42764211
6	-1.29981208	2.84169412	1.64506686	6	2.09363151	0.13917433	2.86879086
6	-1.53866744	2.95122027	-1.18270004	6	2.40936232	-1.11996996	2.36096120
6	-2.49885917	2.32056737	1.00018811	6	-1.97352350	0.92089522	2.80956006
6	-2.61591601	2.37360907	-0.38801730	6	0.36905417	1.71660805	3.06487489
6	-2.91203809	1.12891173	1.72016072	6	-0.97803718	1.98405778	2.75435424
6	-3.15201855	1.23906553	-1.11811137	6	1.41252685	-2.18318725	2.39278507
6	-3.42451286	0.03260212	1.01918674	6	-1.44097877	-2.31550264	-2.27862740
6	-3.54590654	0.08844190	-0.42783082	6	-2.50633287	-1.33593822	-2.15549850
6	-3.02055740	-1.31454039	1.38481998	6	-0.36882684	-1.71665680	-3.06461668
6	-3.21824479	-1.22469890	-0.95723939	6	-2.09352994	-0.13922837	-2.86863995
6	-2.89070010	-2.09162855	0.16292121	6	-0.76931477	-0.38320297	-3.42761230
6	3.54582310	-0.08836643	0.42749840	6	0.18705420	0.64854550	-3.46831751
6	3.42377782	-0.03260635	-1.01948738	6	1.58485115	0.37119326	-3.15856194
6	3.15215921	-1.23882174	1.11834753	6	1.97384870	-0.92085516	-2.80878639
6	2.91291571	-1.12951255	-1.72065043	6	0.97832316	-1.98409307	-2.75397277

6	2.61613965	-2.37339997	0.38830221	6	-0.13872437	1.94802654	-2.94351125
6	2.49928880	-2.32005882	-1.00015819	6	-1.41255379	2.18316579	-2.39270449
6	1.53863311	-2.95103431	1.18265307	6	-2.40918565	1.11978853	-2.36067271

Fullerene C_{70} (D_{5h})

$\mathbf{E_{tot}}$ = -2665.106373 a.u.; $\boldsymbol{\varepsilon_{ZPV}}$ = 1130.85 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 1199.39 kJ mol^{-1};

$\boldsymbol{G_{corr}}$ = 1015.68 kJ mol^{-1}

6	-1.75898552	-1.20777678	3.56584954	6	3.33172274	-1.24695587	-0.92866266
6	-1.77888894	0.19152856	3.60920691	6	2.49681234	-1.94570208	-1.87020469
6	-2.63017297	0.93535507	2.70368195	6	1.52335501	-2.88686204	-1.43478465
6	-1.92955089	2.13172865	2.29123545	6	3.59945917	0.07017341	-1.46330690
6	-0.63851309	2.13037586	2.92759585	6	2.24833584	-1.06058145	-2.98695779
6	-0.54089308	0.93318129	3.73352933	6	2.93989038	0.18937857	-2.74738050
6	-2.11248064	2.69342661	0.99739766	6	2.35167265	1.40222740	-3.12592936
6	-1.04457140	3.48959756	0.49874550	6	-1.85664654	-3.05527878	2.11811852
6	0.24645090	3.48828101	1.13514733	6	-1.97022176	-3.42760348	0.77320594
6	0.50001907	2.69057584	2.28506517	6	-0.79130983	-3.80459213	0.02076799
6	-0.84087753	3.68078542	-0.92051673	6	-0.92555475	-3.30076742	-1.32846367
6	1.24842787	3.67857003	0.10938720	6	-2.17962790	-2.59985685	-1.41664135
6	0.58020020	3.81117606	-1.16891694	6	-2.82082319	-2.67041278	-0.12196133
6	1.14708519	3.25108099	-2.32011628	6	0.20536184	-2.88541245	-2.08440876
6	-0.49400711	-1.91482568	3.65480590	6	-0.04060125	-1.94294882	-3.12085533
6	0.69911480	-1.19355965	3.78352094	6	-1.29465389	-1.24202824	-3.20905972
6	0.67365694	0.25427705	3.81888032	6	-2.33246279	-1.46690083	-2.26281929
6	1.82619715	0.75272965	3.10088086	6	0.99796867	-1.05923676	-3.60325885
6	2.56434298	-0.38004735	2.60720611	6	-1.03146696	0.07503627	-3.74608946
6	1.86815357	-1.57891893	3.01993251	6	0.38889599	0.19205655	-4.00502586
6	1.78007460	1.97492504	2.37492371	6	1.04943037	1.40358686	-3.76787925
6	2.71127939	2.11065412	1.30845380	6	-2.60114169	-1.91260862	2.61615610
6	3.44938517	0.97783285	0.81473422	6	-3.42854619	-1.18917656	1.74876237

6	3.27382135	-0.31719062	1.37606764	6	-3.53563523	-1.57327795	0.35622492
6	2.46298361	2.99968743	0.19477040	6	-3.63030457	-0.37352440	-0.44627696
6	3.65745974	1.16648293	-0.60422707	6	-3.57041979	0.75843453	0.44077960
6	3.05821276	2.42609215	-0.99469244	6	-3.43875146	0.25863430	1.79178262
6	2.41206455	2.54403067	-2.23117805	6	-3.08595490	-0.31049681	-1.75881004
6	-0.55438566	-3.05662704	2.76004601	6	-2.74527001	0.98434436	-2.23873639
6	0.58085346	-3.43016744	2.03065920	6	-2.68545580	2.11632299	-1.35170555
6	1.81015968	-2.67519283	2.16078877	6	-2.96475625	1.98011923	0.03624443
6	2.44673395	-2.60479665	0.86380553	6	-1.74628067	1.17215848	-3.26788020
6	1.61183071	-3.30352759	-0.07774097	6	-1.64951873	3.00409985	-1.83240545
6	0.45905066	-3.80594659	0.63708967	6	-1.06947660	2.43037534	-3.02928329
6	3.21284151	-1.47278690	0.47056586	6	0.30493450	2.54625344	-3.26983809

Radical cation $C_{70}^{+\bullet}$ (D_{5h})

E_{tot} = –2664.833487 a.u.; **ε_{ZPV}** = 1119.25 kJ mol^{-1}; **H_{corr}** = 1190.35 kJ mol^{-1};

G_{corr} = 990.43 kJ mol^{-1}

6	-1.75900376	-1.20933366	3.56831908	6	3.32462311	-1.24165845	-0.92583179
6	-1.77792132	0.18980502	3.61435008	6	2.48577881	-1.94290864	-1.87036383
6	-2.61939430	0.93224150	2.70334411	6	1.51608813	-2.88782907	-1.43910682
6	-1.92554116	2.13493800	2.29391670	6	3.58908391	0.06843868	-1.46481895
6	-0.63704658	2.13303089	2.92759871	6	2.24778724	-1.06012475	-2.99234915
6	-0.54010463	0.93063039	3.74005914	6	2.93890953	0.18893297	-2.75081110
6	-2.10971904	2.69683123	1.00132823	6	2.35077000	1.40233934	-3.12727785
6	-1.04148364	3.49137449	0.50332814	6	-1.85797060	-3.05780721	2.12045407
6	0.24644877	3.48860478	1.13814867	6	-1.97195315	-3.43189144	0.77632254
6	0.50142491	2.69571781	2.28967094	6	-0.79354501	-3.80519533	0.02391938
6	-0.83184308	3.67493629	-0.91719925	6	-0.92941791	-3.30322933	-1.33425844
6	1.25360656	3.68277597	0.10703904	6	-2.17786217	-2.60587835	-1.42205513
6	0.58438772	3.81436753	-1.17031944	6	-2.81633401	-2.67182350	-0.11889002
6	1.14902830	3.25254893	-2.32166934	6	0.20107841	-2.89072251	-2.09055138
6	-0.49578249	-1.91489387	3.65653586	6	-0.04556364	-1.94710505	-3.12443542
6	0.69629520	-1.19239867	3.78765869	6	-1.29383302	-1.24948561	-3.21258593

6	0.66991633	0.25499898	3.82589674	6	-2.33222961	-1.47442186	-2.26840782
6	1.82365441	0.75591022	3.09903383	6	0.99829316	-1.05592394	-3.60530734
6	2.56208348	-0.37669450	2.60677838	6	-1.02595162	0.07521466	-3.74516773
6	1.85918593	-1.57033682	3.01700497	6	0.39108306	0.19378725	-4.00981998
6	1.77974272	1.98011327	2.37871122	6	1.05075896	1.40514529	-3.77094698
6	2.70701170	2.11127234	1.30986321	6	-2.60084867	-1.91349828	2.61602068
6	3.44606781	0.97962946	0.81633854	6	-3.42900324	-1.19120550	1.74872279
6	3.27252626	-0.31479114	1.37726068	6	-3.53487635	-1.57557535	0.35727194
6	2.46375608	3.00734210	0.19261689	6	-3.61808968	-0.37937334	-0.44787979
6	3.64579797	1.17091620	-0.60163546	6	-3.55840278	0.75850844	0.44398871
6	3.05795050	2.43116117	-0.99568719	6	-3.43352127	0.25481310	1.78828931
6	2.41171765	2.54617238	-2.23237514	6	-3.08003783	-0.31799617	-1.76158440
6	-0.55581504	-3.05732322	2.75978017	6	-2.73482537	0.97584563	-2.23686099
6	0.57846010	-3.43277621	2.03009176	6	-2.67491460	2.11407113	-1.34544635
6	1.80246413	-2.67282748	2.15383863	6	-2.95743632	1.98148429	0.04088799
6	2.44090939	-2.59756851	0.86406130	6	-1.74423563	1.17185950	-3.26952910
6	1.60252559	-3.29811049	-0.08140457	6	-1.64592850	2.99757123	-1.83233809
6	0.45553333	-3.81003571	0.63771975	6	-1.06902003	2.42978835	-3.03123546
6	3.20930743	-1.46806979	0.47239703	6	0.30542952	2.54569268	-3.27041483

