Supporting Information

Computational Insights into Diels-Alder Reactions of Paramagnetic Endohedral Metallofullerenes: $M@C_{82}$ (M = Sc, Y, La) and $La@C_{72}$

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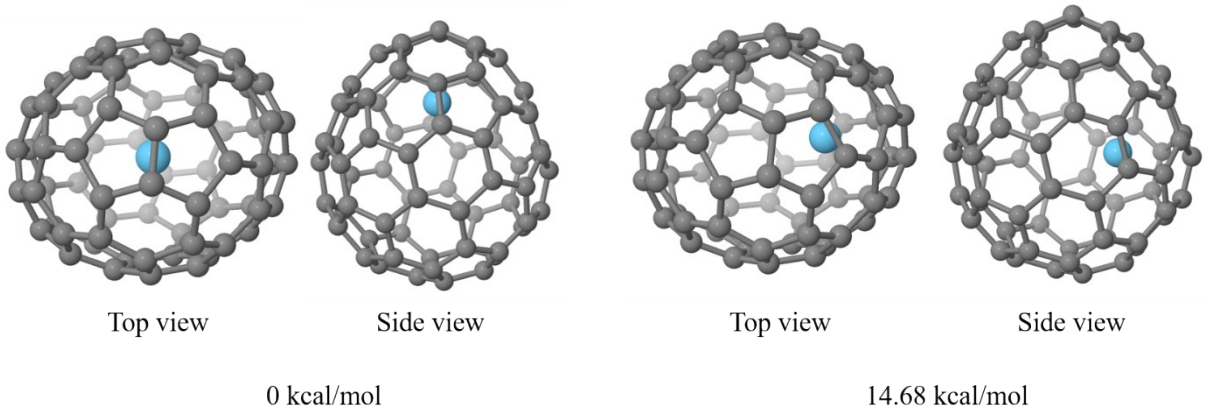

Figure S1. Geometrical structures of La@C_2-C_{72} isomers with different La atom positions.

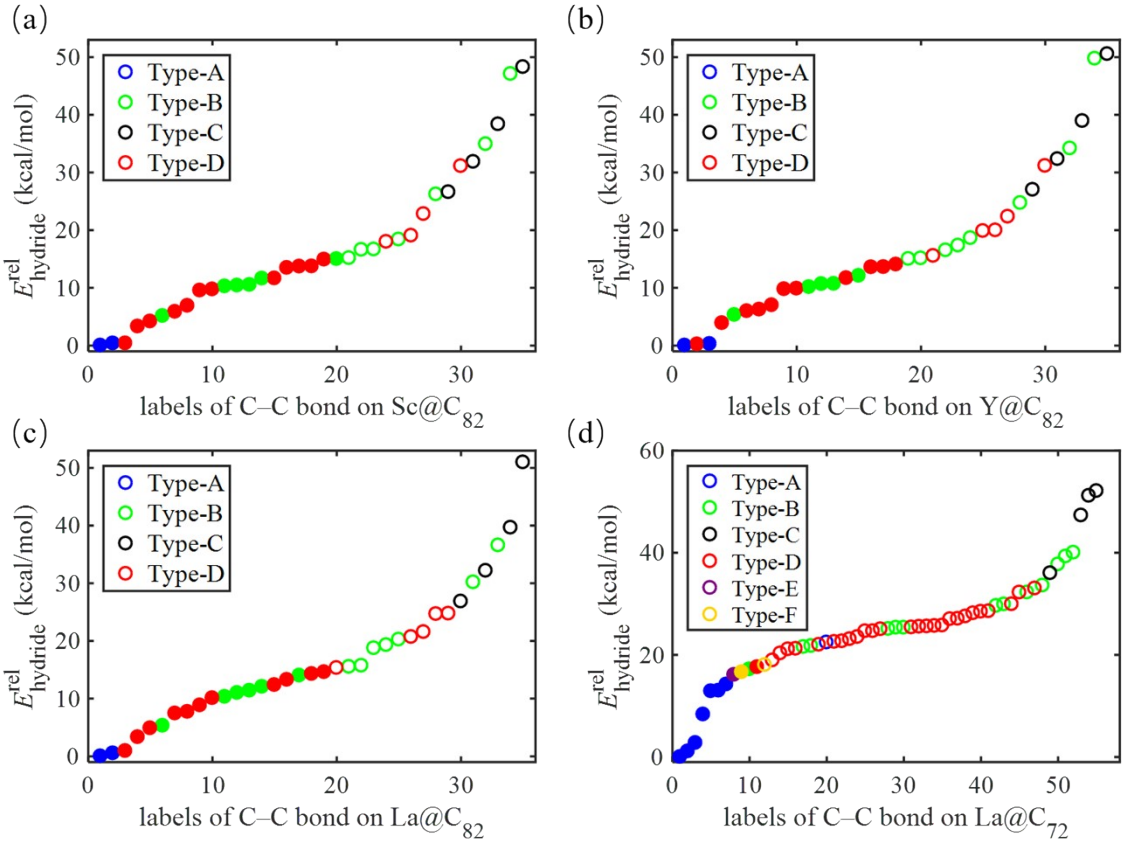

Figure S2. Relative energies of dihydrides for (a) Sc@C_{82}, (b) Y@C_{82}, (c) La@C_{82}, and (d) La@C_{72}. The relative energies are given in kcal/mol.

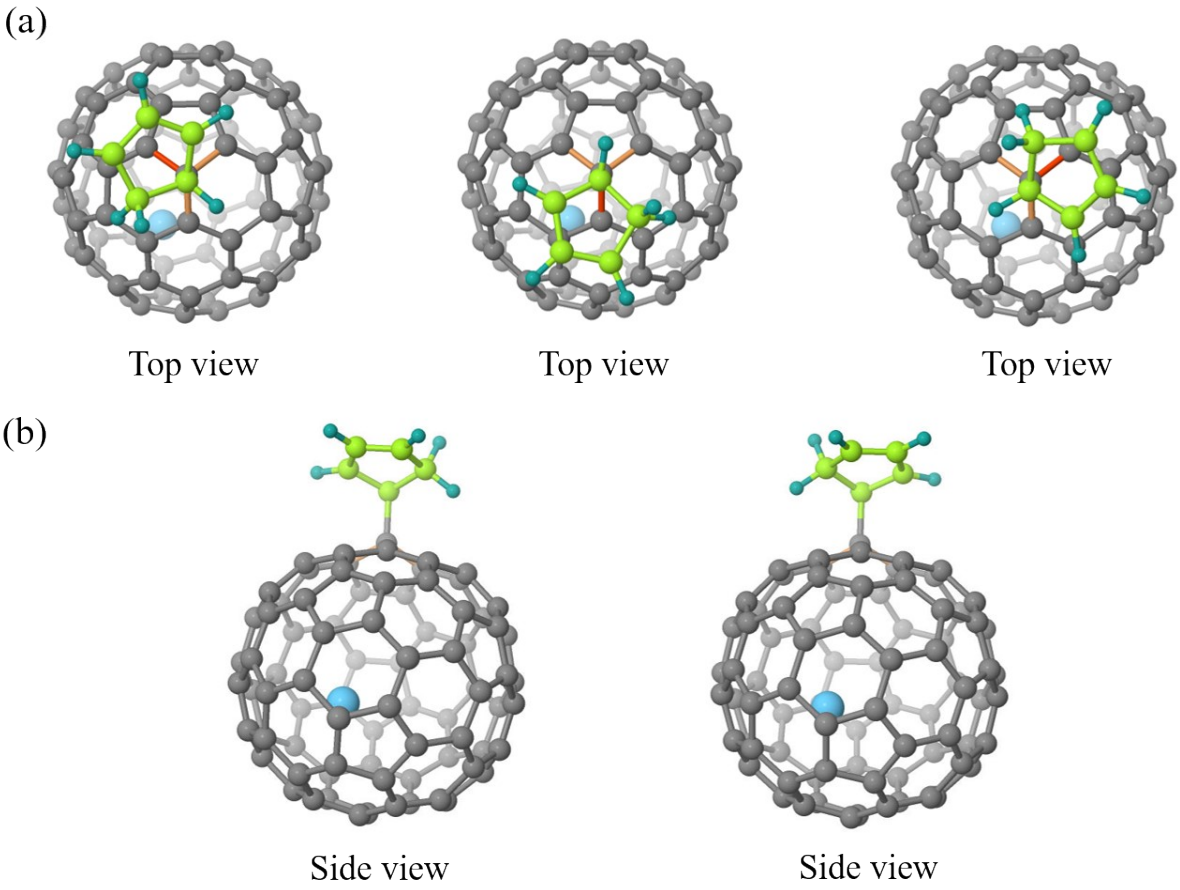

Figure S3. (a) Three intermediate conformers for Cp addition to C_α of $M@C_{82}$ (M = Sc, Y, and La) resulting from C-C single bond rotation. (b) Intermediate conformers for Cp addition to C_α of $M@C_{82}$ (M = Sc, Y, and La) with mirror orientations.

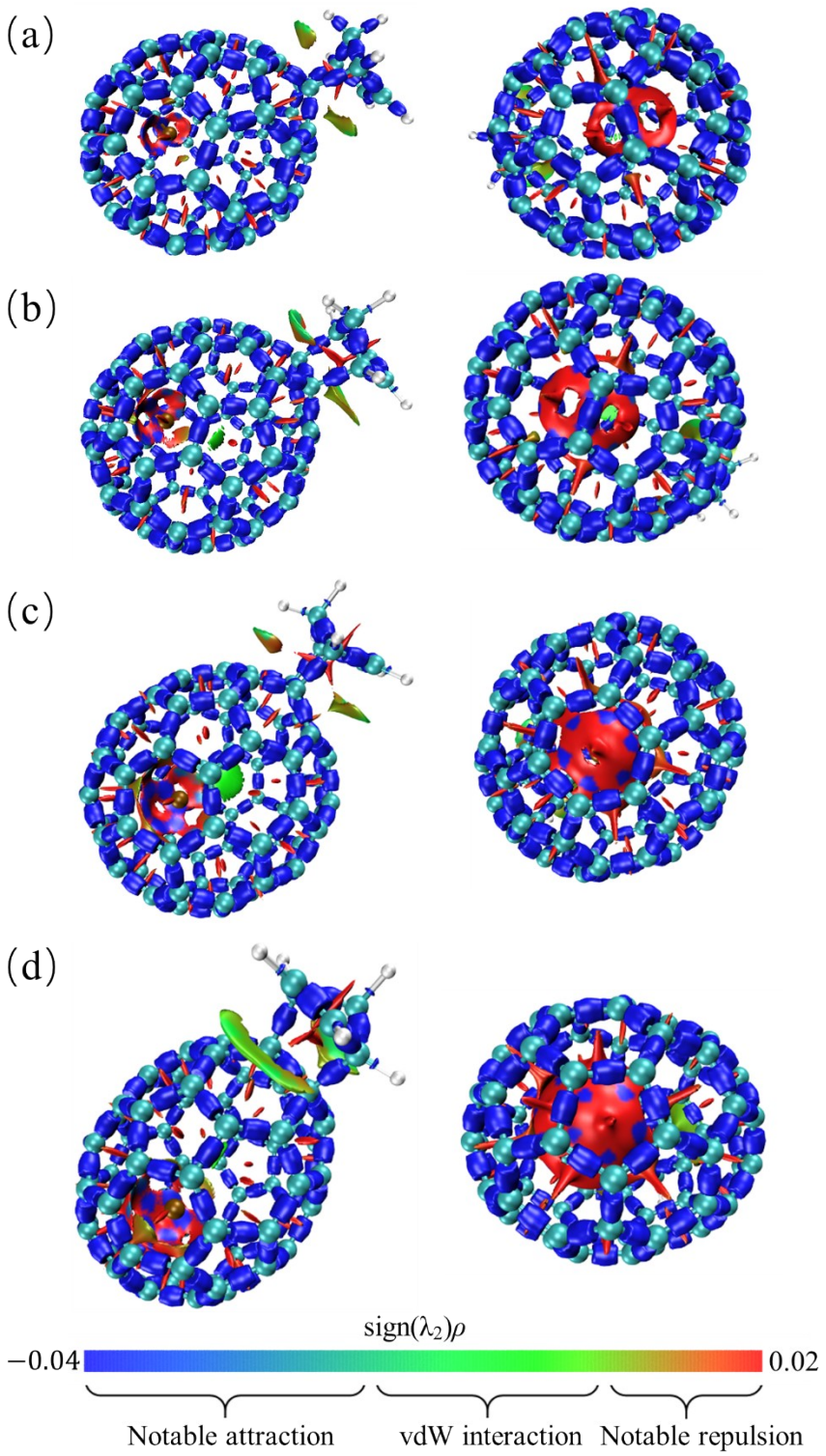

Figure S4. BP86/Def2-svp~SDD calculated isosurface of IRI = 1.0 with $sign(\lambda_2)\rho$ mapped on the isosurface for Cp adducts with (a) Sc@C_{82}, (b) Y@C_{82}, (c) La@C_{82}, and (d) La@C_{72}.

Table S1. Relative energies (in kcal/mol, with isomer **a** as reference) and net charges of M by Mulliken population and Natural Population Analysis of $M@C_{82}$ (M = Sc, Y, and La) isomers.

Isomer	$Sc@C_{82}$			$Y@C_{82}$			$La@C_{82}$		
	ΔE	Mulliken	NBA	ΔE	Mulliken	NBA	ΔE	Mulliken	NBA
a	0.0	0.50	0.73	0.0	1.14	1.03	0.0	0.48	0.89
b	0.4	0.50	0.73	-	-	-	0.9	0.46	0.89
c	4.1	0.50	0.73	-	-	-	-	-	-
d	11.0	0.51	0.74	-	-	-	-	-	-
e	12.7	0.49	0.72	13.8	1.15	1.04	14.6	0.51	0.89
f	26.7	0.49	0.74	28.5	1.15	1.04	28.6	0.50	0.89

*The hyphen (-) indicates that no stable isomer was found.

Table S2. Gibbs free energy barriers ($\Delta G^{\ddagger}$) and reaction energies ($^{\Delta G_R}$) for the reaction of Cp with M@C_{82} (M = Sc, Y, and La) and La@C_{72} in gas-phase, toluene, and *o*-DCB. All the energies are given in kcal/mol.

EMFs	mechanism	type	No. C–C	$\Delta G^{\ddagger}$ (ΔG_R)	$\Delta G^{\ddagger}$ (ΔG_R)	$\Delta G^{\ddagger}$ (ΔG_R)
				gas	toluene	*o*–DCB
Sc@C_{82}	stepwise	B	7–13	11.4, 11.3 (0.6)	15.0, 14.9 (5.6)	14.8, 14.7 (4.7)
		C	13–6	22.1, 26.2 (18.4)	24.9, 29.4 (22.3)	24.9, 29.3 (21.7)
		D	7–14	14.3, 15.2 (4.6)	17.3, 18.5 (9.4)	17.3, 18.3 (8.2)
	concerted	A	1–3	12.4 (-2.4)	14.8 (3.3)	15.3 (2.1)
		B	45–46	15.7 (-1.1)	20.2 (6.2)	19.1 (4.1)
		D	8–15	12.1 (-5.8)	16.5 (-0.4)	16.2 (-1.3)
Y@C_{82}	stepwise	B	7–13	10.3, 10.2 (-0.9)	15.3, 14.8 (5.5)	14.9, 14.3 (4.2)
		C	13–22	19.1, 22.5 (13.7)	24.1, 28.7 (20.4)	23.3, 27.4 (19.0)
		D	7–14	12.7, 13.5 (0.5)	17.6, 18.5 (7.0)	17.2, 18.1 (5.1)
	concerted	A	1–3	11.0 (-3.9)	15.7 (2.1)	16.0 (1.8)
		B	45–46	13.9 (-3.0)	21.1 (6.0)	19.3 (3.8)
		D	8–15	10.8 (-7.2)	16.2 (-1.6)	15.6 (-2.3)
La@C_{82}	stepwise	B	7–13	11.5, 11.7 (1.0)	10.5, 9.0 (-0.5)	11.9, 11.2 (1.1)
		C	13–22	22.0, 27.0 (16.5)	21.3, 25.2 (17.7)	22.6, 27.0 (18.3)
		D	7–14	14.5, 14.2 (3.3)	11.3, 12.7 (3.5)	13.8, 14.3 (3.8)
	concerted	A	1–3	11.2 (-4.0)	13.0 (-2.4)	13.5 (-2.0)
		B	45–46	16.5 (0.1)	16.9 (3.1)	17.1 (3.1)
		D	8–15	12.4 (-5.7)	12.4 (-5.9)	13.3 (-5.1)
La@C_{72}	stepwise	A	33–7	12.3, 13.2 (2.7)	15.4, 16.9 (3.8)	16.3, 17.2 (5.7)
		B	4–5	13.8, 15.1 (3.4)	17.2, 19.4 (10.0)	17.9, 19.2 (9.0)
		C	31–9	17.0, 19.9 (10.7)	20.7, 23.9 (15.3)	20.9, 23.3 (15.2)
		D	33–32	12.3, 10.6 (-2.6)	16.9, 16.2 (3.1)	16.6, 15.0 (2.0)
		F	33–34	13.1, 11.9 (-1.8)	15.9, 17.0 (2.7)	16.7, 16.2 (2.5)
	concerted	A	61–62	8.4 (-11.4)	11.6 (-7.1)	11.7 (-7.4)
		B	3–37	14.7 (-1.0)	18.7 (4.0)	18.5 (3.6)
		E	34–47	14.5 (-8.5)	18.0 (-8.9)	18.3 (-6.1)
		F	34–45	14.0 (-3.4)	18.2 (0.4)	18.0 (0.8)

Cartesian coordinates for most important structures

In the following sections, the DFT optimized Cartesian coordinates of the reactants, reactant complexes (RC), intermediates (INT), transition states (TS) and products (P) for the most important reaction pathways studied in this work are presented.

The total energy in units of Hartree, atomic coordinates in Å, the lowest vibrational frequency ($\tilde{\nu}$) in cm^{-1}, and the number of imaginary frequencies (denoted by NIMAG) are provided for each of the structures below.

1. Sc@C_{2v}-C_{82}

Energy = -3883.77785224

NIMAG = 0 $\tilde{\nu}$ = 46.72

C	-3.575029	-0.715620	-2.411068
C	-2.538985	-1.446790	-3.107764
C	-3.563500	0.669557	-2.412074
C	-3.965349	-1.450861	-1.211773
C	-2.411016	-2.714970	-2.415083
C	-1.405680	-0.781806	-3.677530
C	-2.513219	1.379748	-3.108516
C	-3.939512	1.412343	-1.212441
C	-4.276387	-0.754752	-0.001284
C	-3.237139	-2.693416	-1.213728
C	-1.199019	-3.394069	-2.408918
C	-0.138329	-1.529101	-3.706348
C	-1.392635	0.691864	-3.678910
C	-2.360494	2.644799	-2.417247
C	-3.186037	2.639755	-1.214482
C	-4.262520	0.722630	-0.001301
C	-3.966120	-1.450828	1.209421
C	-2.784677	-3.312085	-0.000773
C	-0.744482	-4.093607	-1.219581
C	-0.061406	-2.828568	-3.101178
C	1.087774	-0.793927	-3.780945
C	-0.112112	1.413466	-3.709878
C	-1.134056	3.299423	-2.412924
C	-2.721591	3.247190	-0.000846
C	-3.940287	1.412372	1.210021
C	-3.576581	-0.715558	2.408955
C	-3.237918	-2.693382	1.211876
C	-1.498878	-4.032145	-0.000340
C	0.695044	-4.034036	-1.222991
C	1.121244	-3.275232	-2.397511
C	2.281805	-1.253551	-3.119396
C	1.100960	0.652776	-3.789493
C	-0.009100	2.710437	-3.105358
C	-0.666183	3.986324	-1.221797
C	-1.419029	3.938236	-0.000435
C	-3.186822	2.639790	1.212508
C	-3.565055	0.669623	2.409926
C	-2.540988	-1.446697	3.106335
C	-2.412568	-2.714908	2.413761
C	-0.745268	-4.093559	1.219382
C	1.434506	-3.967343	0.000612
C	2.292092	-2.466262	-2.359990
C	3.031983	-0.088971	-2.678460
C	2.303908	1.091138	-3.134048
C	1.186317	3.128330	-2.398286
C	0.771869	3.891541	-1.224090
C	-0.666971	3.986318	1.221389
C	-2.362055	2.644865	2.415798
C	-2.515225	1.379823	3.107018
C	-1.408059	-0.781707	3.676821
C	-1.200576	-3.393993	2.408409
C	0.694254	-4.033963	1.223737
C	2.660140	-3.204849	0.001002
C	3.098512	-2.484705	-1.165875
C	3.860402	-0.095851	-1.500810
C	2.339542	2.297403	-2.372044
C	1.499702	3.800355	0.000492
C	0.771092	3.891507	1.224615
C	-1.135618	3.299465	2.412239
C	-1.395015	0.691954	3.678153
C	-0.140708	-1.529001	3.706539
C	-0.063401	-2.828488	3.101416

C	1.119675	-3.275111	2.398522
C	3.097704	-2.484656	1.168188
C	3.852789	-1.322209	-0.732227
C	3.984157	1.152426	-0.742218
C	3.144376	2.271045	-1.162175
C	2.688697	2.981898	0.000857
C	1.184730	3.128283	2.399073
C	-0.011100	2.710487	3.105417
C	-0.114494	1.413538	3.709946
C	1.085326	-0.793861	3.782035
C	2.290606	-2.466172	2.361830
C	3.852125	-1.322211	0.734948
C	3.983160	1.152292	0.744780
C	3.143319	2.270904	1.164185
C	2.337939	2.297296	2.373605
C	1.098500	0.652861	3.790482
C	2.279867	-1.253512	3.121327
C	3.858650	-0.095838	1.503350
C	2.301912	1.091163	3.135793
C	3.030388	-0.088951	2.681016
Sc	2.134755	0.250815	-0.001084

