

Electronic Supplementary Information of

Annulated Boron Substituted *N*-Heterocyclic Carbenes: Theoretical Prediction of Highly Electrophilic Carbenes

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Table S1: PBE0/6-31+G* Calculated C_c-N Bond Lengths (r₁/r₂ in Å), B-B Bond Lengths (r(B-B) in Å) and N-C_c-N Bond Angles (∠N-C_c-N in Degrees) of carbenes 1 – 33.

Molecule	r ₁ /r ₂	r(B-B)	∠N-C _c -N	Ref
1	1.380/1.380 (<i>1.352/1.404</i>)	1.737 (<i>1.731</i>)	108.7 (<i>108.4</i>)	[11c]
2	1.389/1.389	1.682	109.8	
3	1.395/1.377	1.685	110.7	
4	1.371/1.371	1.756	109.5	
5	1.391/1.391	1.663	109.9	
6	1.380/1.380	1.636	110.7	
7	1.353/1.413	1.712	106.8	
8	1.348/1.425	1.712	106.3	
9	1.385/1.385	1.705	105.9	
10	1.390/1.390	1.706	105.3	
11	1.379/1.379	1.700	105.4	
12	1.385/1.376	1.701	105.6	
13	1.407/1.407	1.596	107.0	
14	1.409/1.409	1.604	107.7	
15	1.407/1.407	1.589	107.3	
16	1.363/1.363 (<i>1.366/1.363</i>)	-	114.3 (<i>114.4</i>)	[11a]
17	1.389/1.346	-	113.3	

18	1.391/1.343	-	112.5
19	1.389/1.347	-	111.9
20	1.392/1.344	-	111.9
21	1.332/1.375	-	113.9
22	1.350/1.378	-	114.3
23	1.349/1.381	-	114.2
24	1.355/1.377	-	114.3
25	1.357/1.376	-	114.3
26	1.366/1.358	-	115.5
27	1.370/1.371	-	112.8
28	1.371/1.369	-	111.6
29	1.372/1.371	-	110.5
30	1.372/1.371	-	110.3
31	1.342/1.342	-	114.5
32	1.368/1.368	-	112.5
33	1.372/1.366	-	112.7

Table S2: PBE0/6-31+G* calculated out of plane p_π occupancies of the B atoms [Occ(p_π)] for the five-membered NHCs (1 – 15).

Molecule	Occ(p_π)
1	0.220/0.220
2	0.266/0.266
3	0.311/0.314
4	0.497/0.497
5	0.313/0.313
6	0.423/0.423
7	0.195/0.413
8	0.190/0.407
9	0.366/0.366
10	0.346/0.346
11	0.417/0.417
12	0.382/0.413
13	0.414/0.414
14	0.403/0.403
15	0.456/0.456

Table S3: PBE0/6-31+G* calculated NICS values (in ppm) of all the molecules (1 – 33).^[a]

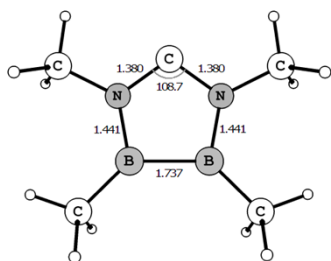
Molecule	NICS (0)	NICS (1)	Molecule	NICS (0)	NICS (1)
1	7.85	-0.05	19	-2.89	-5.19
2	12.68	4.02	20	-2.74	-5.23
3	7.65	3.22	21	-1.49	-2.96
6	-1.21	-4.75	22	-2.33	-4.78
7	10.23	1.91	23	-2.20	-4.71
8	10.24	1.85	24	-2.47	-4.93
9	12.26	3.96	25	-2.73	-5.13
10	13.63	5.10	26	-2.66	-3.80
11	8.46	1.13	27	-3.27	-5.58
12	9.67	1.99	28	-3.64	-5.63
13	8.02	6.49	29	-4.39	-6.13
14	4.33	-11.55	30	-4.08	-6.30
15	8.09	7.40	31	-2.04	-2.88
16	-2.24	-4.59	32	-1.92	-4.37
17	-2.19	-4.62	33	-2.52	-4.88
18	-2.51	-4.86			

^[a]Molecules with very small singlet-triplet gaps (**4** and **5**) are not considered.

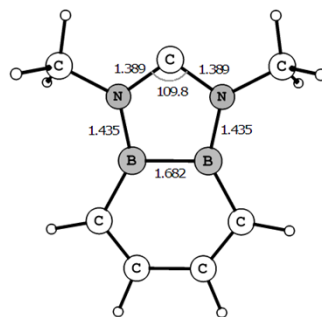
Table S4: PBE0/6-31+G* Calculated C_c-P and P-C_{ph} Bond Lengths (in Å) of the Adducts L-PPh (L=1 – 33).^[a]

Molecule	C _c -P	P-C _{ph}	Molecule	C _c -P	P-C _{ph}
1	1.729	1.839	19	1.736	1.840
2	1.729	1.836	20	1.736	1.835
3	1.727	1.836	21	1.757	1.844
6	1.747	1.836	22	1.756	1.836
7	1.724	1.834	23	1.754	1.837
8	1.720	1.833	24	1.752	1.836
9	1.716	1.833	25	1.748	1.836
10	1.710	1.830	26	1.764	1.835
11	1.726	1.836	27	1.725	1.833
12	1.721	1.835	28	1.725	1.833
13	1.703	1.831	29	1.716	1.836
14	1.699	1.827	30	1.712	1.829
15	1.699	1.830	31	1.748	1.845
16	1.757	1.837	32	1.732	1.835
17	1.744	1.836	33	1.728	1.835
18	1.739	1.834			

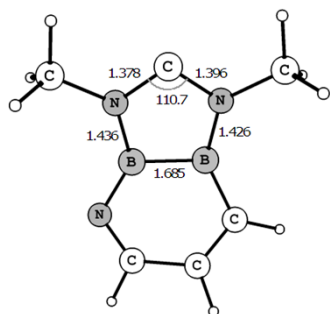
^[a]Molecules with very small singlet-triplet gaps (**4** and **5**) are not considered.