Radical (*o*-$C_2HB_{10}H_{10}$)$^{\bullet}$

$\mathbf{E_{tot}}$ = -331.020412 a.u.; $\boldsymbol{\varepsilon_{ZPV}}$ = 416.47 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 440.07 kJ mol^{-1};

$\mathbf{G_{corr}}$ = 335.34 kJ mol^{-1}

5	-1.55623698	-1.06940055	0.69580191
5	-1.60126722	0.69937223	0.78922909
5	-1.90189588	-0.13246606	-0.76769274
5	-0.33848554	-0.20133257	1.67229939
5	0.09492977	1.27972019	0.78917599
6	-0.84319305	1.19115877	-0.64960861
5	0.13503410	-1.60640967	0.65621626
5	1.16270494	-0.14316681	0.70726752
6	0.67857194	0.66935253	-0.66465551
5	-0.39184439	-0.06713239	-1.73172069

5	-0.82754177	-1.55480421	-0.86092895
5	0.86163712	-0.97626388	-0.85204643
1	-0.35509935	0.18716960	-2.89252853
1	-2.41565609	-1.72166574	1.21023571
1	-2.43274307	1.41105998	1.25535607
1	-0.30882093	-0.20918612	2.86384416
1	0.42884907	2.35628033	1.16734409
1	2.27719617	-0.02943131	1.10972309
1	1.77807558	-1.41056871	-1.47535789
1	-1.03802145	2.15156245	-1.12512684
1	-1.14617682	-2.52649641	-1.47330713
1	-2.93359756	0.02518116	-1.33853889
1	0.52549613	-2.63016677	1.12782085

Radical (9-*o*-$C_2H_2B_{10}H_9$)$^{\bullet}$

$\mathbf{E_{tot}}$ = -331.028979 a.u.;

$\boldsymbol{\varepsilon_{ZPV}}$ = 424.42 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 447.48 kJ mol^{-1}; $\mathbf{G_{corr}}$ = 343.55 kJ mol^{-1}

5	-1.56724942	-1.08525395	0.70704311
5	-1.58915830	0.69538331	0.78624153
5	-1.88948154	-0.13516128	-0.76634365
5	-0.33347148	-0.21165895	1.67294550
5	0.09616913	1.26781166	0.79940373
6	-0.82516140	1.18185437	-0.64925677
5	0.12443989	-1.56627142	0.63714337
5	1.16471839	-0.15414976	0.70678157
6	0.73487425	0.71031314	-0.69875056
5	-0.39277652	-0.08437219	-1.72837245
5	-0.82210803	-1.56304467	-0.85336101
5	0.86477292	-0.98366076	-0.84394628
1	-0.34999135	0.17091464	-2.88793945
1	1.42137349	1.39301562	-1.19671869

1	-2.43422461	-1.72703075	1.21804416
1	-2.41983557	1.41639674	1.24109292
1	-0.30305123	-0.21581705	2.86572266
1	0.43545514	2.34334612	1.17317474
1	2.27972555	-0.03439427	1.10750890
1	1.78087294	-1.41395938	-1.47145426
1	-1.04461014	2.13823795	-1.11836565
1	-1.14136875	-2.53432441	-1.46845925
1	-2.91892052	0.03629835	-1.33878112

$Mn(OAc)_2$(*o*-$C_2HB_{10}H_{10}$) (product **1)**

E_{tot} = -1938.592333 a.u.; **ε_{ZPV}** = 163.7311 kcal/mol; **H_{corr}** = 177.02 kJ mol^{-1}

5	2.76417208	-1.35967636	0.97767675	25	1.40758383	1.46497893	-2.22160172
5	2.60380602	0.31065753	0.38642779	1	2.30013442	-3.53728223	-0.44631219
5	1.72643101	-0.99776745	-0.42726672	1	0.53394961	-0.98602712	-0.47283787
5	4.19827604	-0.29198316	0.87467366	1	4.94692993	-2.80768251	0.96750325
5	4.03425264	0.69977671	-0.59204322	8	2.60822988	1.26260364	-3.89648032
6	2.56209183	0.19260436	-1.32018232	8	1.74956477	3.34220529	-2.03218102
5	4.30081940	-2.00468540	0.36485291	6	1.56336367	0.90356129	-4.51076698
5	5.09446764	-0.73877102	-0.59693515	8	0.50212741	0.83888310	-3.74445415
6	4.01240873	-0.43863139	-1.86192226	6	0.76346183	3.42136621	-1.17549407
5	2.62503147	-1.42804241	-1.89996970	8	0.10761352	2.34844232	-0.95599949
5	2.76626372	-2.43949032	-0.45129257	6	0.46794078	4.70922232	-0.48426884
5	4.22005844	-2.05682158	-1.40835857	6	1.48568928	0.59189236	-5.96737194
1	2.12683058	-1.67918575	-2.95065928	1	0.59610605	5.54829884	-1.17823184
1	4.34041595	-0.05936215	-2.82569265	1	-0.54151922	4.68916464	-0.06158768
1	2.28209805	-1.68294954	2.02022314	1	1.19596231	4.83458281	0.33156773
1	4.75854397	0.15168788	1.82970011	1	2.46992278	0.70945913	-6.43123722
1	4.43135405	1.79786170	-0.81564748	1	1.12752903	-0.43832654	-6.10204697
1	6.25377607	-0.56786788	-0.80691034	1	0.75913393	1.25905347	-6.45139027
1	4.78684425	-2.77785134	-2.16773438	1	2.00572824	1.20646560	0.89718771

[$Mn(OAc)_2$(*o*-$C_2HB_{10}H_{10}$)]$^{\bullet-}$ (radical anion of product **1)**

$\mathbf{E_{tot}}$ = -1938.700719 a.u.;

$\boldsymbol{\varepsilon_{ZPV}}$ = 678.70 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 735.69 kJ mol^{-1}; $\mathbf{G_{corr}}$ = 549.09 kJ mol^{-1}

5	2.71278882	-1.11819458	0.94289613
5	2.60785317	0.53377759	0.29651275
5	1.64091957	-0.74648786	-0.43682095
5	4.18846798	-0.13554311	0.74869651
5	3.99353337	0.81274831	-0.75650829
6	2.44379854	0.41732606	-1.41736877
5	4.19500589	-1.86912489	0.30835208
5	4.99959660	-0.67181337	-0.73209894
6	3.89136815	-0.36963657	-1.96464097
5	2.46235085	-1.25745177	-1.91434836
5	2.60991931	-2.24222612	-0.44117418
5	4.03689909	-1.97546256	-1.45480609
1	1.92281425	-1.56539583	-2.93042517
1	4.20194912	-0.03892437	-2.95217609
1	2.25977635	-1.38863015	2.01913786
1	4.81258488	0.30737004	1.67007041
1	4.47842264	1.86994743	-1.00791121
1	6.16411114	-0.56678510	-0.98002011
1	4.53967571	-2.76284933	-2.20070267
25	1.46114588	1.73128879	-2.55512762
1	2.09071970	-3.31943583	-0.37397298
1	0.44787773	-0.71956986	-0.41209254
1	4.82898664	-2.68476105	0.91618997
8	2.63620234	1.37422144	-4.21125555
8	2.04939151	3.39810300	-1.50401735
6	1.64761007	0.74956739	-4.73604298
8	0.57262284	0.66699070	-4.03976679
6	0.89444649	3.39990306	-0.95169741
8	0.06217710	2.49040294	-1.31307399
6	0.53930265	4.39703035	0.12124088
6	1.74828160	0.11013612	-6.09787798

1	1.07799327	5.33877563	-0.04108340
1	-0.54437423	4.56510210	0.14351338
1	0.84672844	3.98907375	1.09638643
1	2.53468776	0.59307367	-6.69035339
1	2.00439048	-0.95414525	-5.97899151
1	0.78253049	0.16770400	-6.61623573
1	2.09483838	1.46425891	0.84053063

Radical $^{\bullet}C_{60}$ (*o*-$C_2HB_{10}H_{10}$) (*C*$_1$)

E_{tot} = -2615.359310 a.u.