2. Y@C_{2v}-C_{82}

Energy = -3161.44684655

NIMAG = 0 $\tilde{\nu}$ = 50.50

C	-3.575945	-0.715026	-2.410933
C	-2.539540	-1.446000	-3.107483
C	-3.565051	0.670047	-2.411757
C	-3.966757	-1.450630	-1.211816
C	-2.411022	-2.713399	-2.415561
C	-1.405621	-0.779760	-3.676679
C	-2.514774	1.381284	-3.107771
C	-3.942105	1.412557	-1.212382
C	-4.278115	-0.754748	-0.001284
C	-3.237119	-2.692330	-1.213741
C	-1.197692	-3.391155	-2.408645
C	-0.138341	-1.526243	-3.705961
C	-1.393120	0.693658	-3.677701
C	-2.363088	2.645785	-2.416936
C	-3.188714	2.640280	-1.214382
C	-4.265044	0.722784	-0.001301
C	-3.967540	-1.450597	1.209466
C	-2.784007	-3.310249	-0.000767
C	-0.742741	-4.090080	-1.219613
C	-0.060516	-2.825511	-3.101233
C	1.088364	-0.789749	-3.782697
C	-0.113029	1.416269	-3.709034
C	-1.136486	3.301394	-2.411890
C	-2.724317	3.248088	-0.000838
C	-3.942888	1.412586	1.209968
C	-3.577516	-0.714963	2.408824
C	-3.237908	-2.692297	1.211898
C	-1.496990	-4.028985	-0.000334
C	0.697391	-4.031380	-1.223446
C	1.123560	-3.272760	-2.398088
C	2.283825	-1.250943	-3.122673
C	1.100558	0.655970	-3.789949
C	-0.011106	2.714136	-3.104943
C	-0.669540	3.989377	-1.221685
C	-1.422537	3.940967	-0.000423
C	-3.189505	2.640313	1.212422
C	-3.566622	0.670113	2.409616
C	-2.541567	-1.445912	3.106066
C	-2.412596	-2.713338	2.414256
C	-0.743535	-4.090037	1.219434
C	1.436126	-3.964111	0.000626
C	2.295277	-2.464598	-2.362995
C	3.034189	-0.084252	-2.681840
C	2.305729	1.097217	-3.134828
C	1.184695	3.136184	-2.399974
C	0.769847	3.899973	-1.224930
C	-0.670334	3.989383	1.221316
C	-2.364665	2.645851	2.415510
C	-2.516800	1.381362	3.106291
C	-1.408023	-0.779660	3.675983
C	-1.199264	-3.391083	2.408152
C	0.696592	-4.031327	1.224216
C	2.662918	-3.202271	0.001019
C	3.103139	-2.482798	-1.166726
C	3.863383	-0.091934	-1.503472
C	2.341985	2.308444	-2.375944
C	1.497933	3.810431	0.000527
C	0.769057	3.899970	1.225512
C	-1.138059	3.301441	2.411238

C	-1.395521	0.693752	3.676966
C	-0.140752	-1.526140	3.706141
C	-0.062536	-2.825425	3.101476
C	1.121984	-3.272662	2.399121
C	3.102358	-2.482762	1.169061
C	3.860145	-1.321304	-0.734130
C	3.970004	1.157260	-0.741877
C	3.148785	2.287849	-1.165661
C	2.692773	2.996848	0.000914
C	1.183112	3.136197	2.400840
C	-0.013126	2.714202	3.105045
C	-0.115437	1.416352	3.709131
C	1.085888	-0.789666	3.783723
C	2.293751	-2.464513	2.364821
C	3.859561	-1.321299	0.736909
C	3.969244	1.157204	0.744571
C	3.147839	2.287762	1.167792
C	2.340399	2.308420	2.377601
C	1.098082	0.656067	3.790922
C	2.281805	-1.250876	3.124506
C	3.861918	-0.091900	1.506114
C	2.303696	1.097280	3.136579
C	3.032462	-0.084198	2.684215
Y	1.941488	0.214146	-0.000438

3. La@C_{2v}-C_{82}

Energy = -3560.36418947

NIMAG = 0 $\tilde{\nu}$ = 39.25

C	3.610723	0.693927	-2.410984
C	2.567477	1.415058	-3.108130
C	3.611196	-0.691525	-2.410984
C	3.994745	1.433559	-1.211418
C	2.427162	2.681616	-2.416762
C	1.439813	0.737457	-3.679468
C	2.568455	-1.413379	-3.108136
C	3.995735	-1.430899	-1.211424
C	4.312957	0.740705	-0.000322
C	3.253000	2.668695	-1.213723
C	1.206541	3.348164	-2.411018
C	0.164808	1.471417	-3.707680
C	1.440321	-0.736558	-3.679470
C	2.429020	-2.680037	-2.416773
C	3.254853	-2.666551	-1.213736
C	4.313467	-0.737829	-0.000325
C	3.994945	1.433553	1.210830
C	2.794696	3.283196	-0.000190
C	0.745162	4.042172	-1.221181
C	0.074790	2.770469	-3.103820
C	-1.055836	0.721989	-3.784383
C	0.165825	-1.471406	-3.707687
C	1.208865	-3.347432	-2.411030
C	2.796973	-3.281377	-0.000207
C	3.995935	-1.430904	1.210822
C	3.611124	0.693914	2.410459
C	3.253202	2.668688	1.213265
C	1.499212	3.988822	-0.000079
C	-0.695079	3.964959	-1.224519
C	-1.116104	3.203499	-2.399451
C	-2.259221	1.171617	-3.127916
C	-1.055342	-0.722830	-3.784382
C	0.076712	-2.770521	-3.103828
C	0.747966	-4.041773	-1.221199
C	1.501984	-3.987908	-0.000100
C	3.255055	-2.666557	1.213250
C	3.611597	-0.691537	2.410451
C	2.567995	1.415040	3.107781
C	2.427565	2.681604	2.416442
C	0.745366	4.042162	1.221147
C	-1.428021	3.884216	0.000165
C	-2.281310	2.384545	-2.369763
C	-3.004458	-0.001100	-2.682719
C	-2.258417	-1.173299	-3.127923
C	-1.113873	-3.204384	-2.399461
C	-0.692326	-3.965569	-1.224538
C	0.748170	-4.041774	1.221123
C	2.429423	-2.680050	2.416424
C	2.568973	-1.413393	3.107772
C	1.440427	0.737437	3.679306
C	1.206944	3.348148	2.410904
C	-0.694874	3.964946	1.224726
C	-2.635664	3.090694	0.000262
C	-3.083411	2.375338	-1.163336
C	-3.842580	-0.001392	-1.508360
C	-2.279647	-2.386240	-2.369757

C	-1.425340	-3.885348	0.000145
C	-0.692122	-3.965568	1.224704
C	1.209268	-3.347440	2.410881
C	1.440935	-0.736577	3.679300
C	0.165425	1.471396	3.707743
C	0.075309	2.770450	3.103894
C	-1.115698	3.203476	2.399724
C	-3.083191	2.375317	1.163934
C	-3.883665	1.237049	-0.738772
C	-3.882649	-1.239821	-0.738765
C	-3.081738	-2.377624	-1.163345
C	-2.633570	-3.092735	0.000246
C	-1.113467	-3.204385	2.399701
C	0.077230	-2.770534	3.103874
C	0.166442	-1.471423	3.707735
C	-1.055204	0.721973	3.784665
C	-2.280909	2.384520	2.370237
C	-3.883495	1.237037	0.739496
C	-3.882479	-1.239816	0.739476
C	-3.081519	-2.377615	1.163917
C	-2.279246	-2.386240	2.370206
C	-1.054710	-0.722852	3.784656
C	-2.258704	1.171608	3.128409
C	-3.842220	-0.001400	1.509058
C	-2.257900	-1.173322	3.128404
C	-3.003994	-0.001113	2.683324
La	-1.769848	-0.000142	-0.000080

4. La@C_2-C_{72}

Energy = -3177.91691911

NIMAG = 0 $\tilde{\nu}$ = 59.85

C	-3.936981	0.784569	-0.470416
C	-3.955971	-0.428863	0.254416
C	-3.453097	-0.480996	1.606710
C	-2.788052	-1.777936	1.780269
C	-1.753036	-1.960963	2.747202
C	-0.631299	-2.788416	2.347349
C	0.726483	-2.500256	2.793618
C	1.627941	-2.751422	1.699163
C	2.777886	-1.912751	1.446514
C	3.276641	-1.937388	0.108427
C	3.936981	-0.784569	-0.470416
C	3.685355	-0.774677	-1.901395
C	3.414419	0.440737	-2.570806
C	2.429464	0.480608	-3.640471
C	1.679967	1.725892	-3.499949
C	0.336089	1.791297	-3.873703
C	-0.611018	2.525156	-3.053073
C	-1.915187	1.905663	-3.234540
C	-2.870814	1.944531	-2.207214
C	-3.685355	0.774677	-1.901395
C	-3.276641	1.937388	0.108427
C	-2.558314	2.620911	-0.970094
C	-1.259552	3.179459	-0.756845
C	-0.221886	3.084459	-1.794756
C	1.200838	3.031599	-1.404005
C	2.130824	2.401101	-2.294462
C	3.280190	1.664793	-1.794296
C	3.567979	1.658844	-0.420090
C	3.955971	0.428863	0.254416
C	3.453097	0.480996	1.606710
C	2.935863	-0.687731	2.258147
C	2.031336	-0.464805	3.378580
C	0.979729	-1.427289	3.698791
C	-0.163341	-0.702312	4.209634
C	-1.505102	-0.875582	3.677324
C	-2.031336	0.464805	3.378580
C	-2.935863	0.687731	2.258147
C	-2.777886	1.912751	1.446514
C	-1.627941	2.751422	1.699163
C	-0.850574	3.305189	0.607414
C	0.535919	3.300612	0.990650
C	1.570959	3.099538	0.019019
C	2.760267	2.439749	0.484492
C	2.788052	1.777936	1.780269
C	1.753036	1.960963	2.747202
C	1.505102	0.875582	3.677324
C	0.163341	0.702312	4.209634
C	-0.979729	1.427289	3.698791
C	-0.726483	2.500256	2.793618
C	0.631299	2.788416	2.347349
C	-3.567979	-1.658844	-0.420090
C	-2.760267	-2.439749	0.484492
C	-1.570959	-3.099538	0.019019

C	-0.535919	-3.300612	0.990650
C	0.850574	-3.305189	0.607414
C	1.259552	-3.179459	-0.756845
C	2.558314	-2.620911	-0.970094
C	2.870814	-1.944531	-2.207214
C	1.915187	-1.905663	-3.234540
C	1.737997	-0.689756	-4.018889
C	0.338684	-0.616937	-4.416983
C	-0.338684	0.616937	-4.416983
C	-1.737997	0.689756	-4.018889
C	-2.429464	-0.480608	-3.640471
C	-3.414419	-0.440737	-2.570806
C	-3.280190	-1.664793	-1.794296
C	-2.130824	-2.401101	-2.294462
C	-1.200838	-3.031599	-1.404005
C	0.221886	-3.084459	-1.794756
C	0.611018	-2.525156	-3.053073
C	-0.336089	-1.791297	-3.873703
C	-1.679967	-1.725892	-3.499949
La	-0.000000	0.000000	1.726732

5. Cp

Energy = -193.971183286

NIMAG = 0 $\tilde{\nu}$ = 324.34

C	0.062075	0.857039	0.000011
H	1.177527	0.894108	0.000029
H	-0.263829	1.924465	-0.000016
C	-0.478461	0.100615	-1.186259
H	-0.284739	0.371248	-2.233697
C	-1.227813	-0.946744	-0.735652
H	-1.754807	-1.683544	-1.359988
C	-0.478499	0.100660	1.186292
H	-0.284815	0.371333	2.233727
C	-1.227853	-0.946704	0.735700
H	-1.754879	-1.683476	1.360044

6. RC for Type D [5,6] 8-15 concerted mechanism addition between Sc@C_{2v}-C_{82} and Cp

Energy = -4077.76382747

NIMAG = 0 $\tilde{\nu}$ = 7.13

C	-3.610661	-0.695570	-2.340406
C	-2.583556	-1.418589	-3.059258
C	-3.599612	0.688879	-2.326291
C	-3.983116	-1.444009	-1.142766
C	-2.444835	-2.693321	-2.381409
C	-1.459083	-0.746843	-3.639530
C	-2.560925	1.407497	-3.032747
C	-3.964559	1.422496	-1.115584
C	-4.274453	-0.759494	0.079612
C	-3.254094	-2.685040	-1.168183
C	-1.231767	-3.371035	-2.399680
C	-0.191717	-1.492071	-3.694085
C	-1.447484	0.726727	-3.626238
C	-2.397974	2.664844	-2.327876
C	-3.209973	2.649139	-1.115409
C	-4.259939	0.716209	0.095411
C	-3.949236	-1.468845	1.278818
C	-2.783129	-3.315982	0.032479
C	-0.759510	-4.082090	-1.224021
C	-0.105017	-2.797634	-3.102564
C	1.032350	-0.754699	-3.778948
C	-0.168305	1.450393	-3.668410
C	-1.173772	3.322077	-2.336721
C	-2.723754	3.239466	0.099113
C	-3.929479	1.394698	1.306860
C	-3.544610	-0.745663	2.479462
C	-3.219725	-2.711585	1.257724
C	-1.496343	-4.033851	0.006522
C	0.679681	-4.020955	-1.247474
C	1.088129	-3.249693	-2.420280
C	2.236417	-1.219554	-3.138808
C	1.044054	0.692054	-3.773160
C	-0.058236	2.741151	-3.050941
C	-0.689297	3.996896	-1.144486
C	-1.424505	3.933259	0.087474
C	-3.175951	2.626010	1.311196
C	-3.533963	0.640279	2.492468
C	-2.497301	-1.481968	3.153466
C	-2.377284	-2.743550	2.446801
C	-0.725188	-4.107362	1.214742
C	1.436713	-3.966181	-0.033891

C	2.258555	-2.439762	-2.391493
C	2.991711	-0.058772	-2.697498
C	2.255927	1.125125	-3.129740
C	1.146229	3.152956	-2.356190
C	0.748119	3.904450	-1.168620
C	-0.655298	3.973325	1.298994
C	-2.332764	2.617689	2.501079
C	-2.474554	1.344845	3.180952
C	-1.356923	-0.821189	3.714164
C	-1.164180	-3.420901	2.417330
C	0.714381	-4.046422	1.199007
C	2.661415	-3.202285	-0.043451
C	3.081924	-2.469602	-1.209187
C	3.833442	-0.076501	-1.529669
C	2.300605	2.322858	-2.355083
C	1.493965	3.802135	0.045073
C	0.783456	3.880619	1.280294
C	-1.106560	3.274649	2.488712
C	-1.345423	0.652542	3.729512
C	-0.088681	-1.567074	3.717946
C	-0.018265	-2.860839	3.099361
C	1.155555	-3.298922	2.375050
C	3.114990	-2.493381	1.124591
C	3.839591	-1.310505	-0.774181
C	3.968084	1.163748	-0.760176
C	3.121836	2.285452	-1.156720
C	2.683405	2.984776	0.019914
C	1.214087	3.105772	2.440503
C	0.027996	2.679010	3.158961
C	-0.065519	1.375440	3.751028
C	1.137515	-0.831058	3.782830
C	2.324591	-2.488011	2.329585
C	3.861529	-1.325342	0.692659
C	3.992435	1.149639	0.726622
C	3.156569	2.263083	1.169374
C	2.367645	2.276234	2.390096
C	1.149430	0.615458	3.806342
C	2.323013	-1.282614	3.100725
C	3.880714	-0.106831	1.474062
C	2.343265	1.062034	3.139823
C	3.065808	-0.112774	2.661363
Sc	2.132483	0.254646	0.011892
C	-5.861039	3.415149	-2.928734
C	-5.379214	4.567012	-2.088791
C	-5.856909	4.416650	-0.815160
C	-6.624209	2.558983	-1.954317
C	-6.628275	3.175499	-0.732132
H	-6.519637	3.767355	-3.758868
H	-5.031834	2.868300	-3.433732
H	-4.760802	5.392650	-2.466694
H	-5.678837	5.099746	0.027786
H	-7.112626	1.609941	-2.214368
H	-7.109462	2.798107	0.181619

7. TS for Type D [5,6] 8-15 concerted mechanism addition between Sc@C_{2v}-C_{82} and Cp

Energy = -4077.75205633

NIMAG = 1 $\tilde{\nu}$ = -415.30

C	-2.802194	-1.032917	-2.192774
C	-1.767531	-1.761544	-2.895930
C	-2.797954	0.348505	-2.191157
C	-3.196604	-1.789681	-1.001925
C	-1.642342	-3.035810	-2.219435
C	-0.635642	-1.099977	-3.473721
C	-1.734760	1.047122	-2.860636
C	-3.309306	1.144153	-1.025506
C	-3.475027	-1.093253	0.216403
C	-2.467793	-3.025793	-1.015705
C	-0.432019	-3.719552	-2.226504
C	0.627874	-1.850773	-3.520109
C	-0.617979	0.367468	-3.458364
C	-1.571528	2.305784	-2.163763
C	-2.430797	2.343106	-0.995450
C	-3.451996	0.371668	0.229350
C	-3.170216	-1.804678	1.421891
C	-2.004690	-3.658533	0.192342
C	0.027742	-4.432372	-1.046604
C	0.703671	-3.153571	-2.921726
C	1.854818	-1.117274	-3.595090
C	0.661243	1.088916	-3.498398
C	-0.347914	2.967181	-2.180526
C	-1.923791	2.901539	0.230838
C	-3.135193	1.046410	1.422148

C	-2.777185	-1.082328	2.620494
C	-2.448044	-3.053571	1.411739
C	-0.719063	-4.378019	0.177731
C	1.466906	-4.375212	-1.057694
C	1.889307	-3.609345	-2.229708
C	3.051683	-1.584975	-2.942875
C	1.872309	0.328952	-3.596102
C	0.769449	2.381053	-2.883318
C	0.128940	3.646535	-0.991837
C	-0.618706	3.586355	0.231792
C	-2.389118	2.300446	1.438676
C	-2.756950	0.304168	2.618492
C	-1.739824	-1.818114	3.308966
C	-1.617777	-3.084113	2.609336
C	0.042210	-4.451783	1.393063
C	2.214592	-4.319135	0.162108
C	3.062097	-2.803407	-2.192503
C	3.806640	-0.425509	-2.498032
C	3.080512	0.759847	-2.942074
C	1.970784	2.794414	-2.183379
C	1.567769	3.553631	-1.004701
C	0.138846	3.631211	1.449883
C	-1.559098	2.288038	2.630066
C	-1.705555	1.012612	3.309199
C	-0.601951	-1.154443	3.871489
C	-0.404598	-3.762104	2.590746
C	1.481975	-4.393855	1.389012
C	3.441975	-3.559427	0.160729
C	3.876267	-2.832706	-1.003417
C	4.641406	-0.442372	-1.324350
C	3.123471	1.959393	-2.171101
C	2.301642	3.451830	0.217115
C	1.581101	3.537372	1.445269
C	-0.326453	2.942356	2.634704
C	-0.585417	0.320039	3.876110
C	0.663651	-1.903228	3.891291
C	0.736683	-3.200987	3.279839
C	1.915430	-3.644015	2.567205
C	3.887589	-2.848318	1.330922
C	4.633440	-1.674412	-0.565189
C	4.774938	0.800464	-0.558771
C	3.935503	1.924424	-0.966630
C	3.488072	2.629085	0.204304
C	1.994940	2.764130	2.609130
C	0.797822	2.343380	3.316263
C	0.695880	1.040662	3.910037
C	1.890328	-1.169124	3.962854
C	3.086427	-2.836064	2.528779
C	4.640619	-1.684490	0.901703
C	4.782099	0.790243	0.928667
C	3.946722	1.909022	1.360330
C	3.145946	1.928833	2.572705
C	1.907100	0.277609	3.982453
C	3.081365	-1.627458	3.295090
C	4.655961	-0.462741	1.678225
C	3.109737	0.717359	3.326063
C	3.832042	-0.461565	2.859107
Sc	2.925682	-0.091688	0.187845
C	-4.752684	2.801965	-2.585766
C	-4.376476	4.024550	-1.802155
C	-4.946146	3.935577	-0.532811
C	-5.139792	1.829605	-1.480678
C	-5.479710	2.634450	-0.350551
H	-5.675966	3.022151	-3.176534
H	-3.995357	2.442818	-3.309953
H	-3.855330	4.896551	-2.220567
H	-4.924364	4.722714	0.233891
H	-5.651981	0.880240	-1.702840
H	-5.950384	2.264299	0.570465

8. P for Type D [5,6] 8-15 concerted mechanism addition between Sc@C_{2v}-C_{82} and Cp

Energy = -4077.78776644

NIMAG = 0 $\tilde{\nu}$ = 54.23

C	-3.538381	-0.740351	-2.373897
C	-2.495254	-1.465982	-3.060391
C	-3.539523	0.640393	-2.366310
C	-3.943054	-1.501843	-1.187305
C	-2.371921	-2.742245	-2.385657
C	-1.364435	-0.805602	-3.639375
C	-2.465913	1.337692	-2.998356
C	-4.223866	1.459795	-1.281905
C	-4.229040	-0.796270	0.024640