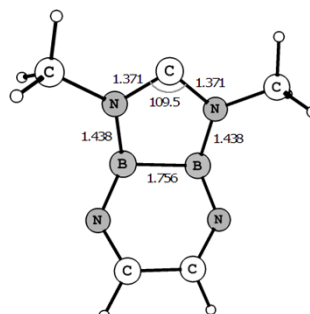
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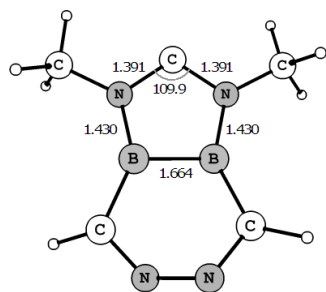
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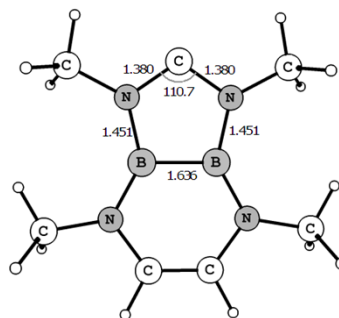
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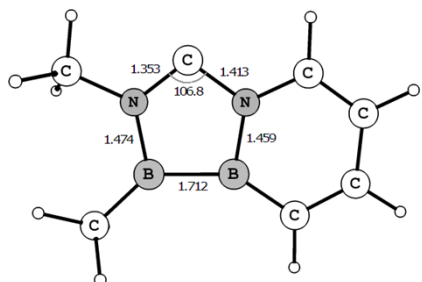
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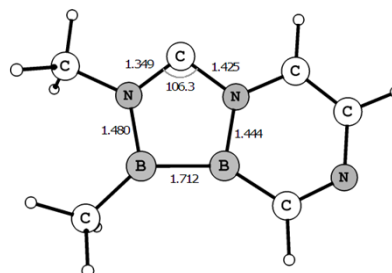
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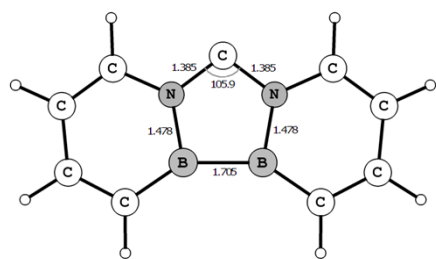
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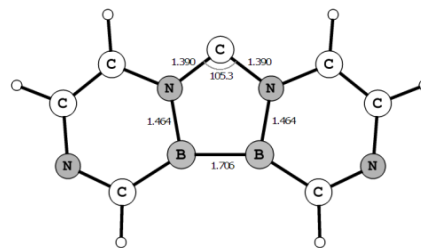
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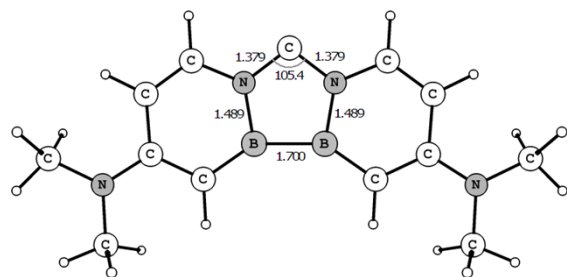
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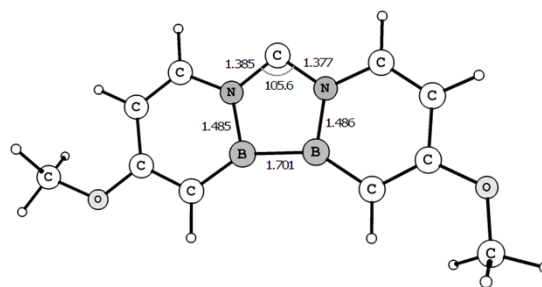
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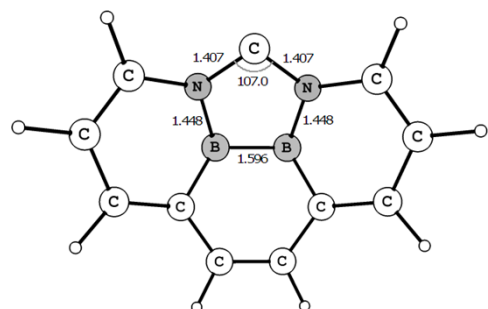
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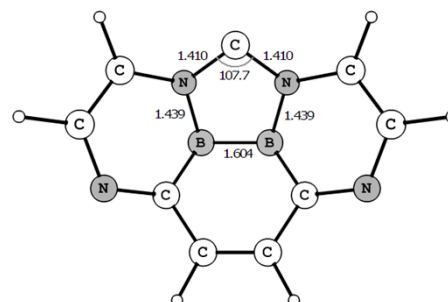
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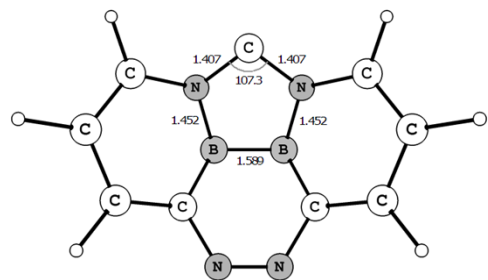
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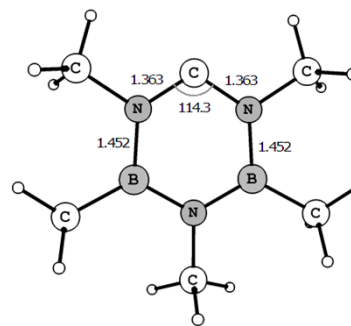
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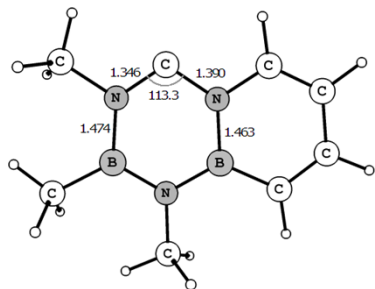
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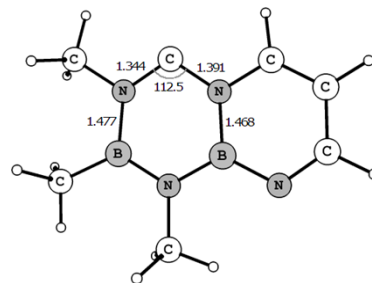
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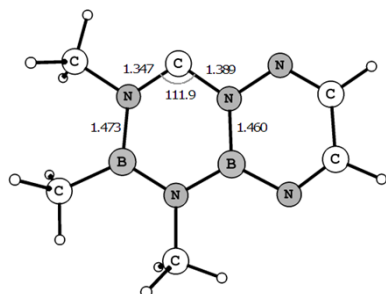
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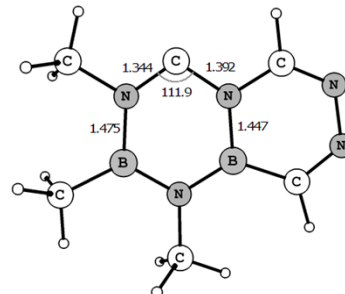
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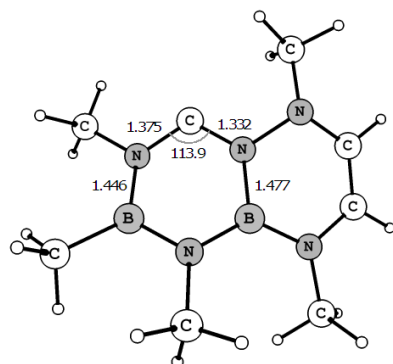
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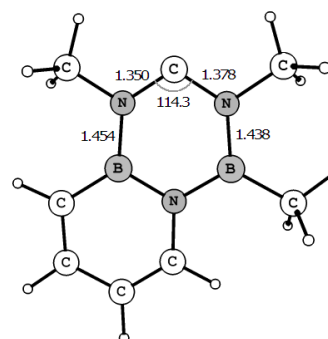
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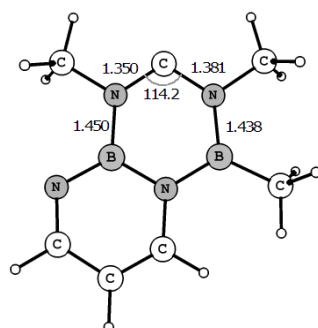
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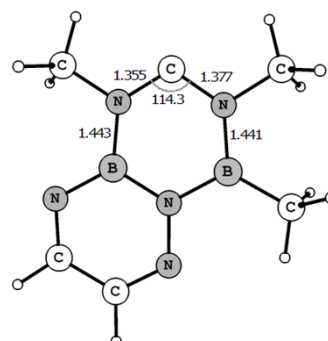
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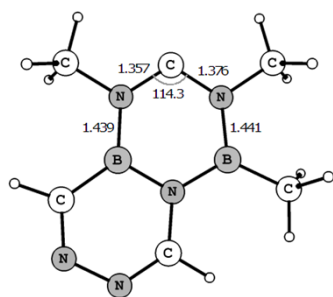
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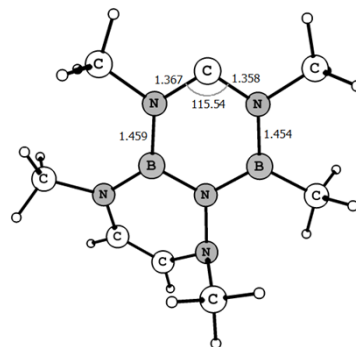
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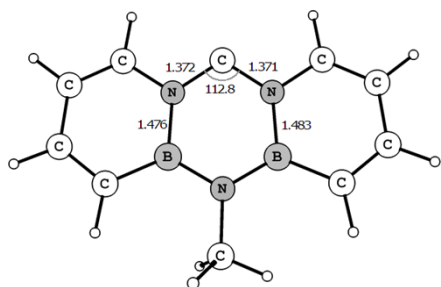
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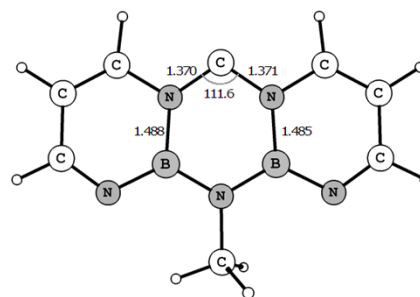
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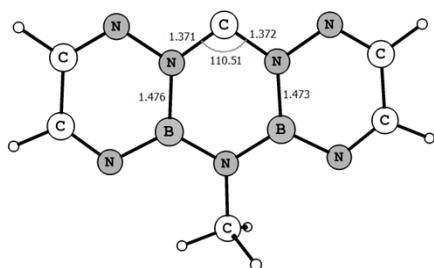
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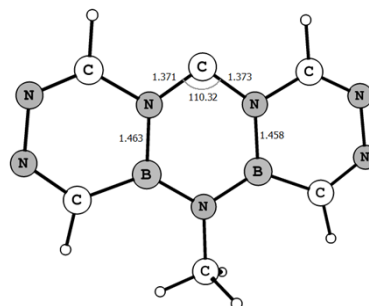
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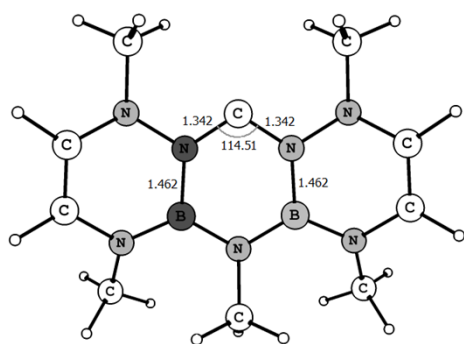
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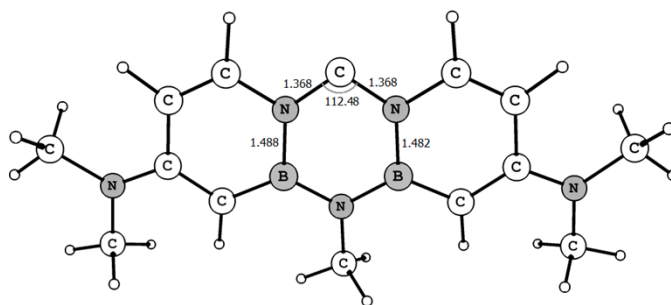
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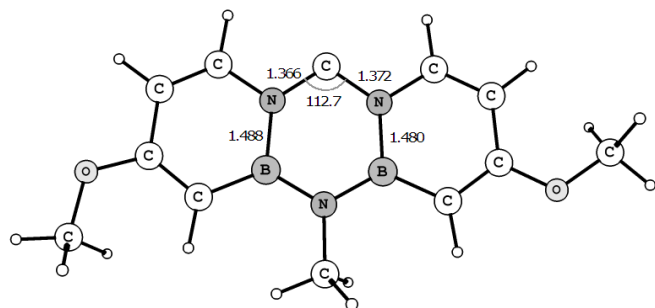
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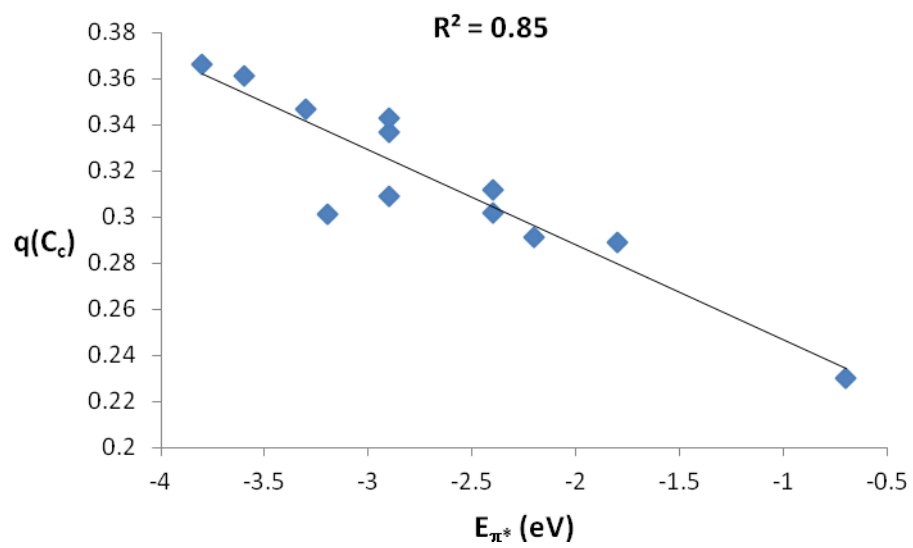