ε_{ZPV} = 1389.00 kJ/mol; **H_{corr}** = 1471.97 kJ mol^{-1}; **G_{corr}** = 1250.94 kJ mol^{-1}

5	4.69184399	-3.47440410	-0.40924698	6	-1.58426523	1.67325795	2.14567208
5	4.79773951	-2.36486006	0.97832900	6	-2.04965687	2.64471006	3.11163402
5	3.26786637	-2.54217434	0.09125329	6	-1.51716280	3.94210243	3.11982107
5	6.13204575	-2.44154859	-0.19879989	6	-1.20041537	4.58789778	4.37858772
5	5.59667397	-0.87915707	0.42374939	6	0.01900704	5.36223459	4.19496584
6	3.86893916	-0.99462521	0.53975618	6	0.96265525	5.43923712	5.22764397
5	5.41274500	-2.66467428	-1.82113409	6	2.37952447	5.34907389	4.92376375
5	5.96617699	-1.05744362	-1.30289590	6	3.01928759	4.59484577	5.98932552
6	4.55404854	-0.27153111	-0.78817135	6	4.05707407	3.70467997	5.69105530
5	3.10353947	-1.15668714	-1.00289786	6	3.97969985	0.14625582	2.88967919
5	3.63584471	-2.71938825	-1.63675451	6	2.57026434	0.70170778	7.25594425
5	4.43028307	-1.22815430	-2.18421388	6	3.01808906	-0.22827785	6.31368589
1	2.10064650	-0.54822445	-1.18492365	6	2.07322097	-1.11353266	5.64999771
1	4.45157146	0.81056851	-0.82936144	6	0.70447463	-1.02487135	5.95760727
1	4.72652292	-4.65399218	-0.23831929	6	0.23985618	-0.05409287	6.92493773
1	4.85902977	-2.63678241	2.13470101	6	0.83012265	2.19442558	7.76000452
1	7.20354223	-2.85685968	0.11707875	6	2.04927087	2.96904111	7.57617760
1	6.14784575	-0.10083656	1.12889051	6	3.12420726	2.04704738	7.26747799
1	6.84027863	-0.38180095	-1.74453020	6	4.11296940	2.40676022	6.34412861
1	4.26731968	-0.66678733	-3.22047687	6	4.58065891	1.43705237	5.37036848
1	2.91083193	-3.33383250	-2.35593653	6	4.03661442	0.14710052	5.35009336
1	2.29394579	-2.93501067	0.64769202	6	2.50824118	-1.29015851	4.28563404

1	5.97962999	-3.24987411	-2.69159174	6	1.56196880	-1.33882833	3.25104928
6	1.38342500	3.27461672	0.93226951	6	0.14006582	-1.25934875	3.56842589
6	1.71209538	1.87809956	0.73145860	6	-0.27919912	-1.10117793	4.89035130
6	2.93728733	1.37742209	1.14879334	6	-1.35738516	-0.17859626	5.20168638
6	3.84358001	2.24415755	1.84782922	6	-1.03539348	0.47170666	6.46038675
6	3.55307651	3.60659432	2.03065157	6	-1.34368730	1.82244039	6.64662409
6	2.29335546	4.13290691	1.56157148	6	-0.39398584	2.70120382	7.30942440
6	-0.03368387	3.36857986	1.23189938	6	1.99629200	4.22102070	6.94968653
6	-0.58795327	2.02336121	1.21779811	6	0.72617072	4.74343252	6.47964334
6	0.47706053	1.10287774	0.90279055	6	-0.44641808	3.99506950	6.65379667
6	0.54415560	-0.13889579	1.55463123	6	-1.42795324	3.92018867	5.58707285
6	3.13683152	-0.08900723	1.61083448	6	-1.98347974	2.57668209	5.58085871
6	4.48092079	1.48969364	2.91387558	6	-2.29132128	1.95194364	4.36880636
6	4.80830097	2.12555075	4.12233591	6	-1.97332847	0.54753411	4.17587709
6	4.48771858	3.52930450	4.31513786	6	-1.53271985	0.37714136	2.80204391
6	3.87340546	4.25574017	3.29019666	6	-0.49534410	-0.50939131	2.51013255
6	2.80142999	5.18535423	3.59952688	6	3.72955251	-0.49877498	4.09046698
6	1.82171226	5.10832930	2.52803111	6	1.78920627	-0.68015116	2.00172257
6	0.45599446	5.19224644	2.82362008	6	1.15332377	0.79436159	7.56684923
6	-0.49073532	4.30949736	2.15853071				

Radical $^{\bullet}C_{60}(9\text{-}o\text{-}C_2H_2B_{10}H_9)$ (C_S)

$\mathbf{E_{tot}}$ = -2615.385343 a.u.

$\boldsymbol{\varepsilon_{ZPV}}$ = 1393.56 kJ/mol; $\mathbf{H_{corr}}$ = 1476.78 kJ/mol; $\mathbf{G_{corr}}$ = 1252.74 kJ/mol

5	3.78405070	-2.74996281	-1.72586334	6	-1.72724283	1.13023758	2.55233407
5	3.37428880	-2.51407719	-0.01374109	6	-2.22862577	2.10846424	3.49247861
5	3.21695018	-1.15780866	-1.16931212	6	-1.90239346	3.46493793	3.34210157
5	4.81717825	-3.45196724	-0.45350215	6	-1.55440784	4.26029158	4.50335932
5	4.89741325	-2.29941702	0.89991772	6	-0.49469697	5.18240261	4.11930656
5	3.90099597	-0.87161773	0.46500489	6	0.53077716	5.48651552	5.02438021
6	5.47444963	-2.60844755	-1.77116311	6	1.90405083	5.57228279	4.55978966
5	6.23875713	-2.40759826	-0.24315253	6	2.76215672	5.01540422	5.59386826

5	5.68000269	-0.81359833	0.30241033	6	3.88724756	4.26183987	5.24110222
5	4.64633322	-0.11122965	-0.97045630	6	4.04133892	0.49448240	2.74155164
5	4.55360413	-1.26253569	-2.31832075	6	3.05011058	1.23094630	7.18759823
6	5.96183443	-1.11244094	-1.34122431	6	3.53239703	0.29313856	6.26952791
1	4.73475933	1.04414928	-1.23711979	6	2.66820264	-0.77610552	5.79050112
1	6.45671892	-0.12591726	0.88341957	6	1.34189379	-0.85693330	6.25258827
1	3.26210213	-3.45844316	-2.52544975	6	0.84136128	0.12066842	7.19379044
1	2.42347884	-3.05123401	0.46289983	6	1.16773009	2.49765849	7.78537178
1	4.98366785	-4.62824774	-0.40524846	6	2.22744489	3.41993976	7.40152025
1	5.04981899	-2.66800833	2.02340317	6	3.39106655	2.63732529	7.03473139
1	7.35214472	-2.80128503	-0.12426665	6	4.21047640	3.04955792	5.97645903
1	6.84539461	-0.73294866	-1.84935892	6	4.71653271	2.07345295	5.02880955
1	4.64168310	-0.95933616	-3.46243358	6	4.37604904	0.72047180	5.16903639
1	2.17090535	-0.70962566	-1.52440667	6	2.97623992	-1.01084042	4.40139771
1	6.07475090	-3.10270572	-2.53131485	6	1.94263196	-1.29322088	3.49204373
6	0.81519496	3.02587938	0.87603486	6	0.56593299	-1.38762844	3.97079563
6	1.32940829	1.67827809	0.74233311	6	0.27295324	-1.16937709	5.31813526
6	2.64924383	1.39604473	1.06325161	6	-0.89360225	-0.38562930	5.68715858
6	3.48717856	2.44518113	1.56959438	6	-0.54105824	0.41519856	6.84696770
6	3.01419425	3.76493549	1.68125618	6	-1.03027916	1.71932149	6.96888399
6	1.64631641	4.06116247	1.32728767	6	-0.16049409	2.78195834	7.44765711
6	-0.55752301	2.94117904	1.33842957	6	1.91635275	4.58923244	6.69551373
6	-0.89996737	1.53415132	1.48854280	6	0.53872263	4.88116026	6.34358692
6	0.25402519	0.75184637	1.11974442	6	-0.48069352	3.99105358	6.71135378
6	0.57589525	-0.40826452	1.84432209	6	-1.54638135	3.67935276	5.77670431
6	3.11071539	0.03403542	1.60754001	6	-1.88783252	2.27460480	5.93496323
6	4.34390402	1.89037097	2.60261178	6	-2.22470665	1.50540304	4.81704426
6	4.70185184	2.67250037	3.71534777	6	-1.71927798	0.14911000	4.69160795
6	4.19064474	4.02677155	3.83991480	6	-1.40851152	-0.08066667	3.29099631
6	3.36484885	4.56120205	2.84476089	6	-0.28680000	-0.83515859	2.94271421
6	2.20217252	5.35194969	3.21065235	6	4.03711128	-0.07486486	4.00664425
6	1.13713717	5.03909588	2.27116966	6	1.93055797	-0.71421307	2.18467593
6	-0.18590809	4.95322418	2.72187972	6	1.67816567	1.14654219	7.65904284

6 -1.05198681 3.88684678 2.24189782

Dimer $[C_{60}(o\text{-}C_2HB_{10}H_{10})]_2$

$\mathbf{E_{tot}}$ = -5230.724858 a.u.