C	-3.206366	-2.733288	-1.190186
C	-1.158620	-3.421534	-2.391186
C	-0.101579	-1.554489	-3.690517
C	-1.349511	0.655822	-3.615244
C	-2.339562	2.618968	-2.373893
C	-3.378167	2.850949	-1.285029
C	-4.227288	0.670687	0.020971
C	-3.914924	-1.498263	1.233350
C	-2.740824	-3.356928	0.024130
C	-0.697737	-4.125023	-1.203749
C	-0.024455	-2.856232	-3.086591
C	1.121769	-0.817185	-3.768136
C	-0.085504	1.380151	-3.677029
C	-1.116282	3.265661	-2.382256
C	-2.679157	3.224335	0.018500
C	-3.885705	1.343513	1.191416
C	-3.528170	-0.767018	2.422318
C	-3.190044	-2.749547	1.237072
C	-1.449716	-4.068803	0.017217
C	0.740298	-4.064282	-1.211748
C	1.160382	-3.299540	-2.386302
C	2.319737	-1.274842	-3.109832
C	1.132343	0.628281	-3.776637
C	0.009846	2.672729	-3.066296
C	-0.633936	3.977338	-1.202389
C	-1.384912	3.904512	0.021890
C	-3.116415	2.605042	1.193176
C	-3.506372	0.620626	2.395762
C	-2.489659	-1.491008	3.121580
C	-2.361635	-2.765037	2.434205
C	-0.690198	-4.130881	1.234509
C	1.484835	-3.997095	0.009444
C	2.331059	-2.488000	-2.351437
C	3.066194	-0.108676	-2.669097
C	2.334944	1.071549	-3.124259
C	1.207440	3.101225	-2.375453
C	0.797317	3.877141	-1.205948
C	-0.623937	3.956096	1.239803
C	-2.306640	2.602735	2.398836
C	-2.457652	1.334871	3.082579
C	-1.356238	-0.819494	3.682263
C	-1.144417	-3.437209	2.427550
C	0.749683	-4.068311	1.234477
C	2.708358	-3.231201	0.006115
C	3.140809	-2.507556	-1.160379
C	3.903103	-0.114349	-1.496484
C	2.366390	2.276216	-2.359902
C	1.537670	3.782506	0.018544
C	0.818919	3.871227	1.243057
C	-1.086294	3.272389	2.422442
C	-1.343249	0.655206	3.673117
C	-0.087849	-1.562300	3.716004
C	-0.008429	-2.865834	3.115265
C	1.174162	-3.305528	2.407615
C	3.144416	-2.508307	1.172588
C	3.891826	-1.340566	-0.727598
C	4.027020	1.136174	-0.738368
C	3.181047	2.253026	-1.153897
C	2.725457	2.962422	0.011541
C	1.232694	3.106263	2.415337
C	0.036316	2.684937	3.119995
C	-0.066354	1.383421	3.715279
C	1.134580	-0.822525	3.788821
C	2.342637	-2.492357	2.369216
C	3.890757	-1.342257	0.737624
C	4.020761	1.131156	0.748526
C	3.183043	2.249041	1.172442
C	2.385050	2.273052	2.385907
C	1.146745	0.624739	3.799419
C	2.331364	-1.280016	3.129328
C	3.894990	-0.117098	1.506102
C	2.350723	1.065607	3.146622
C	3.079324	-0.113616	2.691047
Sc	2.171609	0.246221	-0.027729
C	-5.328658	3.079387	-2.707817
C	-4.508919	3.908189	-1.694116
C	-5.479395	3.968880	-0.524719
C	-5.683621	1.973649	-1.688954
C	-6.182360	2.811825	-0.521719
H	-6.226501	3.623506	-3.060437
H	-4.743345	2.721777	-3.578060
H	-4.072038	4.864359	-2.036614
H	-5.504449	4.763947	0.233264
H	-6.331965	1.144196	-2.026803
H	-6.898150	2.470810	0.238927

9. RC for Type B [6,6] 7-13 stepwise addition between Sc@C_{2v}-C_{82} and Cp

Energy = -4077.76524994

NIMAG = 0 $\tilde{\nu}$ = 15.61

C	-3.383503	-0.733545	-1.991257
C	-2.358981	-1.471833	-2.703171
C	-3.360134	0.649817	-1.989988
C	-3.760285	-1.464651	-0.786637
C	-2.227498	-2.738727	-2.009760
C	-1.225506	-0.812420	-3.275523
C	-2.316443	1.354940	-2.706319
C	-3.715828	1.395486	-0.789075
C	-4.053089	-0.766248	0.427950
C	-3.037335	-2.710920	-0.796913
C	-1.018405	-3.425765	-2.017369
C	0.035629	-1.566392	-3.325339
C	-1.202145	0.659838	-3.277882
C	-2.146575	2.620351	-2.015768
C	-2.955423	2.620324	-0.802885
C	-4.030532	0.710340	0.427046
C	-3.730229	-1.462707	1.635018
C	-2.572688	-3.330473	0.411097
C	-0.552666	-4.124565	-0.832988
C	0.113671	-2.867218	-2.723483
C	1.264832	-0.837485	-3.417687
C	0.079480	1.374229	-3.328024
C	-0.917033	3.270771	-2.028888
C	-2.473421	3.227403	0.404028
C	-3.688986	1.400450	1.633035
C	-3.320982	-0.728173	2.828389
C	-3.008086	-2.708920	1.629224
C	-1.290926	-4.057451	0.396020
C	0.887851	-4.073151	-0.854231
C	1.303921	-3.319695	-2.034900
C	2.465734	-1.303524	-2.772969
C	1.286930	0.608965	-3.428914
C	0.197054	2.675168	-2.735033
C	-0.430192	3.955235	-0.844282
C	-1.167622	3.911834	0.386826
C	-2.927330	2.623651	1.624032
C	-3.302318	0.657115	2.828238
C	-2.280624	-1.464504	3.513381
C	-2.167765	-2.733487	2.820509
C	-0.522593	-4.122069	1.606281
C	1.642646	-4.009082	0.360273
C	2.478702	-2.516194	-2.012672
C	3.228389	-0.142621	-2.343928
C	2.501240	1.041469	-2.790532
C	1.403746	3.086726	-2.042983
C	1.008116	3.852550	-0.864600
C	-0.399897	3.956950	1.599219
C	-2.087780	2.625702	2.816155
C	-2.239130	1.362535	3.510683
C	-1.136450	-0.804663	4.068256
C	-0.959005	-3.418691	2.799762
C	0.917571	-4.070555	1.592696
C	2.872458	-3.253384	0.344507
C	3.300272	-2.537231	-0.828805
C	4.069448	-0.152638	-1.175205
C	2.553165	2.248683	-2.030162
C	1.750696	3.758348	0.351153
C	1.038140	3.854641	1.584438
C	-0.857202	3.273840	2.795963
C	-1.115268	0.668908	4.067624
C	0.126902	-1.558522	4.082464
C	0.189705	-2.858862	3.477922
C	1.361898	-3.313306	2.760983
C	3.329244	-2.534685	1.505354
C	4.065573	-1.378551	-0.405848
C	4.209772	1.095345	-0.419829
C	3.371640	2.218738	-0.830629
C	2.935456	2.933706	0.337534
C	1.462302	3.090938	2.754001
C	0.272436	2.679552	3.475384
C	0.169613	1.383704	4.082152
C	1.358113	-0.829692	4.141484
C	2.536350	-2.510571	2.708494
C	4.084552	-1.376948	1.061392
C	4.230306	1.097540	1.067189
C	3.401142	2.221387	1.495742
C	2.610299	2.253269	2.714651
C	1.379499	0.616501	4.148578
C	2.541285	-1.296580	3.465957
C	4.109456	-0.149469	1.828428

C	2.577037	1.047771	3.478028
C	3.292714	-0.136607	3.014564
Sc	2.367519	0.203162	0.355689
C	-2.400545	2.470615	-5.745336
C	-3.701815	1.886199	-5.262430
C	-3.715161	0.544619	-5.537313
C	-1.649897	1.277224	-6.270167
C	-2.444338	0.168066	-6.156710
H	-2.572627	3.225500	-6.550064
H	-1.845032	3.019805	-4.950899
H	-4.508892	2.470546	-4.800048
H	-4.533446	-0.154243	-5.312310
H	-0.634125	1.318565	-6.686568
H	-2.175524	-0.853736	-6.460613

10. TS1 for Type B [6,6] 7-13 stepwise addition between Sc@C_{2v}-C_{82} and Cp

Energy = -4077.75341217

NIMAG = 1 $\tilde{\nu}$ = -393.98

C	-3.133294	-0.840500	-1.715377
C	-2.104493	-1.584068	-2.427582
C	-3.120243	0.536705	-1.718442
C	-3.512831	-1.566863	-0.510098
C	-1.967012	-2.838021	-1.721096
C	-0.957558	-0.912081	-2.969902
C	-2.153852	1.289032	-2.562843
C	-3.459588	1.273613	-0.527304
C	-3.825112	-0.869045	0.699078
C	-2.784548	-2.807738	-0.510717
C	-0.752373	-3.523436	-1.707010
C	0.307598	-1.665435	-3.003672
C	-0.941287	0.550094	-3.005317
C	-1.915721	2.522098	-1.756224
C	-2.705637	2.503538	-0.545130
C	-3.801820	0.602646	0.691968
C	-3.513600	-1.558966	1.913157
C	-2.331361	-3.421657	0.704903
C	-0.297163	-4.212952	-0.517354
C	0.385336	-2.964783	-2.401676
C	1.534871	-0.936243	-3.091709
C	0.334475	1.259932	-3.015381
C	-0.685876	3.163515	-1.750909
C	-2.250741	3.126550	0.667202
C	-3.478792	1.303226	1.894697
C	-3.116805	-0.815962	3.104854
C	-2.783828	-2.799909	1.917765
C	-1.046701	-4.143369	0.705886
C	1.145564	-4.157583	-0.523747
C	1.572930	-3.413179	-1.703718
C	2.737344	-1.397155	-2.440021
C	1.550109	0.505737	-3.109348
C	0.444963	2.572025	-2.444242
C	-0.209514	3.852927	-0.564288
C	-0.954631	3.819440	0.660372
C	-2.718103	2.529713	1.884877
C	-3.103456	0.569964	3.097907
C	-2.080018	-1.545423	3.803647
C	-1.955690	-2.815572	3.118451
C	-0.291347	-4.201356	1.923340
C	1.887319	-4.085646	0.698279
C	2.745176	-2.605933	-1.673949
C	3.490025	-0.232038	-2.011803
C	2.757960	0.946560	-2.465208
C	1.638936	2.988845	-1.742609
C	1.229252	3.757445	-0.571580
C	-0.199029	3.877994	1.881103
C	-1.894840	2.544161	3.085636
C	-2.048163	1.284432	3.785022
C	-0.942089	-0.876134	4.363561
C	-0.741742	-3.493233	3.108513
C	1.150120	-4.144293	1.923825
C	3.115410	-3.326202	0.691844
C	3.554613	-2.616200	-0.481276
C	4.313553	-0.230394	-0.829765
C	2.797043	2.156485	-1.711493
C	1.962650	3.676518	0.651145
C	1.239895	3.779310	1.878511
C	-0.664952	3.198494	3.074325
C	-0.926451	0.597659	4.354981
C	0.323392	-1.623773	4.392446
C	0.397412	-2.925976	3.794804
C	1.579684	-3.380502	3.091211
C	3.559193	-2.600796	1.853389

C	4.311451	-1.453398	-0.056168
C	4.440082	1.020878	-0.080860
C	3.602375	2.139225	-0.506783
C	3.153052	2.859322	0.653932
C	1.656913	3.026354	3.056091
C	0.459812	2.611853	3.766896
C	0.355764	1.318177	4.377457
C	1.552425	-0.888971	4.458864
C	2.750953	-2.573377	3.046561
C	4.317961	-1.443415	1.411810
C	4.453582	1.033696	1.406630
C	3.612741	2.157038	1.820073
C	2.807483	2.192078	3.030203
C	1.568134	0.555710	4.458904
C	2.742264	-1.354540	3.795866
C	4.333992	-0.210441	2.172697
C	2.770521	0.988848	3.796393
C	3.494516	-0.194135	3.344241
Sc	2.601606	0.118462	0.710253
6	-1.986602	2.341363	-5.040780
6	-3.131039	1.792802	-4.196783
6	-3.498162	0.544208	-4.790841
6	-1.475479	1.105077	-5.716292
6	-2.445234	0.110050	-5.637604
H	-2.429107	3.022564	-5.808931
H	-1.225142	2.938865	-4.500565
H	-3.883499	2.465800	-3.756651
H	-4.386552	-0.044223	-4.524268
H	-0.524527	1.042885	-6.263099
H	-2.384844	-0.878994	-6.113153

11. INT for Type B [6,6] 7-13 stepwise addition between Sc@C_{2v}-C_{82} and Cp

Energy = -4077.75697466

NIMAG = 0 $\tilde{\nu}$ = 43.68

C	-3.361924	-0.770516	-2.045643
C	-2.337212	-1.518721	-2.757871
C	-3.358162	0.606762	-2.056132
C	-3.741993	-1.492966	-0.835946
C	-2.192349	-2.759237	-2.044609
C	-1.177894	-0.838189	-3.294338
C	-2.430222	1.384582	-2.971106
C	-3.676730	1.339815	-0.866818
C	-4.055634	-0.793776	0.370614
C	-3.011180	-2.729728	-0.832225
C	-0.973312	-3.444624	-2.022233
C	0.090124	-1.596461	-3.324464
C	-1.152556	0.604890	-3.319902
C	-2.145043	2.598010	-2.095122
C	-2.924537	2.572526	-0.886594
C	-4.027756	0.676433	0.358457
C	-3.746528	-1.479031	1.588237
C	-2.558776	-3.340607	0.385068
C	-0.521314	-4.132363	-0.834957
C	0.165979	-2.892503	-2.719040
C	1.316677	-0.870279	-3.418465
C	0.107043	1.315582	-3.347190
C	-0.916788	3.233986	-2.091081
C	-2.476271	3.203605	0.326497
C	-3.703906	1.380800	1.554796
C	-3.347755	-0.731835	2.774814
C	-3.013687	-2.718402	1.596478
C	-1.271956	-4.060404	0.389384
C	0.923147	-4.079841	-0.840156
C	1.354251	-3.343901	-2.022489
C	2.521506	-1.330471	-2.761464
C	1.330774	0.566780	-3.443627
C	0.218596	2.635054	-2.780711
C	-0.439009	3.926006	-0.905939
C	-1.183785	3.899027	0.318694
C	-2.945193	2.611525	1.543799
C	-3.333397	0.654046	2.763777
C	-2.310437	-1.459484	3.477745
C	-2.186986	-2.731175	2.799102
C	-0.519517	-4.117305	1.605963
C	1.662987	-4.004782	0.382333
C	2.526906	-2.537059	-1.993341
C	3.270582	-0.165919	-2.336275
C	2.535927	1.011064	-2.798046
C	1.406603	3.051541	-2.083067
C	0.997247	3.826291	-0.912572
C	-0.428881	3.960603	1.539610
C	-2.125753	2.629725	2.745022

C	-2.279111	1.371449	3.447675
C	-1.173054	-0.786810	4.034686
C	-0.970802	-3.405814	2.788749
C	0.924131	-4.059150	1.607476
C	2.891920	-3.246362	0.375634
C	3.334888	-2.541230	-0.799187
C	4.102498	-0.157270	-1.157659
C	2.570186	2.219491	-2.046255
C	1.731532	3.750750	0.308901
C	1.010175	3.860231	1.536993
C	-0.895368	3.284821	2.733737
C	-1.157617	0.687256	4.020948
C	0.093109	-1.533319	4.067382
C	0.167233	-2.836396	3.473419
C	1.351253	-3.292257	2.770353
C	3.333738	-2.517201	1.535376
C	4.094461	-1.377981	-0.378139
C	4.221876	1.097733	-0.414022
C	3.378611	2.212392	-0.844950
C	2.923309	2.934332	0.313980
C	1.426819	3.112468	2.717315
C	0.229129	2.699901	3.428334
C	0.124578	1.407796	4.042160
C	1.322521	-0.798022	4.134608
C	2.523505	-2.485547	2.726824
C	4.093422	-1.362282	1.090336
C	4.221553	1.113192	1.073848
C	3.380077	2.237595	1.482063
C	2.576312	2.277119	2.693052
C	1.336893	0.645456	4.127354
C	2.512971	-1.265068	3.473117
C	4.100284	-0.126209	1.844679
C	2.540312	1.076978	3.463249
C	3.266399	-0.106221	3.019341
Sc	2.380645	0.188799	0.338472
C	-2.233852	2.475789	-5.324303
C	-3.229113	1.800441	-4.351771
C	-3.644467	0.565820	-5.075587
C	-1.790412	1.331956	-6.186936
C	-2.709274	0.279905	-6.078434
H	-2.785499	3.223833	-5.943331
H	-1.409224	3.031531	-4.833242
H	-4.064234	2.443628	-4.012670
H	-4.476137	-0.080530	-4.764569
H	-0.916695	1.357597	-6.853383
H	-2.684847	-0.645043	-6.672577

12. TS2 for Type B [6,6] 7-13 stepwise addition between Sc@C_{2v}-C_{82} and Cp

Energy = -4077.75635178

NIMAG = 1 $\tilde{\nu}$ = -117.53

C	-3.146340	-0.848826	-1.699182
C	-2.117525	-1.592427	-2.419052
C	-3.149601	0.526363	-1.710290
C	-3.508786	-1.573473	-0.488084
C	-1.967898	-2.840171	-1.708723
C	-0.975369	-0.916933	-2.967667
C	-2.242850	1.309359	-2.637548
C	-3.462447	1.257509	-0.515591
C	-3.817085	-0.876746	0.722223
C	-2.775326	-2.810421	-0.491248
C	-0.750573	-3.524041	-1.700617
C	0.291245	-1.666836	-3.007714
C	-0.973419	0.541981	-3.054830
C	-1.947500	2.519854	-1.761982
C	-2.713156	2.490766	-0.543238
C	-3.796719	0.592355	0.710625
C	-3.494454	-1.562656	1.936055
C	-2.311980	-3.420860	0.722171
C	-0.284622	-4.209137	-0.514057
C	0.379268	-2.964683	-2.404908
C	1.515309	-0.936015	-3.112618
C	0.303179	1.251991	-3.032883
C	-0.718886	3.155664	-1.764679
C	-2.255219	3.121578	0.665799
C	-3.468451	1.298709	1.907582
C	-3.090032	-0.814225	3.121612
C	-2.758961	-2.799680	1.937675
C	-1.024478	-4.138065	0.715161
C	1.158707	-4.149411	-0.531896
C	1.574704	-3.408210	-1.717225
C	2.726701	-1.391015	-2.471082
C	1.522474	0.504307	-3.133080

C	0.412827	2.564986	-2.467017
C	-0.232626	3.848674	-0.584306
C	-0.965838	3.820957	0.646613
C	-2.712024	2.528536	1.888212
C	-3.082089	0.571807	3.110451
C	-2.044947	-1.537777	3.814635
C	-1.921171	-2.808474	3.132224
C	-0.260036	-4.190829	1.926748
C	1.909296	-4.070760	0.684061
C	2.744578	-2.596963	-1.700165
C	3.477744	-0.222103	-2.053219
C	2.734277	0.951551	-2.500128
C	1.608015	2.987972	-1.776404
C	1.205768	3.758898	-0.604349
C	-0.200137	3.888634	1.861370
C	-1.881285	2.551332	3.082928
C	-2.023913	1.293250	3.786724
C	-0.904502	-0.861375	4.362513
C	-0.703724	-3.480441	3.113043
C	1.181661	-4.128306	1.915667
C	3.134425	-3.306609	0.665829
C	3.562451	-2.599319	-0.513351
C	4.304867	-0.212397	-0.873879
C	2.773406	2.162465	-1.751119
C	1.950670	3.687957	0.611956
C	1.238771	3.794287	1.845704
C	-0.653415	3.211083	3.059720
C	-0.894677	0.612458	4.349316
C	0.363762	-1.603368	4.382543
C	0.438152	-2.906684	3.788129
C	1.617441	-3.359546	3.076380
C	3.585312	-2.576084	1.821235
C	4.318473	-1.433084	-0.097473
C	4.431133	1.040634	-0.130087
C	3.587187	2.154399	-0.553750
C	3.145545	2.877037	0.608108
C	1.669494	3.048309	3.022541
C	0.479124	2.630678	3.744288
C	0.384931	1.338265	4.358698
C	1.591125	-0.863308	4.436067
C	2.784786	-2.548142	3.019989
C	4.339098	-1.417934	1.370721
C	4.463722	1.060779	1.356949
C	3.619816	2.182284	1.772795
C	2.822703	2.218349	2.988917
C	1.601175	0.580601	4.431720
C	2.776699	-1.326318	3.764315
C	4.359745	-0.181792	2.128315
C	2.796398	1.016615	3.757553
C	3.521195	-0.164669	3.301821
Sc	2.609301	0.125686	0.705389
C	-2.002654	2.283490	-4.969947
C	-3.085732	1.750388	-4.012027
C	-3.552312	0.509244	-4.677972
C	-1.491560	0.994595	-5.538469
C	-2.536671	0.044067	-5.509968
H	-2.497189	2.880754	-5.772649
H	-1.237313	2.931661	-4.500544
H	-3.866662	2.461913	-3.686312
H	-4.470205	-0.032267	-4.412274
H	-0.531557	0.877498	-6.060742
H	-2.512742	-0.940147	-5.998746

