Electronic Supplementary Information

Theoretical Study of the Regio- and Stereoselctivity of the Intramolecular Povarov Reaction yielding 5*H*-chromeno[2,3-c] acridine derivatives

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Contents

Table S1. B3LYP/6-31G(d,p) total (E, in a.u.) and relative (ΔE, in kcal mol^{-1}) energies in gas phase of the stationary points involved in the *trans* and *cis* stereoisomeric channels of the IMADA reaction of ATCI **3**.

	Non-catalysed reaction	
	E	ΔE
3	-1021.486188	
TS-tf	-1021.430982	34.6
TS-cf	-1021.430246	35.1
TS-b	-1021.382279	65.2
trans-**4**	-1021.478530	4.8
cis-**4**	-1021.476399	6.1
10	-1021.391336	59.5

Table S2. MPW1B95/6-31G(d,p) total (E, in a.u.) and relative (ΔE, in kcal mol^{-1}) energies in the presence of BF$_3$ catalyst of the stationary points involved in the *trans* and *cis* stereoisomeric channels of the IMADA reaction of ATCI **3-B** and of the 1,3-hydrogen shift for the favored *trans* channel.
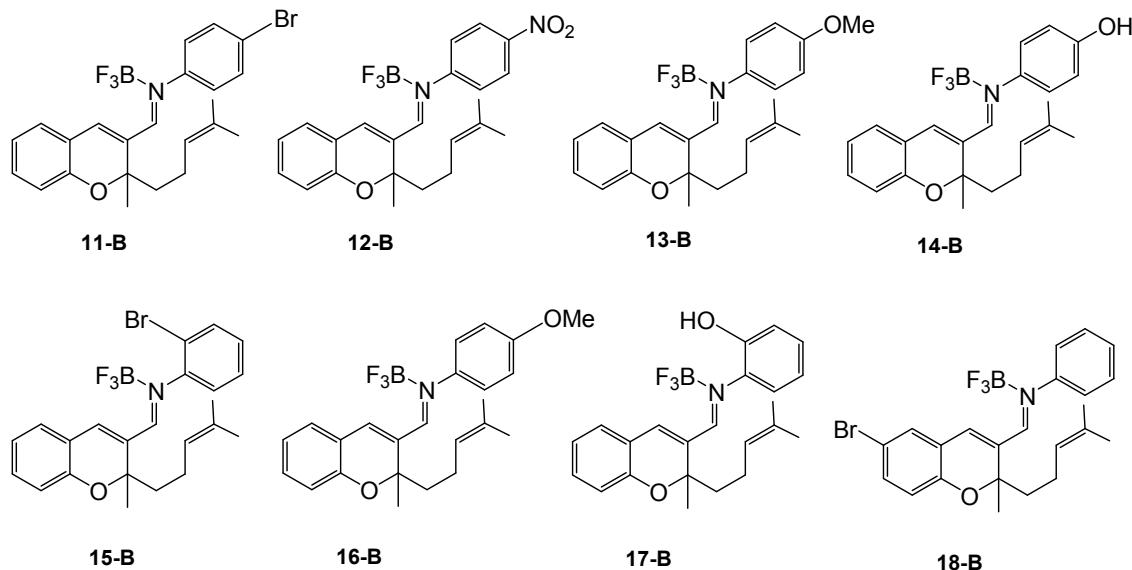
	IMADA reaction			1,3-hydrogen shift	
	E	ΔE[a]		E	ΔE
3-B	-1345.460306		*trans*-**4**+**11**	-1271.534301	
TS-tf-B	-1345.419862	25.4	**TS-6**	-1271.497047	23.4[b]
TS-cf-B	-1345.418785	26.1	**IN1**	-1271.506761	17.3[b]
TS-b-B	-1345.388107	45.3	*trans*-**5**+**11**	-1271.580025	-28.7[b]
trans-**4-B**	-1345.468388	-5.1	**TS-5-tf**	-1021.045397	74.7[c]
cis-**4-B**	-1345.481828	-13.5	*trans*-**5**	-1021.238425	-46.4[c]
10-B	-1345.406934	33.5			

[a] Relative to reactant **3-B**
[b] Relative to *trans*-**4**+**11** complex
[c] Relative to *trans*-**4**
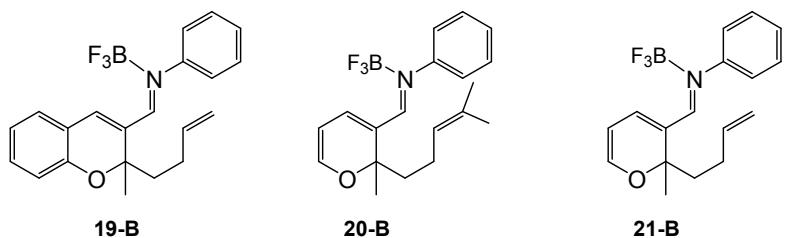
a) Experimental reactants

11-B **12-B** **13-B** **14-B**

15-B **16-B** **17-B** **18-B**

b) Non-experimental (reduced) reactants

19-B **20-B** **21-B**

Scheme S1: Structures of experimental **11B-18B** and non-experimental (reduced) **19B-21B** derivatives of ATCI **3-B**.

Table S3. B3LYP/6-31G(d,p) total (E, in a.u.) and relative (ΔE, in kcal mol^{-1}) energies of the stationary points involved in the *trans* and *cis* stereoisomeric pathways associated with the BF$_3$ catalysed IMADA reaction of the experimental **11B-18B** and non-experimental (reduced) **19B-21B** derivatives of ATCI **3-B**.

	E	ΔE[a]
Experimental derivatives		
11-B	-3917.171684	
TS-tf-B-11	-3917.123859	**30.0**
TS-cf-B-11	-3917.114742	**35.7**
trans-**11-B**	-3917.166969	3.0
cis-**11-B**	-3917.158362	8.4
12-B	-1550.568076	
TS-tf-B-12	-1550.521669	**29.1**
TS-cf-B-12	-1550.510878	**35.9**
trans-**12-B**	-1550.561402	4.2
cis-**12-B**	-1550.552497	9.8
13-B	-1460.594675	
TS-tf-B-13	-1460.547062	**29.9**
TS-cf-B-13	-1460.539029	**34.9**
trans-**13-B**	-1460.586942	4.9
cis-**13-B**	-1460.578494	10.2
14-B	-1421.289533	
TS-tf-B-14	-1421.241573	**30.1**
TS-cf-B-14	-1421.233508	**35.2**
trans-**14-B**	-1421.283596	3.7
cis-**14-B**	-1421.275109	9.1
15-B	-3917.167284	
TS-tf-B-15	-3917.118631	**30.5**
TS-cf-B-15	-3917.109317	**36.4**
trans-**15-B**	-3917.150760	10.4
cis-**15-B**	-3917.146640	13.0
16-B	-1460.590149	
TS-tf-B-16	-1460.539740	**31.6**
TS-cf-B-16	-1460.529814	**37.9**
trans-**16-B**	-1460.580656	6.0
cis-**16-B**	-1460.572111	11.3
17-B	-1421.284620	
TS-tf-B-17	-1421.235729	**30.7**
TS-cf-B-17	-1421.228901	**35.0**
trans-**17-B**	-1421.281259	2.1
cis-**17-B**	-1421.264563	12.6

Table S3 (continued)

18-B	-3917.170524	
TS-tf-B-18	-3917.123514	**29.5**
TS-cf-B-18	-3917.114683	**35.0**
trans-**18-B**	-3917.168977	1.0
cis-**18-B**	-3917.161627	5.6
Non-experimental (Reduced Models)		
19-B	-1267.428057	
TS-tf-B-19	-1267.379887	**30.2**
TS-cf-B-19	-1267.369909	**36.4**
trans-**19-B**	-1267.436371	-5.2
cis-**19-B**	-1267.431164	-1.9
20-B	-1192.408212	
TS-tf-B-20	-1192.356364	**32.5**
TS-cf-B-20	-1192.347797	**37.9**
trans-**20-B**	-1192.400372	4.9
cis-**20-B**	-1192.392673	9.7
21-B	-1113.767045	
TS-tf-B-21	-1113.711778	**34.6**
TS-cf-B-21	-1113.706212	**38.1**
trans-**21-B**	-1113.770929	-2.4
cis-**21-B**	-1113.767741	-0.4

[a] Relative to reactants **X-B** (X=11-21)

Table S4. B3LYP/6-31G(d,p) electronic chemical potential μ, chemical hardness η, global electrophilicity ω, and global nucleophilicity N indices, in eV units, of ATCI **3-B** and its derivatives **11B-21B**.