$\boldsymbol{\varepsilon_{ZPV}}$ = 2785.28 kJ/mol; $\mathbf{H_{corr}}$ = 2953.35 kJ mol^{-1};

5	4.98925877	7.98969364	1.84369743	6	11.75982380	16.68928337	7.70330286
5	4.41010332	9.64767456	1.55282223	6	12.18375492	15.71521187	6.71558332
5	5.66371584	8.94175529	0.51037645	6	11.70709515	14.39848804	6.78573608
5	4.69831991	9.08845043	3.21682048	6	10.15511990	12.85953331	5.91134405
5	5.19053173	10.71042347	2.73541331	6	9.13172245	12.71468067	4.98226118
6	5.80175209	10.55959702	1.11664236	6	7.76108837	12.73425388	5.43315983
5	6.14664078	8.04072571	3.19449186	6	7.45702028	12.90772533	6.79099131
5	6.27345896	9.72493362	3.73547387	6	6.36886501	13.78021145	7.17944908
6	6.85814238	10.56755638	2.37400746	6	6.76442862	14.49043369	8.38402367
5	7.23199606	9.58018112	1.02186084	6	6.40250063	15.82978916	8.55713177
5	6.74358988	7.95634794	1.51434779	6	7.36003208	16.78075409	9.09808540
5	7.53008413	9.03513813	2.68584681	6	9.61462212	18.41063499	8.46230984
1	8.09371853	9.93574333	0.28997254	6	8.27915096	18.85089302	8.10597515
1	7.46198988	11.46676254	2.47512889	6	7.17213964	18.04776955	8.41524982
1	4.28021622	7.05884886	1.61370003	6	6.09877682	17.88601494	7.45149040
1	3.36441565	9.98445034	1.09842360	6	5.62475586	16.51303673	7.53575087
1	3.79571557	8.96458435	3.98525906	6	5.25048304	15.83110619	6.37456560
1	4.76840782	11.76980305	3.05717754	6	5.62656498	14.43878651	6.18998575
1	6.55752468	10.13920212	4.81260586	6	5.94817972	14.24314404	4.79186392
1	8.66096687	8.99843121	3.05276203	6	6.99884129	13.41679096	4.41630888
1	7.31459093	7.01659584	1.05499816	6	11.30915737	13.70604134	5.58521843
1	5.46651125	8.78785229	-0.64978194	6	9.19206429	13.36322403	3.66619253
1	6.29402542	7.14443111	3.96670079	6	9.02630520	14.96464920	9.25687695
5	11.68625164	10.68283844	0.76499075	6	3.27019167	11.53885078	-2.83689499
5	11.51588631	11.38627911	2.39410615	6	3.69868684	11.48297882	-1.46019602
5	10.54486752	12.01114273	1.04584885	6	5.03162622	11.29993439	-1.15279269
5	13.13249302	10.98482800	1.76256394	6	5.99500704	11.21080685	-2.19946122
5	12.88118649	12.48318291	2.64897490	6	5.59926081	11.22977161	-3.54663277

6	11.30212307	13.07094574	2.14081740	6	4.20403862	11.40091896	-3.87322640
5	13.14887142	11.37061501	0.01783359	6	2.20060205	12.51504517	-2.94019771
5	13.87706375	12.49257755	1.18707192	6	1.96030569	13.06641388	-1.61682010
6	12.68020344	13.67792034	1.44340253	6	2.88249993	12.43646049	-0.69516712
5	11.28777409	13.50980759	0.46677300	6	3.46782684	13.16779041	0.32949188
5	11.54219437	12.00784683	-0.42531565	6	5.69125700	11.81027031	0.14984778
5	12.90071297	13.12282085	-0.15450510	6	7.19934654	11.89284229	-1.76852608
1	10.71295452	14.50367737	0.17858735	6	7.96837330	12.57747555	-2.71712208
1	12.94454861	14.69708729	1.71783590	6	7.54850912	12.62668419	-4.10745716
1	11.28074551	9.58474064	0.53930026	6	6.38689709	11.96457672	-4.51796579
1	10.98309135	10.90212536	3.34054494	6	5.47244978	12.60256863	-5.44509649
1	13.78401470	10.12121868	2.26234841	6	4.11633396	12.25418377	-5.04261208
1	13.30312157	12.81633186	3.70216560	6	3.09306121	13.20391178	-5.13797808
1	15.01136494	12.82904911	1.31147039	6	2.11298180	13.33255959	-4.07060719
1	13.37462807	13.88448429	-0.93587571	6	1.64089513	14.42418385	-1.47453547
1	11.05459309	11.87162971	-1.50439322	6	1.55874074	15.27660465	-2.64845586
1	9.36473179	11.94953060	1.10602212	6	1.79215562	14.74267960	-3.91974664
1	13.83043098	10.77519321	-0.75784749	6	2.58075118	15.48426723	-4.89007378
6	8.48552132	17.19902229	2.57972693	6	3.38287401	14.53445053	-5.63986254
6	8.86163807	15.82825947	2.31929946	6	4.68737698	14.86954212	-6.03013229
6	10.13950443	15.41353226	2.65449858	6	5.75086117	13.88586617	-5.92945480
6	11.05380821	16.35816765	3.25535512	6	6.96030140	14.57350254	-5.51121616
6	10.71706772	17.70643616	3.43352294	6	7.84235668	13.95399952	-4.61620283
6	9.39253902	18.14130211	3.08021903	6	7.01541758	12.38938522	-0.42441827
6	7.10846996	17.23767853	3.02926421	6	7.89893866	16.62692070	-2.07550073
6	6.62277412	15.89871883	3.08779168	6	7.94511700	15.78299236	-0.95204389
6	7.59469795	14.93078709	2.38156056	6	7.00227022	15.92229080	0.10790113
6	7.91260386	13.78236103	3.32086754	6	5.98557854	16.85253525	-0.00155544
6	10.49023724	13.98406887	3.15084624	6	5.89871931	17.71455765	-1.15496540
6	11.83218288	15.68561840	4.28081083	6	6.42378426	17.67424583	-3.56654525
6	12.24852848	16.37383080	5.43383598	6	7.22680855	16.72286415	-4.32244015
6	11.87501431	17.76391029	5.61856270	6	8.13879585	16.07851219	-3.39677238
6	11.12321663	18.41592598	4.63600588	6	8.43915939	14.71963120	-3.53642845

6	10.03578949	19.29730988	5.02243280	6	8.51346684	13.86084938	-2.36668706
6	8.96259117	19.12635612	4.05991411	6	8.26384354	14.37524128	-1.08858645
6	7.63114786	19.16137123	4.48740673	6	6.88696671	14.61146927	0.91236055
6	6.67821074	18.20731354	3.95017695	6	5.41647959	14.22715282	1.00579393
6	5.76949549	15.53000736	4.10950327	6	4.35041714	15.23512363	0.88787258
6	5.33417988	16.49747849	5.08730841	6	4.61771488	16.51097679	0.40997303
6	5.77502060	17.82645607	5.00775242	6	3.70391393	17.16785240	-0.49957177
6	6.16765881	18.53239822	6.21268606	6	4.49441910	17.90583420	-1.47173154
6	7.31974173	19.36322403	5.88891315	6	4.08676815	17.97073555	-2.80685210
6	8.35428524	19.51937675	6.81901264	6	5.06899643	17.84515381	-3.87301087
6	9.73768425	19.48956299	6.37818480	6	6.64362097	15.98291302	-5.35766888
6	10.51743317	18.80586052	7.39581013	6	5.23846626	16.16406059	-5.67694473
6	11.57054710	17.96281433	7.02247000	6	4.46533871	17.07809830	-4.94683313
6	11.39248371	14.33086872	4.35684919	6	3.11204481	16.73313904	-4.54993963
6	10.40990257	14.93543625	8.81078625	6	2.87439537	17.28616714	-3.22675228
6	10.81308270	13.99762535	7.85645437	6	2.11141300	16.57540321	-2.29467869
6	9.85739803	13.04455471	7.31535816	6	2.53078747	16.51548004	-0.90479827
6	8.52585125	13.06976223	7.75326681	6	2.24199510	15.18860340	-0.40101820
6	8.10423279	14.04895973	8.74048138	6	3.13791847	14.56521988	0.48114038
6	8.64806843	16.35601616	9.44195557	6	7.54768276	13.62379074	-0.08032904
6	9.79564571	17.18293762	9.11514378	6	4.88650894	12.99257469	0.67586857
6	10.88670444	16.30777740	8.72794628	6	6.84808254	17.61090851	-2.18109608

Dimer [C_{60} (9-*o*-$C_2H_2B_{10}H_9$)]$_2$

E_{tot} = -5230.779906 a.u.