13. P for Type B [6,6] 7-13 stepwise addition between Sc@C_{2v}-C_{82} and Cp

Energy = -4077.77729729

NIMAG = 0 $\tilde{\nu}$ = 72.97

C	-3.358992	-0.744683	-2.050296
C	-2.302614	-1.487390	-2.750486
C	-3.386902	0.628515	-2.071038
C	-3.714688	-1.474389	-0.841555
C	-2.171082	-2.746614	-2.046034
C	-1.192574	-0.850496	-3.338670
C	-2.535800	1.450525	-3.017524
C	-3.696285	1.346999	-0.860597
C	-4.036798	-0.789044	0.372166
C	-2.984508	-2.715485	-0.840425
C	-0.965771	-3.442258	-2.047146
C	0.068135	-1.585087	-3.358477
C	-1.253205	0.658253	-3.689343
C	-2.183049	2.610659	-2.099144
C	-2.944572	2.577326	-0.878270

C	-4.021807	0.677261	0.364457
C	-3.719663	-1.481418	1.583990
C	-2.533230	-3.336352	0.371357
C	-0.504623	-4.134047	-0.857382
C	0.160976	-2.882501	-2.747258
C	1.296336	-0.852689	-3.461744
C	0.091851	1.356349	-3.400617
C	-0.951451	3.232217	-2.094493
C	-2.486489	3.202001	0.334166
C	-3.701151	1.380152	1.567246
C	-3.322386	-0.736748	2.775599
C	-2.986077	-2.719217	1.586381
C	-1.248426	-4.059398	0.366685
C	0.937044	-4.073108	-0.871475
C	1.352846	-3.323450	-2.053426
C	2.495181	-1.302925	-2.809516
C	1.294148	0.598161	-3.465668
C	0.184984	2.631399	-2.793422
C	-0.464034	3.918942	-0.912566
C	-1.198330	3.898871	0.317823
C	-2.946068	2.608619	1.554048
C	-3.316192	0.649140	2.767849
C	-2.279822	-1.461029	3.469593
C	-2.151814	-2.730163	2.782133
C	-0.487147	-4.113142	1.582623
C	1.683871	-3.993040	0.346746
C	2.519100	-2.510976	-2.035297
C	3.247286	-0.132858	-2.381546
C	2.505542	1.039058	-2.821799
C	1.379747	3.063782	-2.095395
C	0.975117	3.833244	-0.928996
C	-0.433682	3.968119	1.533716
C	-2.116921	2.629800	2.751662
C	-2.260188	1.369449	3.450693
C	-1.140988	-0.786207	4.022857
C	-0.935165	-3.404065	2.767867
C	0.952868	-4.051966	1.576281
C	2.905957	-3.224916	0.331184
C	3.333122	-2.513828	-0.846482
C	4.065571	-0.127092	-1.199373
C	2.546047	2.248838	-2.074278
C	1.719235	3.769209	0.288491
C	1.004400	3.874869	1.520557
C	-0.889267	3.289250	2.731283
C	-1.131936	0.687423	4.013931
C	0.127159	-1.528110	4.043779
C	0.204348	-2.830814	3.447368
C	1.386042	-3.283559	2.740339
C	3.354750	-2.495873	1.488428
C	4.087185	-1.348964	-0.425575
C	4.191969	1.122601	-0.450331
C	3.356487	2.239176	-0.873392
C	2.915623	2.961224	0.286647
C	1.433590	3.126009	2.696631
C	0.242205	2.707610	3.416489
C	0.147569	1.413944	4.027725
C	1.353716	-0.787749	4.099588
C	2.551913	-2.471517	2.686439
C	4.111927	-1.337070	1.042474
C	4.234763	1.143016	1.035602
C	3.390028	2.263718	1.451809
C	2.588288	2.297092	2.664757
C	1.364050	0.656829	4.100739
C	2.541988	-1.249595	3.431696
C	4.137142	-0.102416	1.805670
C	2.560679	1.093973	3.431369
C	3.287650	-0.087461	2.973302
SC	2.377575	0.191888	0.425071
C	-2.164734	2.274448	-5.269157
C	-3.333532	1.931948	-4.323534
C	-3.886247	0.678905	-4.977523
C	-1.595193	0.842362	-5.260457
C	-2.842625	0.024840	-5.539145
H	-2.517201	2.577680	-6.274649
H	-1.469984	3.039582	-4.870102
H	-4.056847	2.732167	-4.082123
H	-4.923766	0.327204	-4.889030
H	-0.707650	0.630354	-5.884533
H	-2.852357	-0.971519	-6.002113

14. RC for Type D [5,6] 8-15 concerted mechanism addition between Y@C_{2v}-C_{82} and Cp

Energy = -3355.43517565

NIMAG = 0 $\tilde{\nu}$ = 6.71

C	-3.617759	-0.774741	-2.321894
C	-2.587678	-1.496907	-3.037671
C	-3.619792	0.609696	-2.324456
C	-3.977086	-1.512265	-1.113338
C	-2.433047	-2.761247	-2.346044
C	-1.472056	-0.820857	-3.631886
C	-2.591804	1.330173	-3.045177
C	-3.985452	1.354306	-1.120721
C	-4.268181	-0.815935	0.102411
C	-3.235391	-2.745969	-1.127920
C	-1.212596	-3.426809	-2.362294
C	-0.198367	-1.554432	-3.685095
C	-1.474434	0.652587	-3.636298
C	-2.437302	2.596728	-2.356892
C	-3.242246	2.587853	-1.139689
C	-4.267711	0.660079	0.100288
C	-3.929505	-1.507498	1.308276
C	-2.751387	-3.357350	0.077561
C	-0.726846	-4.118605	-1.181197
C	-0.095544	-2.851526	-3.078614
C	1.019060	-0.805797	-3.787916
C	-0.202580	1.388224	-3.694881
C	-1.219060	3.265786	-2.379848
C	-2.754815	3.197718	0.064708
C	-3.936748	1.356303	1.301484
C	-3.524160	-0.765750	2.497455
C	-3.187294	-2.742906	1.297926
C	-1.457030	-4.062581	0.052926
C	0.712266	-4.045695	-1.214049
C	1.106980	-3.285146	-2.398390
C	2.232111	-1.253430	-3.150485
C	1.016545	0.639991	-3.798410
C	-0.101869	2.688241	-3.094144
C	-0.735112	3.960712	-1.199639
C	-1.462888	3.905017	0.037190
C	-3.194640	2.594690	1.286584
C	-3.526711	0.620201	2.493560
C	-2.465923	-1.484102	3.174040
C	-2.337862	-2.752303	2.482831
C	-0.678599	-4.114076	1.257553
C	1.474850	-3.968822	-0.005075
C	2.271003	-2.465238	-2.388591
C	2.979157	-0.078377	-2.727234
C	2.230007	1.094782	-3.167478
C	1.103010	3.123723	-2.413592
C	0.704147	3.886303	-1.231848
C	-0.687185	3.966955	1.243618
C	-2.344623	2.608831	2.471430
C	-2.469966	1.343630	3.167004
C	-1.327987	-0.805066	3.719769
C	-1.117499	-3.417631	2.453901
C	0.760981	-4.041145	1.233270
C	2.693728	-3.194634	-0.030898
C	3.102935	-2.473177	-1.208735
C	3.829615	-0.075156	-1.564216
C	2.268998	2.307489	-2.411374
C	1.457972	3.806900	-0.020434
C	0.753510	3.892301	1.218685
C	-1.124459	3.277605	2.443373
C	-1.330492	0.668573	3.717078
C	-0.052980	-1.538523	3.725820
C	0.026642	-2.838849	3.122958
C	1.201749	-3.275505	2.397716
C	3.149052	-2.468143	1.126837
C	3.855510	-1.302859	-0.793274
C	3.940120	1.176506	-0.807585
C	3.099492	2.297773	-1.217002
C	2.660445	3.005086	-0.042756
C	1.198063	3.134823	2.386498
C	0.019670	2.702134	3.114872
C	-0.057546	1.404226	3.722955
C	1.167426	-0.789446	3.777264
C	2.364163	-2.455514	2.338450
C	3.885283	-1.299647	0.677383
C	3.971483	1.180237	0.678662
C	3.146904	2.303664	1.116229
C	2.363050	2.318560	2.341785
C	1.165079	0.656343	3.781716
C	2.354816	-1.240101	3.095559
C	3.892109	-0.068622	1.444385
C	2.353239	1.108373	3.103127
C	3.084714	-0.066824	2.638098
Y	1.936871	0.218505	-0.014846
C	-5.913915	3.306464	-2.943157

C	-5.430850	4.474693	-2.126907
C	-5.895072	4.342283	-0.846302
C	-6.662629	2.461991	-1.947473
C	-6.658302	3.098203	-0.735465
H	-6.582320	3.641160	-3.772682
H	-5.086350	2.756072	-3.447032
H	-4.821249	5.297710	-2.524313
H	-5.712947	5.040138	-0.016418
H	-7.147930	1.506058	-2.187281
H	-7.128296	2.733065	0.189015

15. TS for Type D [5,6] 8-15 concerted mechanism addition between Y@C_{2v}-C_{82} and Cp

Energy = -3355.42334143

NIMAG = 1 $\tilde{\nu}$ = -415.38

C	-2.803222	-1.061196	-2.176853
C	-1.767097	-1.789837	-2.878223
C	-2.805730	0.320081	-2.184356
C	-3.191207	-1.812291	-0.980167
C	-1.633887	-3.058458	-2.194523
C	-0.639530	-1.126191	-3.463678
C	-1.747493	1.019708	-2.861266
C	-3.318102	1.121084	-1.022868
C	-3.468929	-1.109132	0.234467
C	-2.455595	-3.044511	-0.988049
C	-0.419339	-3.735878	-2.200449
C	0.627040	-1.871155	-3.509704
C	-0.628794	0.341222	-3.457964
C	-1.588688	2.283179	-2.173868
C	-2.446223	2.325565	-1.003829
C	-3.452854	0.356178	0.237377
C	-3.157311	-1.811077	1.443698
C	-1.985343	-3.666578	0.222722
C	0.047710	-4.438141	-1.017594
C	0.711150	-3.169374	-2.903209
C	1.851118	-1.131648	-3.595794
C	0.646723	1.068802	-3.507491
C	-0.368051	2.950423	-2.198275
C	-1.936424	2.893339	0.217664
C	-3.135164	1.040242	1.424589
C	-2.763158	-1.078809	2.635766
C	-2.428140	-3.056307	1.439457
C	-0.695373	-4.379356	0.208738
C	1.487297	-4.375925	-1.034107
C	1.902329	-3.615885	-2.212386
C	3.053481	-1.591280	-2.945822
C	1.861113	0.313740	-3.604931
C	0.750155	2.366298	-2.901475
C	0.108676	3.641226	-1.016472
C	-0.635116	3.585465	0.209856
C	-2.395349	2.298404	1.430690
C	-2.749331	0.307719	2.624443
C	-1.719820	-1.805340	3.325459
C	-1.594043	-3.074869	2.634790
C	0.069961	-4.441398	1.422120
C	2.237888	-4.308055	0.183417
C	3.072783	-2.805456	-2.186918
C	3.804895	-0.423349	-2.511177
C	3.071788	0.757183	-2.957995
C	1.952028	2.793508	-2.210141
C	1.548836	3.559531	-1.034143
C	0.126361	3.641791	1.425071
C	-1.561196	2.297404	2.619183
C	-1.698941	1.026147	3.306650
C	-0.582682	-1.131946	3.879548
C	-0.376580	-3.746486	2.616334
C	1.510237	-4.378413	1.413568
C	3.463257	-3.543752	0.173046
C	3.892372	-2.823608	-0.998300
C	4.643601	-0.429625	-1.338988
C	3.112662	1.967106	-2.198553
C	2.287471	3.470831	0.186840
C	1.570148	3.559723	1.417491
C	-0.331384	2.957911	2.615293
C	-0.573089	0.342508	3.874289
C	0.686241	-1.874372	3.900840
C	0.763843	-3.175732	3.298372
C	1.943805	-3.618863	2.585359
C	3.911041	-2.823546	1.338065
C	4.648120	-1.659495	-0.570962
C	4.757093	0.819690	-0.578977
C	3.930391	1.949429	-0.995711

C	3.483213	2.658067	0.175572
C	1.991367	2.795157	2.586041
C	0.798050	2.369992	3.297809
C	0.704705	1.069842	3.900168
C	1.910494	-1.133167	3.966010
C	3.112077	-2.806868	2.540445
C	4.660211	-1.659852	0.899662
C	4.769531	0.819534	0.907955
C	3.949223	1.949573	1.338526
C	3.150233	1.968118	2.553991
C	1.919819	0.312804	3.974640
C	3.102895	-1.592238	3.299078
C	4.668146	-0.429927	1.668854
C	3.120779	0.756342	3.311916
C	3.847400	-0.423814	2.853269
Y	2.734032	-0.114872	0.181927
C	-4.770312	2.763033	-2.587910
C	-4.391565	3.988148	-1.809336
C	-4.961595	3.904866	-0.539369
C	-5.154040	1.795044	-1.477873
C	-5.493852	2.604333	-0.350901
H	-5.695359	2.981476	-3.176545
H	-4.015200	2.401036	-3.313013
H	-3.872608	4.859222	-2.232371
H	-4.939675	4.695427	0.223802
H	-5.663425	0.842930	-1.694642
H	-5.962972	2.237692	0.572311

16. P for Type D [5,6] 8-15 concerted mechanism addition between Y@C_{2v}-C_{82} and Cp

Energy = -3355.45911849

NIMAG = 0 $\tilde{\nu}$ = 48.11

C	-3.535736	-0.725399	-2.381246
C	-2.492312	-1.452948	-3.066192
C	-3.533953	0.655214	-2.372334
C	-3.944867	-1.487273	-1.196550
C	-2.372870	-2.729368	-2.393155
C	-1.358581	-0.794002	-3.642277
C	-2.457028	1.351094	-3.000841
C	-4.218918	1.475231	-1.288812
C	-4.231171	-0.782147	0.015643
C	-3.209315	-2.719724	-1.199043
C	-1.159846	-3.410685	-2.396823
C	-0.097402	-1.545334	-3.693031
C	-1.340479	0.667262	-3.616562
C	-2.329675	2.631390	-2.376016
C	-3.369810	2.865136	-1.289263
C	-4.226113	0.685071	0.013087
C	-3.920523	-1.485459	1.224366
C	-2.746595	-3.344618	0.015638
C	-0.702228	-4.115366	-1.209620
C	-0.023700	-2.847576	-3.090295
C	1.128317	-0.809856	-3.771026
C	-0.075032	1.389410	-3.676556
C	-1.104751	3.276144	-2.381586
C	-2.672098	3.235895	0.015364
C	-3.884891	1.356253	1.184549
C	-3.533715	-0.755870	2.414040
C	-3.197030	-2.738081	1.228347
C	-1.455895	-4.058425	0.010164
C	0.736906	-4.059075	-1.215663
C	1.160372	-3.294698	-2.388872
C	2.326127	-1.272721	-3.113223
C	1.141353	0.634799	-3.776478
C	0.021558	2.682176	-3.064886
C	-0.623736	3.987493	-1.201627
C	-1.376857	3.914936	0.021274
C	-3.112915	2.616692	1.188735
C	-3.509013	0.631725	2.388806
C	-2.497380	-1.482982	3.114071
C	-2.371028	-2.756227	2.427028
C	-0.698728	-4.123182	1.228760
C	1.478858	-3.994447	0.007352
C	2.334254	-2.486905	-2.354491
C	3.075069	-0.106537	-2.671245
C	2.346416	1.077119	-3.121970
C	1.219000	3.110571	-2.373614
C	0.808655	3.887657	-1.203446
C	-0.617691	3.963580	1.240459
C	-2.305176	2.611604	2.395393
C	-2.459592	1.343771	3.077271
C	-1.362832	-0.813589	3.676495

C	-1.153793	-3.430146	2.421181
C	0.742150	-4.065554	1.231585
C	2.705663	-3.232441	0.006686
C	3.143134	-2.509736	-1.159936
C	3.904582	-0.115788	-1.492822
C	2.379986	2.285687	-2.359078
C	1.547027	3.792672	0.023108
C	0.826091	3.881050	1.247222
C	-1.083064	3.279173	2.421159
C	-1.346785	0.661147	3.668356
C	-0.096432	-1.558870	3.712218
C	-0.018250	-2.861890	3.111324
C	1.166347	-3.304970	2.405955
C	3.143837	-2.512457	1.175409
C	3.896934	-1.345283	-0.725126
C	4.015034	1.134080	-0.730519
C	3.193530	2.266109	-1.151109
C	2.738838	2.974347	0.017645
C	1.236584	3.113702	2.420721
C	0.037287	2.690146	3.120584
C	-0.068684	1.387308	3.713737
C	1.128291	-0.820620	3.788894
C	2.337370	-2.495304	2.372183
C	3.897069	-1.348392	0.743965
C	4.014063	1.130258	0.755969
C	3.195001	2.261797	1.182643
C	2.391274	2.281261	2.394831
C	1.142768	0.625615	3.799508
C	2.325927	-1.281967	3.132417
C	3.901356	-0.120384	1.514449
C	2.350741	1.067138	3.149389
C	3.077211	-0.114837	2.695256
Y	1.979455	0.213128	-0.000035
C	-5.317759	3.098973	-2.714704
C	-4.498007	3.925169	-1.699063
C	-5.469744	3.986500	-0.530876
C	-5.676911	1.993031	-1.697668
C	-6.175150	2.830884	-0.530066
H	-6.213765	3.645325	-3.068655
H	-4.731590	2.740882	-3.584230
H	-4.058699	4.880761	-2.040192
H	-5.494129	4.780495	0.228305
H	-6.326613	1.165472	-2.037610
H	-6.892376	2.490692	0.229647

17. RC for Type B [6,6] 7-13 stepwise addition between Y@C_{2v}-C_{82} and Cp

Energy = -3355.43676691

NIMAG = 0 $\tilde{\nu}$ = 15.77

C	-3.453824	-0.714667	-2.013283
C	-2.424511	-1.452140	-2.718934
C	-3.430891	0.668616	-2.014967
C	-3.832630	-1.442798	-0.807087
C	-2.291565	-2.715194	-2.022855
C	-1.290209	-0.789980	-3.290856
C	-2.387583	1.375416	-2.730667
C	-3.793269	1.417535	-0.817981
C	-4.129614	-0.741460	0.404842
C	-3.104204	-2.686164	-0.811160
C	-1.078411	-3.398190	-2.026079
C	-0.028051	-1.539684	-3.337154
C	-1.269328	0.682035	-3.296443
C	-2.223617	2.643214	-2.043424
C	-3.036817	2.644597	-0.833711
C	-4.110627	0.735374	0.398982
C	-3.809188	-1.432483	1.615779
C	-2.640636	-3.297920	0.400831
C	-0.614548	-4.088605	-0.836907
C	0.052489	-2.838482	-2.731807
C	1.200980	-0.805498	-3.435281
C	0.011194	1.400810	-3.343131
C	-0.996517	3.297367	-2.052889
C	-2.559639	3.259139	0.371719
C	-3.772915	1.430671	1.603004
C	-3.404598	-0.692660	2.807863
C	-3.081575	-2.675751	1.616236
C	-1.354005	-4.018491	0.391736
C	0.827131	-4.030616	-0.854238
C	1.247103	-3.282807	-2.036925
C	2.403901	-1.270068	-2.791859
C	1.220704	0.639853	-3.435074
C	0.122648	2.704620	-2.754213
C	-0.514746	3.990618	-0.871505

C	-1.257944	3.950578	0.355739
C	-3.015292	2.656181	1.591807
C	-3.386528	0.692493	2.801373
C	-2.363481	-1.423374	3.497614
C	-2.245115	-2.693254	2.811158
C	-0.591208	-4.077762	1.606419
C	1.568493	-3.950935	0.364027
C	2.421312	-2.479108	-2.027861
C	3.162449	-0.102466	-2.352363
C	2.433267	1.078519	-2.790449
C	1.323276	3.129224	-2.064381
C	0.924606	3.900918	-0.889164
C	-0.491283	4.000598	1.567910
C	-2.178284	2.665287	2.785483
C	-2.327582	1.404423	3.484541
C	-1.221671	-0.756921	4.053778
C	-1.032319	-3.374489	2.797304
C	0.850076	-4.019572	1.596491
C	2.780602	-3.163277	0.349119
C	3.240115	-2.469775	-0.825349
C	4.001443	-0.107139	-1.180654
C	2.478565	2.295705	-2.037028
C	1.673787	3.823051	0.328285
C	0.947867	3.911091	1.558853
C	-0.950115	3.316956	2.763665
C	-1.202605	0.716351	4.045789
C	0.042797	-1.506375	4.076707
C	0.111475	-2.808672	3.477619
C	1.291891	-3.259971	2.764075
C	3.262936	-2.459509	1.508417
C	4.089546	-1.355175	-0.414803
C	4.032407	1.125352	-0.417819
C	3.297609	2.301772	-0.848930
C	2.884353	3.035674	0.320202
C	1.368358	3.149387	2.732603
C	0.180843	2.730219	3.448311
C	0.080761	1.435708	4.059616
C	1.273403	-0.771702	4.143187
C	2.466297	-2.457265	2.725784
C	4.104682	-1.348722	1.071737
C	4.046727	1.131896	1.053067
C	3.319532	2.311864	1.487281
C	2.522102	2.315965	2.690619
C	1.292239	0.673388	4.129148
C	2.462581	-1.241726	3.478822
C	4.031300	-0.093747	1.827869
C	2.491432	1.105967	3.455755
C	3.212436	-0.078271	3.013840
Y	2.088732	-0.370300	0.347426
C	-2.460119	2.478896	-5.772196
C	-3.769902	1.916076	-5.286902
C	-3.801161	0.572660	-5.551157
C	-1.724919	1.271362	-6.286341
C	-2.534637	0.173970	-6.165599
H	-2.620778	3.229316	-6.583455
H	-1.898364	3.027295	-4.981625
H	-4.569425	2.515017	-4.830087
H	-4.629240	-0.113186	-5.321924
H	-0.708238	1.295983	-6.701916
H	-2.279502	-0.853652	-6.461686