	μ	η	ω	N
Experimental derivatives				
3-B	-4.24	3.52	2.54	3.11
11-B	-4.34	3.38	2.78	3.09
12-B	-4.60	3.22	3.27	3.30
13-B	-4.10	3.36	2.49	3.07
14-B	-4.13	3.38	2.51	3.28
15-B	-4.35	3.39	2.79	3.24
16-B	-4.14	3.38	2.54	2.91
17-B	-4.18	3.40	2.57	3.35
18-B	-4.36	3.34	2.84	3.09
Non-experimental derivatives				
19-B	-4.27	3.51	2.59	3.10
20-B	-4.15	3.50	2.46	3.22
21-B	-4.21	3.54	2.50	3.14

Atomic coordinates (in Å) of equilibrium geometries of the calculated structures at the B3LYP/6-31G(d,p) and MPW1B95/6-31G(d,p) level.

3
E(RB3LYP)= -1021.486188 a.u.

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8           2.87101400      0.33635900      1.42408900
6           1.52235800      0.81598800      1.10466100
6           1.73147100      2.08556300      0.23607300
6           0.50504100      2.95146000     -0.12224000
6           0.95789000      1.16132600      2.48561400
6          -2.44401000      1.79112800     -2.44884900
6          -2.64387900      2.93033200     -0.19045100
1           2.23466900      1.78011500     -0.68923300
1           2.44725600      2.70610500      0.78832900
1           0.90816200      3.90983400     -0.48322300
1          -0.06116200      3.20007800      0.78084900
1          -0.01416800      1.65388300      2.42020800
1           1.64890500      1.83856900      2.99456600
1           0.85234600      0.25748600      3.09119200
1          -3.09010300      0.95760400     -2.14524700
1          -1.74316300      1.42101800     -3.20194500
1          -3.09533200      2.53580200     -2.92565300
1          -3.27298200      3.73165600     -0.59957300
1          -2.11184100      3.33831600      0.67142700
1          -3.32879700      2.15148700      0.16884500
6           2.87122900     -1.14099600     -0.47770000
6           3.61983700     -1.90308800     -1.38955100
1           3.09279300     -2.50160900     -2.12795800
6           5.01055800     -1.90029100     -1.34734100
1           5.57961000     -2.48859500     -2.05997700
6           5.67064900     -1.14355100     -0.37218400
1           6.75593500     -1.14265300     -0.32982000
6           4.95032100     -0.38158600      0.54770200
1           5.44707300      0.20736700      1.31139100
6           3.55672600     -0.37119200      0.48592400
6           1.42941300     -1.16347300     -0.39643800
1           0.87329100     -1.92095100     -0.94157500
6           0.74666500     -0.29379600      0.38757800
6          -3.56014500     -1.88198900     -0.88869800
1          -3.06474500     -2.14012300     -1.81917800
6          -4.94177300     -1.98723700     -0.75414800
1          -5.53856200     -2.32997000     -1.59466700
6          -5.55938800     -1.66875400      0.45848100
1          -6.63538100     -1.76546200      0.56707400
6          -4.77905100     -1.24714400      1.53669600
1          -5.24732900     -1.02284700      2.49113300
6          -3.39664900     -1.12398000      1.40453000
6          -2.76935100     -1.42361900      0.18012900
6          -0.70732000     -0.39830900      0.52654400
1          -1.20512300      0.37766200      1.11776200
6          -0.38740500      2.38456500     -1.19620200
1           0.14947500      1.95671100     -2.04402000
6          -1.72853900      2.37997800     -1.25679100
7          -1.38332000     -1.34278300     -0.02457800
1          -2.79359700     -0.83088700      2.25861000
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3-B
E(RB3LYP)=-1346.069196 a.u.

8	-3.02143700	0.78909700	-1.51404200
6	-1.68919100	1.16858300	-1.03638600
6	-1.91928100	2.20605600	0.09785800
6	-0.74822300	3.11990800	0.50708700
6	-1.05624400	1.80961900	-2.27165400
6	2.76034000	2.11875300	1.96480000
6	2.19094200	4.13394700	0.52253600
1	-2.28884800	1.67217300	0.98051200
1	-2.73976000	2.84401400	-0.25141000
1	-1.17150100	3.84039400	1.22354900
1	-0.43630800	3.72479600	-0.35129900
1	-0.06770600	2.21888300	-2.05470600
1	-1.69472200	2.62803500	-2.61367100
1	-0.97279700	1.08189300	-3.08357700
1	3.64388400	1.91574700	1.34629400
1	2.39597800	1.16491300	2.35162500
1	3.11135100	2.72256300	2.81300000
1	2.51974200	4.85797900	1.28010000
1	1.43312000	4.62458200	-0.09192400
1	3.06693200	3.93603200	-0.10885700
6	-3.13285700	-1.02283900	0.06704700
6	-3.93250100	-1.94423200	0.76863500
1	-3.44661300	-2.67496100	1.40896900
6	-5.31532600	-1.91617800	0.64763600
1	-5.92722000	-2.62087500	1.20079100
6	-5.91554600	-0.97969800	-0.20599100
1	-6.99633200	-0.96116500	-0.31146200
6	-5.14653200	-0.06515800	-0.92208300
1	-5.59888300	0.65999900	-1.58980300
6	-3.75846100	-0.07432100	-0.77129600
6	-1.69468400	-1.07210000	0.05588900
1	-1.20798000	-1.96158100	0.43989000
6	-0.95907700	-0.08370900	-0.52530900
6	3.20908300	-2.34964600	-0.64681100
1	2.65187200	-3.18307700	-0.23524800
6	4.47063000	-2.52920500	-1.20808300
1	4.90596000	-3.52348200	-1.23374500
6	5.17429300	-1.44254900	-1.73318700
1	6.15991700	-1.58823000	-2.16443600
6	4.61110100	-0.16716200	-1.68942500
1	5.15930100	0.68609600	-2.07735100
6	3.34636200	0.02387600	-1.13201600
6	2.64281700	-1.07098000	-0.62138200
6	0.45600100	-0.23749400	-0.75963100
1	0.84162500	0.23569100	-1.66124600
6	0.43182200	2.43230700	1.15310400
1	0.20248200	1.52082000	1.70106200
6	1.70448400	2.86639300	1.18391800
7	1.32324400	-0.92035700	-0.06554000
1	2.91960800	1.01932000	-1.06034300
5	1.10462000	-1.56972900	1.46177800
9	0.62439000	-2.85702100	1.25463200
9	2.34814100	-1.53768900	2.03892900
9	0.19890100	-0.76164900	2.12132600

TS-tf
E(RB3LYP)=-1021.430982 a.u.