ε_{ZPV} = 2795.58 kJ/mol; **H_{corr}** = 2963.77 kJ/mol;

5	-2.78711867	-6.07966375	0.22647710	6	4.23403502	2.67043114	6.01596785
5	-3.17196131	-4.35379982	0.05107823	6	4.65438461	1.71492302	5.00855589
5	-2.07103777	-5.15646076	-1.09129667	6	4.18607759	0.39337900	5.06241512
6	-2.75424814	-4.99806118	1.56091177	6	2.62922859	-1.13677740	4.18358517
5	-2.19228792	-3.43578935	1.22701430	6	1.59375703	-1.27427959	3.26712036
5	-1.69759834	-3.48482275	-0.48706433	6	0.22720751	-1.27601862	3.73510909

6	-1.56275558	-6.10562563	1.43358147	6	-0.06003186	-1.12335694	5.09946203
5	-1.18673110	-4.58363056	2.13663435	6	-1.14873242	-0.26318395	5.51583815
5	-0.47727209	-3.66323543	0.80883145	6	-0.74026352	0.43228233	6.72418451
5	-0.40507090	-4.71932745	-0.63028634	6	-1.10805714	1.76689136	6.92434788
5	-1.07412326	-6.30513000	-0.17836659	6	-0.14856604	2.71515179	7.46788883
5	-0.09190369	-5.38567209	0.98910177	6	2.08906889	4.36832523	6.83045816
1	0.47581118	-4.63476610	-1.42993498	6	0.74649537	4.80597162	6.49781609
1	0.34436184	-2.83732605	1.02715755	6	-0.35262999	3.99245286	6.80911446
1	-3.59859848	-6.94591379	0.23562633	6	-1.43556464	3.83851910	5.85497618
1	-4.31024313	-4.05935955	-0.12861978	6	-1.90045929	2.46126676	5.92307615
1	-3.49837780	-5.17845726	2.33317137	6	-2.28415704	1.79559040	4.75452185
1	-2.69412756	-2.53785563	1.82088268	6	-1.90490746	0.40762061	4.54362249
1	-1.02472365	-4.54920244	3.31175733	6	-1.60290229	0.23401155	3.13776660
1	0.91318369	-5.85203171	1.42067063	6	-0.54967159	-0.57660085	2.73691630
1	-0.72452366	-7.38653946	-0.52849787	6	3.77904773	-0.28414500	3.85589361
1	-2.40387559	-5.40180111	-2.20703459	6	1.63305318	-0.59133375	1.96686220
1	-1.61048758	-6.93815899	2.13130641	6	1.53043807	0.90648305	7.57617235
5	4.24982595	-3.32581997	-1.09123683	6	-4.18766451	-2.52738953	-4.50804520
5	4.00324535	-2.66411161	0.54221398	6	-3.78156710	-2.55810571	-3.12385917
5	3.14537740	-1.95708990	-0.85675848	6	-2.44757581	-2.70129204	-2.79079461
5	5.63790703	-3.12021923	0.00599854	6	-1.46713054	-2.80190444	-3.82250738
5	5.39993858	-1.62399149	0.92949665	6	-1.84278703	-2.80965424	-5.17736578
5	3.82667494	-0.88574660	0.40515012	6	-3.23487902	-2.66483498	-5.52886343
6	5.70011806	-2.61679697	-1.61294723	6	-5.26928234	-1.56735897	-4.64130497
5	6.49860287	-1.63637912	-0.44795859	6	-5.54087782	-1.00260174	-3.32958412
5	5.39253616	-0.26617649	-0.21768451	6	-4.62189102	-1.60558689	-2.38519573
5	4.00629377	-0.47015619	-1.32100141	6	-4.06554222	-0.85121316	-1.35995746
5	4.23726273	-1.97158110	-2.24220681	6	-1.81983721	-2.16596580	-1.49514639
6	5.56084490	-0.99541205	-1.73732042	6	-0.28148147	-2.09521198	-3.38175058
1	3.57939601	0.47955126	-1.89287257	6	0.49633867	-1.41163099	-4.32729721
1	5.87263441	0.81153286	-0.06744243	6	0.09563634	-1.38735759	-5.72449398
1	3.97225809	-4.40458775	-1.50730157	6	-1.05036771	-2.07242155	-6.14413786
1	3.43428278	-3.30457139	1.37182474	6	-1.95929980	-1.46108258	-7.09482098

1	6.28879833	-4.06302929	0.32477874	6	-3.31624913	-1.82562864	-6.70920515
1	5.85578632	-1.51037538	2.02230048	6	-4.35209608	-0.89298189	-6.83392572
1	7.67918968	-1.53545606	-0.51895106	6	-5.35139084	-0.76577044	-5.78423548
1	6.12223816	-0.52413398	-2.54076552	6	-5.88270187	0.35168579	-3.21004438
1	4.04738140	-2.08015990	-3.40870976	6	-5.95708227	1.18716180	-4.39686680
1	1.97852683	-2.09080744	-1.01834559	6	-5.69734383	0.64053702	-5.65802526
1	6.34735346	-3.09536362	-2.34386992	6	-4.90403748	1.38212919	-6.62479210
6	0.89428747	3.24363351	0.94260561	6	-4.07510662	0.43552038	-7.34921122
6	1.27527094	1.87856472	0.65747517	6	-2.77011538	0.78618985	-7.72370386
6	2.55733418	1.46258569	0.97669607	6	-1.69334948	-0.17973225	-7.59180069
6	3.47470880	2.40634394	1.57485723	6	-0.50185895	0.53245205	-7.16365528
6	3.13360190	3.75169802	1.77460456	6	0.37575611	-0.06122775	-6.24613762
6	1.80218816	4.18461514	1.44514382	6	-0.50481766	-1.57964039	-2.05124736
6	-0.47752160	3.26626945	1.40975618	6	0.34954804	2.64517212	-3.73994279
6	-0.95806175	1.92285097	1.44829667	6	0.38919002	1.81691718	-2.60513377
6	0.01527364	0.97142780	0.72135091	6	-0.57112700	1.95544136	-1.55832565
6	0.34810874	-0.18622512	1.64077771	6	-1.60077763	2.86711478	-1.69829917
6	2.91304493	0.03614099	1.44734490	6	-1.68227720	3.71231818	-2.86517382
6	4.26741648	1.72318256	2.57766795	6	-1.11780143	3.64871359	-5.26800728
6	4.69871092	2.39425015	3.73666453	6	-0.28808802	2.70006847	-5.99876595
6	4.31817627	3.77897525	3.94749236	6	0.61955678	2.08267474	-5.05077648
6	3.54961967	4.44210529	2.98431325	6	0.94467193	0.72757447	-5.16814899
6	2.46184659	5.31064320	3.40014195	6	1.01689172	-0.11579412	-3.98502517
6	1.37811875	5.15032482	2.44756007	6	0.73214293	0.41271490	-2.71841621
6	0.05235730	5.17108822	2.89174390	6	-0.67897147	0.65169954	-0.74146450
6	-0.90179765	4.21903896	2.35103536	6	-2.14514399	0.24731603	-0.65979362
6	-1.79378152	1.53267241	2.47810888	6	-3.22342229	1.23635423	-0.81408393
6	-2.22151089	2.48203492	3.47728300	6	-2.97018719	2.51156259	-1.30123365
6	-1.78819835	3.81491399	3.41407275	6	-3.87812853	3.13929462	-2.23751593
6	-1.38550997	4.50401211	4.62509966	6	-3.08314705	3.87588096	-3.20752478
6	-0.24270479	5.34753132	4.30023003	6	-3.47100449	3.91835213	-4.55033207
6	0.80193102	5.49539280	5.22073174	6	-2.46992850	3.79419255	-5.59896564
6	2.17999530	5.48028708	4.76234818	6	-0.84268826	1.93854463	-7.03436708

6	2.97644806	4.78512383	5.75891209	6	-2.24530172	2.09371424	-7.37872839
6	4.02914381	3.95406532	5.35833263	6	-3.04416633	3.00516534	-6.67328978
6	3.82853842	0.36597574	2.63665938	6	-4.39762068	2.64350033	-6.29223967
6	2.90840006	0.89279783	7.11269379	6	-4.66575527	3.21113157	-4.98043060
6	3.30527425	-0.02737714	6.13763571	6	-5.43130159	2.50006580	-4.05050278
6	2.34821630	-0.97817904	5.59588289	6	-5.03550434	2.46522260	-2.65329552
6	1.02188683	-0.96866912	6.05089760	6	-5.31120157	1.14033532	-2.13673973
6	0.60682815	-0.00700392	7.05731726	6	-4.42113018	0.54321200	-1.23159671
6	1.14636588	2.29258728	7.78836346	6	0.00837168	-0.33508003	-1.71457100
6	2.28526497	3.13134265	7.46092701	6	-2.64741063	-0.99833667	-0.99233431
6	3.37650800	2.26867676	7.04631281	6	-0.71507186	3.61009574	-3.87551284

Radical $^{\bullet}C_{70}$-*a*-(*o*-$C_2HB_{10}H_{10}$)

$\mathbf{E_{tot}}$ = -2996.168245 a.u.; $\boldsymbol{\varepsilon_{ZPV}}$ = 1552.33 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 1645.91 kJ mol^{-1}