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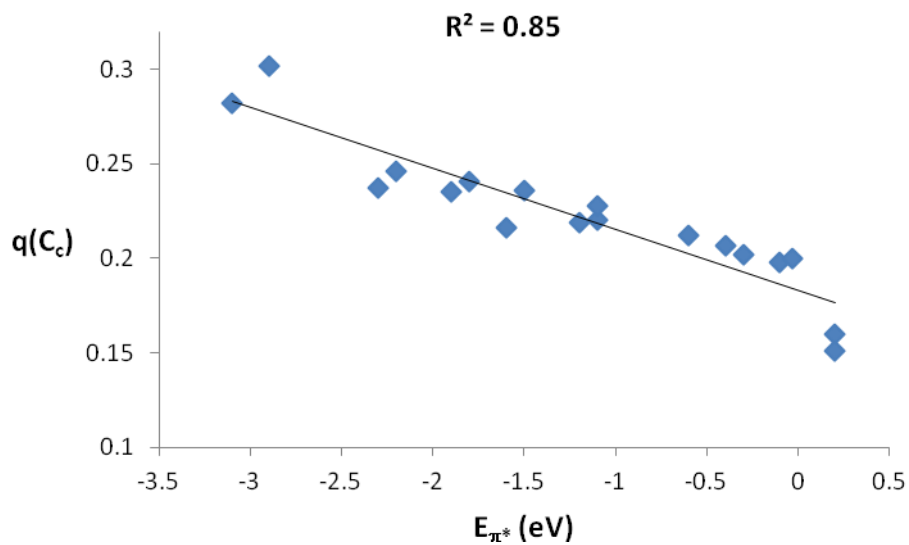


33

Fig. S1: Optimized singlet state geometries of all the molecules (1 – 33).



(a)



(b)

Fig. S2: Correlation plot between $q(C_c)$ and E_{π^*} for (a) five- (omitting the point corresponding to **3**) and (b) six-membered *B*-NHCs.

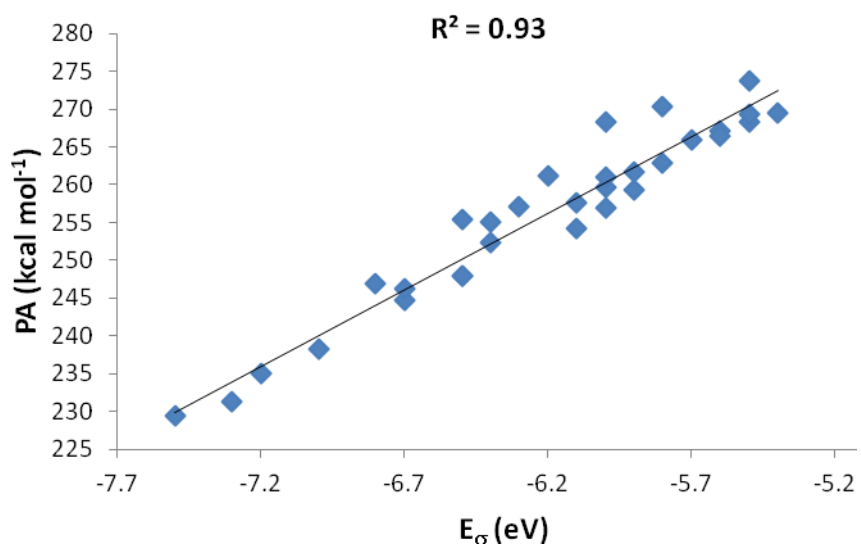
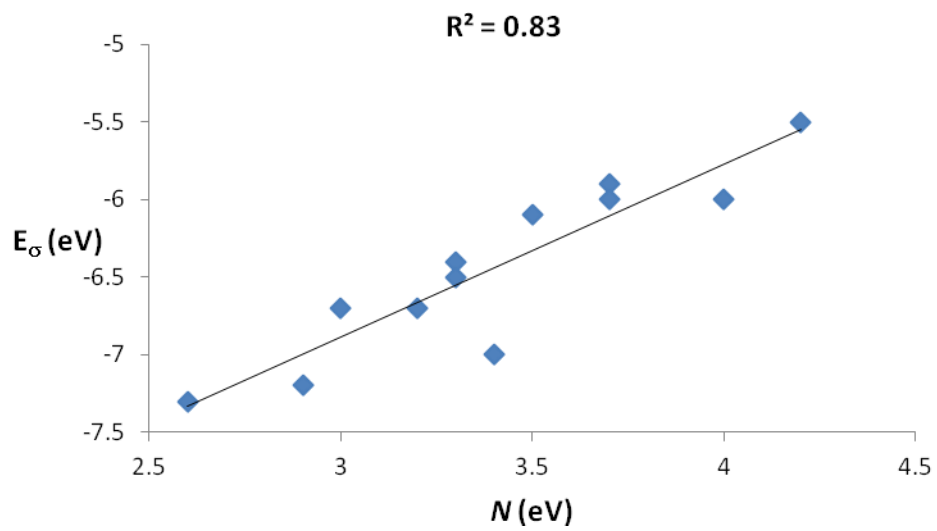
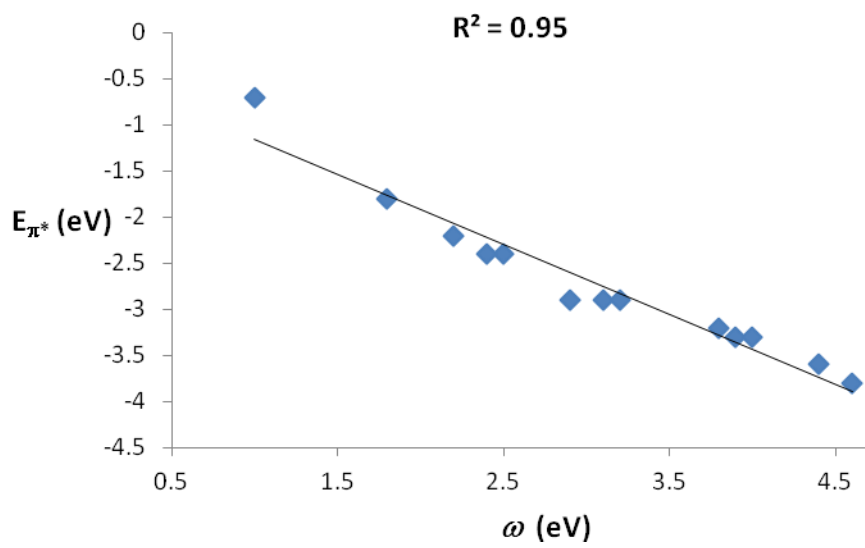


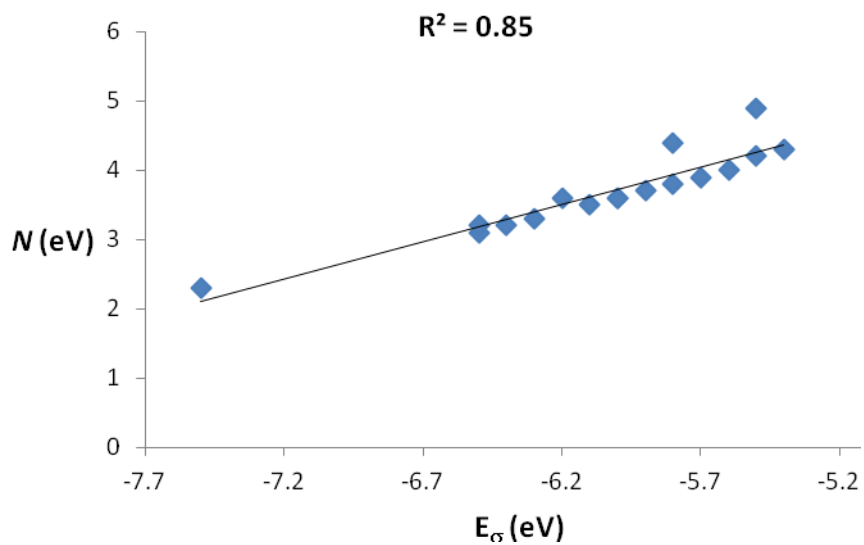
Fig. S3: Correlation plot between E_{σ} and PA values for **1** – **33**.