8	3.04817400	1.32038100	-0.00333000
6	1.67470700	1.31505000	0.48987500
6	1.01736300	2.44683900	-0.32726400
6	-0.50683100	2.53946600	-0.21594000
6	1.74528600	1.64500600	1.99185400
6	-3.25866300	0.54987200	-2.00172800
6	-3.44948200	2.42295700	-0.28520700
1	1.28920800	2.27835500	-1.37529200
1	1.47658500	3.39692900	-0.03207300
1	-0.83741000	3.41657700	-0.78836000
1	-0.80360800	2.73901500	0.82172700
1	0.75017100	1.75579800	2.43243500
1	2.29591300	2.57909100	2.13879000
1	2.26431000	0.84500100	2.52693100
1	-4.28499900	0.23259200	-1.79309200
1	-2.67094500	-0.32486900	-2.29008600
1	-3.29243400	1.22645700	-2.86937500
1	-3.35833400	3.28896300	-0.95853800
1	-3.11849000	2.75446500	0.70277700
1	-4.51114600	2.17018900	-0.22657500
6	3.14141100	-1.08878900	-0.12856900
6	3.93710600	-2.23413400	-0.27048300
1	3.45100500	-3.20575600	-0.30564600
6	5.32388600	-2.13656800	-0.36826100
1	5.92728600	-3.03213500	-0.47791100
6	5.93042900	-0.87808200	-0.32811600
1	7.01037600	-0.79161100	-0.40566400
6	5.15967500	0.27687800	-0.18409300
1	5.61269700	1.26230900	-0.15355800
6	3.77314300	0.16844300	-0.08243200
6	1.69326600	-1.12200400	-0.03417100
1	1.16796300	-2.06245000	-0.16772900
6	0.97798000	-0.01805500	0.25017100
6	-3.09791700	-2.52906300	-0.06125300
1	-2.48096000	-3.33431900	-0.44758800
6	-4.46379600	-2.63037900	-0.00230100
1	-4.95654600	-3.53844100	-0.33846200
6	-5.24837300	-1.55370800	0.49729800
1	-6.32840400	-1.65508300	0.55147500
6	-4.63325700	-0.40985400	0.95303700
1	-5.22672900	0.38693700	1.39341400
6	-3.22384800	-0.25595500	0.86538700
6	-2.42298500	-1.33839000	0.36540800
6	-0.50515700	-0.07068200	0.42960000
1	-0.83505900	0.47003900	1.32818500
6	-1.21085800	1.29122400	-0.74550000
1	-0.73172500	0.88623300	-1.63689500
6	-2.63921400	1.26941700	-0.82888600
7	-1.10216200	-1.25211600	0.14832700
1	-2.76219800	0.50054500	1.48890700

TS-tf-B
E(RB3LYP)=-1346.020772 a.u.

8	-3.22039100	1.43641300	0.30027400
6	-1.87554500	1.61649300	-0.21480000
6	-1.26824600	2.64644800	0.74644900
6	0.22268700	2.88025300	0.51451600
6	-2.00178700	2.16040700	-1.65155200
6	3.37130700	1.03298600	1.63020000
6	3.10142900	2.95532800	-0.01589000
1	-1.43285300	2.28198500	1.76627400
1	-1.81941200	3.58769600	0.64773300
1	0.56694800	3.67487000	1.18729300
1	0.39253500	3.25240000	-0.50255900
1	-1.02455200	2.35293900	-2.10480000
1	-2.57280000	3.09416400	-1.64973200
1	-2.52276100	1.43322700	-2.27988100
1	4.39200400	0.92282900	1.25462000
1	2.96726700	0.05725900	1.90746500
1	3.42625600	1.63480700	2.55365700
1	3.07420400	3.81164700	0.67758500
1	2.56404200	3.26640200	-0.91444300
1	4.14865100	2.77536900	-0.26679300
6	-3.21702500	-0.87465100	-0.36947000
6	-3.96183800	-2.02356300	-0.67323800
1	-3.43243200	-2.94273800	-0.90908800
6	-5.35440500	-1.99497600	-0.66109700
1	-5.91930600	-2.89105600	-0.89757400
6	-6.01962200	-0.81015700	-0.33109800
1	-7.10524100	-0.78301200	-0.31379400
6	-5.30044800	0.34634800	-0.02601700
1	-5.79831100	1.27409100	0.23570800
6	-3.90768400	0.31044200	-0.05456400
6	-1.76529300	-0.85338400	-0.31097100
1	-1.23672000	-1.79953400	-0.34562600
6	-1.09172300	0.30636700	-0.19130600
6	3.13106900	-2.08796200	-0.52779700
1	2.68288900	-2.94619900	-0.04712400
6	4.42497600	-2.14199300	-0.99349700
1	4.99384600	-3.05878800	-0.86956700
6	5.02161400	-1.03274800	-1.63389700
1	6.04437600	-1.09457000	-1.99234900
6	4.26818500	0.10482000	-1.84766100
1	4.68344500	0.94147200	-2.40255100
6	2.93987700	0.18547500	-1.38513100
6	2.35306600	-0.90130400	-0.67427400
6	0.41207400	0.37691000	-0.28235700
1	0.64139600	0.82053300	-1.25456300
6	1.05295000	1.61164800	0.77333000
1	0.78749300	1.14647300	1.72620800
6	2.49323500	1.76712500	0.66761800
7	1.11608600	-0.81724200	-0.08122400
1	2.34189800	1.01002400	-1.74500200
5	0.82519200	-1.72455000	1.26188500
9	0.33066100	-2.95014000	0.84501400
9	2.04072100	-1.87226300	1.93476900
9	-0.05931700	-1.00560100	2.05031500

TS-cf
E(RB3LYP)=-1021.430246 a.u.

8	-2.88817800	1.09651500	-0.79913400
6	-1.47396700	0.74696400	-0.95416000
6	-0.77450700	2.11576500	-0.79403900
6	0.74348400	2.07074800	-0.58935000
6	-1.30782700	0.15331300	-2.35949200
1	-1.23735300	2.60500800	0.07109100
1	-1.01851000	2.72973300	-1.66811000
1	1.11019800	3.10406300	-0.52948500
1	1.23527600	1.61535500	-1.45423100
1	-0.26458500	-0.10864800	-2.54298100
1	-1.65929200	0.87187300	-3.10686700
1	-1.90233000	-0.76086100	-2.44721000
6	-3.32610000	-0.78312000	0.64894100
6	-4.28033300	-1.60327700	1.26457900
1	-3.94136800	-2.38727900	1.93744000
6	-5.64170200	-1.42384700	1.02482700
1	-6.37012600	-2.06742200	1.50785000
6	-6.05994400	-0.40780400	0.16136300
1	-7.11855300	-0.25867600	-0.03073300
6	-5.12728000	0.42016000	-0.46508000
1	-5.43376600	1.21550800	-1.13636600
6	-3.76614700	0.23056700	-0.22383900
6	-1.89315200	-0.90399600	0.86555600
1	-1.54721500	-1.59637000	1.63108200
6	-1.00410400	-0.22011600	0.12464700
6	0.46832900	-0.41051000	0.33744700
6	1.13430000	1.31608900	0.68228500
7	1.18417700	-0.88503400	-0.71967500
6	2.76538100	1.33295700	2.59838500
1	2.72566700	2.36827100	2.96858500
1	2.01445700	0.76518200	3.15751100
1	3.75689000	0.94284900	2.84644700
6	3.58402600	1.90689000	0.25157600
1	4.57468000	1.55390800	0.54990300
1	3.44848100	1.68395800	-0.80772200
1	3.57840100	3.00297700	0.36165000
1	0.65251400	-0.85171200	1.32717000
1	0.45151900	1.51532000	1.51270300
6	2.48624900	-1.13896900	-0.50065600
6	3.31415800	-1.42949900	-1.63405800
6	3.12497000	-1.00823500	0.77644200
6	4.67351500	-1.56221400	-1.50392300
1	2.82150400	-1.52120500	-2.59704900
6	4.52577600	-1.19126200	0.88552400
1	2.53312200	-1.08923300	1.67881800
6	5.29491700	-1.42913900	-0.23262000
1	5.28465000	-1.77195600	-2.37737400
1	4.99201500	-1.14709400	1.86660600
1	6.37054500	-1.55056100	-0.14402400
6	2.49985500	1.31189100	1.11166300

TS-cf-B
E(RB3LYP)=-1346.011914 a.u.