18. TS1 for Type B [6,6] 7-13 stepwise addition between Y@C_{2v}-C_{82} and Cp

Energy = -3355.42486363

NIMAG = 1 $\tilde{\nu}$ = -397.56

C	-3.127177	-0.851801	-1.720366
C	-2.094594	-1.595287	-2.427412
C	-3.114652	0.525202	-1.726762
C	-3.508534	-1.575340	-0.513529
C	-1.955820	-2.845300	-1.718829
C	-0.947025	-0.920264	-2.969774
C	-2.148838	1.278540	-2.571149
C	-3.459878	1.265385	-0.538620
C	-3.824163	-0.874802	0.693153
C	-2.775061	-2.813325	-0.508679
C	-0.737119	-3.526835	-1.700819
C	0.318956	-1.669619	-3.000160
C	-0.932983	0.541311	-3.007832
C	-1.915837	2.513848	-1.767243
C	-2.709894	2.497047	-0.558606
C	-3.804294	0.597108	0.681408
C	-3.514665	-1.559609	1.910799
C	-2.322471	-3.419767	0.710498

C	-0.283230	-4.207803	-0.506307
C	0.398928	-2.967135	-2.395078
C	1.546250	-0.935398	-3.093809
C	0.341599	1.255222	-3.014176
C	-0.688346	3.158702	-1.758561
C	-2.259038	3.127022	0.652048
C	-3.484657	1.302534	1.882188
C	-3.122023	-0.811721	3.101250
C	-2.779696	-2.797510	1.920918
C	-1.033344	-4.135490	0.716830
C	1.160679	-4.146863	-0.509346
C	1.591352	-3.407849	-1.691054
C	2.750589	-1.394796	-2.443354
C	1.559078	0.505041	-3.099653
C	0.447049	2.570220	-2.447841
C	-0.216404	3.856673	-0.575423
C	-0.966874	3.826507	0.645914
C	-2.727752	2.530909	1.869856
C	-3.109042	0.574037	3.088264
C	-2.084252	-1.535771	3.804072
C	-1.954956	-2.806729	3.124856
C	-0.282763	-4.188348	1.938160
C	1.889518	-4.059944	0.716104
C	2.762902	-2.600094	-1.674186
C	3.499233	-0.223013	-2.004713
C	2.766436	0.952633	-2.450996
C	1.635725	3.000106	-1.749707
C	1.222986	3.773880	-0.580913
C	-0.211923	3.889355	1.865828
C	-1.906282	2.551956	3.071834
C	-2.057580	1.294511	3.775625
C	-0.948477	-0.860353	4.365163
C	-0.737233	-3.480310	3.121213
C	1.159571	-4.125533	1.941984
C	3.100147	-3.268935	0.709972
C	3.569713	-2.580725	-0.463561
C	4.324877	-0.217046	-0.822361
C	2.800075	2.172953	-1.705577
C	1.963533	3.708862	0.642960
C	1.228128	3.802683	1.868026
C	-0.678933	3.209649	3.058449
C	-0.934660	0.612956	4.349399
C	0.318084	-1.603816	4.402282
C	0.397281	-2.907933	3.809624
C	1.587161	-3.359079	3.108801
C	3.570065	-2.558755	1.870647
C	4.410936	-1.460963	-0.050237
C	4.343244	1.019479	-0.067486
C	3.607716	2.191053	-0.512779
C	3.179104	2.928858	0.649909
C	1.641464	3.051101	3.049086
C	0.447432	2.629804	3.755381
C	0.346234	1.337542	4.370625
C	1.546496	-0.863764	4.477001
C	2.758950	-2.552681	3.078765
C	4.413967	-1.447217	1.436610
C	4.343899	1.033876	1.403355
C	3.606545	2.213737	1.824077
C	2.797305	2.220602	3.019970
C	1.560025	0.579634	4.455190
C	2.742437	-1.332440	3.824635
C	4.328215	-0.187589	2.184335
C	2.764453	1.013705	3.789504
C	3.493959	-0.168972	3.360940
Y	2.400157	-0.484264	0.700052
C	-1.976423	2.320150	-5.053008
C	-3.123177	1.777126	-4.208560
C	-3.492317	0.526972	-4.798174
C	-1.467844	1.080679	-5.724757
C	-2.439126	0.087515	-5.642175
H	-2.415701	3.001008	-5.823183
H	-1.213609	2.916661	-4.513406
H	-3.874641	2.453575	-3.772025
H	-4.381913	-0.058896	-4.529990
H	-0.516871	1.015098	-6.271159
H	-2.380367	-0.903341	-6.114224

19. INT for Type B [6,6] 7-13 stepwise addition between Y@C_{2v}-C_{82} and Cp

Energy = -3355.42862008

NIMAG = 0 $\tilde{\nu}$ = 46.95

C	-3.433303	-0.750399	-2.064286
C	-2.405638	-1.499820	-2.772267

C	-3.430011	0.626516	-2.078787
C	-3.814950	-1.469419	-0.852823
C	-2.259512	-2.735957	-2.056641
C	-1.245721	-0.816284	-3.308382
C	-2.502775	1.404842	-2.994673
C	-3.753548	1.363427	-0.892139
C	-4.131801	-0.767278	0.351059
C	-3.079077	-2.703394	-0.843647
C	-1.036592	-3.418072	-2.030433
C	0.023240	-1.570949	-3.335604
C	-1.221695	0.626232	-3.334651
C	-2.221991	2.620930	-2.120579
C	-3.006132	2.598062	-0.914444
C	-4.106961	0.703137	0.334008
C	-3.824889	-1.447216	1.572375
C	-2.627276	-3.306615	0.377203
C	-0.585586	-4.095951	-0.837938
C	0.101100	-2.865166	-2.726779
C	1.249492	-0.840179	-3.435685
C	0.036443	1.340510	-3.359311
C	-0.996368	3.260120	-2.113458
C	-2.561866	3.236368	0.296634
C	-3.786652	1.412870	1.528184
C	-3.430226	-0.694830	2.757340
C	-3.087031	-2.683624	1.586215
C	-1.336396	-4.020887	0.386584
C	0.860414	-4.038517	-0.840055
C	1.294545	-3.308511	-2.024086
C	2.456892	-1.298702	-2.780459
C	1.261300	0.595512	-3.447647
C	0.143767	2.664179	-2.799116
C	-0.522933	3.960951	-0.931851
C	-1.273277	3.938337	0.289206
C	-3.032053	2.645375	1.514300
C	-3.416114	0.690880	2.740317
C	-2.391549	-1.417022	3.464065
C	-2.263656	-2.689974	2.791781
C	-0.588164	-4.072207	1.606678
C	1.587464	-3.948472	0.385979
C	2.467595	-2.501690	-2.009195
C	3.202834	-0.126897	-2.346837
C	2.467184	1.046866	-2.798748
C	1.325989	3.093089	-2.105300
C	0.913830	3.874294	-0.937060
C	-0.518899	4.004593	1.509361
C	-2.214066	2.670240	2.716561
C	-2.365404	1.414079	3.423784
C	-1.256585	-0.738316	4.022145
C	-1.043540	-3.360167	2.787275
C	0.856258	-4.009803	1.611565
C	2.799275	-3.158641	0.378722
C	3.273420	-2.476618	-0.797162
C	4.030135	-0.114103	-1.163861
C	2.496046	2.266198	-2.055690
C	1.655155	3.815466	0.285494
C	0.920819	3.916281	1.511259
C	-0.986533	3.328946	2.703484
C	-1.242935	0.735386	4.001320
C	0.010647	-1.480717	4.062604
C	0.089687	-2.785688	3.473780
C	1.281301	-3.238710	2.773302
C	3.266018	-2.443049	1.537055
C	4.114810	-1.355244	-0.386938
C	4.041236	1.125290	-0.413825
C	3.303716	2.294105	-0.865585
C	2.871780	3.035987	0.295045
C	1.334064	3.169865	2.695435
C	0.139484	2.750840	3.402404
C	0.037841	1.460127	4.020983
C	1.239363	-0.740046	4.137269
C	2.453175	-2.432487	2.743719
C	4.110936	-1.333805	1.100049
C	4.037403	1.146032	1.056433
C	3.298129	2.327619	1.471423
C	2.489027	2.339033	2.668280
C	1.251502	0.702238	4.108327
C	2.435114	-1.209946	3.486000
C	4.020072	-0.071194	1.841822
C	2.456996	1.134759	3.441413
C	3.187840	-0.048231	3.019660
Y	2.098631	-0.382527	0.339042
C	-2.303199	2.490699	-5.350907
C	-3.296834	1.814220	-4.376595
C	-3.710686	0.577289	-5.099282
C	-1.864450	1.349938	-6.220526
C	-2.779219	0.295062	-6.106794

H	-2.854076	3.243730	-5.964510
H	-1.475268	3.041863	-4.859946
H	-4.134341	2.457054	-4.042182
H	-4.539123	-0.071668	-4.785081
H	-0.995533	1.379235	-6.893077
H	-2.755954	-0.628897	-6.702636

20. TS2 for Type B [6,6] 7-13 stepwise addition between Y@C_{2v}-C_{82} and Cp

Energy = -3355.42726383

NIMAG = 1 $\tilde{\nu}$ = -122.15

C	-3.137114	-0.834626	-1.723380
C	-2.105403	-1.578176	-2.439257
C	-3.136791	0.540565	-1.728920
C	-3.509208	-1.563314	-0.517470
C	-1.963558	-2.828696	-1.733844
C	-0.957253	-0.902438	-2.976434
C	-2.221957	1.325909	-2.646560
C	-3.455898	1.267441	-0.532835
C	-3.823715	-0.870914	0.693774
C	-2.778691	-2.802052	-0.520990
C	-0.747299	-3.515238	-1.720275
C	0.307028	-1.654881	-3.011561
C	-0.951546	0.557382	-3.059732
C	-1.929462	2.531311	-1.764060
C	-2.702602	2.498699	-0.550491
C	-3.799699	0.598305	0.688329
C	-3.510617	-1.562620	1.906798
C	-2.324450	-3.418012	0.692896
C	-0.290564	-4.205566	-0.533459
C	0.388193	-2.955574	-2.414628
C	1.535021	-0.925996	-3.107544
C	0.327563	1.264348	-3.024587
C	-0.698536	3.163875	-1.755197
C	-2.250837	3.123560	0.664128
C	-3.477803	1.298961	1.890565
C	-3.111675	-0.819920	3.098280
C	-2.778069	-2.801232	1.908153
C	-1.038010	-4.137900	0.691474
C	1.153529	-4.151153	-0.541987
C	1.579480	-3.406117	-1.721369
C	2.741138	-1.388653	-2.461374
C	1.545564	0.513749	-3.120573
C	0.436410	2.575323	-2.453709
C	-0.218669	3.851845	-0.569808
C	-0.960178	3.820983	0.656326
C	-2.717561	2.526784	1.881024
C	-3.100102	0.566084	3.092282
C	-2.073002	-1.548905	3.794769
C	-1.947837	-2.816571	3.108237
C	-0.281671	-4.197091	1.907765
C	1.895096	-4.078227	0.679772
C	2.751806	-2.598675	-1.695692
C	3.492126	-0.221127	-2.030994
C	2.756410	0.957991	-2.478559
C	1.629279	2.997030	-1.756092
C	1.220709	3.764090	-0.582253
C	-0.202097	3.881808	1.876095
C	-1.894273	2.542752	3.080794
C	-2.044004	1.282450	3.777987
C	-0.933554	-0.877117	4.352583
C	-0.731209	-3.490732	3.093901
C	1.160819	-4.139586	1.906913
C	3.122680	-3.316527	0.672506
C	3.563431	-2.606621	-0.501005
C	4.322270	-0.219886	-0.851912
C	2.795808	2.171256	-1.728999
C	1.957638	3.686617	0.639492
C	1.238062	3.788108	1.870037
C	-0.664366	3.199921	3.067802
C	-0.919729	0.596307	4.344944
C	0.332471	-1.622092	4.378850
C	0.407588	-2.923083	3.779334
C	1.591110	-3.376343	3.073621
C	3.569811	-2.592626	1.834435
C	4.328974	-1.447478	-0.077920
C	4.426124	1.030880	-0.098641
C	3.604243	2.160080	-0.525984
C	3.155063	2.876697	0.639385
C	1.658524	3.034471	3.046741
C	0.462541	2.614546	3.757735
C	0.361930	1.319161	4.366344
C	1.562107	-0.884922	4.447507

C	2.762482	-2.569024	3.031720
C	4.336211	-1.438382	1.394798
C	4.438953	1.041736	1.388276
C	3.616941	2.175888	1.807296
C	2.813308	2.203553	3.019591
C	1.575686	0.558190	4.447238
C	2.753122	-1.350436	3.783618
C	4.343439	-0.202407	2.157777
C	2.779472	0.995600	3.782777
C	3.505468	-0.187252	3.332920
Y	2.415836	0.056677	0.691120
C	-1.959920	2.310059	-4.970719
C	-3.054143	1.776079	-4.026229
C	-3.517014	0.539150	-4.701755
C	-1.444168	1.020957	-5.534757
C	-2.493177	0.073750	-5.523305
H	-2.444694	2.908852	-5.778165
H	-1.199208	2.956564	-4.491560
H	-3.835744	2.488173	-3.703554
H	-4.439186	-0.000892	-4.448142
H	-0.478955	0.903429	-6.047294
H	-2.466249	-0.908866	-6.015135

21. P for Type B [6,6] 7-13 stepwise addition between Y@C_{2v}-C_{82} and Cp

Energy = -3355.44803751

NIMAG = 0 $\tilde{\nu}$ = 34.05

C	-3.428090	-0.735149	-2.085922
C	-2.368977	-1.478479	-2.780474
C	-3.450849	0.638359	-2.102112
C	-3.793216	-1.467299	-0.880972
C	-2.245518	-2.739775	-2.080063
C	-1.252199	-0.842362	-3.359777
C	-2.591923	1.461230	-3.041291
C	-3.765963	1.354246	-0.891724
C	-4.120005	-0.784353	0.332853
C	-3.066395	-2.710341	-0.878891
C	-1.041095	-3.437830	-2.075292
C	0.005465	-1.580162	-3.374322
C	-1.306275	0.666985	-3.706196
C	-2.241699	2.618010	-2.117518
C	-3.009258	2.582250	-0.901414
C	-4.100488	0.682151	0.329471
C	-3.811873	-1.480858	1.544683
C	-2.623523	-3.335002	0.333847
C	-0.589057	-4.134288	-0.884822
C	0.091178	-2.879462	-2.766900
C	1.238329	-0.850560	-3.470330
C	0.038602	1.360722	-3.407052
C	-1.007124	3.235021	-2.102375
C	-2.556493	3.202193	0.315796
C	-3.785669	1.380613	1.536390
C	-3.419066	-0.740520	2.741055
C	-3.081881	-2.720476	1.548055
C	-1.339856	-4.060952	0.335116
C	0.853213	-4.079407	-0.890458
C	1.278982	-3.327598	-2.067785
C	2.431412	-1.308150	-2.812151
C	1.239752	0.598901	-3.468153
C	0.131585	2.634438	-2.796802
C	-0.524937	3.918172	-0.916688
C	-1.266682	3.896411	0.309419
C	-3.025513	2.606683	1.530982
C	-3.408770	0.645313	2.736431
C	-2.383150	-1.469687	3.439149
C	-2.254437	-2.736532	2.749012
C	-0.586398	-4.120190	1.555607
C	1.591678	-4.003515	0.332950
C	2.448030	-2.519620	-2.042199
C	3.183620	-0.139764	-2.372744
C	2.449825	1.037177	-2.815660
C	1.325209	3.066425	-2.093259
C	0.915205	3.833504	-0.926036
C	-0.509271	3.960333	1.530051
C	-2.203620	2.622425	2.733288
C	-2.354304	1.361193	3.427445
C	-1.244585	-0.799135	4.000878
C	-1.039171	-3.413405	2.739960
C	0.854399	-4.063909	1.558502
C	2.816529	-3.238500	0.326818
C	3.256997	-2.526895	-0.846210
C	4.009281	-0.141194	-1.193238
C	2.491523	2.250043	-2.069369

C	1.651843	3.763584	0.296637
C	0.930372	3.866427	1.525764
C	-0.973464	3.279025	2.721680
C	-1.230930	0.673926	3.995463
C	0.020935	-1.544584	4.028573
C	0.097968	-2.845896	3.428622
C	1.282962	-3.300175	2.727478
C	3.261995	-2.514693	1.489484
C	4.022787	-1.369415	-0.420580
C	4.115793	1.108215	-0.437451
C	3.299157	2.238469	-0.863957
C	2.850139	2.955385	0.298849
C	1.349445	3.111824	2.702446
C	0.152433	2.692618	3.412437
C	0.050914	1.396903	4.019721
C	1.250183	-0.807797	4.098430
C	2.453539	-2.492723	2.686462
C	4.031281	-1.361014	1.052142
C	4.133614	1.119583	1.048905
C	3.312294	2.253915	1.467888
C	2.505014	2.280819	2.677251
C	1.264632	0.636001	4.101440
C	2.443636	-1.273864	3.438755
C	4.041854	-0.125997	1.818510
C	2.469423	1.072900	3.440198
C	3.196666	-0.111135	2.989637
Y	2.109119	0.124097	0.377019
C	-2.203145	2.290286	-5.287477
C	-3.379253	1.947322	-4.351277
C	-3.930020	0.697342	-5.013031
C	-1.637149	0.857010	-5.279936
C	-2.883926	0.042678	-5.569392
H	-2.548388	2.597891	-6.294163
H	-1.509548	3.052515	-4.880927
H	-4.102540	2.748484	-4.113043
H	-4.968592	0.347740	-4.931921
H	-0.745462	0.644650	-5.897979
H	-2.892503	-0.952425	-6.035083

22. RC for Type D [5,6] 8-15 concerted mechanism addition between La@C_{2v}-C_{82} and Cp

Energy = -3752.85303654

NIMAG = 0 $\tilde{\nu}$ = 9.87

C	3.678488	0.689696	-2.293052
C	2.647296	1.393597	-3.024895
C	3.687224	-0.694596	-2.272496
C	4.027329	1.448766	-1.094707
C	2.481729	2.667915	-2.355233
C	1.538622	0.700737	-3.613882
C	2.667647	-1.433229	-2.986614
C	4.051869	-1.417566	-1.055534
C	4.315945	0.773891	0.133686
C	3.277742	2.677309	-1.132807
C	1.257030	3.326203	-2.389394
C	0.261046	1.425263	-3.684839
C	1.549041	-0.772420	-3.593530
C	2.517838	-2.689939	-2.278537
C	3.317503	-2.656456	-1.058178
C	4.323978	-0.701907	0.155242
C	3.967886	1.482619	1.326851
C	2.783939	3.304174	0.060643
C	0.761678	4.032550	-1.221073
C	0.147333	2.731877	-3.101743
C	-0.951487	0.666101	-3.779607
C	0.281712	-1.517092	-3.644385
C	1.304526	-3.367219	-2.296041
C	2.827438	-3.250633	0.153374
C	3.991206	-1.381030	1.365556
C	3.561302	0.757606	2.525914
C	3.217561	2.712815	1.293078
C	1.485012	4.000140	0.018414
C	-0.677061	3.946432	-1.258993
C	-1.063249	3.165418	-2.432426
C	-2.173346	1.115483	-3.159046
C	-0.941231	-0.778157	-3.759706
C	0.186335	-2.808170	-3.024333
C	0.818725	-4.047171	-1.107434
C	1.541255	-3.967652	0.131042
C	3.257346	-2.624438	1.367140
C	3.570572	-0.628279	2.543379