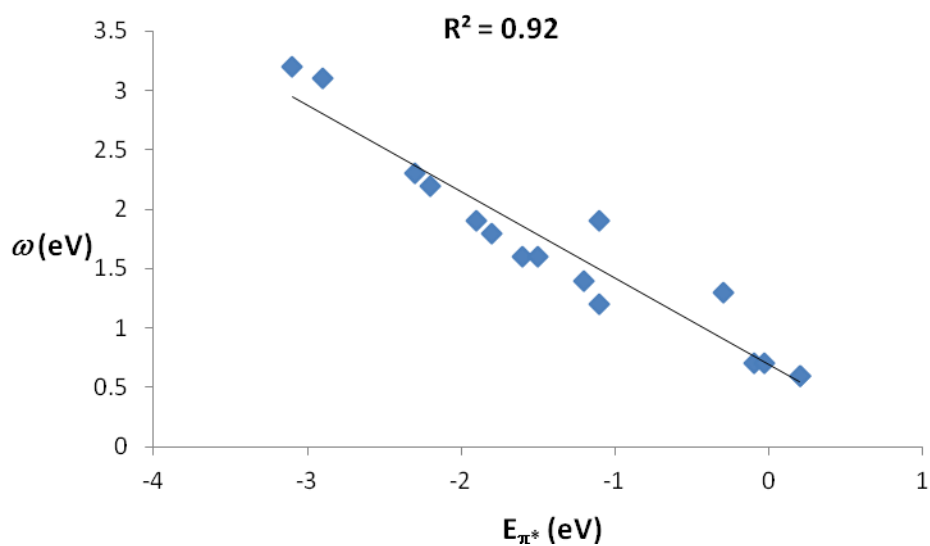
(a)



(b)



(c)



(d)

Fig. S4: Correlation plot between (a) N and E_{σ} (omitting the point corresponding to **13**), (b) ω and E_{π^*} of five-membered and (c) N and E_{σ} (omitting the points corresponding to **31**), (d) ω and E_{π^*} (omitting the points corresponding to **23** and **24**) of six-membered B-NHCs.

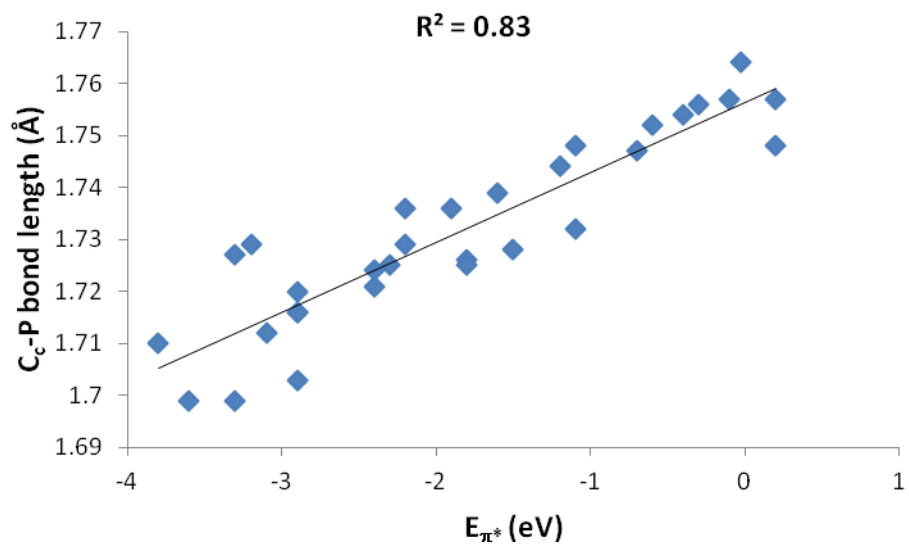


Fig. S5: Correlation plot between C_c-P bond length and E_{π*} values for **1 – 33**.

Cartesian coordinates of **1** – **33** along with their total energies (in hartrees) including zero point vibrational correction.

1, T.E. = -356.361027

7	1.121381000	-0.662810000	0.001319000
5	0.868511000	0.755973000	0.001066000
5	-0.868535000	0.755943000	-0.001531000
7	-1.121367000	-0.662846000	-0.001410000
6	0.000005000	-1.467725000	0.000062000
6	2.420343000	-1.317238000	0.002321000
1	2.997463000	-1.040563000	0.891688000
1	2.264199000	-2.398143000	0.001861000
1	2.999058000	-1.039987000	-0.885816000
6	-2.420359000	-1.317201000	-0.002255000
1	-2.999425000	-1.038884000	0.885309000
1	-2.997079000	-1.041517000	-0.892198000
1	-2.264317000	-2.398123000	-0.000524000
6	-1.982182000	1.855043000	0.002170000
1	-1.880281000	2.484311000	0.899258000
1	-1.838788000	2.546680000	-0.840756000
1	-3.012900000	1.483835000	-0.033073000
6	1.982212000	1.855035000	-0.002248000
1	3.013019000	1.483628000	0.027800000
1	1.877112000	2.488912000	-0.895642000
1	1.841852000	2.542378000	0.844759000

2, T.E. = -431.240016

5	0.209671000	-0.841129000	0.000099000
5	0.209688000	0.841099000	0.000091000
6	1.559359000	1.585286000	0.000027000
6	2.629008000	0.746300000	-0.000052000
6	2.629017000	-0.746320000	- 0.000041000

6	1.559372000	-1.585304000	0.000031000
7	-1.194510000	-1.136439000	0.000050000
6	-1.992716000	0.000035000	-0.000055000
7	-1.194524000	1.136424000	0.000032000
1	1.753691000	2.658405000	0.000019000
1	3.634701000	1.172281000	-0.000128000
1	3.634714000	-1.172291000	-0.000098000
1	1.753705000	-2.658423000	0.000030000
6	-1.855752000	-2.431205000	-0.000044000
1	-1.578169000	-3.008123000	-0.889276000
1	-1.578149000	-3.008246000	0.889099000
1	-2.936824000	-2.274205000	-0.000028000
6	-1.855684000	2.431238000	-0.000033000
1	-2.936766000	2.274309000	-0.000335000
1	-1.578292000	3.008113000	0.889285000
1	-1.577799000	3.008272000	-0.889091000

3, T.E. = -447.295024

5	-0.263709000	0.799907000	-0.351107000
5	-0.179496000	-0.882849000	-0.364021000
6	-1.510609000	-1.610104000	-0.085471000
6	-2.510045000	-0.756648000	0.264560000
6	-2.482050000	0.734707000	0.129977000
7	-1.506051000	1.511151000	-0.187590000
7	1.096632000	1.173317000	-0.080354000
6	1.900072000	0.077121000	0.144347000
7	1.209175000	-1.105029000	-0.125126000
1	-1.726838000	-2.679504000	-0.093658000
1	-3.484419000	-1.146092000	0.565028000
1	-3.475178000	1.189847000	0.239953000
6	1.641836000	2.498712000	0.164955000

1	1.532324000	3.124470000	-0.726490000
1	1.118996000	2.985088000	0.995044000
1	2.701140000	2.399271000	0.412010000
6	1.906735000	-2.357595000	0.115591000
1	2.969518000	-2.144704000	0.252772000
1	1.526276000	-2.854367000	1.015807000
1	1.780281000	-3.032529000	-0.737096000

4, T.E. = -463.356188

5	-0.224371000	0.877859000	-0.472550000
5	-0.224303000	-0.877893000	-0.472542000
6	-2.473771000	-0.733025000	0.273476000
6	-2.473860000	0.732867000	0.273402000
7	1.144530000	1.119893000	-0.103598000
6	1.904221000	0.000071000	0.115607000
7	1.144631000	-1.119812000	-0.103639000
1	-3.457287000	-1.206532000	0.325080000
1	-3.457454000	1.206246000	0.324657000
6	1.715307000	2.427967000	0.184207000
1	1.596387000	3.098407000	-0.672725000
1	1.229218000	2.879877000	1.055682000
1	2.778446000	2.289183000	0.393001000
6	1.715524000	-2.427840000	0.184146000
1	2.778659000	-2.288971000	0.392901000
1	1.229503000	-2.879786000	1.055640000
1	1.596624000	-3.098290000	-0.672780000
7	-1.457033000	-1.399212000	-0.157835000
7	-1.457164000	1.399101000	-0.157930000

5, T.E. = -463.266625

5	-0.237077000	0.827923000	0.079976000
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5	-0.237082000	-0.827921000	-0.080134000
6	-1.629846000	-1.491690000	0.064452000
6	-1.629861000	1.491675000	-0.064518000
7	1.158297000	1.137806000	0.045695000
6	1.957444000	0.000000000	0.000038000
7	1.158295000	-1.137797000	-0.045750000
1	-1.882066000	-2.494366000	0.415265000
1	-1.882150000	2.494426000	-0.415079000
6	1.823550000	2.431058000	0.086039000
1	1.699248000	2.961999000	-0.864574000
1	1.408215000	3.048181000	0.888954000
1	2.889511000	2.273570000	0.264156000
6	1.823550000	-2.431052000	-0.085987000
1	2.889526000	-2.273573000	-0.264020000
1	1.699168000	-2.961959000	0.864634000
1	1.408279000	-3.048201000	-0.888915000
7	-2.581702000	-0.618930000	0.250836000
7	-2.581740000	0.618916000	-0.250748000

6, T.E. = -543.074050

5	0.817977000	0.080982000	-0.001022000
5	-0.817956000	0.080967000	-0.000960000
7	-1.501844000	-1.155958000	-0.000206000
6	-0.678591000	-2.286915000	-0.000089000
6	0.678580000	-2.286913000	-0.000025000
7	1.501851000	-1.155971000	-0.000118000
7	1.135476000	1.496495000	-0.000350000
6	-0.000006000	2.280812000	0.000304000
7	-1.135456000	1.496499000	-0.000168000
1	-1.191343000	-3.244789000	-0.000083000
1	1.191324000	-3.244792000	0.000026000