8	-3.04219400	-1.02796300	1.01139700
6	-1.74669400	-0.36419900	1.19768800
6	-0.97596700	-1.38638400	2.06096200
6	0.54394400	-1.34127400	1.90306400
6	-2.00919300	0.92474400	1.98857000
1	-1.33319400	-2.38459500	1.78332800
1	-1.25313700	-1.23337400	3.10866900
1	0.99178100	-2.05180400	2.60761000
1	0.93944600	-0.35007700	2.14933500
1	-1.07927900	1.37125200	2.33841100
1	-2.63451500	0.66465300	2.84899400
1	-2.52409500	1.66658500	1.37750100
6	-3.37591700	0.04573700	-1.10443200
6	-4.26912500	0.48822100	-2.08959900
1	-3.87341700	0.93392200	-2.99862300
6	-5.64456300	0.35957400	-1.90993800
1	-6.32899600	0.71120200	-2.67537700
6	-6.13794600	-0.23160200	-0.74227300
1	-7.20937800	-0.33797700	-0.59942900
6	-5.26682300	-0.68052500	0.25104300
1	-5.63175600	-1.14165600	1.16270200
6	-3.89228600	-0.52912000	0.07199300
6	-1.93070600	0.05688600	-1.24265200
1	-1.51811500	0.22992200	-2.23457700
6	-1.10975500	-0.13772400	-0.19217800
6	0.37172800	-0.22910300	-0.48823700
6	0.90662600	-1.72609900	0.46469100
7	1.24340300	0.81713900	-0.22710800
5	0.82110200	2.21982300	0.50960500
9	1.65200100	3.20345000	0.00933200
9	-0.49379300	2.47213300	0.18508400
9	1.01642100	2.03534400	1.88612900
6	2.38352700	-3.25898200	-0.88199500
1	2.28103600	-4.24035900	-0.39427500
1	1.61317800	-3.20761600	-1.65695700
1	3.37094000	-3.23448500	-1.34917000
6	3.37246900	-1.98446700	1.08919000
1	4.31235300	-1.84887100	0.54434400
1	3.22966000	-1.14372000	1.76692800
1	3.48892700	-2.89513600	1.69843600
1	0.49242600	-0.65031300	-1.48587600
1	0.16081300	-2.38839100	0.01580100
6	2.56227500	0.64129900	-0.61671200
6	3.60323800	1.35399400	0.04738300
6	2.94453600	-0.31050200	-1.59379600
6	4.92572700	1.11869800	-0.26505700
1	3.34567900	2.06569300	0.81725700
6	4.29457400	-0.50876200	-1.92499200
1	2.19599200	-0.78976100	-2.21127300
6	5.28887900	0.18314700	-1.25532800
1	5.69916100	1.66174600	0.26996200
1	4.54843100	-1.21311900	-2.71199600
1	6.33459900	0.02350500	-1.49967000
6	2.21779200	-2.18538200	0.15820500

TS-b
E(RB3LYP)=-1021.382279 a.u.

6	-4.92076900	-1.57220000	-0.97086600
6	-5.21697100	-1.15293800	0.33004200
6	-4.26736900	-0.46589800	1.08810900
6	-3.01826900	-0.19975900	0.53001300
6	-2.69311200	-0.62707200	-0.76683000
6	-3.66195500	-1.31509100	-1.51060800
8	-2.07074400	0.41933700	1.28881100
6	-1.04051100	1.23020600	0.62429000
6	-0.47104300	0.44804100	-0.59105000
6	-1.33733700	-0.37634100	-1.22286000
6	-0.12354000	1.47998700	1.84715100
6	1.26385200	2.12303700	1.67264600
6	2.21416400	1.45754100	0.71752800
6	0.89185100	0.54764800	-1.34175600
6	-1.75107100	2.52021000	0.16836900
6	2.14045700	1.66521700	-0.69816800
6	1.72458400	-1.10330200	0.80679100
6	2.01239500	-1.36189700	-0.57302900
7	1.56800500	-0.62945400	-1.60472700
6	2.41900700	-1.79810500	1.82327800
6	3.37810800	-2.73633000	1.50482500
6	3.64644300	-3.03783600	0.14252400
6	2.98260800	-2.38235600	-0.86342700
6	3.45963300	1.34623300	-1.41540500
6	1.65434700	3.05151900	-1.16973900
1	-5.66515000	-2.10367600	-1.55538000
1	-6.19473900	-1.35665800	0.75673300
1	-4.47687600	-0.13426400	2.09968700
1	-3.41480600	-1.65267700	-2.51388600
1	-1.00891400	-0.90014300	-2.11674800
1	-0.00822100	0.52077500	2.35654400
1	-0.70360100	2.10456600	2.53535200
1	1.71932200	2.14952200	2.66833700
1	1.13662700	3.17297200	1.37348100
1	3.12604900	1.04103200	1.12699400
1	0.68475800	1.05280200	-2.29241900
1	-1.05860500	3.26217500	-0.23064800
1	-2.27492100	2.96399000	1.02050900
1	-2.48229900	2.29264800	-0.61118000
1	2.16550600	-1.60862000	2.86337200
1	3.90521500	-3.27147200	2.28919000
1	4.39097400	-3.79112000	-0.10030500
1	3.19388300	-2.57808500	-1.90999100
1	3.31598100	1.24860900	-2.49432400
1	3.90993700	0.42109000	-1.05372700
1	4.16801700	2.16352500	-1.23128300
1	1.62924200	3.08171200	-2.26270800
1	2.35447900	3.82316200	-0.83163000
1	0.66404300	3.31680700	-0.80936400
1	0.80100300	-0.61028900	1.05502400

TS-b-B
E(RB3LYP)=-1345.984982 a.u.