C	2.495154	1.479871	3.185431
C	2.362787	2.735978	2.474039
C	0.701407	4.066919	1.219444
C	-1.439619	3.876689	-0.051932
C	-2.222001	2.337970	-2.418422
C	-2.921249	-0.055397	-2.717913
C	-2.156749	-1.227504	-3.126282
C	-1.017564	-3.239948	-2.342584
C	-0.620422	-3.982581	-1.147668
C	0.758834	-4.014679	1.333641
C	2.401313	-2.625058	2.547467
C	2.515329	-1.347692	3.223363
C	1.358530	0.802154	3.736722
C	1.138178	3.393901	2.429746
C	-0.737783	3.980762	1.188721
C	-2.642003	3.076890	-0.070570
C	-3.053972	2.340516	-1.233765
C	-3.779675	-0.045378	-1.560670
C	-2.188342	-2.429109	-2.351849
C	-1.384392	-3.889865	0.057580
C	-0.681951	-3.949816	1.300447
C	1.186176	-3.302383	2.523939
C	1.369081	-0.671210	3.756546
C	0.079375	1.527573	3.724757
C	-0.005415	2.818112	3.102481
C	-1.181632	3.232147	2.362687
C	-3.112044	2.373037	1.090974
C	-3.847946	1.199006	-0.811283
C	-3.832128	-1.269602	-0.776872
C	-3.020390	-2.410164	-1.167120
C	-2.597451	-3.107155	0.016403
C	-1.136277	-3.174945	2.452821
C	0.034314	-2.723365	3.179851
C	0.100370	-1.414916	3.765773
C	-1.136783	0.770263	3.780004
C	-2.338763	2.403792	2.314372
C	-3.885729	1.219659	0.661837
C	-3.869962	-1.249476	0.696615
C	-3.078620	-2.378637	1.157819
C	-2.305135	-2.364509	2.381564
C	-1.126418	-0.673816	3.800257
C	-2.326785	1.201612	3.088976
C	-3.856995	-0.003884	1.448190
C	-2.310151	-1.141101	3.121926
C	-3.053660	0.018635	2.644553
La	-1.728499	-0.015578	0.003927
C	5.997036	-3.392907	-2.835631
C	5.537912	-4.535747	-1.971051
C	6.010109	-4.347292	-0.700398
C	6.739812	-2.499294	-1.879316
C	6.754694	-3.088500	-0.643805
H	6.664950	-3.749597	-3.656319
H	5.157723	-2.875369	-3.354558
H	4.938089	-5.382575	-2.331480
H	5.845030	-5.015251	0.157158
H	7.208412	-1.546054	-2.159584
H	7.226186	-2.680969	0.262003

23. TS for Type D [5,6] 8-15 concerted mechanism addition between La@C_{2v}-C_{82} and Cp

Energy = -3752.84119288

NIMAG = 1 $\tilde{\nu}$ = -414.00

C	2.809754	1.055820	-2.170290
C	1.772634	1.767996	-2.886594
C	2.821087	-0.325476	-2.160654
C	3.183527	1.823735	-0.979756
C	1.625468	3.043707	-2.219547
C	0.654210	1.088719	-3.472445
C	1.773538	-1.041285	-2.836951
C	3.332744	-1.109184	-0.987226
C	3.457689	1.136831	0.244968
C	2.438540	3.050198	-1.007206
C	0.405657	3.712243	-2.243015
C	-0.617430	1.823297	-3.535797
C	0.653799	-0.378411	-3.448725
C	1.619709	-2.298205	-2.135934
C	2.471610	-2.321515	-0.960373
C	3.452419	-0.328385	0.264623
C	3.133196	1.850512	1.443923
C	1.955019	3.681961	0.193240
C	-0.074632	4.423444	-1.070874
C	-0.715361	3.128297	-2.946817
C	-1.835497	1.072273	-3.620096

C	-0.616046	-1.116386	-3.496610
C	0.405179	-2.975212	-2.160396
C	1.955743	-2.878121	0.264668
C	3.131416	-1.001145	1.457296
C	2.736371	1.129218	2.641692
C	2.394025	3.089816	1.420191
C	0.659443	4.383948	0.162108
C	-1.513815	4.346790	-1.095984
C	-1.916471	3.570303	-2.267420
C	-3.048917	1.529217	-2.987486
C	-1.835086	-0.371647	-3.605243
C	-0.713600	-2.407825	-2.877339
C	-0.074840	-3.656746	-0.973920
C	0.661134	-3.581460	0.256079
C	2.401726	-2.265148	1.473226
C	2.731489	-0.257488	2.645581
C	1.682472	1.855494	3.315371
C	1.551973	3.115930	2.609794
C	-0.113853	4.454993	1.370404
C	-2.267485	4.280569	0.117683
C	-3.080522	2.750281	-2.243482
C	-3.800274	0.362440	-2.542196
C	-3.048820	-0.814192	-2.960607
C	-1.915484	-2.835755	-2.189269
C	-1.514941	-3.586157	-1.002248
C	-0.109373	-3.629240	1.465872
C	1.559012	-2.256776	2.655656
C	1.682304	-0.976263	3.329135
C	0.546494	1.179511	3.869604
C	0.329281	3.778631	2.576333
C	-1.553801	4.377532	1.352129
C	-3.476520	3.491028	0.108259
C	-3.901844	2.757793	-1.052181
C	-4.647926	0.375712	-1.376563
C	-3.082227	-2.016437	-2.188564
C	-2.265833	-3.489753	0.211548
C	-1.553433	-3.558348	1.447173
C	0.335085	-2.927447	2.651094
C	0.547381	-0.294858	3.880726
C	-0.727938	1.912302	3.873241
C	-0.811245	3.206415	3.257025
C	-1.991545	3.628928	2.528922
C	-3.937669	2.785230	1.272728
C	-4.693846	1.617501	-0.623808
C	-4.708278	-0.851375	-0.595964
C	-3.903958	-1.994648	-0.996176
C	-3.472476	-2.695672	0.182555
C	-1.988250	-2.782344	2.602895
C	-0.804365	-2.340171	3.318086
C	-0.725189	-1.031847	3.903912
C	-1.947214	1.161022	3.936326
C	-3.153017	2.806827	2.488269
C	-4.717613	1.635244	0.848271
C	-4.732141	-0.834302	0.879082
C	-3.939655	-1.968301	1.330173
C	-3.152597	-1.962863	2.546039
C	-1.945983	-0.283156	3.954627
C	-3.141735	1.602200	3.259655
C	-4.696311	0.410742	1.631987
C	-3.140761	-0.740725	3.287672
C	-3.880632	0.425003	2.820314
La	-2.581488	0.339893	0.169012
C	4.802824	-2.758428	-2.521524
C	4.418637	-3.970707	-1.725586
C	4.986761	-3.869216	-0.455430
C	5.177612	-1.773380	-1.423707
C	5.515544	-2.565464	-0.284064
H	5.732771	-2.986486	-3.098560
H	4.053474	-2.408228	-3.258108
H	3.903306	-4.848966	-2.137996
H	4.963129	-4.648659	0.318990
H	5.682623	-0.821422	-1.650989
H	5.980126	-2.184321	0.635563

24. P for Type D [5,6] 8-15 concerted mechanism addition between La@C_{2v}-C_{82} and Cp

Energy = -3752.87692143

NIMAG = 0 $\tilde{\nu}$ = 23.10

C	3.597642	0.676729	-2.329331
C	2.556597	1.391465	-3.030562
C	3.605104	-0.703936	-2.310415
C	3.987593	1.449690	-1.145231
C	2.420212	2.671698	-2.368285

C	1.434258	0.719714	-3.614929
C	2.541058	-1.412287	-2.946342
C	4.284278	-1.511470	-1.214060
C	4.265168	0.754985	0.074970
C	3.242881	2.676582	-1.164580
C	1.202047	3.344149	-2.391176
C	0.168223	1.460966	-3.685093
C	1.426337	-0.741232	-3.578621
C	2.416065	-2.689547	-2.313690
C	3.445924	-2.907441	-1.214074
C	4.270995	-0.712212	0.082295
C	3.936589	1.464301	1.275402
C	2.761649	3.305600	0.040719
C	0.726009	4.052413	-1.213582
C	0.078051	2.766959	-3.093420
C	-1.051257	0.714746	-3.770458
C	0.166625	-1.473492	-3.645796
C	1.196905	-3.343862	-2.328100
C	2.736775	-3.275671	0.085305
C	3.921140	-1.378155	1.254053
C	3.541726	0.739801	2.465564
C	3.203058	2.711150	1.262643
C	1.465466	4.008945	0.015806
C	-0.712760	3.982115	-1.234968
C	-1.118652	3.206740	-2.406796
C	-2.262902	1.172063	-3.132952
C	-1.053626	-0.728666	-3.759075
C	0.072989	-2.763218	-3.027458
C	0.707978	-4.051554	-1.148764
C	1.447732	-3.965920	0.081337
C	3.160358	-2.645470	1.259203
C	3.526499	-0.648119	2.448947
C	2.492016	1.463622	3.148740
C	2.363720	2.731047	2.452114
C	0.694921	4.076930	1.226216
C	-1.463921	3.914324	-0.019441
C	-2.286350	2.389246	-2.382592
C	-3.013139	0.004759	-2.689133
C	-2.264298	-1.172899	-3.113506
C	-1.127515	-3.195552	-2.346707
C	-0.724835	-3.962540	-1.167218
C	0.674464	-4.011991	1.291590
C	2.338412	-2.638059	2.455792
C	2.475169	-1.363882	3.130414
C	1.356080	0.788916	3.702778
C	1.141372	3.396322	2.428791
C	-0.745709	4.005408	1.212685
C	-2.676041	3.129761	-0.028412
C	-3.102422	2.397458	-1.189608
C	-3.854391	0.015499	-1.519846
C	-2.294353	-2.377367	-2.344227
C	-1.480204	-3.865746	0.049532
C	-0.769965	-3.940873	1.281281
C	1.121540	-3.315535	2.472650
C	1.350717	-0.685941	3.704271
C	0.083996	1.524686	3.718537
C	0.002536	2.823308	3.109759
C	-1.179171	3.249942	2.386559
C	-3.130489	2.416306	1.134315
C	-3.889249	1.252446	-0.761940
C	-3.920711	-1.217178	-0.744269
C	-3.117189	-2.359006	-1.149928
C	-2.682464	-3.064264	0.025011
C	-1.199052	-3.167308	2.443555
C	-0.011699	-2.730172	3.154205
C	0.077604	-1.421825	3.737780
C	-1.136153	0.776056	3.783485
C	-2.342771	2.430122	2.346866
C	-3.908308	1.265538	0.708043
C	-3.940937	-1.204551	0.731242
C	-3.147994	-2.340928	1.176458
C	-2.359408	-2.342436	2.392115
C	-1.139805	-0.668672	3.797534
C	-2.332627	1.222851	3.114080
C	-3.892906	0.040025	1.487513
C	-2.338543	-1.120908	3.135253
C	-3.076031	0.048941	2.674035
La	-1.780520	-0.078506	0.017087
C	5.410819	-3.136075	-2.616887
C	4.586394	-3.961554	-1.604479
C	5.546127	-4.007651	-0.425707
C	5.750408	-2.020521	-1.603638
C	6.242594	-2.846667	-0.425140
H	6.314816	-3.677872	-2.957183
H	4.831463	-2.788485	-3.495177
H	4.157848	-4.922706	-1.943438

H	5.568092	-4.796461	0.338870
H	6.397397	-1.190236	-1.942040
H	6.949118	-2.495584	0.339585

25. RC for Type B [6,6] 7-13 stepwise addition between La@C_{2v}-C_{82} and Cp

Energy = -3752.85449635

NIMAG = 0 $\tilde{\nu}$ = 15.75

C	3.528392	0.775416	-1.999289
C	2.495486	1.504597	-2.708226
C	3.523695	-0.608001	-2.009693
C	3.889522	1.500964	-0.786151
C	2.342073	2.762144	-2.005409
C	1.373571	0.832244	-3.291851
C	2.494248	-1.323042	-2.736921
C	3.886755	-1.359617	-0.814612
C	4.186792	0.795899	0.423472
C	3.146367	2.735406	-0.788221
C	1.121345	3.430740	-2.012873
C	0.102268	1.567000	-3.340850
C	1.371496	-0.639716	-3.306894
C	2.341175	-2.596959	-2.059131
C	3.145161	-2.595650	-0.843203
C	4.186264	-0.680992	0.408794
C	3.848866	1.475934	1.635799
C	2.666686	3.335203	0.423671
C	0.640273	4.109378	-0.823440
C	0.001530	2.861293	-2.729513
C	-1.116545	0.818228	-3.446139
C	0.100595	-1.373811	-3.367305
C	1.122057	-3.266579	-2.082550
C	2.666795	-3.222484	0.355332
C	3.849277	-1.387593	1.606412
C	3.444662	0.723933	2.820392
C	3.106482	2.710282	1.638288
C	1.372684	4.041395	0.409457
C	-0.800189	4.033548	-0.851361
C	-1.202032	3.286399	-2.040621
C	-2.331321	1.261317	-2.807435
C	-1.117788	-0.625880	-3.461519
C	0.001010	-2.682898	-2.788530
C	0.640732	-3.971726	-0.908065
C	1.373519	-3.929130	0.325751
C	3.106337	-2.622044	1.582494
C	3.445015	-0.661320	2.806182
C	2.389936	1.437964	3.506842
C	2.260979	2.710698	2.826830
C	0.599455	4.083800	1.618130
C	-1.552628	3.938536	0.359928
C	-2.366186	2.466616	-2.038030
C	-3.084814	0.085107	-2.389620
C	-2.332317	-1.082327	-2.831781
C	-1.201086	-3.123138	-2.108078
C	-0.799710	-3.896306	-0.935080
C	0.599750	-3.996725	1.533055
C	2.261220	-2.648462	2.770229
C	2.389804	-1.390072	3.477054
C	1.252442	0.754432	4.050352
C	1.040740	3.377773	2.807664
C	-0.840704	4.007740	1.597043
C	-2.759938	3.145572	0.331550
C	-3.189788	2.444066	-0.846533
C	-3.933923	0.072674	-1.225337
C	-2.366257	-2.303183	-2.086875
C	-1.553769	-3.828081	0.277876
C	-0.840509	-3.921520	1.513456
C	1.041095	-3.315758	2.736816
C	1.252303	-0.718779	4.034428
C	-0.021510	1.488447	4.065919
C	-0.101861	2.793781	3.475577
C	-1.281190	3.234446	2.755961
C	-3.229350	2.419726	1.479555
C	-3.994160	1.301029	-0.446236
C	-3.981727	-1.168096	-0.471139
C	-3.187707	-2.308409	-0.896539
C	-2.763623	-3.039956	0.266016
C	-1.280613	-3.172662	2.687964
C	-0.101663	-2.746408	3.416582
C	-0.021905	-1.453823	4.034328
C	-1.242797	0.738227	4.112585
C	-2.444901	2.415907	2.697232
C	-4.020084	1.285582	1.028510
C	-4.007517	-1.183882	1.001378

C	-3.226858	-2.333020	1.428603
C	-2.443991	-2.352505	2.645116
C	-1.243305	-0.705427	4.097035
C	-2.434552	1.194646	3.441027
C	-3.986702	0.040876	1.783270
C	-2.435384	-1.147770	3.416016
C	-3.173828	0.028158	2.973564
La	-1.869610	0.104858	0.322731
C	2.613359	-2.402580	-5.784847
C	3.906688	-1.814057	-5.286007
C	3.910947	-0.468997	-5.543485
C	1.856425	-1.208624	-6.299187
C	2.641140	-0.094706	-6.166450
H	2.797051	-3.145124	-6.598425
H	2.057062	-2.966889	-5.001723
H	4.715438	-2.397902	-4.825947
H	4.722196	0.233409	-5.304452
H	0.843808	-1.252994	-6.722837
H	2.366256	0.928701	-6.459337

26. TS1 for Type B [6,6] 7-13 stepwise addition between La@C_{2v}-C_{82} and Cp

Energy = -3752.84253039

NIMAG = 1 $\tilde{\nu}$ = -394.83

C	3.126656	0.903744	-1.691694
C	2.089874	1.638393	-2.401717
C	3.132658	-0.473242	-1.706867
C	3.489354	1.624428	-0.477471
C	1.929737	2.882528	-1.686072
C	0.955244	0.952183	-2.956288
C	2.183453	-1.233683	-2.563736
C	3.478687	-1.216401	-0.520968
C	3.805624	0.920269	0.726905
C	2.740488	2.853044	-0.470345
C	0.702969	3.548929	-1.672528
C	-0.320282	1.685579	-2.989568
C	0.960929	-0.509243	-3.004156
C	1.960119	-2.476921	-1.769094
C	2.744354	-2.457424	-0.554307
C	3.804964	-0.551645	0.705823
C	3.478264	1.593595	1.946207
C	2.271405	3.446859	0.748994
C	0.231451	4.217261	-0.477523
C	-0.421583	2.978444	-2.378027
C	-1.536816	0.936020	-3.091037
C	-0.304200	-1.239420	-3.024237
C	0.740869	-3.138109	-1.774440
C	2.292779	-3.100305	0.649276
C	3.486488	-1.268839	1.899999
C	3.086473	0.832996	3.128891
C	2.727712	2.822045	1.958650
C	0.974279	4.147173	0.750158
C	-1.211374	4.136555	-0.491226
C	-1.623449	3.398286	-1.679857
C	-2.753264	1.373169	-2.445587
C	-1.530745	-0.503402	-3.111874
C	-0.396805	-2.559651	-2.468396
C	0.269510	-3.848724	-0.598518
C	1.009669	-3.815930	0.629193
C	2.745035	-2.506617	1.874400
C	3.092491	-0.552788	3.107547
C	2.034552	1.539457	3.828433
C	1.893774	2.813196	3.156059
C	0.213254	4.182532	1.965589
C	-1.951222	4.033374	0.727010
C	-2.784897	2.574267	-1.670837
C	-3.494987	0.191969	-2.027585
C	-2.739388	-0.969609	-2.478043
C	-1.586297	-3.006353	-1.779791
C	-1.171082	-3.782075	-0.613733
C	0.247308	-3.897281	1.843929
C	1.915405	-2.545914	3.070247
C	2.045132	-1.291042	3.782243
C	0.903514	0.845928	4.376388
C	0.668092	3.472024	3.147140
C	-1.228193	4.099984	1.957607
C	-3.156371	3.234800	0.707059
C	-3.598188	2.540645	-0.471035
C	-4.328934	0.168002	-0.852091
C	-2.760736	-2.193282	-1.740618
C	-1.917851	-3.728889	0.605410
C	-1.193937	-3.826649	1.835497
C	0.696495	-3.219983	3.044624

C	0.909203	-0.627233	4.351956
C	-0.372925	1.572911	4.405413
C	-0.464988	2.880126	3.822360
C	-1.654359	3.319422	3.115134
C	-3.616989	2.505009	1.856431
C	-4.397680	1.394478	-0.068691
C	-4.357602	-1.074589	-0.106071
C	-3.570722	-2.213830	-0.546891
C	-3.135701	-2.952961	0.608729
C	-1.627250	-3.088085	3.017219
C	-0.442196	-2.658644	3.736573
C	-0.362161	-1.368449	4.358261
C	-1.591246	0.816092	4.458174
C	-2.815469	2.496932	3.064120
C	-4.413746	1.371736	1.407445
C	-4.372432	-1.098975	1.364946
C	-3.588644	-2.252137	1.778741
C	-2.793515	-2.271771	2.986487
C	-1.586398	-0.625378	4.434830
C	-2.790210	1.270134	3.798386
C	-4.360688	0.119632	2.153093
C	-2.783784	-1.069800	3.761902
C	-3.531991	0.103822	3.334198
La	-2.252875	0.266210	0.703269
C	2.043200	-2.261738	-5.051997
C	3.175516	-1.707160	-4.195538
C	3.530483	-0.448177	-4.775090
C	1.521270	-1.025757	-5.719630
C	2.477331	-0.019099	-5.624265
H	2.498478	-2.930856	-5.823195
H	1.285397	-2.873014	-4.522037
H	3.934075	-2.375201	-3.758377
H	4.409425	0.148999	-4.496929
H	0.573265	-0.970560	-6.272241
H	2.407471	0.973652	-6.090732

27. INT for Type B [6,6] 7-13 stepwise addition between La@C_{2v}-C_{82} and Cp

Energy = -3752.84613926

NIMAG = 0 $\tilde{\nu}$ = 16.72

C	3.506999	0.813936	-2.050157
C	2.474967	1.554904	-2.760321
C	3.521767	-0.562868	-2.073799
C	3.870758	1.529630	-0.831331
C	2.308090	2.784888	-2.037411
C	1.327734	0.860077	-3.308592
C	2.611253	-1.346636	-3.001500
C	3.846396	-1.303486	-0.889984
C	4.188322	0.823398	0.369934
C	3.119578	2.754319	-0.819239
C	1.077173	3.452211	-2.015210
C	0.049333	1.598874	-3.337747
C	1.323099	-0.582455	-3.345820
C	2.339757	-2.572198	-2.137904
C	3.114511	-2.547336	-0.925873
C	4.182442	-0.647072	0.343003
C	3.864239	1.491508	1.593258
C	2.651859	3.344586	0.402147
C	0.609148	4.117106	-0.821841
C	-0.049421	2.888376	-2.722245
C	-1.166491	0.853231	-3.445737
C	0.074056	-1.312241	-3.383349
C	1.122178	-3.227422	-2.144383
C	2.669756	-3.198776	0.278009
C	3.863234	-1.368790	1.530298
C	3.470613	0.726151	2.770193
C	3.110769	2.718523	1.610024
C	1.352960	4.043570	0.406979
C	-0.835978	4.039358	-0.833919
C	-1.252018	3.310133	-2.024591
C	-2.385911	1.289351	-2.795187
C	-1.159708	-0.581251	-3.472709
C	-0.020535	-2.641041	-2.834009
C	0.649546	-3.941416	-0.970277
C	1.390140	-3.916607	0.256763
C	3.124061	-2.610598	1.503018
C	3.475020	-0.659577	2.744349
C	2.418124	1.430766	3.474178
C	2.278705	2.706676	2.809366
C	0.594827	4.077354	1.621559
C	-1.573795	3.933319	0.384934
C	-2.415436	2.487442	-2.017711
C	-3.125054	0.108423	-2.382597