6	2.418817000	2.172114000	0.000120000
1	3.003121000	1.912548000	0.891882000
1	3.004341000	1.911238000	-0.890447000
1	2.240524000	3.250368000	-0.000748000
6	-2.418822000	2.172074000	0.000358000
1	-2.240566000	3.250335000	0.001853000
1	-3.003482000	1.912979000	-0.891302000
1	-3.003967000	1.910675000	0.891029000
6	-2.934911000	-1.399096000	0.000376000
1	-3.236802000	-1.964024000	-0.890256000
1	-3.235677000	-1.966130000	0.890021000
1	-3.467285000	-0.446482000	0.001794000
6	2.934862000	-1.399132000	0.000586000
1	3.236681000	-1.965354000	-0.889274000
1	3.467295000	-0.446569000	0.000554000
1	3.235971000	-1.964861000	0.890975000

7, T.E. = -431.291086

7	-1.657196000	-0.613297000	-0.009856000
5	-1.316091000	0.820598000	-0.021620000
6	-0.621123000	-1.483923000	0.004558000
7	0.562584000	-0.711541000	0.000616000
6	1.768309000	-1.341061000	0.010857000
6	2.919592000	-0.600423000	0.008851000
6	2.863192000	0.820937000	-0.003348000
6	1.674508000	1.527133000	-0.013867000
5	0.394063000	0.737784000	-0.012395000
1	1.743918000	-2.427210000	0.020257000
1	3.878230000	-1.109055000	0.016805000
1	3.815610000	1.352847000	-0.004233000
1	1.730733000	2.614569000	-0.022821000

6	-2.403951000	1.939318000	0.010432000
1	-2.503506000	2.272198000	1.057609000
1	-2.098121000	2.831826000	-0.547749000
1	-3.404250000	1.637158000	-0.321739000
6	-3.006541000	-1.159126000	-0.007756000
1	-3.568902000	-0.789511000	0.856133000
1	-3.541274000	-0.870020000	-0.918968000
1	-2.943922000	-2.247978000	0.041099000

8, T.E. = -447.316886

7	-1.650593000	-0.619070000	-0.008939000
5	-1.307416000	0.820118000	-0.020703000
6	-0.622167000	-1.491228000	0.004948000
7	0.567923000	-0.707718000	0.000559000
6	1.784100000	-1.309766000	0.009990000
6	2.906642000	-0.520805000	0.007668000
7	2.882631000	0.838792000	-0.003042000
6	1.722199000	1.475217000	-0.012354000
5	0.401793000	0.726986000	-0.011777000
1	1.803471000	-2.395712000	0.019045000
1	3.890175000	-0.981642000	0.014753000
1	1.818316000	2.562954000	-0.020336000
6	-2.387494000	1.942324000	0.008762000
1	-2.441006000	2.321233000	1.043543000
1	-2.094780000	2.809081000	-0.595779000
1	-3.401561000	1.636998000	-0.273201000
6	-3.003617000	-1.158294000	-0.006803000
1	-3.560281000	-0.790479000	0.861152000
1	-3.537318000	-0.859135000	-0.914915000
1	-2.946611000	-2.247542000	0.034832000

9, T.E. = -506.215095

6	-3.318367000	0.959228000	0.000018000
6	-3.456408000	-0.464750000	0.000016000
6	-2.358955000	-1.270245000	-0.000001000
7	-1.105721000	-0.711010000	-0.000018000
5	-0.852555000	0.745417000	-0.000024000
6	-2.098514000	1.597066000	-0.000002000
1	-4.240962000	1.541079000	0.000037000
1	-4.444329000	-0.913779000	0.000029000
1	-2.396267000	-2.355530000	-0.000002000
1	-2.092462000	2.685564000	0.000000000
6	0.000000000	-1.545048000	-0.000013000
7	1.105721000	-0.711010000	-0.000010000
6	2.358955000	-1.270245000	0.000010000
6	3.456408000	-0.464750000	0.000017000
6	3.318367000	0.959228000	0.000011000
6	2.098514000	1.597066000	-0.000007000
5	0.852555000	0.745417000	-0.000019000
1	2.396267000	-2.355529000	0.000013000
1	4.444329000	-0.913779000	0.000029000
1	4.240962000	1.541079000	0.000020000
1	2.092462000	2.685564000	-0.000012000

10, T.E. = -538.263224

7	3.327039000	-0.981961000	0.000001000
6	3.433028000	0.383315000	0.000001000
6	2.370997000	1.237753000	0.000000000
7	1.104826000	0.711345000	-0.000001000
5	0.853208000	-0.730833000	-0.000001000
6	2.139648000	-1.550092000	0.000000000
1	4.444122000	0.778792000	0.000002000

1	2.456327000	2.319827000	-0.000001000
1	2.168788000	-2.641228000	0.000000000
6	0.000000000	1.555077000	0.000000000
7	-1.104826000	0.711345000	-0.000001000
6	-2.370997000	1.237753000	0.000000000
6	-3.433028000	0.383315000	0.000001000
7	-3.327039000	-0.981961000	0.000001000
6	-2.139648000	-1.550092000	0.000000000
5	-0.853208000	-0.730833000	-0.000001000
1	-2.456327000	2.319827000	0.000001000
1	-4.444122000	0.778792000	0.000002000
1	-2.168788000	-2.641228000	-0.000001000

11, T.E. = -773.715579

6	3.338736000	0.250853000	-0.000021000
6	3.451901000	-1.194818000	-0.000016000
6	2.357869000	-1.998246000	-0.000005000
7	1.096578000	-1.471858000	0.000003000
5	0.849993000	-0.003811000	0.000064000
6	2.071590000	0.849229000	0.000085000
1	4.423963000	-1.671531000	0.000003000
1	2.424130000	-3.083002000	0.000006000
1	2.011687000	1.933680000	0.000161000
6	0.000007000	-2.307400000	-0.000024000
7	-1.096573000	-1.471866000	-0.000009000
6	-2.357863000	-1.998246000	-0.000014000
6	-3.451896000	-1.194818000	-0.000021000
6	-3.338738000	0.250853000	-0.000037000
6	-2.071583000	0.849221000	0.000090000
5	-0.849999000	-0.003829000	0.000065000
1	-2.424135000	-3.083001000	0.000011000

1	-4.423949000	-1.671545000	0.000036000
1	-2.011668000	1.933671000	0.000188000
7	4.492318000	0.984888000	-0.000122000
7	-4.492315000	0.984884000	-0.000145000
6	4.413460000	2.428991000	-0.000031000
1	3.886737000	2.801324000	-0.888822000
1	3.887182000	2.801276000	0.889050000
1	5.421663000	2.846163000	-0.000278000
6	5.795553000	0.353272000	0.000036000
1	5.948599000	-0.269696000	0.891190000
1	5.948579000	-0.270106000	-0.890825000
1	6.565399000	1.126395000	-0.000152000
6	-4.413476000	2.428985000	-0.000009000
1	-5.421688000	2.846138000	-0.000431000
1	-3.887354000	2.801262000	0.889170000
1	-3.886611000	2.801333000	-0.888703000
6	-5.795557000	0.353274000	0.000040000
1	-5.948647000	-0.269585000	0.891262000
1	-6.565398000	1.126401000	-0.000296000
1	-5.948541000	-0.270213000	-0.890749000

12, T.E. = -734.970817

6	-3.419810000	-0.227174000	0.000001000
6	-3.470425000	1.212217000	0.000002000
6	-2.334231000	1.949314000	0.000001000
7	-1.109028000	1.328192000	0.000000000
5	-0.953232000	-0.149399000	-0.000001000
6	-2.231526000	-0.933366000	0.000000000
1	-4.442668000	1.692399000	0.000003000
1	-2.321535000	3.035243000	0.000002000
1	-2.257984000	-2.019365000	-0.000001000

6	0.038349000	2.088744000	0.000000000
7	1.086555000	1.183297000	-0.000001000
6	2.370764000	1.644987000	-0.000002000
6	3.418812000	0.775981000	-0.000003000
6	3.188392000	-0.642975000	-0.000003000
6	1.915094000	-1.187306000	-0.000003000
5	0.744234000	-0.261834000	-0.000002000
1	2.493354000	2.724473000	-0.000002000
1	4.423518000	1.179926000	-0.000004000
1	1.855366000	-2.273640000	-0.000003000
8	4.223412000	-1.509200000	-0.000004000
8	-4.651628000	-0.772241000	0.000001000
6	5.554124000	-1.030525000	0.000008000
1	5.767685000	-0.437362000	-0.897386000
1	5.767666000	-0.437357000	0.897403000
1	6.185460000	-1.920341000	0.000018000
6	-4.763758000	-2.182298000	0.000000000
1	-4.301894000	-2.613888000	-0.895745000
1	-4.301892000	-2.613890000	0.895742000
1	-5.833751000	-2.394521000	0.000001000

13, T.E. = -582.263802

6	-2.753212000	0.871253000	-0.333143000
6	-3.189068000	-0.497319000	-0.437010000
6	-2.375319000	-1.576861000	-0.186736000
7	-1.131129000	-1.353723000	0.361542000
5	-0.798199000	-0.004005000	0.767940000
6	-1.518693000	1.182504000	0.211965000
1	-3.394821000	1.624283000	-0.797572000
1	-4.168348000	-0.695479000	-0.863231000
1	-2.636008000	-2.595233000	-0.460624000

6	-0.000002000	-2.116435000	0.018395000
7	1.131130000	-1.353723000	0.361545000
6	2.375316000	-1.576862000	-0.186738000
6	3.189068000	-0.497320000	-0.437012000
6	2.753213000	0.871250000	-0.333142000
6	1.518694000	1.182501000	0.211968000
5	0.798201000	-0.004007000	0.767944000
1	2.636002000	-2.595233000	-0.460631000
1	4.168345000	-0.695482000	-0.863236000
1	3.394821000	1.624282000	-0.797571000
6	0.689407000	2.383909000	0.057339000
6	-0.689404000	2.383911000	0.057337000
1	1.177750000	3.330926000	-0.178753000
1	-1.177745000	3.330929000	-0.178755000