6	-4.82871900	-2.30624400	0.12390100
6	-5.42847800	-1.19830000	0.73155400
6	-4.71658400	-0.01013600	0.90549100
6	-3.39840100	0.05767200	0.46020800
6	-2.77139700	-1.04597300	-0.13726800
6	-3.50407800	-2.23038600	-0.30083200
8	-2.67868500	1.19617300	0.68540600
6	-1.59827500	1.54661200	-0.23948700
6	-0.73190500	0.28923600	-0.51638500
6	-1.37115900	-0.90318500	-0.49133300
6	-0.96748100	2.70367100	0.57420200
6	0.37281000	3.32389100	0.13342700
6	1.53555300	2.39191700	-0.00726800
6	0.73516100	0.15993300	-0.99935700
6	-2.28264600	2.05628800	-1.52292700
6	1.75125200	1.59231700	-1.17619500
6	1.17945800	0.40515800	1.76006800
6	1.81266500	-0.61761900	0.99486700
7	1.51605500	-0.80026900	-0.32997400
6	1.59778800	0.69495800	3.07172300
6	2.62904800	-0.01787100	3.65054900
6	3.23442800	-1.06473800	2.92075000
6	2.84518700	-1.37090600	1.63497800
6	3.20983400	1.13555200	-1.32483900
6	1.28684700	2.20005400	-2.51871500
1	-5.39020400	-3.22550400	-0.00854700
1	-6.45905200	-1.25644000	1.06916300
1	-5.16327700	0.85837300	1.37788900
1	-3.02085800	-3.08954600	-0.75794600
1	-0.82142500	-1.80986000	-0.73208900
1	-0.87774400	2.35981500	1.60684000
1	-1.71390500	3.50414500	0.59596900
1	0.62046000	4.09394100	0.87102800
1	0.22822900	3.84301600	-0.82293700
1	2.33891100	2.46962400	0.71627600
1	0.70520900	-0.13699300	-2.04464600
1	-1.57621200	2.48280900	-2.23635900
1	-3.01099300	2.82916400	-1.25901900
1	-2.80733200	1.23781100	-2.02157700
1	1.07229500	1.46090500	3.63533200
1	2.94893600	0.19576000	4.66564900
1	4.03293900	-1.64177400	3.37823800
1	3.33759000	-2.15615600	1.08229300
1	3.29665900	0.35040800	-2.07688900
1	3.62337300	0.75886000	-0.38791600
1	3.81390100	1.99403800	-1.64018200
1	1.51095400	1.49705100	-3.32459100
1	1.83703900	3.12571900	-2.71621400
1	0.22345100	2.42270400	-2.55495700
5	2.03945500	-2.04310800	-1.26554400
9	3.31973900	-2.42157300	-0.90342600
9	2.02566100	-1.57159300	-2.58075600
9	1.11017000	-3.05672200	-1.07742900
1	0.22529100	0.77775000	1.43129700

trans-**4**
E(RB3LYP)=-1021.478530 a.u.

8	-3.01408700	-1.29653500	-0.34853100
6	-1.68942100	-1.36429000	0.25061900
6	-0.94602500	-2.37712400	-0.63714200
6	0.54997300	-2.46211300	-0.32521900
6	-1.86781300	-1.86707100	1.69486100
6	3.48550200	-1.15905300	-1.62674700
6	3.27148600	-2.32309000	0.58698200
1	-1.09079900	-2.06046600	-1.67629600
1	-1.42052000	-3.35927800	-0.53247800
1	1.01136300	-3.18993400	-1.00265300
1	0.69375100	-2.85488000	0.68779500
1	-0.90676600	-1.98858100	2.20317500
1	-2.38592800	-2.83120300	1.69418000
1	-2.46294500	-1.15043000	2.26769100
1	4.57275500	-1.24634000	-1.53783700
1	3.26703400	-0.25631300	-2.20611700
1	3.12670900	-2.01987700	-2.20194200
1	3.06923300	-3.26897000	0.07785900
1	2.78749700	-2.35860300	1.56888600
1	4.35178800	-2.27784000	0.75569300
6	-3.14495300	1.08472200	0.00601400
6	-3.95364200	2.22666400	0.07337600
1	-3.48149200	3.19199500	0.23795000
6	-5.33774000	2.13628900	-0.07121700
1	-5.95086800	3.03037400	-0.01501800
6	-5.92800900	0.89006900	-0.29538800
1	-7.00489700	0.81038900	-0.41285900
6	-5.14314800	-0.26246000	-0.36587000
1	-5.58178900	-1.23901200	-0.54295600
6	-3.76125800	-0.16197000	-0.21109500
6	-1.69312600	1.11398200	0.11767000
1	-1.17814100	2.06880900	0.11562200
6	-0.97877600	-0.01742400	0.22262600
6	2.99186300	2.65767400	-0.18117300
1	2.32717200	3.47311400	-0.44772600
6	4.33595200	2.79684100	-0.16349900
1	4.78926600	3.75109800	-0.41712100
6	5.20727700	1.68494300	0.18967900
1	6.28102900	1.85015900	0.19717900
6	4.70505600	0.47897600	0.50854000
1	5.37578200	-0.33033900	0.78320900
6	3.22841000	0.19840000	0.53709200
6	2.36188000	1.38601700	0.14692000
6	0.53294600	-0.01819800	0.40191100
1	0.74763300	-0.27682300	1.45971100
6	1.24115600	-1.09547000	-0.47331900
1	1.07116300	-0.76031100	-1.50493200
6	2.79976300	-1.11462200	-0.24708600
7	1.07634900	1.29859100	0.11664000
1	2.96612500	-0.01476100	1.58953000

trans-**4**-**B**
E(RB3LYP)=-1346.065708 a.u.

6	5.08898400	-1.88812900	-1.36189900
6	5.79796400	-0.69739800	-1.18470200
6	5.14741300	0.45459200	-0.73909300
6	3.77986700	0.40996100	-0.47332500
6	3.04506800	-0.77571700	-0.65607700
6	3.72002600	-1.92012700	-1.10010400
8	3.16183900	1.57074300	-0.09947400
6	1.89773100	1.52267300	0.61804200
6	1.04872400	0.32865000	0.18934900
6	1.61346000	-0.74074700	-0.38837000
6	1.22696000	2.86392600	0.23505200
6	-0.29169800	2.92554000	0.47209800
6	-0.97230800	1.71498900	-0.19043900
6	-0.42178800	0.46870500	0.53815900
6	2.21797100	1.43965900	2.12139800
6	-2.51751800	1.70433200	-0.30007800
6	-2.82316200	0.38855700	-1.10221800
6	-2.25036000	-0.83514500	-0.39857100
7	-1.18272800	-0.77481100	0.34902600
6	-4.25284700	0.21791600	-1.54693000
6	-4.87360600	-0.97254700	-1.55651600
6	-4.17603500	-2.15908800	-1.09924600
6	-2.93586600	-2.10759600	-0.55997900
6	-2.99035200	2.93235200	-1.09938900
6	-3.22441700	1.68024100	1.06930000
1	5.59900900	-2.78354100	-1.70287200
1	6.86439000	-0.66291700	-1.38774900
1	5.67999800	1.38884400	-0.59496300
1	3.15616900	-2.83931300	-1.23578100
1	1.02674200	-1.62490700	-0.61614700
1	1.41897300	3.00947500	-0.83352700
1	1.73360300	3.67970200	0.76172900
1	-0.66385600	3.86578500	0.05441500
1	-0.52107000	2.94711600	1.54498800
1	-0.60257600	1.68011500	-1.22585000
1	-0.48026100	0.65572500	1.61755600
1	1.31521800	1.51929700	2.73370000
1	2.89636000	2.25358600	2.39455000
1	2.69352500	0.48382600	2.35415100
1	-4.74648500	1.09422100	-1.95204400
1	-5.88721200	-1.06824000	-1.93289400
1	-4.67280500	-3.12089000	-1.18975500
1	-2.43573900	-2.99987800	-0.21203500
1	-4.07816200	2.95509500	-1.20473600
1	-2.54876100	2.95825000	-2.10231200
1	-2.70856900	3.85564700	-0.58726700
1	-4.31049500	1.64002500	0.93620400
1	-2.99578600	2.58652800	1.63855800
1	-2.93735200	0.81819600	1.67778600
5	-0.82810700	-2.00834500	1.43505500
9	-2.01781400	-2.25224600	2.09187600
9	0.13875500	-1.50371500	2.27125900
9	-0.40304400	-3.08933800	0.67805700
1	-2.25628700	0.48181000	-2.04787600

cis-**4**
E(RB3LYP)=-1021.476399 a.u.