5	-1.73306215	-4.96340561	-0.05992717	6	1.64036703	-1.21675849	-1.46349001
6	-0.34837812	-4.07651091	-0.61420202	6	1.10565209	-1.98043621	-0.38381487
5	-0.12321149	-5.21296072	0.64672476	6	1.81248450	-1.58842206	0.79309666
6	-1.42265868	-4.69040966	-1.71964800	6	-0.31841642	-2.51503849	-0.36352590
5	0.23578386	-4.63238287	-2.14472532	6	1.99380386	5.53489447	-0.40717793
5	1.08832514	-5.02024078	-0.63945663	6	1.94634104	4.89504766	-1.65219927
5	-2.00538754	-6.22184706	-1.28174281	6	2.75773382	3.72097802	-1.89867651
5	-0.79278302	-6.01838732	-2.56773853	6	0.67499691	4.68152094	-2.31226730
5	0.81735128	-6.27927208	-1.86191642	6	0.70977622	3.39476371	-2.97144794
5	0.59362513	-6.64568901	-0.12818225	6	1.99848938	2.79983282	-2.71762156
5	-1.15381730	-6.60501719	0.23159552	6	2.14819384	1.39457703	-2.59069920
5	-0.56974620	-7.26869106	-1.32361758	6	1.03729081	0.59755081	-2.99888182
1	1.35015368	-7.34033871	0.47763687	6	-0.25004762	1.19559062	-3.24599934
1	1.71950173	-6.69833088	-2.51837087	6	-0.45867670	2.59504271	-3.10336137
1	-2.61154008	-4.35282469	0.45220476	6	-1.26735389	0.23824129	-2.87550759
1	-2.05645323	-3.95291924	-2.20718169	6	-0.62242407	-0.96626854	-2.40344739
1	0.58128422	-3.81225586	-2.93029141	6	0.81718117	-0.72594881	-2.47984624
1	-1.10379565	-6.13666725	-3.71009517	6	-1.17672253	-1.70609665	-1.36741555

1	-0.66992772	-8.42470551	-1.59733701	6	0.76415604	5.99129105	0.21697496
1	2.11389875	-4.46162367	-0.41789037	6	-0.46212709	5.78890419	-0.42984378
1	-1.66896367	-7.26009035	1.08354795	6	-0.50520003	5.11914444	-1.71268630
1	0.08299077	-4.78585720	1.73756254	6	-1.61706054	5.34226370	0.32070357
1	-3.13443947	-6.47815847	-1.55562639	6	-2.37568760	4.42296267	-0.50163549
6	2.16983724	5.15463257	1.90196419	6	-1.68707478	4.28485584	-1.75755715
6	2.29105854	4.15057230	2.87066674	6	-1.70494413	3.05835676	-2.47660470
6	1.12607372	3.70693779	3.60807204	6	-2.65313029	2.08963251	-2.04690719
6	3.10183835	2.97936511	2.60823417	6	-3.33950996	2.22572780	-0.79083788
6	2.44949460	1.82711375	3.19354320	6	-3.09739137	3.33705878	0.06485089
6	1.22670186	2.27850556	3.81010032	6	-3.55795312	0.89592701	-0.26306024
6	0.07127972	1.45055008	3.85110021	6	-3.02184582	-0.06796910	-1.19892001
6	0.26434049	0.08414604	3.50733256	6	-2.45464087	0.67642647	-2.29240751
6	1.48633254	-0.37225786	2.89665294	6	-2.36883020	-1.22401023	-0.72952420
6	2.54524183	0.53938955	2.60524774	6	0.87281603	5.75617695	1.64425945
6	1.15954971	-1.46651900	2.02075458	6	-0.24898143	5.32860470	2.36629081
6	-0.28113112	-1.70475996	2.08395100	6	-1.51261353	5.11644125	1.69157803
6	-0.81927705	-0.73005563	3.00572467	6	-0.11866673	4.28417301	3.36045194
6	-0.99793166	-2.08876920	0.96079576	6	-1.30078542	3.45078444	3.31081772
6	2.86361456	5.02087402	0.63446230	6	-2.16401768	3.96537876	2.28091478
6	3.65327311	3.89019871	0.38834783	6	-2.98715019	3.09905910	1.51092279
6	3.77150083	2.85294962	1.39228702	6	-3.12727547	1.76752412	1.99379027
6	3.59576464	3.22952080	-0.89921296	6	-2.26635218	1.25485480	3.02502584
6	3.69772339	1.80128086	-0.68921733	6	-1.24210107	2.05899596	3.59611106
6	3.80711913	1.56862938	0.72613436	6	-2.06860662	-0.15784007	2.77624297
6	3.25009441	0.40424174	1.32444525	6	-2.80755377	-0.52837455	1.59849453
6	2.83464813	-0.62013692	0.43566072	6	-3.45239854	0.67033100	1.10793054
6	2.72981977	-0.39094812	-0.96986932	6	-2.25854349	-1.45788968	0.69555402
6	3.02905703	0.87527013	-1.53714263				

Radical $^{\bullet}C_{70}$-*b*-(*o*-$C_2HB_{10}H_{10}$)

$\mathbf{E_{tot}}$ = -2996.167610 a.u.; $\boldsymbol{\varepsilon_{ZPV}}$ = 1551.92 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 1645.54 kJ mol^{-1}

6	23.98654175	-5.04811192	0.17769241	6	23.73908424	-1.72186816	-1.49060392

6	23.03715515	-4.15237713	-0.84682113	6	22.86279678	-2.60344529	-0.57315397
5	24.58661079	-4.71650839	-1.38947201	6	23.41030502	-2.15269113	0.80067801
5	22.28599358	-5.23265553	0.27636790	6	21.40753746	-2.17898345	-0.70362794
5	21.73483849	-5.12651014	-1.40553856	6	25.55381012	4.73071337	-0.02079880
5	23.14974594	-4.79660606	-2.42958713	6	25.56813049	4.13700247	-1.28861201
5	23.38985825	-6.62028265	0.40717527	6	26.08748817	2.79533195	-1.45665741
5	21.95440102	-6.71123362	-0.63490665	6	24.41853905	4.25903273	-2.16203547
5	22.49125671	-6.44648981	-2.31818390	6	24.24579620	3.01082253	-2.87339067
5	24.25679016	-6.18667507	-2.30791473	6	25.27882004	2.10902619	-2.43862748
5	24.80646324	-6.30044031	-0.62036383	6	25.04225731	0.70893115	-2.35489917
5	23.51486397	-7.37625790	-1.19721675	6	23.85853958	0.22745050	-2.97283173
1	24.97404099	-6.47893763	-3.21376443	6	22.82906342	1.12721896	-3.41284943
1	21.92645645	-6.93147898	-3.24968505	6	22.95616531	2.53337431	-3.23710012
1	24.44404221	-4.48925400	0.99091053	6	21.55774498	0.45096588	-3.27370453
1	21.72636604	-4.75358295	1.20713139	6	21.79457092	-0.87741148	-2.76747608
1	20.69896126	-4.58607388	-1.62258291	6	23.23229027	-1.00924802	-2.56146836
1	21.01462173	-7.38055563	-0.33618930	6	20.91963959	-1.43166435	-1.82131135
1	23.70477676	-8.54840565	-1.30450249	6	24.38920593	5.48094320	0.41304809
1	23.07095909	-4.03232861	-3.33773708	6	23.28371811	5.60235500	-0.43919501
1	25.89968491	-6.57214832	-0.23736842	6	23.29906845	4.97615862	-1.74437642
1	25.45895195	-3.92043519	-1.49712610	6	21.94119644	5.45751190	0.08463225
1	23.52760887	-7.10706854	1.48402727	6	21.13342285	4.76862192	-0.89808792
6	25.22404480	4.30352449	2.26547003	6	21.97317314	4.46874285	-2.02786851
6	24.92166519	3.29923654	3.19303012	6	21.77610588	3.29253912	-2.80182481
6	23.57244682	3.16257191	3.70310044	6	20.55836868	2.58886409	-2.58273864
6	25.44351387	1.96043730	3.01023340	6	19.71543121	2.89207673	-1.45323586
6	24.43323708	1.01325798	3.42402124	6	20.07537651	3.89798713	-0.51538539
6	23.27585793	1.75403130	3.84963799	6	19.07225800	1.66480625	-1.03903568
6	21.96195602	1.24535954	3.65352416	6	19.50677681	0.59993315	-1.91966927
6	21.86357117	-0.12343639	3.27870345	6	20.43274307	1.17887521	-2.86764884
6	23.01874352	-0.86050010	2.84818459	6	19.74094391	-0.67923695	-1.40452528
6	24.30057144	-0.25299922	2.78884435	6	24.18555260	5.21697235	1.82491910
6	22.59192657	-1.83875751	1.87215054	6	22.88436508	5.08531427	2.32821131