14, T.E. = -614.315555

7	-2.669268000	0.922146000	-0.368263000
6	-3.127833000	-0.369522000	-0.448852000
6	-2.382490000	-1.505247000	-0.216622000
7	-1.138313000	-1.362942000	0.368613000
5	-0.802079000	-0.058205000	0.874347000
6	-1.510378000	1.115911000	0.239828000
1	-4.119256000	-0.483323000	-0.877668000
1	-2.692025000	-2.491488000	-0.547862000
6	0.000000000	-2.066133000	-0.075414000
7	1.138313000	-1.362942000	0.368613000
6	2.382490000	-1.505247000	-0.216622000
6	3.127833000	-0.369522000	-0.448852000
7	2.669268000	0.922146000	-0.368263000
6	1.510378000	1.115911000	0.239829000
5	0.802079000	-0.058206000	0.874347000

1	2.692024000	-2.491488000	-0.547862000
1	4.119256000	-0.483323000	-0.877668000
6	0.688242000	2.313700000	0.022555000
6	-0.688242000	2.313700000	0.022555000
1	1.196855000	3.220760000	-0.303872000
1	-1.196855000	3.220760000	-0.303872000

15, T.E. = -614.291724

6	-2.543419000	0.924708000	-0.455147000
6	-3.048959000	-0.413882000	-0.589108000
6	-2.320908000	-1.524327000	-0.235491000
7	-1.132906000	-1.359867000	0.449917000
5	-0.794729000	-0.033873000	0.936416000
6	-1.388757000	1.158311000	0.265830000
1	-3.019362000	1.714788000	-1.038470000
1	-3.974928000	-0.569832000	-1.134367000
1	-2.588137000	-2.530347000	-0.546079000
6	-0.000002000	-2.105843000	0.077380000
7	1.132904000	-1.359869000	0.449915000
6	2.320904000	-1.524331000	-0.235495000
6	3.048957000	-0.413886000	-0.589110000
6	2.543420000	0.924704000	-0.455145000
6	1.388760000	1.158309000	0.265834000
5	0.794729000	-0.033875000	0.936417000
1	2.588130000	-2.530350000	-0.546086000
1	3.974925000	-0.569837000	-1.134370000
1	3.019365000	1.714786000	-1.038466000
7	0.634249000	2.360365000	0.105547000
7	-0.634243000	2.360365000	0.105536000

16, T.E. = -450.983839

7	-0.000078000	1.138143000	-0.020096000
5	1.238977000	0.423062000	0.009053000
7	1.144908000	-1.025427000	0.000182000
6	0.000192000	-1.764744000	-0.013493000
7	-1.144656000	-1.025651000	0.000174000
5	-1.238975000	0.422790000	0.009093000
6	-0.000494000	2.596188000	-0.038631000
1	-0.881795000	2.977379000	-0.560208000
1	-0.003286000	3.010479000	0.978054000
1	0.883226000	2.977942000	-0.555614000
6	2.631252000	1.173676000	0.035711000
1	2.854715000	1.616092000	-0.946682000
1	2.630436000	2.006366000	0.750603000
1	3.477028000	0.528382000	0.288109000
6	2.368674000	-1.827155000	-0.005880000
1	3.004801000	-1.568169000	-0.859105000
1	2.942098000	-1.678778000	0.916074000
1	2.075788000	-2.875533000	-0.078957000
6	-2.368313000	-1.827552000	-0.005891000
1	-2.075311000	-2.875858000	-0.079487000
1	-2.941497000	-1.679640000	0.916293000
1	-3.004713000	-1.568261000	-0.858819000
6	-2.631333000	1.173211000	0.035741000
1	-2.855803000	1.613702000	-0.947294000
1	-3.476738000	0.528180000	0.290098000
1	-2.630043000	2.007254000	0.749040000

17, T.E. = -525.909417

7	1.481197000	-1.103132000	-0.000020000
6	0.297322000	-1.744381000	-0.000007000
7	-0.794630000	-0.884791000	0.000009000

5	-0.747564000	0.577578000	-0.000016000
7	0.560449000	1.174801000	-0.000025000
5	1.715920000	0.352013000	0.000017000
1	-1.939427000	-2.615206000	0.000042000
6	-2.016021000	-1.532560000	0.000029000
6	-2.081596000	1.312802000	-0.000024000
6	-3.228147000	0.569301000	0.000007000
6	-3.196110000	-0.861511000	0.000035000
1	-2.172937000	2.397691000	-0.000048000
1	-4.205566000	1.052356000	0.000010000
1	-4.120656000	-1.429976000	0.000054000
6	2.636385000	-2.004621000	-0.000062000
1	3.253908000	-1.845538000	-0.890152000
1	3.253816000	-1.845741000	0.890130000
1	2.258362000	-3.027619000	-0.000193000
6	3.180442000	0.951021000	0.000099000
1	3.344800000	1.590989000	-0.877771000
1	3.344615000	1.591121000	0.877907000
1	3.976048000	0.202263000	0.000239000
6	0.646850000	2.629379000	-0.000046000
1	0.157202000	3.048752000	-0.886506000
1	0.157224000	3.048782000	0.886412000
1	1.686957000	2.959450000	-0.000066000

18, T.E. = -541.972085

7	-1.463805000	-1.093459000	-0.000039000
6	-0.294958000	-1.755932000	-0.000041000
7	0.801738000	-0.900315000	-0.000019000
5	0.780869000	0.567523000	-0.000032000
7	-0.514081000	1.182209000	-0.000058000
5	-1.675092000	0.368836000	-0.000021000

1	1.975757000	-2.611583000	-0.000024000
6	2.025381000	-1.526506000	0.000005000
7	2.006419000	1.306901000	-0.000011000
6	3.109444000	0.620900000	0.000049000
6	3.181306000	-0.811701000	0.000048000
1	4.056963000	1.171921000	0.000086000
1	4.140080000	-1.319302000	0.000083000
6	-2.643714000	-1.960414000	-0.000003000
1	-3.257380000	-1.779321000	0.888379000
1	-3.257234000	-1.779616000	-0.888543000
1	-2.300344000	-2.995609000	0.000184000
6	-3.145529000	0.939928000	0.000100000
1	-3.186976000	2.032865000	-0.000355000
1	-3.711184000	0.592392000	-0.875150000
1	-3.710728000	0.593149000	0.875946000
6	-0.603066000	2.641173000	-0.000047000
1	-1.133547000	3.000286000	0.888255000
1	0.404405000	3.060682000	-0.000155000
1	-1.133787000	3.000295000	-0.888215000

19, T.E. = -557.978497

7	-1.441980000	-1.091055000	0.000000000
6	-0.271900000	-1.759258000	0.000009000
7	0.817874000	-0.898513000	0.000001000
5	0.782438000	0.561351000	-0.000005000
7	-0.502605000	1.181853000	-0.000010000
5	-1.665031000	0.364706000	-0.000010000
7	1.998044000	-1.571188000	0.000009000
7	2.015951000	1.305626000	-0.000007000
6	3.088824000	0.589446000	-0.000004000
6	3.077728000	-0.856004000	0.000007000

1	4.065064000	1.086836000	-0.000007000
1	4.010626000	-1.414923000	0.000009000
6	-2.619301000	-1.963617000	-0.000014000
1	-3.233487000	-1.785093000	0.888607000
1	-3.233266000	-1.785363000	-0.888845000
1	-2.269659000	-2.996462000	0.000177000
6	-3.134588000	0.934664000	0.000012000
1	-3.179802000	2.027511000	-0.000259000
1	-3.698827000	0.584790000	-0.875099000
1	-3.698561000	0.585253000	0.875486000
6	-0.593943000	2.641082000	-0.000001000
1	-1.125886000	2.997694000	0.888130000
1	0.410757000	3.066826000	-0.000006000
1	-1.125897000	2.997705000	-0.888121000

20, T.E. = -557.955291

7	-1.449986000	-1.098813000	0.000000000
6	-0.271152000	-1.744270000	0.000009000
7	0.805189000	-0.860849000	0.000001000
5	0.755144000	0.585191000	-0.000003000
7	-0.532462000	1.196533000	-0.000005000
5	-1.684862000	0.357756000	-0.000010000
6	2.050639000	-1.455190000	0.000005000
6	2.153003000	1.225321000	-0.000005000
7	3.249721000	0.523916000	-0.000003000
7	3.191598000	-0.851510000	0.000002000
6	-2.617583000	-1.984664000	-0.000006000
1	-3.232619000	-1.812991000	0.888857000
1	-3.232436000	-1.813220000	-0.889042000
1	-2.257212000	-3.013822000	0.000156000
6	-3.161327000	0.906954000	0.000001000

1	-3.227569000	1.998524000	-0.000241000
1	-3.719953000	0.547766000	-0.874877000
1	-3.719743000	0.548181000	0.875188000
6	-0.668084000	2.650799000	0.000004000
1	-1.208255000	2.994397000	0.887958000
1	0.314172000	3.125908000	0.000047000
1	-1.208186000	2.994417000	-0.887985000
1	2.034027000	-2.542211000	0.000010000
1	2.344969000	2.299683000	-0.000010000

21, T.E. = -637.611359

7	1.710019000	-1.139286000	-0.276054000
6	0.470002000	-1.709301000	-0.110572000
7	-0.505701000	-0.828837000	0.105188000
5	-0.382663000	0.643018000	0.079712000
7	0.953560000	1.136637000	0.252925000
5	2.045146000	0.239286000	0.003353000
6	-2.765712000	0.685003000	-0.336504000
6	-2.853116000	-0.621991000	-0.055198000
1	-3.626349000	1.242848000	-0.686989000
1	-3.791802000	-1.154828000	-0.150718000
6	2.769729000	-2.095223000	-0.588130000
1	3.271440000	-1.834152000	-1.527222000
1	3.522346000	-2.135758000	0.208078000
1	2.311031000	-3.079767000	-0.692419000
6	3.548693000	0.726820000	0.077434000
1	3.671454000	1.772163000	-0.229185000
1	3.925355000	0.659354000	1.109675000
1	4.225156000	0.124036000	-0.536343000
6	1.233107000	2.491229000	0.715533000
1	1.511737000	3.168186000	-0.102846000