8	-2.88697600	1.16813000	-0.71434100
6	-1.49678100	0.76556400	-0.90822800
6	-0.73119500	2.10205000	-0.89940500
6	0.78924800	1.94946000	-0.76557900
6	-1.40352400	0.04227100	-2.26080500
1	-1.11252600	2.68317300	-0.05135500
1	-0.98341000	2.66176700	-1.80694000
1	1.23265500	2.94964600	-0.75578100
1	1.19788200	1.43446700	-1.64130800
1	-0.38046800	-0.28596400	-2.45561100
1	-1.74260800	0.70693700	-3.06212900
1	-2.03860200	-0.84824200	-2.25070000
6	-3.32723900	-0.74484500	0.68701600
6	-4.28067400	-1.58981200	1.26900500
1	-3.94312200	-2.38174800	1.93325600
6	-5.64034000	-1.42393700	1.00915800
1	-6.36745800	-2.08831800	1.46546000
6	-6.05950700	-0.39396700	0.16305300
1	-7.11694500	-0.25496100	-0.04266300
6	-5.12791300	0.45993400	-0.42949000
1	-5.43414500	1.26637900	-1.08762500
6	-3.76870900	0.28054100	-0.17264100
6	-1.89615600	-0.83454600	0.94370900
1	-1.55681700	-1.49794600	1.73730800
6	-1.01079500	-0.12739700	0.22502200
6	0.48086200	-0.21953300	0.46698500
6	1.15718800	1.18551900	0.52306300
7	1.13604300	-1.03700300	-0.55654000
6	2.91505400	1.53419800	2.31100900
1	2.66432100	2.59600700	2.40786000
1	2.28328900	0.97888500	3.01356700
1	3.95665200	1.41343500	2.62706900
6	3.58754800	1.89372200	-0.07488200
1	4.63654900	1.80565000	0.22150500
1	3.51267200	1.56891600	-1.11632800
1	3.32328900	2.95422600	-0.03028200
1	0.61716300	-0.70120300	1.45122400
1	0.68476000	1.72577700	1.35383400
6	2.41426900	-1.14190600	-0.40382300
6	3.18889600	-1.91322500	-1.36483700
6	3.11871800	-0.47386600	0.76603900
6	4.52570700	-2.05875100	-1.22486900
1	2.63961600	-2.35820900	-2.18839600
6	4.60018900	-0.71600200	0.81315400
1	2.69436900	-0.93460300	1.67628500
6	5.24148900	-1.45504100	-0.10980200
1	5.09011600	-2.63842900	-1.95006200
1	5.15239000	-0.28963100	1.64648500
1	6.31238400	-1.62057900	-0.03151300
6	2.69391600	1.05766200	0.86170600

cis-**4**-**B**
E(RB3LYP)=-1346.057091 a.u.

8	-3.02092000	-1.14868400	1.02739500
6	-1.66612300	-0.61111900	1.14989900
6	-0.88654200	-1.78595400	1.76857900
6	0.62832400	-1.69103000	1.57152700
6	-1.73435500	0.58309700	2.11186900
1	-1.25098700	-2.70389300	1.29315000
1	-1.13535400	-1.85725000	2.83249000
1	1.08917400	-2.56418500	2.04024400
1	1.03455600	-0.80920100	2.08121000
1	-0.74260700	0.96588000	2.35913700
1	-2.23326900	0.25857500	3.03065400
1	-2.29465800	1.40629500	1.66691800
6	-3.41196600	0.06902400	-1.00804200
6	-4.33857700	0.59945000	-1.91525400
1	-3.97262600	1.08952500	-2.81394300
6	-5.70766300	0.50483400	-1.67364000
1	-6.41607400	0.92488000	-2.38059700
6	-6.16215000	-0.13890000	-0.51885900
1	-7.22798900	-0.21958800	-0.32587400
6	-5.25761700	-0.67528900	0.39848700
1	-5.59204400	-1.17872000	1.29945900
6	-3.88890200	-0.56189300	0.15660700
6	-1.97363800	0.07640600	-1.21531900
1	-1.60222700	0.36267700	-2.19729300
6	-1.11460600	-0.24099500	-0.23280600
6	0.37441300	-0.32377300	-0.52480100
6	0.95606300	-1.64555500	0.06662100
7	1.21851600	0.82482400	-0.08318200
6	2.49536300	-3.01252400	-1.40197700
1	2.12254300	-3.94630100	-0.96877300
1	1.86745300	-2.77535000	-2.26819500
1	3.51111300	-3.20467900	-1.76176700
6	3.35974000	-2.27914500	0.83386800
1	4.38576900	-2.43607300	0.49050400
1	3.38274600	-1.51091300	1.61147700
1	3.02279900	-3.21331200	1.29100900
1	0.46702600	-0.36850600	-1.62076500
1	0.36579200	-2.44266100	-0.40140700
6	2.50996900	0.66289000	-0.25261200
6	3.47608700	1.61187300	0.25981900
6	2.99675300	-0.55115700	-1.00928600
6	4.79387400	1.46496200	-0.02646500
1	3.12701800	2.41737900	0.88810300
6	4.46583700	-0.56968800	-1.29654200
1	2.48961000	-0.49854600	-1.98841100
6	5.30003400	0.38447200	-0.84741600
1	5.50270900	2.18086100	0.37998000
1	4.84108500	-1.39410900	-1.89488700
1	6.36054100	0.34987200	-1.07660800
6	2.45234400	-1.88778500	-0.34828200
5	0.66744000	2.34848400	0.36761600
9	-0.66874100	2.41751500	0.07989400
9	0.95486200	2.45188700	1.72295300
9	1.40259800	3.23586500	-0.39358400

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10
E(RB3LYP)=-1021.391335 a.u.
8                -2.45686400     1.26276800    -0.40466900
6                -1.07651400     0.82568400    -0.61606500
6                -0.38341400     2.25024100    -0.62405500
6                 1.17155600     2.33674300    -0.73672600
6                -1.01818800     0.19183600    -2.02488700
7                 1.46685700    -1.60712500     0.35021400
6                 0.62875400     1.71592200     2.16636300
6                 2.73835100     0.47776600     2.15537500
1                -0.73450300     2.77642300     0.26231700
1                -0.84572100     2.77131900    -1.46827100
1                 1.53904400     3.23755600    -0.23261600
1                 1.46450300     2.42488700    -1.79036100
1                -0.00481200    -0.11555000    -2.29781400
1                -1.37229500     0.91303600    -2.76799400
1                -1.65201800    -0.69701200    -2.06952900
1                 0.68629000     1.43665600     3.22340300
1                -0.42955800     1.74743500     1.91333200
1                 1.04016600     2.72707700     2.08063700
1                 3.27679700     1.42520100     2.27211400
1                 3.43441600    -0.24475400     1.73252200
1                 2.47846200     0.12601600     3.15941100
6                -3.12389600    -0.90636900     0.36332100
6                -4.15656900    -1.83273000     0.56600200
1                -3.92554000    -2.78328900     1.04023300
6                -5.46137100    -1.54015000     0.17489000
1                -6.25282700    -2.26601400     0.33289200
6                -5.74829900    -0.30336400    -0.41201100
1                -6.76501400    -0.06786300    -0.71279400
6                -4.73610100     0.63343000    -0.62379300
1                -4.93825900     1.59853700    -1.07640300
6                -3.43051200     0.32168200    -0.24612500
6                -1.75677200    -1.09070100     0.82003200
1                -1.56893400    -1.91942800     1.49912300
6                -0.73516800    -0.28380100     0.46767500
6                 3.52345100    -2.23614500    -0.68960400
1                 3.23589800    -3.28293600    -0.68255800
6                 4.81125600    -1.84748200    -0.86501900
1                 5.57370600    -2.59692400    -1.06176300
6                 5.23915600    -0.45932400    -0.71239300
1                 6.30457300    -0.24699500    -0.70368800
6                 4.33665200     0.53167200    -0.57215600
1                 4.64226000     1.56889800    -0.46121900
6                 2.87644000     0.20483800    -0.71789900
1                 2.73137300     0.16510800    -1.81739100
6                 2.52468900    -1.24282500    -0.29125900
6                 0.64727400    -0.60246800     1.10621000
1                 0.42798500    -1.11163100     2.05352700
6                 1.69587700     1.01871100    -0.18314300
1                 0.97259400     0.38847700    -0.67718400
6                 1.44473600     0.69908600     1.33458800
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10-B
E(RB3LYP)=-1345.986425 a.u.