6	21.14826393	-1.71514189	1.70963812	6	21.74530220	5.20416164	1.44150150
6	20.71538544	-0.64085710	2.56671572	6	22.57455063	4.03736973	3.27741742
6	20.59573174	-1.85256720	0.42624101	6	21.24913406	3.53101754	2.98916864
6	26.07151794	4.00328779	1.12475395	6	20.73591995	4.25406075	1.85543299
6	26.57831764	2.70968723	0.95594513	6	19.86914444	3.63047361	0.91515899
6	26.25591087	1.67071509	1.91365862	6	19.31855011	2.37737131	1.29919755
6	26.58333206	2.09501982	-0.35659748	6	19.83502579	1.65117788	2.43243122
6	26.27659988	0.69106513	-0.20541003	6	20.90857697	2.16871262	3.21071649
6	26.07504082	0.42863917	1.19776022	6	19.70880508	0.24027684	2.15352345
6	25.14646149	-0.55167741	1.63571835	6	19.10806465	0.08263974	0.84729773
6	24.63956070	-1.44208539	0.64019656	6	18.87657166	1.41098785	0.31825504
6	24.83929634	-1.17786562	-0.76202995	6	19.53924561	-0.94091058	-0.00248193
6	25.55400467	-0.02139480	-1.19801450				

Radical $^{\bullet}C_{70}$-*c*-(*o*-$C_2HB_{10}H_{10}$)

$\mathbf{E_{tot}}$ = -2996.166374 a.u.; $\boldsymbol{\varepsilon_{ZPV}}$ = 1552.80 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 1646.25 kJ mol^{-1}

6	22.36917877	-11.16217518	-0.21681847	6	23.25575447	-7.74754143	1.00583124
6	22.81372261	-10.16256523	-1.46704757	6	22.20951080	-8.17957401	0.13165146
5	24.01961136	-11.11527729	-0.66094315	6	22.82094765	-8.59617424	-1.22576761
5	21.26749420	-10.93735695	-1.50841177	6	20.94615746	-7.61473274	0.25894824
5	22.29347801	-10.85426712	-2.95234942	6	26.88152504	-2.28936577	-0.95230502
5	23.98895836	-10.95387554	-2.42913485	6	26.73339462	-2.74825430	0.36245957
5	21.51263618	-12.52620602	-0.74932551	6	26.84283447	-4.16290379	0.65436262
5	21.48114014	-12.37298775	-2.51851273	6	25.67770386	-2.22298670	1.20318377
5	23.17285538	-12.38936710	-3.09198213	6	25.15798187	-3.29724240	2.02015877
5	24.24329948	-12.54514694	-1.67212415	6	25.87621880	-4.49711370	1.67795181
5	23.20995522	-12.63471794	-0.22810005	6	25.23946953	-5.76778126	1.71046221
5	22.68908882	-13.42845535	-1.73020709	6	23.97902107	-5.82731199	2.36508870
1	25.31087303	-13.07409286	-1.70347977	6	23.26419258	-4.63077116	2.71536922
1	23.47696304	-12.81051636	-4.16534281	6	23.79065132	-3.34411573	2.40830898
1	22.11231041	-10.65458870	0.71022117	6	21.85018730	-4.91709661	2.61200404
1	20.30997276	-10.26346207	-1.31375432	6	21.68919563	-6.30165625	2.21457863
1	21.97634888	-10.10959625	-3.82246113	6	23.00827408	-6.85352802	2.05246997

1	20.56052589	-12.77740002	-3.15832138	6	20.67556572	-6.66424131	1.31900001
1	22.63739395	-14.61746979	-1.80154967	6	25.97765350	-1.27624428	-1.46799159
1	24.82032585	-10.27881813	-2.94617438	6	24.96434784	-0.76508194	-0.64745373
1	23.48601913	-13.11715508	0.82390207	6	24.80999756	-1.24946940	0.70780671
1	24.77659416	-10.55505466	0.05985369	6	23.63167381	-0.55910569	-1.17838013
1	20.64215279	-12.93461037	-0.04854662	6	22.66915703	-0.89948988	-0.15151918
6	26.41635704	-2.80523372	-3.19561028	6	23.39802551	-1.32442677	1.01407218
6	25.82380867	-3.75903606	-4.03195286	6	22.87649536	-2.32031274	1.88591301
6	24.48822212	-3.54261994	-4.55024099	6	21.50611115	-2.65917873	1.70820832
6	25.93590736	-5.16939688	-3.72268677	6	20.77722359	-2.23349905	0.54186761
6	24.69045830	-5.82108736	-4.06604195	6	21.40174866	-1.45695078	-0.47401565
6	23.79490089	-4.80562115	-4.58091640	6	19.80355644	-3.25522232	0.22666845
6	22.39161873	-4.88705587	-4.36499929	6	19.92033195	-4.31899929	1.20152318
6	21.90245819	-6.12532711	-3.87779450	6	20.98468590	-3.94618821	2.11152887
6	22.79505157	-7.13668442	-3.34635687	6	19.77087402	-5.65413380	0.80548900
6	24.20801544	-6.93397141	-3.33744144	6	25.69148254	-1.59370875	-2.85478806
6	22.10780334	-7.85703897	-2.33390307	6	24.40377426	-1.38597655	-3.36504149
6	20.80098152	-7.29547882	-2.18070865	6	23.35730362	-0.86288774	-2.50933337
6	20.66895866	-6.21822405	-3.14800215	6	23.79228401	-2.37498307	-4.22565317
6	20.19476700	-7.18175793	-0.92236793	6	22.38003159	-2.44459033	-3.91733694
6	27.15330315	-3.23362684	-2.02046204	6	22.10996246	-1.51083159	-2.85655475
6	27.26557922	-4.59982443	-1.73041010	6	21.11020851	-1.77391863	-1.87902737
6	26.64014053	-5.58015060	-2.59337807	6	20.21518898	-2.84191704	-2.16311717
6	27.10638237	-5.06868601	-0.37038559	6	20.48444557	-3.77418804	-3.22490263
6	26.40432739	-6.33575249	-0.40239677	6	21.65459061	-3.66226912	-4.02628326
6	26.11438751	-6.64985228	-1.77418172	6	19.96472168	-5.06306982	-2.82323074
6	24.94564438	-7.37363958	-2.14057970	6	19.35378456	-4.93318701	-1.51696599
6	24.24152374	-8.01011181	-1.08896911	6	19.52761078	-3.55908489	-1.10653198
6	24.49261475	-7.64826918	0.25536308	6	19.47932625	-5.97368860	-0.57981074
6	25.51074791	-6.71464443	0.62488866				

Radial $^{\bullet}C_{70}$-*d*-(*o*-$C_2HB_{10}H_{10}$)

$\mathbf{E_{tot}}$ = -2996.165688 a.u.; $\boldsymbol{\varepsilon_{ZPV}}$ = 1553.01 kJ mol^{-1}; $\mathbf{H_{corr}}$ = 1646 kJ mol^{-1}

6	23.66210175	-10.98983479	-0.14576466	6	22.20108795	-7.75624895	0.85988587
6	23.37799835	-10.03470802	-1.47598124	6	21.09426880	-7.85611153	-0.07185485
5	24.97174263	-10.64553928	-1.19317567	6	21.63682365	-8.12018490	-1.36852658
5	22.14125443	-11.12039185	-0.91398704	6	19.95758438	-7.05017948	0.09896277
5	22.51011467	-10.94682789	-2.64143443	6	26.97501945	-3.22242236	-0.85334855
5	24.25545883	-10.66482830	-2.81526732	6	26.70321655	-3.68561888	0.44065452
5	23.00149536	-12.54533577	-0.30100316	6	26.47496223	-5.09323359	0.67912108
5	22.27771187	-12.56039906	-1.92449188	6	25.78760910	-2.95575094	1.29648387
5	23.58894539	-12.28442287	-3.10214639	6	25.01943016	-3.90748739	2.06603885
5	25.11873436	-12.09064102	-2.20099282	6	25.44290543	-5.22885942	1.67585754
5	24.74719620	-12.25427818	-0.47167262	6	24.53035355	-6.31889057	1.65511346
5	23.89532471	-13.27230167	-1.65382576	6	23.28750038	-6.10772800	2.30688381
1	26.18720436	-12.39146137	-2.63502121	6	22.85877800	-4.78357744	2.70076823
1	23.55381393	-12.72916317	-4.20795393	6	23.67149353	-3.64766788	2.44524646
1	23.67257118	-10.46223164	0.80522645	6	21.42292023	-4.73231125	2.56997442
1	21.19712639	-10.65481853	-0.36904657	6	20.95766068	-6.02548742	2.10961556
1	21.73446655	-10.36163235	-3.32714319	6	22.12403297	-6.86234617	1.94187629
1	21.29908562	-13.19852257	-2.16017485	6	19.89392662	-6.11035490	1.20477045
1	24.08621979	-14.44856739	-1.69246078	6	26.34506035	-2.00869131	-1.33437550
1	24.66075706	-9.89312935	-3.62221837	6	25.46378517	-1.30479336	-0.50144309
1	25.49718857	-12.56947517	0.39643615	6	25.17976379	-1.78977382	0.83335114
1	25.80005646	-9.88434410	-0.81834650	6	24.22537231	-0.77937716	-1.03389084
1	22.57048035	-13.05805016	0.68235147	6	23.19307518	-0.92162228	-0.02721760
6	26.44632721	-3.52933550	-3.12429023	6	23.78258705	-1.54514420	1.12528765
6	25.66806030	-4.28230572	-4.01124239	6	23.02904892	-2.42097092	1.95595539
6	24.42709732	-3.74354672	-4.52835989	6	21.62026596	-2.42363882	1.75604570
6	25.44266891	-5.69098330	-3.75945067	6	21.03057480	-1.79976976	0.59956205
6	24.09022522	-6.01744938	-4.12641859	6	21.83445740	-1.16058111	-0.38191891
6	23.45942116	-4.81636572	-4.60730696	6	19.85354042	-2.56121182	0.23621339
6	22.07496262	-4.58825588	-4.40189266	6	19.70240402	-3.65213180	1.17415023
6	21.30971336	-5.71240902	-3.96735787	6	20.80834770	-3.56701779	2.10657096
6	21.93410873	-6.91096020	-3.49974132	6	19.24717331	-4.90208101	0.73055655