1	0.364236000	2.909498000	1.229840000
1	2.060140000	2.480262000	1.431804000
7	-1.787481000	-1.351572000	0.463708000
7	-1.559654000	1.397149000	-0.188053000
6	-1.893634000	-2.792226000	0.449277000
1	-1.713987000	-3.227508000	-0.544776000
1	-1.165445000	-3.226374000	1.136352000
1	-2.905347000	-3.032599000	0.789365000
6	-1.625825000	2.799497000	-0.547848000
1	-0.637653000	3.185872000	-0.795565000
1	-2.254663000	2.921454000	-1.438663000
1	-2.054720000	3.414307000	0.256340000

22, T.E. = -525.911684

7	1.927335000	0.150865000	0.000017000
5	1.074506000	-1.007333000	0.000040000
7	-0.355683000	-0.739149000	-0.000044000
5	-0.817784000	0.633889000	0.000025000
7	0.206924000	1.665641000	-0.000020000
6	1.543835000	1.474856000	-0.000029000
6	-1.275559000	-1.763439000	-0.000116000
6	-2.319368000	0.878147000	0.000097000
6	-3.142785000	-0.213720000	0.000068000
6	-2.618026000	-1.542611000	-0.000065000
1	-4.226652000	-0.097349000	0.000145000
1	-3.288900000	-2.396145000	-0.000132000
1	-0.876554000	-2.772450000	-0.000228000
1	-2.774029000	1.866703000	0.000201000
6	1.627370000	-2.486070000	0.000091000
1	1.274836000	-3.043662000	-0.878699000
1	2.718122000	-2.547959000	0.000596000

1	1.273978000	-3.043992000	0.878317000
6	3.381202000	-0.029315000	-0.000007000
1	3.833944000	0.963020000	-0.000114000
1	3.711289000	-0.574788000	0.890553000
1	3.711244000	-0.574976000	-0.890477000
6	-0.218723000	3.063545000	-0.000043000
1	-0.818247000	3.286081000	-0.889694000
1	-0.817416000	3.286367000	0.890102000
1	0.677075000	3.686515000	-0.000543000

23, T.E. = -541.970856

7	1.888917000	0.230071000	-0.000003000
5	1.110636000	-0.978535000	-0.000009000
7	-0.332121000	-0.785092000	-0.000011000
5	-0.869304000	0.566042000	-0.000008000
7	0.090393000	1.652392000	-0.000018000
6	1.434907000	1.534327000	-0.000012000
6	-1.233939000	-1.817174000	-0.000007000
7	-2.277638000	0.811289000	0.000007000
6	-3.047050000	-0.236044000	0.000013000
6	-2.575452000	-1.589035000	0.000004000
1	-4.131879000	-0.079507000	0.000027000
1	-3.272199000	-2.420711000	0.000007000
6	1.811737000	-2.390759000	0.000000000
1	2.467243000	-2.496053000	-0.874864000
1	2.467272000	-2.496025000	0.874847000
1	1.139414000	-3.253389000	0.000025000
6	3.348367000	0.121303000	0.000019000
1	3.755045000	1.133367000	-0.000032000
1	3.704020000	-0.411034000	0.889165000
1	3.704042000	-0.411136000	-0.889055000

6	-0.427201000	3.022206000	0.000002000
1	-1.046499000	3.196712000	-0.884406000
1	-1.046037000	3.196865000	0.884707000
1	0.428902000	3.698374000	-0.000264000
1	-0.831050000	-2.824557000	-0.000013000

24, T.E. = -557.982330

7	1.874271000	0.228524000	0.000024000
5	1.094592000	-0.983293000	-0.000005000
7	-0.344260000	-0.762266000	-0.000011000
5	-0.874469000	0.578247000	0.000029000
7	0.080510000	1.659832000	-0.000037000
6	1.429621000	1.531450000	-0.000021000
7	-1.157239000	-1.846339000	-0.000050000
7	-2.296186000	0.796647000	0.000086000
6	-3.003933000	-0.284647000	0.000067000
6	-2.433549000	-1.611891000	-0.000020000
1	-4.096945000	-0.208348000	0.000129000
1	-3.074693000	-2.490080000	-0.000054000
6	1.733367000	-2.414022000	-0.000058000
1	2.379956000	-2.559137000	-0.876168000
1	2.379841000	-2.559196000	0.876131000
1	0.976951000	-3.202518000	-0.000143000
6	3.332978000	0.102623000	0.000089000
1	3.754157000	1.108720000	-0.000060000
1	3.678366000	-0.436352000	0.888866000
1	3.678413000	-0.436640000	-0.888492000
6	-0.428544000	3.033398000	-0.000082000
1	-1.044670000	3.214623000	-0.885554000
1	-1.043941000	3.214953000	0.885834000
1	0.432643000	3.702954000	-0.000541000

25, T.E. = -557.956431

7	1.891995000	0.216996000	0.000095000
5	1.095998000	-0.984516000	-0.000035000
7	-0.343239000	-0.755281000	-0.000108000
5	-0.843445000	0.590008000	-0.000065000
7	0.111459000	1.666688000	-0.000141000
6	1.461129000	1.523762000	-0.000033000
6	-1.283101000	-1.758007000	-0.000156000
6	-2.372585000	0.688667000	0.000174000
7	-3.136204000	-0.367582000	0.000263000
7	-2.569655000	-1.618671000	-0.000014000
1	-0.916140000	-2.779758000	-0.000334000
1	-2.934986000	1.623516000	0.000442000
6	1.766275000	-2.406971000	-0.000092000
1	2.419459000	-2.525719000	-0.874985000
1	2.419331000	-2.525901000	0.874866000
1	1.073576000	-3.252685000	-0.000233000
6	3.350966000	0.083255000	0.000233000
1	3.776335000	1.087352000	0.000534000
1	3.694156000	-0.456156000	0.889380000
1	3.694372000	-0.455713000	-0.889090000
6	-0.373722000	3.047191000	-0.000166000
1	-0.980478000	3.244274000	-0.890194000
1	-0.978597000	3.244987000	0.890994000
1	0.495941000	3.705910000	-0.001307000

26, T.E. = -637.611880

7	2.158083000	0.684624000	-0.088758000
5	1.571385000	-0.642918000	-0.178741000
7	0.152836000	-0.677682000	-0.058500000

5	-0.630198000	0.530334000	0.020062000
7	0.136310000	1.763768000	0.156676000
6	1.498671000	1.856287000	0.103759000
7	-2.054460000	0.394835000	-0.141589000
6	-2.490485000	-0.827058000	-0.673480000
6	-1.751502000	-1.940264000	-0.628287000
1	-3.450932000	-0.812124000	-1.184169000
1	-2.088509000	-2.874564000	-1.067432000
6	2.453557000	-1.933590000	-0.354145000
1	3.196450000	-1.812400000	-1.152566000
1	3.026774000	-2.155684000	0.557683000
1	1.839306000	-2.809047000	-0.584552000
6	3.610551000	0.816724000	-0.185197000
1	3.863790000	1.863976000	-0.012694000
1	4.112385000	0.192128000	0.561966000
1	3.966009000	0.519475000	-1.178516000
6	-0.506721000	3.066213000	0.326499000
1	-1.210133000	3.273082000	-0.486099000
1	-1.032274000	3.131932000	1.286254000
1	0.285865000	3.815936000	0.312285000
7	-0.474515000	-1.959015000	-0.013481000
6	-3.103784000	1.390526000	-0.010807000
1	-2.829446000	2.158426000	0.709413000
1	-3.339234000	1.875473000	-0.969341000
1	-4.015954000	0.910504000	0.361081000
6	-0.521545000	-2.475779000	1.350313000
1	-0.964806000	-3.476418000	1.320038000
1	0.496212000	-2.559477000	1.743861000
1	-1.121675000	-1.842362000	2.023820000

27, T.E. = -600.831192

6	3.704302000	0.315840000	-0.000102000
6	2.636203000	1.163212000	0.000053000
5	1.231452000	0.566126000	0.000066000
7	1.135639000	-0.907127000	-0.000009000
6	2.299451000	-1.667712000	-0.000104000
6	3.532802000	-1.108849000	-0.000197000
7	0.002979000	1.292118000	0.000129000
6	-0.011667000	-1.658770000	0.000105000
7	-1.148778000	-0.893705000	0.000122000
5	-1.236376000	0.586751000	-0.000040000
6	-2.645069000	1.181346000	-0.000374000
1	-2.848262000	2.250408000	-0.000774000
6	-3.714329000	0.336836000	-0.000290000
6	-3.548331000	-1.088550000	0.000102000
6	-2.317233000	-1.649699000	0.000270000
1	4.724009000	0.700838000	-0.000156000
1	2.829423000	2.234492000	0.000129000
1	2.122604000	-2.738062000	-0.000135000
1	4.399774000	-1.761943000	-0.000323000
1	-4.732397000	0.725947000	-0.000564000
1	-4.417176000	-1.739113000	0.000214000
1	-2.143437000	-2.720464000	0.000457000
6	0.055490000	2.748401000	0.000265000
1	0.580691000	3.119374000	0.887491000
1	0.579850000	3.119616000	-0.887362000
1	-0.949056000	3.173189000	0.000832000