C	-2.366691	-1.051117	-2.838378
C	-1.203317	-3.087007	-2.149721
C	-0.788492	-3.870661	-0.984741
C	0.628560	-4.001282	1.471777
C	2.298318	-2.653846	2.699375
C	2.428627	-1.400591	3.415287
C	1.287993	0.733947	4.019170
C	1.050708	3.362504	2.800210
C	-0.848916	3.995033	1.614893
C	-2.780552	3.135844	0.364021
C	-3.228420	2.448868	-0.816726
C	-3.958856	0.077381	-1.205572
C	-2.383612	-2.274314	-2.104067
C	-1.536255	-3.824508	0.233203
C	-0.812331	-3.929063	1.463616
C	1.079006	-3.328435	2.673936
C	1.293377	-0.739573	3.989071
C	0.011094	1.460121	4.052179
C	-0.080954	2.768518	3.473668
C	-1.272395	3.209992	2.767248
C	-3.239901	2.402159	1.511386
C	-4.029992	1.302041	-0.417703
C	-3.977471	-1.167301	-0.465197
C	-3.193583	-2.306396	-0.913607
C	-2.756342	-3.051083	0.239667
C	-1.244824	-3.195950	2.648739
C	-0.059049	-2.768915	3.368386
C	0.021966	-1.480645	3.994010
C	-1.207502	0.702870	4.104886
C	-2.434217	2.388255	2.716796
C	-4.039847	1.271964	1.059141
C	-3.986631	-1.197927	1.004549
C	-3.205553	-2.355455	1.412355
C	-2.409809	-2.378763	2.619943
C	-1.202028	-0.737399	4.073959
C	-2.406444	1.158810	3.446428
C	-3.976572	0.015243	1.797268
C	-2.400682	-1.179992	3.399973
C	-3.148950	-0.005568	2.978945
La	-1.874747	0.209347	0.328643
C	2.442128	-2.416211	-5.366733
C	3.421586	-1.735963	-4.381051
C	3.824254	-0.488392	-5.090521
C	1.992868	-1.272857	-6.227147
C	2.894444	-0.208225	-6.100086
H	3.006744	-3.155231	-5.984879
H	1.619281	-2.983401	-4.885679
H	4.264251	-2.370869	-4.044846
H	4.643281	0.167579	-4.766414
H	1.126859	-1.306072	-6.903211
H	2.862626	0.720747	-6.687606

28. TS2 for Type B [6,6] 7-13 stepwise addition between La@C_{2v}-C_{82} and Cp

Energy = -3752.84593510

NIMAG = 1 $\tilde{\nu}$ = -118.31

C	3.128075	0.864954	-1.721627
C	2.089211	1.599215	-2.436821
C	3.138313	-0.510035	-1.727980
C	3.492750	1.595585	-0.514560
C	1.934989	2.847497	-1.731290
C	0.948565	0.911317	-2.977613
C	2.233946	-1.303468	-2.647849
C	3.465279	-1.236287	-0.533162
C	3.812464	0.904920	0.695640
C	2.747703	2.826207	-0.517007
C	0.710062	3.520632	-1.718101
C	-0.323303	1.649263	-3.013509
C	0.956370	-0.547253	-3.059164
C	1.952720	-2.513799	-1.766813
C	2.727057	-2.475269	-0.553420
C	3.803087	-0.564475	0.688168
C	3.492806	1.592048	1.910317
C	2.285956	3.434817	0.697946
C	0.245548	4.201861	-0.529052
C	-0.417832	2.949619	-2.414491
C	-1.541344	0.906751	-3.114200
C	-0.315560	-1.267419	-3.026831
C	0.729477	-3.157724	-1.757876
C	2.279744	-3.107900	0.659524
C	3.487147	-1.270843	1.888647
C	3.100000	0.842992	3.099358
C	2.744809	2.821690	1.912549

C	0.991029	4.141550	0.695639
C	-1.200838	4.127835	-0.538813
C	-1.615584	3.378339	-1.717459
C	-2.758935	1.354380	-2.472273
C	-1.539306	-0.532075	-3.120056
C	-0.412170	-2.581539	-2.457433
C	0.254547	-3.855015	-0.575207
C	0.997532	-3.820680	0.648990
C	2.739250	-2.505951	1.876112
C	3.099899	-0.543065	3.090345
C	2.051945	1.560909	3.795468
C	1.913497	2.827085	3.113227
C	0.233835	4.195266	1.914552
C	-1.939286	4.045865	0.682172
C	-2.778551	2.555789	-1.698456
C	-3.503465	0.179444	-2.054603
C	-2.751996	-0.988723	-2.482104
C	-1.596675	-3.015296	-1.763444
C	-1.184632	-3.784392	-0.590501
C	0.236473	-3.890625	1.865641
C	1.914276	-2.533129	3.075563
C	2.051617	-1.273652	3.774756
C	0.918738	0.873800	4.350391
C	0.688704	3.492046	3.099812
C	-1.208146	4.116487	1.908433
C	-3.154343	3.256236	0.680059
C	-3.579065	2.538235	-0.490040
C	-4.268967	0.166351	-0.840737
C	-2.776008	-2.203073	-1.729691
C	-1.935571	-3.728565	0.627607
C	-1.204892	-3.814644	1.857177
C	0.691978	-3.205080	3.057895
C	0.918293	-0.599553	4.338383
C	-0.352924	1.605157	4.367799
C	-0.444244	2.907091	3.778558
C	-1.638367	3.342565	3.069174
C	-3.649954	2.560944	1.844472
C	-4.360244	1.395314	-0.069904
C	-4.313866	-1.063009	-0.097328
C	-3.587850	-2.231041	-0.541597
C	-3.162804	-2.967454	0.625942
C	-1.634228	-3.066306	3.032850
C	-0.443295	-2.632214	3.744776
C	-0.354421	-1.336127	4.346165
C	-1.575694	0.851684	4.411471
C	-2.815664	2.537636	3.033573
C	-4.440282	1.405464	1.401201
C	-4.340938	-1.067334	1.366369
C	-3.601610	-2.250445	1.792077
C	-2.798428	-2.249316	2.988741
C	-1.576350	-0.583665	4.398756
C	-2.787948	1.306195	3.767778
C	-4.389869	0.148057	2.151529
C	-2.782744	-1.027881	3.741716
C	-3.553797	0.139702	3.339064
La	-2.174305	0.515194	1.053870
C	1.986340	-2.278177	-4.978029
C	3.072672	-1.742329	-4.025262
C	3.533720	-0.500433	-4.693931
C	1.470023	-0.990603	-5.544891
C	2.513269	-0.037763	-5.521494
H	2.478260	-2.874793	-5.782755
H	1.224233	-2.927176	-4.504519
H	3.856585	-2.452151	-3.703098
H	4.451517	0.043327	-4.432544
H	0.506982	-0.875663	-6.061952
H	2.484996	0.946094	-6.010762

29. P for Type B [6,6] 7-13 stepwise addition between La@C_{2v}-C_{82} and Cp

Energy = -3752.86680119

NIMAG = 0 $\tilde{\nu}$ = 35.59

C	3.482535	0.709799	-2.140072
C	2.414801	1.441488	-2.834466
C	3.516484	-0.663353	-2.155363
C	3.839931	1.445903	-0.935501
C	2.278275	2.701967	-2.134791
C	1.306044	0.792374	-3.414682
C	2.667595	-1.495086	-3.094700
C	3.840372	-1.376609	-0.945284
C	4.173232	0.766588	0.278288
C	3.097981	2.680453	-0.933361
C	1.065043	3.385941	-2.130929

C	0.040250	1.515095	-3.430779
C	1.375265	-0.716216	-3.759543
C	2.329552	-2.656073	-2.170844
C	3.098671	-2.612446	-0.955330
C	4.169209	-0.699892	0.274884
C	3.858523	1.460103	1.490746
C	2.648063	3.299813	0.279917
C	0.605451	4.075301	-0.939308
C	-0.059695	2.814785	-2.823994
C	-1.181789	0.769746	-3.528939
C	0.037540	-1.424945	-3.461586
C	1.102576	-3.285529	-2.154187
C	2.651987	-3.239077	0.261365
C	3.861493	-1.402519	1.481365
C	3.473378	0.715159	2.686148
C	3.112699	2.690841	1.493985
C	1.355875	4.011972	0.280199
C	-0.838502	4.000087	-0.945293
C	-1.253713	3.242104	-2.121463
C	-2.385450	1.213060	-2.875538
C	-1.170250	-0.679784	-3.521241
C	-0.042989	-2.701317	-2.851647
C	0.626558	-3.976340	-0.969758
C	1.370860	-3.948986	0.254089
C	3.114303	-2.636412	1.475162
C	3.475235	-0.670771	2.680247
C	2.428085	1.433732	3.383380
C	2.285108	2.698204	2.695895
C	0.602016	4.066500	1.503238
C	-1.573415	3.916703	0.277572
C	-2.411434	2.417944	-2.099600
C	-3.129521	0.037533	-2.445737
C	-2.380398	-1.129312	-2.870225
C	-1.227551	-3.144016	-2.149092
C	-0.813233	-3.910005	-0.981266
C	0.611214	-4.020680	1.471688
C	2.291463	-2.662140	2.677487
C	2.429253	-1.400471	3.371658
C	1.296346	0.748156	3.943479
C	1.061138	3.364939	2.687576
C	-0.838442	3.988179	1.501698
C	-2.785521	3.123440	0.278200
C	-3.209450	2.401264	-0.889873
C	-3.895368	0.027858	-1.234391
C	-2.406852	-2.342289	-2.118623
C	-1.563814	-3.860629	0.237935
C	-0.830051	-3.945187	1.465722
C	1.068971	-3.333671	2.662605
C	1.296820	-0.725006	3.935635
C	0.024563	1.479205	3.962419
C	-0.069589	2.780465	3.370814
C	-1.265651	3.215132	2.665849
C	-3.278051	2.429588	1.444827
C	-3.989199	1.259403	-0.465565
C	-3.942998	-1.200009	-0.487247
C	-3.219789	-2.369353	-0.928642
C	-2.792930	-3.103501	0.237971
C	-1.257351	-3.194527	2.640190
C	-0.065207	-2.759458	3.350012
C	0.024117	-1.462163	3.948231
C	-1.197359	0.725539	4.009752
C	-2.441903	2.409272	2.633028
C	-4.067658	1.272789	1.005079
C	-3.968993	-1.201037	0.976805
C	-3.230131	-2.382658	1.404156
C	-2.423055	-2.378020	2.597564
C	-1.198059	-0.710421	4.002059
C	-2.412200	1.178998	3.369433
C	-4.016241	0.017251	1.759235
C	-2.405260	-1.155772	3.348613
C	-3.177839	0.011840	2.944469
La	-1.802250	0.380289	0.657478
C	2.290758	-2.327585	-5.340876
C	3.462609	-1.972527	-4.403672
C	4.000820	-0.716751	-5.064756
C	1.709965	-0.900375	-5.334009
C	2.948304	-0.073376	-5.622352
H	2.640128	-2.631936	-6.347171
H	1.604419	-3.096362	-4.934498
H	4.193937	-2.766045	-4.164498
H	5.035558	-0.355724	-4.982488
H	0.815736	-0.697637	-5.951390
H	2.947050	0.921444	-6.088777

30. RC for Type A [6,6] 61-62

concerted mechanism addition between La@C_2-C_{72} and Cp

Energy = -3371.90393245

NIMAG = 0 $\tilde{\nu}$ = 22.13

C	-3.947317	0.776437	-0.120283
C	-3.976906	-0.445776	0.589660
C	-3.499133	-0.513673	1.950166
C	-2.835159	-1.811617	2.120073
C	-1.818605	-2.005414	3.104360
C	-0.688526	-2.827236	2.715159
C	0.660462	-2.542817	3.190421
C	1.582302	-2.779762	2.109833
C	2.735743	-1.936708	1.888331
C	3.259269	-1.945277	0.559349
C	3.928425	-0.784462	0.005356
C	3.705281	-0.758561	-1.429797
C	3.442218	0.465382	-2.090866
C	2.480070	0.517663	-3.179221
C	1.723217	1.763100	-3.035912
C	0.386209	1.826870	-3.427974
C	-0.575171	2.547907	-2.616260
C	-1.875252	1.930391	-2.830093
C	-2.851579	1.957519	-1.821723
C	-3.670909	0.784587	-1.546343
C	-3.299058	1.923063	0.485274
C	-2.562448	2.620548	-0.570790
C	-1.268689	3.179041	-0.327055
C	-0.211080	3.097942	-1.345747
C	1.203088	3.042322	-0.931381
C	2.149439	2.421585	-1.813806
C	3.289843	1.679100	-1.301099
C	3.552761	1.657417	0.077966
C	3.931001	0.420185	0.745070
C	3.403862	0.455748	2.088372
C	2.876490	-0.721357	2.716959
C	1.951762	-0.513220	3.823407
C	0.895355	-1.480236	4.112985
C	-0.258048	-0.762900	4.611349
C	-1.589537	-0.931394	4.052380
C	-2.112182	0.412571	3.759988
C	-2.995674	0.647694	2.625604
C	-2.825073	1.882588	1.832229
C	-1.681518	2.720170	2.116296
C	-0.885246	3.289025	1.045865
C	0.494623	3.280764	1.453823
C	1.547367	3.092711	0.498364
C	2.728395	2.427336	0.977248
C	2.733397	1.749608	2.264789
C	1.681079	1.919869	3.215391
C	1.418044	0.823572	4.128290
C	0.067116	0.642392	4.634009
C	-1.067383	1.371828	4.110685
C	-0.799561	2.456331	3.223562
C	0.565835	2.751559	2.805119
C	-3.574478	-1.666905	-0.092528
C	-2.783009	-2.458293	0.817434
C	-1.584525	-3.111529	0.366031
C	-0.567471	-3.323204	1.354607
C	0.826243	-3.321660	0.997331
C	1.260033	-3.179100	-0.357557
C	2.561943	-2.616334	-0.539794
C	2.897103	-1.923668	-1.762846
C	1.957792	-1.870728	-2.805152
C	1.792526	-0.646662	-3.577052
C	0.402976	-0.573911	-4.012762
C	-0.276825	0.662353	-4.012219
C	-1.681229	0.725197	-3.625684
C	-2.382481	-0.449407	-3.279526
C	-3.384574	-0.423065	-2.226355
C	-3.261130	-1.655714	-1.461369
C	-2.102717	-2.386065	-1.949653
C	-1.188279	-3.026973	-1.048571
C	0.240646	-3.073033	-1.412390
C	0.651696	-2.493891	-2.655093
C	-0.280311	-1.751601	-3.483902
C	-1.631862	-1.697296	-3.138894
La	-0.049796	-0.031991	2.142879
C	-0.803975	-0.393387	-6.940763
H	-1.318046	-0.636599	-7.902405
H	-1.495934	-0.752869	-6.146572
C	0.557254	-1.032876	-6.892415
H	0.732896	-2.117162	-6.906497
C	1.510670	-0.047966	-6.888857
H	2.598963	-0.202565	-6.874123
C	-0.504331	1.078900	-6.860056

H	-1.269667	1.866814	-6.849674
C	0.855164	1.256334	-6.868340
H	1.380733	2.221476	-6.837361

31. TS for Type A [6,6] 61-62 concerted mechanism addition between La@C_2-C_{72} and CP

Energy = -3371.89819425

NIMAG = 1 $\tilde{\nu}$ = -246.30

C	-3.968173	0.766428	0.559382
C	-3.992720	-0.455594	1.270612
C	-3.512500	-0.522054	2.629764
C	-2.847454	-1.819632	2.799726
C	-1.829314	-2.012640	3.782746
C	-0.699978	-2.835468	3.393007
C	0.650221	-2.550388	3.865037
C	1.570238	-2.789907	2.783724
C	2.722931	-1.946634	2.557495
C	3.244258	-1.957708	1.227529
C	3.911967	-0.797006	0.668008
C	3.687711	-0.774805	-0.765988
C	3.415589	0.448160	-1.431480
C	2.455928	0.497627	-2.519808
C	1.689758	1.747160	-2.372245
C	0.355607	1.804924	-2.757058
C	-0.596052	2.515171	-1.936082
C	-1.896055	1.903406	-2.148354
C	-2.876179	1.941869	-1.142592
C	-3.696902	0.774212	-0.866693
C	-3.318406	1.914282	1.163973
C	-2.583877	2.609102	0.106188
C	-1.289658	3.168479	0.346701
C	-0.232587	3.081276	-0.670773
C	1.178603	3.029609	-0.264008
C	2.118471	2.402793	-1.151540
C	3.260084	1.660857	-0.641626
C	3.530044	1.644249	0.736812
C	3.912799	0.409301	1.405813
C	3.389686	0.446911	2.749986
C	2.864478	-0.729636	3.383255
C	1.942822	-0.519603	4.491308
C	0.886862	-1.486154	4.785299
C	-0.265463	-0.768310	5.284774
C	-1.598381	-0.937680	4.729097
C	-2.122121	0.406155	4.436376
C	-3.008022	0.640387	3.304176
C	-2.840417	1.874872	2.509848
C	-1.696710	2.713507	2.791223
C	-0.903200	3.282198	1.718356
C	0.478272	3.273230	2.121848
C	1.528418	3.083517	1.163490
C	2.710128	2.416777	1.638210
C	2.718839	1.740788	2.926315
C	1.669663	1.912732	3.880361
C	1.409345	0.817870	4.795536
C	0.059582	0.637110	5.304876
C	-1.076279	1.365655	4.783911
C	-0.811181	2.449634	3.895413
C	0.553252	2.744539	3.473029
C	-3.589254	-1.676236	0.587972
C	-2.797885	-2.467871	1.497994
C	-1.600947	-3.123322	1.046369
C	-0.581729	-3.334003	2.033274
C	0.811659	-3.334077	1.673726
C	1.242132	-3.191458	0.317920
C	2.543954	-2.629128	0.131798
C	2.876788	-1.935650	-1.092013
C	1.928189	-1.874067	-2.126981
C	1.763942	-0.661652	-2.906137
C	0.386846	-0.612052	-3.434974
C	-0.313434	0.671237	-3.439237
C	-1.707453	0.708747	-2.951471
C	-2.409700	-0.459768	-2.605826
C	-3.405167	-0.433789	-1.548704
C	-3.275659	-1.663760	-0.781437
C	-2.118573	-2.394808	-1.270865
C	-1.206213	-3.038959	-0.367963
C	0.218136	-3.082083	-0.731346
C	0.622834	-2.490934	-1.971743
C	-0.303613	-1.759303	-2.807519
C	-1.650867	-1.710867	-2.462267
La	-0.062959	-0.041094	2.815135
C	-0.813654	-0.391221	-5.846556
H	-1.100129	-0.515802	-6.920033

H	-1.639901	-0.810179	-5.240550
C	0.544783	-1.019292	-5.649582
H	0.726971	-2.102989	-5.678283
C	1.509789	-0.027974	-5.924512
H	2.592025	-0.200161	-6.005950
C	-0.489255	1.066965	-5.617065
H	-1.240575	1.869154	-5.645658
C	0.883562	1.238947	-5.902593
H	1.401431	2.205883	-5.969882

32. P for Type A [6,6] 61-62 concerted mechanism addition between La@C_2-C_{72} and Cp

Energy = -3371.93530662

NIMAG = 0 $\tilde{\nu}$ = 62.61

C	-3.920355	0.800002	-0.472308
C	-3.942507	-0.422569	0.238732
C	-3.463615	-0.489064	1.597649
C	-2.799455	-1.786959	1.769051
C	-1.782769	-1.981010	2.753636
C	-0.654013	-2.806094	2.366535
C	0.696226	-2.522147	2.839243
C	1.617750	-2.765719	1.760274
C	2.770992	-1.923192	1.533236
C	3.294198	-1.936752	0.203488
C	3.963313	-0.777178	-0.358235
C	3.738291	-0.757685	-1.791647
C	3.457563	0.462167	-2.460125
C	2.502288	0.505972	-3.552473
C	1.727539	1.759434	-3.405892
C	0.402536	1.833000	-3.796791
C	-0.539127	2.521672	-2.960807
C	-1.843185	1.920499	-3.175504
C	-2.826992	1.971617	-2.171642
C	-3.648240	0.808576	-1.897515
C	-3.270075	1.947868	0.133611
C	-2.534134	2.639805	-0.923988
C	-1.238424	3.195158	-0.683297
C	-0.180704	3.097521	-1.696871
C	1.226319	3.046194	-1.293537
C	2.158409	2.411147	-2.182280
C	3.300677	1.673894	-1.672623
C	3.577314	1.664071	-0.294716
C	3.961601	0.431075	0.377069
C	3.438457	0.470935	1.720609
C	2.912105	-0.704776	2.356309
C	1.990388	-0.491894	3.463234
C	0.933043	-1.456917	3.758036
C	-0.218889	-0.737353	4.255939
C	-1.551746	-0.905936	3.699586
C	-2.074281	0.438767	3.405754
C	-2.959044	0.673746	2.273429
C	-2.791255	1.908043	1.479510
C	-1.646647	2.745775	1.761235
C	-0.852212	3.312377	0.687973
C	0.529561	3.300625	1.090654
C	1.579373	3.107400	0.132755
C	2.760074	2.439436	0.606471
C	2.768498	1.765491	1.895650
C	1.719820	1.940295	2.849780
C	1.458067	0.846858	3.766232
C	0.107703	0.667855	4.275198
C	-1.027448	1.397455	3.754020
C	-0.760914	2.480604	2.864770
C	0.604088	2.773221	2.442186
C	-3.536360	-1.642411	-0.444082
C	-2.748680	-2.435550	0.467894
C	-1.552492	-3.093976	0.020157
C	-0.534839	-3.306691	1.007877
C	0.859296	-3.310339	0.650278
C	1.290579	-3.166248	-0.704956
C	2.593767	-2.607561	-0.891172
C	2.927984	-1.915675	-2.115058
C	1.977894	-1.843798	-3.149402
C	1.828051	-0.651736	-3.944535
C	0.475877	-0.655782	-4.640704
C	-0.287914	0.766550	-4.637418
C	-1.665675	0.742536	-3.988005
C	-2.355272	-0.420378	-3.640577
C	-3.346357	-0.398060	-2.580235
C	-3.214220	-1.624899	-1.812035
C	-2.055418	-2.352162	-2.297773
C	-1.152540	-3.004375	-1.392056
C	0.266761	-3.047377	-1.751090