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8              2.83275100    -1.57908700    -0.15850300
6              1.43129700    -1.32381300    -0.48004700
6              0.87501300    -2.78509200    -0.23144900
6             -0.65926300    -3.03451500    -0.34720200
6              1.36682400    -0.97830400    -1.98570900
7             -1.43974600     0.97225800     0.04917100
6             -0.22978000    -1.84178800     2.40122000
6             -2.46310600    -0.87205000     2.15991900
1              1.24258200    -3.10395100     0.74239100
1              1.40742100    -3.40699400    -0.95725400
1             -0.96492000    -3.85763600     0.30775300
1             -0.91525700    -3.33449100    -1.37098200
1              0.34022400    -0.82480100    -2.33211200
1              1.80856900    -1.79040100    -2.57143000
1              1.91769300    -0.05763500    -2.19013800
1             -0.34953700    -1.39055100     3.39091700
1              0.83126200    -1.79410100     2.16467100
1             -0.52540900    -2.89182600     2.48965400
1             -2.88453600    -1.83928500     2.45417600
1             -3.23533200    -0.33102300     1.61346800
1             -2.27038800    -0.30565300     3.07615300
5             -1.39541700     2.63075100     0.13156800
9             -1.36082300     3.08199400    -1.17336200
9             -0.26107900     2.96187200     0.85152200
9             -2.55044600     3.00461100     0.79428300
6              3.27310900     0.75277000     0.15291600
6              4.20683500     1.79931800     0.17208900
1              3.87076800     2.79891200     0.43439400
6              5.54439600     1.56098900    -0.13402800
1              6.25942300     2.37741100    -0.12161300
6              5.96444200     0.26347000    -0.44672200
1              7.00798400     0.07245800    -0.67943900
6              5.05284800    -0.79246500    -0.47145300
1              5.35919100    -1.80516500    -0.71157800
6              3.71290500    -0.53684800    -0.18409000
6              1.88367600     0.89859600     0.54964100
1              1.59463700     1.83028100     1.02301400
6              0.95082300    -0.05903700     0.36126600
6             -3.58253300     1.13237100    -1.07903400
1             -3.47407000     2.18848100    -1.27978500
6             -4.78568700     0.50911300    -1.18387300
1             -5.64318800     1.08967700    -1.51323200
6             -5.00256800    -0.88261700    -0.82206100
1             -6.01812700    -1.26530600    -0.79964400
6             -3.95108800    -1.67500000    -0.53991400
1             -4.06801800    -2.73191000    -0.31821300
6             -2.56058900    -1.13012300    -0.70427100
1             -2.38995600    -1.23784300    -1.79698300
6             -2.45886200     0.38714400    -0.52789200
6             -0.46242900     0.22312900     0.95618500
1             -0.32119900     0.92368700     1.77968500
6             -1.30641500    -1.69228800    -0.04254700
1             -0.63807000    -1.09166500    -0.64031300
6             -1.13273500    -1.08693000     1.39712900
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trans-**4**+**11** complex
E(RB3LYP)= -1272.152041 a.u.

6	-1.48118200	4.41897900	-1.58702500
6	-0.53733300	3.49708400	-0.85253700
6	-0.97211100	2.60043700	0.04811300
7	-2.32275300	2.41943900	0.37650200
6	-3.21395100	3.52594900	0.02887900
6	-2.94167700	3.96165000	-1.41527500
6	-2.77831100	-1.07397000	0.23240900
6	-4.20980700	-1.40423700	0.57776400
6	-4.72226100	-1.17254700	1.79837600
6	-3.87647500	-0.68034900	2.87858800
6	-2.53920900	-0.55948100	2.72411800
6	-1.88068900	-0.93059600	1.46667800
7	-0.60226800	-1.05999900	1.49012400
6	-2.12189800	-1.95724800	-0.87056000
1	-1.88714200	-0.28040400	3.54612500
1	-4.33572200	-0.45478600	3.83754100
1	-5.77379900	-1.35472400	2.00095800
1	-4.85306700	-1.76249200	-0.22047300
1	-2.82153000	-0.04207500	-0.16990200
1	-4.25024900	3.19171400	0.14526300
1	-3.06401400	4.38898900	0.69984900
1	-3.63700900	4.75953900	-1.69747400
1	-3.13951000	3.10882100	-2.07503400
1	-1.36448400	5.45349100	-1.22973600
1	-1.23089500	4.44952300	-2.65596100
1	0.52420600	3.54503900	-1.07315300
1	-0.29069500	1.91808900	0.54844200
1	-2.46840400	2.05123400	1.30848900
6	-2.16031600	-3.43821800	-0.44263400
1	-3.19581500	-3.78563800	-0.36829000
1	-1.65258300	-4.08260600	-1.16693000
1	-1.69506900	-3.59588700	0.53490200
6	-2.87463900	-1.78700500	-2.20428500
1	-2.41499100	-2.39024400	-2.99248600
1	-3.91836000	-2.10680600	-2.12911300
1	-2.86639300	-0.74146300	-2.53271700
6	1.67328700	-2.08072800	-1.94089100
1	2.21319000	-2.14123400	-2.89134500
1	1.94847000	-2.97345300	-1.36877900
6	0.14764500	-2.04875900	-2.18879200
1	-0.18250000	-3.07678600	-2.37197300
1	-0.06300200	-1.49760500	-3.11085200
6	-0.66838500	-1.41438100	-1.02859700
1	-0.77943700	-0.34403300	-1.24731300
6	0.11129700	-1.50571400	0.30054000
1	0.33734500	-2.57308000	0.47765500
6	5.58029000	-0.07083200	-0.15204300
6	4.19076400	0.90621700	2.06694600
6	5.55159500	1.17370800	1.92853200
6	6.24475700	0.67635800	0.82141600
1	6.10042600	-0.46532400	-1.01878800
1	3.64729100	1.26873900	2.93594700
1	6.07129000	1.75714800	2.68223500

1	7.30672100	0.87517500	0.70956100
8	3.59572300	−1.08373900	−0.96520700
6	2.10809300	−0.25900900	1.23971000
1	1.62144600	−0.19178100	2.20763200
6	1.46554700	−0.81677900	0.20054400
6	3.49907000	0.15931200	1.10334200
6	4.21427700	−0.31600900	−0.01700600
6	2.16895200	−0.86497700	−1.15175500
6	2.00624600	0.44696000	−1.94026500
1	2.43980400	1.27845500	−1.37853700
1	2.52584700	0.36721500	−2.90097500
1	0.95655600	0.68618900	−2.12522800

TS-6
E(RB3LYP)= -1272.134988 a.u.