28, T.E. = -632.952110

6	3.553783000	0.420158000	-0.000009000
7	2.510888000	1.187725000	0.000015000
5	1.226116000	0.550550000	-0.000001000

7	1.130503000	-0.930925000	-0.000015000
6	2.314126000	-1.648749000	-0.000010000
6	3.513697000	-1.020343000	-0.000006000
7	0.001432000	1.270986000	-0.000005000
6	-0.005249000	-1.698518000	-0.000007000
7	-1.135932000	-0.925670000	0.000000000
5	-1.227311000	0.559123000	-0.000010000
7	-2.514034000	1.194584000	-0.000034000
6	-3.558130000	0.430212000	-0.000038000
6	-3.520455000	-1.010768000	0.000028000
6	-2.322258000	-1.640597000	0.000030000
1	4.542627000	0.892796000	0.000042000
1	2.185576000	-2.726893000	-0.000008000
1	4.432175000	-1.597946000	0.000001000
1	-4.545938000	0.904975000	-0.000015000
1	-4.439811000	-1.586934000	0.000064000
1	-2.195725000	-2.718950000	0.000057000
6	0.021805000	2.733567000	0.000024000
1	0.548200000	3.106066000	0.883364000
1	0.548705000	3.106090000	-0.883000000
1	-1.003740000	3.105760000	-0.000249000

29, T.E. = -664.965570

6	-3.516770000	0.380809000	-0.000012000
5	-1.217639000	0.542688000	-0.000016000
7	-1.124363000	-0.927404000	0.000008000
6	-3.385211000	-1.064235000	0.000023000
7	-0.001375000	1.271801000	-0.000020000
6	0.005454000	-1.706565000	0.000007000
7	1.129827000	-0.922327000	-0.000004000
5	1.218777000	0.551327000	-0.000001000

6	3.521093000	0.391348000	0.000019000
6	3.392225000	-1.054344000	-0.000017000
1	-4.531781000	0.793056000	-0.000038000
1	-4.270916000	-1.695610000	0.000040000
1	4.535082000	0.806032000	0.000044000
1	4.279185000	-1.683987000	-0.000039000
6	-0.022422000	2.735544000	0.000011000
1	-0.547517000	3.108127000	-0.883721000
1	-0.546779000	3.108110000	0.884194000
1	1.002423000	3.109494000	-0.000389000
7	-2.257548000	-1.694616000	0.000027000
7	-2.509167000	1.182334000	-0.000034000
7	2.266240000	-1.686510000	-0.000028000
7	2.511870000	1.189487000	0.000023000

30, T.E. = -664.916646

6	-2.658559000	1.071849000	0.000016000
5	-1.209703000	0.558699000	-0.000017000
7	-1.121287000	-0.897020000	-0.000011000
6	-2.323641000	-1.598382000	-0.000001000
7	-0.002258000	1.307337000	-0.000042000
6	0.009305000	-1.675840000	-0.000020000
7	1.131191000	-0.886939000	-0.000016000
5	1.213020000	0.574018000	-0.000018000
6	2.664789000	1.086018000	0.000026000
1	2.943039000	2.141087000	0.000080000
6	2.336914000	-1.584744000	-0.000014000
1	-2.931282000	2.128615000	0.000047000
1	-2.215202000	-2.679980000	-0.000014000
1	2.230379000	-2.666517000	-0.000048000
6	-0.041343000	2.768487000	-0.000027000

1	-0.561135000	3.140252000	-0.888427000
1	-0.560301000	3.140266000	0.888857000
1	0.969198000	3.179266000	-0.000518000
7	-3.688644000	0.279906000	0.000039000
7	-3.504757000	-1.089891000	0.000017000
7	3.695842000	0.296536000	0.000050000
7	3.516188000	-1.074344000	0.000007000

31, T.E. = -824.242347

6	-3.575456000	-0.379185000	0.433849000
5	-1.237585000	-0.646076000	-0.062397000
7	-1.128532000	0.811637000	-0.083774000
6	-3.455378000	0.951854000	0.347580000
7	-0.000008000	-1.369412000	0.022849000
6	0.000019000	1.537435000	-0.079575000
7	1.128584000	0.811637000	-0.083584000
5	1.237574000	-0.646103000	-0.062249000
6	3.575562000	-0.379370000	0.433705000
6	3.455484000	0.951685000	0.347575000
1	-4.436378000	-0.850461000	0.899459000
1	-4.220783000	1.618163000	0.731219000
1	4.436556000	-0.850654000	0.899176000
1	4.221038000	1.617909000	0.731068000
6	-0.000011000	-2.742724000	0.518216000
1	-0.883195000	-2.915772000	1.139402000
1	-0.000118000	-3.488644000	-0.286748000
1	0.883295000	-2.915843000	1.139208000
7	-2.356178000	1.548293000	-0.272243000
7	-2.544455000	-1.220488000	-0.025124000
7	2.356187000	1.548306000	-0.271756000
7	2.544389000	-1.220623000	-0.024997000

6	2.229466000	2.980163000	-0.116246000
1	1.562416000	3.386431000	-0.877238000
1	1.834062000	3.271031000	0.869431000
1	3.230782000	3.397788000	-0.255111000
6	2.951866000	-2.529257000	-0.486023000
1	3.327698000	-3.158286000	0.335431000
1	2.116686000	-3.045986000	-0.961073000
1	3.751999000	-2.434587000	-1.232353000
6	-2.229421000	2.980183000	-0.116835000
1	-1.834342000	3.271144000	0.868939000
1	-1.562103000	3.386300000	-0.877667000
1	-3.230677000	3.397822000	-0.256110000
6	-2.952073000	-2.529366000	-0.485295000
1	-2.117089000	-3.046314000	-0.960429000
1	-3.327524000	-3.157979000	0.336658000
1	-3.752518000	-2.435117000	-1.231342000

32, T.E. = -868.323720

6	-3.737477000	0.006057000	0.018884000
6	-2.623896000	0.829951000	0.009554000
5	-1.238797000	0.229887000	0.001533000
7	-1.134219000	-1.248221000	0.001152000
6	-2.305637000	-1.986464000	0.007873000
6	-3.537379000	-1.431750000	0.015967000
7	-0.002835000	0.951980000	-0.007754000
6	0.006330000	-2.003112000	-0.006147000
7	1.139872000	-1.237917000	-0.013304000
5	1.242325000	0.246672000	-0.014117000
6	2.634624000	0.837545000	-0.018044000
1	2.795559000	1.910786000	-0.007828000
6	3.745635000	0.012377000	-0.028403000

6	3.544597000	-1.424905000	-0.025272000
6	2.312454000	-1.976405000	-0.018427000
7	-5.023239000	0.483147000	0.033171000
1	-2.770433000	1.905788000	0.006235000
1	-2.148961000	-3.060513000	0.006036000
1	-4.383476000	-2.107812000	0.020616000
7	5.033986000	0.487198000	-0.046706000
1	4.389267000	-2.102625000	-0.028814000
1	2.154126000	-3.050108000	-0.016280000
6	-0.056852000	2.403852000	-0.009461000
1	-0.598204000	2.775006000	-0.888492000
1	-0.569020000	2.778892000	0.885373000
1	0.946481000	2.832621000	-0.027501000
6	-5.237437000	1.910158000	0.011951000
1	-6.308130000	2.118417000	0.049550000
1	-4.764684000	2.395731000	0.876596000
1	-4.828070000	2.369070000	-0.900118000
6	-6.163805000	-0.405535000	-0.023281000
1	-6.174496000	-1.010303000	-0.940828000
1	-6.198530000	-1.083734000	0.839494000
1	-7.077941000	0.190461000	-0.008814000
6	6.169261000	-0.401208000	0.080765000
1	6.221581000	-1.117851000	-0.748697000
1	7.085851000	0.190890000	0.057971000
1	6.157003000	-0.963611000	1.025481000
6	5.251609000	1.912984000	-0.002222000
1	4.758213000	2.412370000	-0.846372000
1	4.867740000	2.359150000	0.928036000
1	6.321366000	2.120002000	-0.067064000

33, T.E. = -829.581975

6	-3.634483000	0.372285000	0.000107000
6	-2.492340000	1.126636000	0.000056000
5	-1.152646000	0.426263000	-0.000012000
7	-1.165585000	-1.054087000	0.000001000
6	-2.382228000	-1.712445000	0.000056000
6	-3.572997000	-1.067735000	0.000106000
7	0.133873000	1.051958000	-0.000094000
6	-0.080728000	-1.893963000	-0.000034000
7	1.107062000	-1.219400000	-0.000050000
5	1.315753000	0.253390000	-0.000054000
6	2.755312000	0.746969000	-0.000008000
1	3.012903000	1.801624000	0.000045000
6	3.761108000	-0.178903000	0.000000000
6	3.484357000	-1.593551000	-0.000037000
6	2.218775000	-2.056546000	-0.000054000
1	-2.619802000	2.206811000	0.000075000
1	-2.298764000	-2.794393000	0.000069000
1	-4.474048000	-1.668927000	0.000174000
1	4.319017000	-2.286032000	-0.000041000
1	1.972571000	-3.112995000	-0.000072000
6	0.188367000	2.506336000	-0.000119000
1	-0.309551000	2.915601000	-0.886797000
1	-0.308602000	2.915626000	0.887087000
1	1.220955000	2.858384000	-0.000696000
8	-4.823531000	1.020574000	0.000203000
8	5.086580000	0.083582000	0.000049000
6	-6.028568000	0.283384000	-0.000176000
1	-6.120383000	-0.341139000	-0.897446000
1	-6.120868000	-0.341261000	0.896963000
1	-6.827648000	1.026589000	-0.000332000
6	5.493119000	1.435308000	0.000095000

1	5.132301000	1.956087000	-0.895668000
1	5.132318000	1.956026000	0.895901000
1	6.584068000	1.420546000	0.000087000