6	23.35322380	-7.01759434	-3.42492437	6	26.01578140	-2.19791913	-2.73585558
6	21.08490372	-7.48808575	-2.46570373	6	24.82048988	-1.67764056	-3.24739146
6	19.92185783	-6.63935995	-2.31488943	6	23.90899277	-0.96146089	-2.37872577
6	20.06969643	-5.53866243	-3.23861217	6	24.01122856	-2.46690106	-4.15323162
6	19.35437202	-6.42785454	-1.05360842	6	22.61666679	-2.22612333	-3.85361695
6	27.03514671	-4.16456270	-1.95941949	6	22.55313110	-1.29573870	-2.75817466
6	26.81445885	-5.52564812	-1.72444952	6	21.50385857	-1.35567296	-1.79951310
6	25.99853516	-6.29419136	-2.63466883	6	20.39305687	-2.18037677	-2.13119507
6	26.52769852	-6.00603771	-0.38444927	6	20.45820999	-3.11387062	-3.22389936
6	25.58174324	-7.07666159	-0.46718949	6	21.63448334	-3.24395895	-4.01324749
6	25.22902870	-7.25298548	-1.87410080	6	19.64732552	-4.26087523	-2.87741804
6	23.96162033	-7.67117596	-2.28221107	6	19.06237030	-4.03441477	-1.57078493
6	23.12978745	-8.47582150	-1.27017760	6	19.53982925	-2.74793005	-1.10986924
6	23.42491913	-7.98276138	0.17672838	6	18.91802025	-5.09576941	-0.66989684
6	24.59505844	-7.28400850	0.54598415				

$^{\bullet}C_{70}$-*e*-(*o*-$C_2HB_{10}H_{10}$)

E_{tot} = -2996.147735 a.u.; ε_{ZPV} = 1551.46 kJ/mol; H_{corr} = 1645.12 kJ/mol

6	26.15234947	-4.28705835	-3.32917047	6	24.03573990	-1.32768595	0.64476615
6	25.24129295	-5.14681053	-3.96066046	6	23.31843567	-1.97013044	1.69265437
6	23.98719025	-4.62290478	-4.46289921	6	21.89868355	-1.90457904	1.61898267
6	24.97049332	-6.45804834	-3.41966176	6	21.23410797	-1.47157276	0.41937912
6	23.55226326	-6.74332237	-3.58677077	6	21.97382545	-1.09280491	-0.73735708
6	22.95634842	-5.60806990	-4.23841667	6	19.98388672	-2.19004178	0.31714484
6	21.61105919	-5.23393917	-3.98634171	6	19.86182785	-3.06863952	1.46281242
6	20.83356285	-6.18055296	-3.27119565	6	21.05952835	-2.89365721	2.26014113
6	21.44164276	-7.31299353	-2.62508655	6	19.29162788	-4.33868551	1.31823957
6	22.82732201	-7.55199289	-2.69129324	6	25.83536339	-2.87913704	-3.18332458
6	20.64346695	-7.62583542	-1.44835472	6	24.62590599	-2.37878394	-3.68293929
6	19.55401802	-6.68207169	-1.36832893	6	23.84769630	-1.43985510	-2.90222216
6	19.67931747	-5.78550673	-2.49994969	6	23.68624496	-3.26809621	-4.33482885
6	19.12934685	-6.18308496	-0.12773676	6	22.34404755	-2.86356449	-3.97671270
6	26.82024193	-4.72375822	-2.11796212	6	22.44376183	-1.73563969	-3.09052587

6	26.55477142	-5.99543667	-1.59898770	6	21.49224281	-1.52890635	-2.05209994
6	25.61263657	-6.88493347	-2.25670004	6	20.30573654	-2.31275082	-2.11593509
6	26.36325073	-6.16991138	-0.18233804	6	20.20648956	-3.44051266	-3.00261593
6	25.32206535	-7.16326094	0.01283397	6	21.28981209	-3.81024814	-3.84776020
6	24.89686203	-7.62997055	-1.25757074	6	19.36842346	-4.43364477	-2.36691403
6	23.56377411	-8.32517433	-1.53453779	6	18.92970657	-3.91643143	-1.08628786
6	22.71908760	-8.22314453	-0.26395199	6	19.52639008	-2.60621500	-0.93251735
6	23.18744087	-7.74138117	0.98713344	6	18.81681252	-4.77362251	0.01583144
6	24.45451164	-7.10181952	1.14509380	6	23.00369453	-11.04356956	-1.10949719
6	22.04476929	-7.33686638	1.78612173	6	23.82298660	-9.85683346	-1.93881440
6	20.85541534	-7.53502035	0.99952310	5	24.66719246	-10.82440567	-0.77635550
6	21.29054451	-8.05532265	-0.28674170	5	22.54519081	-10.72455311	-2.72532868
6	19.80079269	-6.61864948	1.08151782	5	24.07669258	-10.37679672	-3.55257630
6	26.92223549	-3.58497763	-1.22391820	5	25.38562775	-10.44759655	-2.35294056
6	26.75302124	-3.76580358	0.15425128	5	22.62542343	-12.37860107	-2.08196330
6	26.46308708	-5.08319998	0.67962086	5	23.33953476	-11.99353123	-3.66338539
6	25.96518326	-2.82316971	0.92160249	5	25.10121536	-11.82673264	-3.43223214
6	25.21910095	-3.55392885	1.92446411	5	25.46782684	-12.09897900	-1.70542085
6	25.52617073	-4.94899845	1.77358663	5	23.93453789	-12.44127750	-0.87886822
6	24.55627632	-5.95510626	2.04790044	5	24.20427513	-13.06456757	-2.52146602
6	23.39232445	-5.52515936	2.74684381	1	26.49876785	-12.54809570	-1.31039441
6	23.08396721	-4.13011885	2.89829445	1	25.88232613	-12.08093739	-4.29673243
6	23.93306351	-3.12467003	2.35723877	1	22.32377243	-10.68044567	-0.34279618
6	21.64286995	-3.98988676	2.89213777	1	21.52301407	-10.15570927	-2.91840124
6	21.05188370	-5.30518293	2.75278282	1	24.08032036	-9.54956150	-4.40606260
6	22.14422226	-6.24885321	2.64792776	1	22.83741188	-12.36774445	-4.67739439
6	19.89950180	-5.48121309	1.97699046	1	24.32509422	-14.23447037	-2.71731043
6	26.31251335	-2.44335175	-1.88187075	1	26.28220177	-9.66992664	-2.39013290
6	25.55952835	-1.53035569	-1.13422632	1	23.78555298	-13.03689003	0.14035328
6	25.38063812	-1.72688317	0.29027748	1	24.96753883	-10.30737877	0.24955748
6	24.30475616	-1.02389181	-1.65248108	1	21.59195709	-12.93136787	-1.87666404
6	23.37224197	-0.89439178	-0.55532622				

$^{\bullet}Mn(OAc)_2$

E_{tot} = -1607.506405 a.u.

ε_{ZPV} = 261.92 kJ/mol; **H_{corr}** = 291.64 kJ/mol; **G_{corr}** = 161.54 kJ/mol

25	-1.88651240	-2.01159048	-0.26993597
8	-1.01426864	-3.11399603	-1.64591599
8	-2.74682069	-0.88968378	1.09726560
6	-0.04125838	-3.29600668	-0.82051587
6	-3.70748448	-0.68557703	0.26256466
6	1.16858208	-4.09441328	-1.18938220
6	-4.86509085	0.20182946	0.59380221
8	-3.60322452	-1.27033317	-0.88118583
8	-0.15863393	-2.73254347	0.33267897
1	1.61203051	-4.54384661	-0.29409519
1	0.90671533	-4.85868359	-1.92924500
1	1.91010690	-3.41717458	-1.63925600
1	-5.75058126	-0.10205242	0.02507565
1	-5.05947304	0.18196066	1.67186117
1	-4.60711575	1.23311675	0.30957070

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