C	0.666560	-2.446556	-2.991069
C	-0.247671	-1.738241	-3.842801
C	-1.584208	-1.676133	-3.492293
La	-0.014995	-0.010243	1.788655
C	-0.719373	-0.341802	-6.730175
H	-0.791213	-0.373776	-7.835275
H	-1.626799	-0.793660	-6.281058
C	0.601272	-0.946591	-6.212391
H	0.803136	-2.013595	-6.417602
C	1.611746	0.061535	-6.735226
H	2.667681	-0.157114	-6.947104
C	-0.401025	1.074012	-6.203362
H	-1.128648	1.880115	-6.409429
C	1.012639	1.275090	-6.718928
H	1.476421	2.251014	-6.919297

33. RC for Type D [5,6] 33-32 stepwise addition between La@C_2-C_{72} and Cp

Energy = -3371.90195800

NIMAG = 0 $\tilde{\nu}$ = 14.16

C	-4.146746	0.977544	-0.880586
C	-4.188705	-0.240345	-0.164741
C	-3.700471	-0.308615	1.192487
C	-3.054493	-1.615186	1.363293
C	-2.031341	-1.817860	2.339273
C	-0.914921	-2.654001	1.942934
C	0.440095	-2.385200	2.403427
C	1.349600	-2.644291	1.320036
C	2.514478	-1.820006	1.085289
C	3.026433	-1.842441	-0.248733
C	3.706955	-0.694221	-0.813330
C	3.468631	-0.670621	-2.246840
C	3.220158	0.552689	-2.910422
C	2.246371	0.612480	-3.989437
C	1.511647	1.866458	-3.847740
C	0.172539	1.952164	-4.234259
C	-0.773278	2.692465	-3.418295
C	-2.083373	2.091451	-3.616984
C	-3.048553	2.135264	-2.598834
C	-3.881081	0.974156	-2.309423
C	-3.477390	2.117548	-0.287225
C	-2.739790	2.799036	-1.353741
C	-1.436189	3.339713	-1.124010
C	-0.389585	3.238617	-2.152308
C	1.028346	3.164637	-1.747989
C	1.959263	2.527899	-2.633453
C	3.093952	1.773428	-2.127127
C	3.367786	1.754133	-0.750210
C	3.733123	0.514528	-0.080447
C	3.216559	0.563865	1.266758
C	2.674978	-0.601058	1.902553
C	1.764612	-0.374799	3.014519
C	0.704191	-1.329741	3.326728
C	-0.438143	-0.591960	3.826676
C	-1.776804	-0.743353	3.280009
C	-2.283436	0.606395	2.985012
C	-3.173908	0.848714	1.857183
C	-2.992621	2.077284	1.056016
C	-1.834975	2.900155	1.325490
C	-1.039871	3.451951	0.245213
C	0.342983	3.426867	0.641654
C	1.385088	3.218816	-0.321165
C	2.560951	2.539740	0.151537
C	2.567653	1.869059	1.442796
C	1.524438	2.057892	2.399426
C	1.253718	0.968732	3.317858
C	-0.094149	0.809228	3.839507
C	-1.222424	1.552319	3.321394
C	-0.947337	2.629157	2.426735
C	0.418079	2.903401	1.995017
C	-3.810245	-1.470838	-0.844024
C	-3.022328	-2.268846	0.063241
C	-1.836521	-2.940186	-0.395555
C	-0.813586	-3.160478	0.584181
C	0.576426	-3.180589	0.215598
C	1.000883	-3.051099	-1.143404
C	2.309487	-2.508741	-1.339449
C	2.642314	-1.827706	-2.568916
C	1.697451	-1.769518	-3.605380
C	1.543776	-0.546106	-4.383112
C	0.149688	-0.452237	-4.794637
C	-0.511871	0.790237	-4.792679
C	-1.914004	0.878626	-4.407900

C	-2.624318	-0.285100	-4.044541
C	-3.619371	-0.240028	-2.984425
C	-3.508915	-1.471282	-2.215373
C	-2.364142	-2.218723	-2.709289
C	-1.451118	-2.867316	-1.814130
C	-0.025220	-2.935849	-2.190844
C	0.383671	-2.372976	-3.441429
C	-0.545817	-1.621655	-4.266161
C	-1.892374	-1.541026	-3.905393
La	-0.243519	0.120602	1.352422
C	2.637208	-1.339476	6.021911
C	3.881840	-1.040547	5.229768
C	4.150122	-2.101078	4.409921
C	2.205311	-2.689278	5.512150
C	3.113445	-3.123240	4.586145
H	2.849939	-1.369753	7.117591
H	1.851364	-0.557631	5.904012
H	4.468536	-0.116360	5.323409
H	4.996996	-2.183481	3.713460
H	1.317477	-3.230254	5.866997
H	3.077117	-4.077375	4.040788

34. TS1 for Type D [5,6] 33-32 stepwise addition between La@C_2-C_{72} and Cp

Energy = -3371.89028860

NIMAG = 1 $\tilde{\nu}$ = -437.43

C	-4.330319	1.076806	-0.975805
C	-4.351477	-0.141752	-0.260415
C	-3.841166	-0.210341	1.088406
C	-3.181774	-1.513527	1.248041
C	-2.147076	-1.714694	2.209185
C	-1.016015	-2.516809	1.786763
C	0.335760	-2.235356	2.222068
C	1.225004	-2.485521	1.127719
C	2.396241	-1.671719	0.871773
C	2.877278	-1.689092	-0.472137
C	3.536730	-0.532124	-1.051900
C	3.273681	-0.509007	-2.480570
C	3.003526	0.713768	-3.138610
C	2.009066	0.767413	-4.199643
C	1.267363	2.015854	-4.043663
C	-0.079582	2.091839	-4.405477
C	-1.015491	2.823229	-3.571252
C	-2.325006	2.211861	-3.747738
C	-3.269553	2.245513	-2.710568
C	-4.089530	1.077647	-2.408564
C	-3.655858	2.219951	-0.393145
C	-2.944403	2.911251	-1.471089
C	-1.641840	3.465300	-1.264431
C	-0.613490	3.371591	-2.312408
C	0.812781	3.307331	-1.934330
C	1.731338	2.678528	-2.836970
C	2.882366	1.931698	-2.352512
C	3.181065	1.913548	-0.981257
C	3.566003	0.674147	-0.319315
C	3.071699	0.716966	1.037699
C	2.558711	-0.454161	1.691614
C	1.685391	-0.245021	2.833375
C	0.677480	-1.281202	3.280328
C	-0.521511	-0.486946	3.670107
C	-1.863647	-0.642749	3.146171
C	-2.385321	0.704524	2.849565
C	-3.300004	0.945506	1.741149
C	-3.142840	2.178871	0.938966
C	-1.990984	3.015271	1.188456
C	-1.221751	3.583147	0.096517
C	0.169275	3.564603	0.466322
C	1.195282	3.363618	-0.513712
C	2.385921	2.692339	-0.064739
C	2.417464	2.012864	1.221959
C	1.383342	2.181186	2.189851
C	1.142733	1.084922	3.104804
C	-0.189740	0.912326	3.655037
C	-1.324120	1.652167	3.155922
C	-1.078729	2.739921	2.266494
C	0.271242	3.028489	1.812974
C	-3.974990	-1.368173	-0.949352
C	-3.168062	-2.163316	-0.056566
C	-1.982838	-2.815841	-0.538667
C	-0.937114	-3.012256	0.420987
C	0.440411	-3.021054	0.029853
C	0.842642	-2.901140	-1.336135
C	2.145916	-2.357691	-1.553760

C	2.449068	-1.671130	-2.787767
C	1.485731	-1.619704	-3.808016
C	1.308001	-0.395264	-4.580707
C	-0.093938	-0.311931	-4.967972
C	-0.765566	0.925290	-4.952973
C	-2.160931	1.002198	-4.543515
C	-2.856551	-0.168088	-4.169344
C	-3.831992	-0.132453	-3.091846
C	-3.698649	-1.364837	-2.325771
C	-2.557278	-2.102041	-2.841721
C	-1.622561	-2.742371	-1.963139
C	-0.202653	-2.798402	-2.364475
C	0.179800	-2.232416	-3.622127
C	-0.770456	-1.487349	-4.428770
C	-2.111461	-1.417811	-4.043991
La	-0.394430	0.167195	1.174241
C	2.046252	-1.042109	5.606378
C	3.419405	-0.902198	5.018908
C	3.734813	-2.059075	4.321013
C	1.476828	-2.223845	4.832691
C	2.591280	-2.909392	4.274880
H	2.135523	-1.345654	6.678873
H	1.433321	-0.117786	5.601944
H	4.084062	-0.043948	5.188947
H	4.699913	-2.273091	3.840261
H	0.575748	-2.754442	5.177499
H	2.545245	-3.883845	3.769124

35. INT for Type D [5,6] 33-32 stepwise addition between La@C_2-C_{72} and Cp

Energy = -3371.89874166

NIMAG = 0 $\tilde{\nu}$ = 47.13

C	-4.120805	0.948006	-0.787375
C	-4.134620	-0.266904	-0.065894
C	-3.619847	-0.331761	1.279393
C	-2.948090	-1.633481	1.438758
C	-1.919791	-1.839009	2.401382
C	-0.776989	-2.624550	1.972157
C	0.571848	-2.337647	2.399926
C	1.451022	-2.581535	1.296714
C	2.630693	-1.783820	1.028994
C	3.094494	-1.799808	-0.314804
C	3.751423	-0.637761	-0.907488
C	3.482429	-0.620534	-2.332575
C	3.205110	0.600130	-2.994672
C	2.201926	0.647793	-4.048682
C	1.457111	1.894965	-3.892760
C	0.106779	1.965637	-4.245627
C	-0.824390	2.696166	-3.407371
C	-2.134685	2.079609	-3.573779
C	-3.069244	2.113379	-2.529366
C	-3.888387	0.944741	-2.219422
C	-3.440389	2.094109	-0.212382
C	-2.740106	2.787687	-1.296191
C	-1.438004	3.347288	-1.099610
C	-0.416521	3.250981	-2.154336
C	1.013106	3.190105	-1.785239
C	1.925283	2.560469	-2.690873
C	3.084792	1.817523	-2.211569
C	3.390173	1.805080	-0.843052
C	3.782205	0.565451	-0.178118
C	3.293936	0.608654	1.183118
C	2.795166	-0.564649	1.855316
C	1.923755	-0.358756	2.983628
C	0.959945	-1.456623	3.557906
C	-0.286680	-0.608511	3.853618
C	-1.623088	-0.763305	3.335927
C	-2.149099	0.584571	3.025844
C	-3.068288	0.823009	1.922344
C	-2.918904	2.057722	1.114442
C	-1.767950	2.899264	1.353956
C	-1.008712	3.472827	0.257021
C	0.384563	3.453823	0.617794
C	1.405293	3.251070	-0.366036
C	2.601025	2.584300	0.074384
C	2.632549	1.892978	1.358094
C	1.603289	2.057565	2.328601
C	1.374792	0.954546	3.240425
C	0.045074	0.785630	3.804873
C	-1.081701	1.528429	3.308735
C	-0.847983	2.623843	2.423464
C	0.493825	2.913095	1.962812
C	-3.755489	-1.494259	-0.754924

C	-2.943417	-2.286436	0.136038
C	-1.758683	-2.933811	-0.351064
C	-0.707160	-3.113011	0.602782
C	0.665590	-3.115590	0.202917
C	1.060968	-3.012662	-1.165534
C	2.362567	-2.471810	-1.391707
C	2.654643	-1.784115	-2.628863
C	1.687698	-1.739658	-3.643583
C	1.500901	-0.516532	-4.419436
C	0.096334	-0.439801	-4.798451
C	-0.580107	0.795013	-4.784477
C	-1.972488	0.868264	-4.366736
C	-2.664240	-0.302878	-3.984966
C	-3.632289	-0.265956	-2.902768
C	-3.489469	-1.495301	-2.131341
C	-2.348277	-2.232113	-2.652715
C	-1.407453	-2.866812	-1.778243
C	0.010393	-2.919940	-2.187625
C	0.383575	-2.355230	-3.447890
C	-0.572773	-1.615521	-4.250720
C	-1.912624	-1.549224	-3.857712
La	-0.219737	0.019745	1.317545
C	2.160411	-1.227294	5.824553
C	3.625374	-1.183468	5.488002
C	3.958172	-2.285292	4.689339
C	1.591977	-2.239623	4.795109
C	2.803773	-2.998309	4.341332
H	2.017843	-1.620928	6.859533
H	1.658316	-0.237184	5.805116
H	4.330081	-0.435166	5.877667
H	4.978108	-2.545845	4.369969
H	0.776818	-2.880874	5.188626
H	2.765037	-3.902853	3.719349

36. TS2 for Type D [5,6] 33-32 stepwise addition between La@C_2-C_{72} and Cp

Energy = -3371.89609419

NIMAG = 1 $\tilde{\nu}$ = -200.65

C	-4.309532	1.057300	-1.022710
C	-4.339030	-0.151463	-0.291897
C	-3.847534	-0.205305	1.064019
C	-3.186236	-1.506458	1.247851
C	-2.169872	-1.700553	2.227966
C	-1.022299	-2.491766	1.827716
C	0.319814	-2.203380	2.279072
C	1.218593	-2.456266	1.195655
C	2.400687	-1.654557	0.939984
C	2.893277	-1.691098	-0.398206
C	3.560358	-0.540294	-0.988188
C	3.316591	-0.535621	-2.419850
C	3.052255	0.678885	-3.096040
C	2.069189	0.718477	-4.168166
C	1.323893	1.968178	-4.036089
C	-0.019374	2.037500	-4.414194
C	-0.964870	2.777327	-3.599224
C	-2.272380	2.161635	-3.783612
C	-3.226915	2.206320	-2.756950
C	-4.051323	1.041246	-2.450979
C	-3.639853	2.208080	-0.445961
C	-2.918013	2.889467	-1.523411
C	-1.618564	3.449329	-1.308588
C	-0.578198	3.342615	-2.343840
C	0.844604	3.284905	-1.948900
C	1.772964	2.646293	-2.833582
C	2.920127	1.905724	-2.326163
C	3.201706	1.904966	-0.952352
C	3.577322	0.671837	-0.271098
C	3.066064	0.729619	1.080341
C	2.550442	-0.431299	1.746319
C	1.717658	-0.224488	2.928469
C	0.682256	-1.314036	3.430595
C	-0.557628	-0.459236	3.693770
C	-1.886673	-0.617218	3.153773
C	-2.405000	0.726990	2.826404
C	-3.305419	0.955194	1.705816
C	-3.139832	2.181409	0.889784
C	-1.993634	3.024137	1.142810
C	-1.213825	3.585199	0.054645
C	0.173539	3.567724	0.439933
C	1.211038	3.359149	-0.524746
C	2.397320	2.694347	-0.053330
C	2.413981	2.026639	1.240076
C	1.362662	2.189133	2.188319

C	1.118438	1.101053	3.110485
C	-0.220524	0.932282	3.640735
C	-1.343206	1.672445	3.123921
C	-1.091364	2.754703	2.229774
C	0.259390	3.037859	1.790073
C	-3.951830	-1.385632	-0.962455
C	-3.156583	-2.170389	-0.049323
C	-1.962713	-2.820939	-0.509043
C	-0.927207	-2.991589	0.465050
C	0.452597	-2.999995	0.091358
C	0.872312	-2.909257	-1.271516
C	2.178708	-2.373998	-1.480692
C	2.494667	-1.701544	-2.720392
C	1.544263	-1.664349	-3.751944
C	1.373446	-0.449027	-4.542043
C	-0.023808	-0.373157	-4.946683
C	-0.697768	0.863095	-4.954282
C	-2.097862	0.942818	-4.562549
C	-2.797415	-0.223815	-4.182674
C	-3.785544	-0.176209	-3.118386
C	-3.659036	-1.398479	-2.334168
C	-2.509600	-2.140704	-2.827773
C	-1.585048	-2.766733	-1.929770
C	-0.160064	-2.825382	-2.313094
C	0.236144	-2.275947	-3.573404
C	-0.705053	-1.542673	-4.400368
C	-2.051195	-1.470704	-4.032398
La	-0.425736	0.142640	1.166385
C	1.924044	-0.939729	5.554333
C	3.200363	-0.747193	4.784802
C	3.578708	-2.004683	4.240147
C	1.292829	-2.077743	4.723299
C	2.483020	-2.856712	4.267309
H	2.149456	-1.309574	6.582321
H	1.291337	-0.036094	5.652879
H	3.849278	0.136996	4.858526
H	4.553936	-2.230392	3.785454
H	0.476559	-2.654421	5.197459
H	2.441726	-3.873412	3.853403

37. P for Type D [5,6] 33-32 stepwise addition between La@C_2-C_{72} and Cp

Energy = -3371.92031797

NIMAG = 0 $\tilde{\nu}$ = 58.73

C	-4.103113	0.940331	-0.848868
C	-4.136155	-0.271023	-0.122866
C	-3.646700	-0.331888	1.234585
C	-2.991797	-1.634191	1.417071
C	-1.979968	-1.839525	2.402787
C	-0.830067	-2.633852	2.006668
C	0.514147	-2.353682	2.469917
C	1.409981	-2.578227	1.376791
C	2.589114	-1.768345	1.117707
C	3.087942	-1.816785	-0.222694
C	3.760127	-0.674381	-0.806785
C	3.522666	-0.665635	-2.242384
C	3.261534	0.551416	-2.911565
C	2.280786	0.598020	-3.984070
C	1.537895	1.849144	-3.846280
C	0.195444	1.922902	-4.227932
C	-0.749638	2.662113	-3.411561
C	-2.058397	2.050387	-3.601185
C	-3.016444	2.093831	-2.577566
C	-3.842146	0.929302	-2.276758
C	-3.432430	2.088568	-0.267622
C	-2.706556	2.770272	-1.339999
C	-1.405702	3.329357	-1.120924
C	-0.363200	3.222341	-2.153884
C	1.058966	3.160150	-1.755749
C	1.987477	2.523850	-2.643193
C	3.129936	1.777294	-2.134801
C	3.411030	1.769721	-0.762291
C	3.779717	0.535293	-0.087995
C	3.273402	0.590726	1.267237
C	2.761015	-0.564093	1.919247
C	2.068400	-0.385958	3.275105
C	0.859460	-1.494740	3.648367
C	-0.358801	-0.608042	3.862208
C	-1.688825	-0.755764	3.323305
C	-2.201886	0.590446	2.996574
C	-3.098321	0.824509	1.878782
C	-2.928535	2.054007	1.066996

C	-1.786499	2.896441	1.324143
C	-1.004283	3.460106	0.242838
C	0.386262	3.431897	0.630790
C	1.422419	3.228647	-0.332111
C	2.605771	2.555355	0.147441
C	2.641574	1.906534	1.443011
C	1.571753	2.039851	2.381711
C	1.329432	0.968598	3.309258
C	-0.006185	0.776070	3.791495
C	-1.134396	1.525929	3.290300
C	-0.878020	2.606280	2.404760
C	0.471749	2.890518	1.973810
C	-3.753954	-1.504373	-0.796824
C	-2.961672	-2.292915	0.115272
C	-1.765634	-2.937362	-0.343004
C	-0.731620	-3.105395	0.635296
C	0.647005	-3.104715	0.264250
C	1.069029	-3.023230	-1.100505
C	2.376443	-2.497237	-1.307662
C	2.699907	-1.828540	-2.547956
C	1.749736	-1.785459	-3.580114
C	1.582975	-0.566877	-4.365286
C	0.186839	-0.485722	-4.771429
C	-0.483867	0.752547	-4.773400
C	-1.885245	0.834502	-4.384868
C	-2.587137	-0.331923	-4.009916
C	-3.579099	-0.287051	-2.948567
C	-3.456848	-1.511354	-2.168904
C	-2.306967	-2.252856	-2.662113
C	-1.384609	-2.879911	-1.762581
C	0.040360	-2.939884	-2.143808
C	0.440097	-2.394058	-3.405144
C	-0.498633	-1.655601	-4.230705
C	-1.845089	-1.582426	-3.865689
La	-0.233226	-0.056335	1.322053
C	2.108790	-0.975350	5.641111
C	3.080369	-0.663163	4.484239
C	3.667854	-2.040097	4.217431
C	1.466204	-2.189439	4.933964
C	2.700689	-2.950811	4.479554
H	2.646872	-1.265911	6.564810
H	1.397680	-0.156607	5.868205
H	3.791849	0.173779	4.610018
H	4.653647	-2.227380	3.769344
H	0.697822	-2.762049	5.485640
H	2.739939	-4.033098	4.293705