6	-2.19583000	3.51863400	-1.99435400
6	-1.13429600	3.10426800	-1.00928800
6	-1.36391900	2.29966100	0.03007000
7	-2.67069100	1.73542300	0.30240700
6	-3.80599400	2.37647100	-0.42021100
6	-3.43575200	2.61937000	-1.88126100
6	-2.62307700	-1.02314500	0.52419500
6	-4.03274200	-1.05648500	0.78742600
6	-4.58754300	-0.55525200	1.94371000
6	-3.71060300	-0.11021800	2.98012600
6	-2.34871100	-0.17701900	2.84477600
6	-1.70967000	-0.71006600	1.64687400
7	-0.40164900	-0.76150800	1.62510900
6	-2.01209500	-1.84988000	-0.62235600
1	-1.68548300	0.10641900	3.65713700
1	-4.13514700	0.26657400	3.90869800
1	-5.66297200	-0.53424700	2.08579800
1	-4.69469100	-1.43045000	0.00940300
1	-2.66310600	0.50765600	0.18197200
1	-4.66240200	1.70676500	-0.31748900
1	-4.04276600	3.32240800	0.08017300
1	-4.29258500	3.06453500	-2.39628800
1	-3.23799000	1.65559000	-2.36382100
1	-2.46700500	4.57091700	-1.82573300
1	-1.79270700	3.47643700	-3.01288900
1	-0.12115300	3.46773800	-1.15232400
1	-0.59729700	1.94606400	0.71058000
1	-2.84330100	1.74312800	1.31403600
6	-2.00469300	-3.33826100	-0.19402600
1	-3.03227100	-3.68658800	-0.04643800
1	-1.54195600	-3.98729800	-0.94575900
1	-1.47454400	-3.47870300	0.75163600
6	-2.81939600	-1.71767800	-1.92885500
1	-2.36841100	-2.31230800	-2.72891400
1	-3.84784100	-2.07296400	-1.81391900
1	-2.85966600	-0.67659200	-2.27220600
6	1.74089600	-2.02254400	-1.82132700
1	2.24772100	-2.14415900	-2.78460000
1	2.02485400	-2.88327800	-1.20667400
6	0.20857300	-1.98331100	-2.01924500
1	-0.13474800	-3.01363300	-2.15602000
1	-0.02395500	-1.46654300	-2.95687500
6	-0.56848100	-1.29968300	-0.85784900
1	-0.70189300	-0.24333300	-1.13001600
6	0.25627600	-1.30949100	0.45206800
1	0.49921800	-2.36996600	0.66231100
6	5.71064900	0.08811400	-0.29430600
6	4.39595400	1.20147700	1.90431300
6	5.75154500	1.45881300	1.70412800
6	6.40793400	0.89347500	0.60756700
1	6.20149800	-0.36092800	-1.15172600
1	3.88234300	1.61538000	2.76864500
1	6.29588900	2.08618500	2.40345900

1	7.46559200	1.08301900	0.44795500
8	3.70192900	−0.96979100	−0.97819400
6	2.28529900	−0.00902200	1.22271300
1	1.82126100	0.12075800	2.19545800
6	1.60926700	−0.63732900	0.24673600
6	3.67108700	0.39694500	1.01403000
6	4.35021800	−0.14726300	−0.09830100
6	2.26704300	−0.76790400	−1.12036600
6	2.07218200	0.49552600	−1.98056600
1	2.50544200	1.36397200	−1.47711700
1	2.57233100	0.36685600	−2.94640700
1	1.01393900	0.70228800	−2.15762700

IN1
E(RB3LYP)= -1272.135132 a.u.

6	-2.31746700	3.98467100	-1.66121800
6	-1.25019000	3.28557100	-0.86042200
6	-1.46626400	2.24116900	-0.06578500
7	-2.82286100	1.69900200	0.12079800
6	-3.93964900	2.58155300	-0.34089400
6	-3.61520100	3.16396200	-1.71304300
6	-2.56392100	-1.40145300	0.52439200
6	-3.95859400	-1.32966800	0.58491600
6	-4.66131600	-0.59737900	1.55832400
6	-3.91390500	0.05352900	2.55383000
6	-2.52407100	0.04810800	2.52246900
6	-1.76540700	-0.66773100	1.50877400
7	-0.44818000	-0.52762200	1.50895700
6	-1.83683100	-2.31227700	-0.47674900
1	-1.94397000	0.53543600	3.30131900
1	-4.42364400	0.58358500	3.35681600
1	-5.74597400	-0.59845000	1.57576900
1	-4.54134800	-1.87748900	-0.15184200
1	-2.88665500	0.74925800	-0.29863800
1	-4.84256500	1.96878900	-0.33149800
1	-4.04654300	3.37171400	0.40799200
1	-4.45504600	3.77952400	-2.04850400
1	-3.51164000	2.34609000	-2.43629600
1	-2.50625000	4.97598900	-1.22535900
1	-1.94876500	4.17295300	-2.67597800
1	-0.22965900	3.65021700	-0.93499600
1	-0.72256300	1.67871300	0.49615800
1	-2.92995200	1.43335300	1.13792700
6	-1.71805200	-3.72841200	0.14202000
1	-2.71608300	-4.12160700	0.36029700
1	-1.22126800	-4.42893800	-0.53858700
1	-1.16286800	-3.71316700	1.08373100
6	-2.61050900	-2.43339600	-1.80675300
1	-2.06262400	-3.04908400	-2.52569400
1	-3.58633200	-2.90786400	-1.66972500
1	-2.77625600	-1.45068900	-2.26480000
6	1.76735000	-1.76778900	-2.06920300
1	1.57391600	-1.35385800	-3.06531400
1	2.61731900	-2.44703700	-2.17675200
6	0.52994000	-2.55362100	-1.58650600
1	0.85901000	-3.38860900	-0.95620500
1	0.04013800	-3.00309500	-2.45651400
6	-0.43434100	-1.68534500	-0.76250200
1	-0.63082300	-0.75585200	-1.32120800
6	0.29641800	-1.32309200	0.55002300
1	0.53251100	-2.30053400	1.01811600
6	5.67337000	0.38048900	-0.44716800
6	4.48001300	1.07854700	1.98049300
6	5.79890100	1.45112900	1.72367100
6	6.39545400	1.09339200	0.51152200
1	6.11716600	0.09210800	-1.39466400
1	4.01405800	1.33220400	2.92955900
1	6.36186200	2.00787200	2.46675500

1	7.42455500	1.37434300	0.30630200
8	3.67863800	−0.70519000	−1.12664700
5	2.38635800	−0.14130300	1.26978100
1	1.96790200	−0.09941700	2.27121700
6	1.66153800	−0.68711000	0.27781600
6	3.73315500	0.36100000	1.03554300
6	4.34870500	0.02916600	−0.18933200
6	2.22061400	−0.61088600	−1.14131400
6	1.86784500	0.75548100	−1.76687000
1	2.24684000	1.57067100	−1.14412000
1	2.31559700	0.83419100	−2.76352600
1	0.78447900	0.87071300	−1.86175000

trans-**5**+**11** complex
E(RB3LYP)= -1272.192387 a.u.

6	3.31988700	4.41769300	-0.43137600
6	2.27562600	3.51072500	-1.03787200
6	2.35375800	2.17215800	-0.94261800
7	3.38018300	1.49688400	-0.27523800
6	4.59772400	2.26734300	-0.03411000
6	4.22394900	3.63819300	0.54198100
6	2.23837100	-1.98280300	-0.02082500
6	3.50207500	-2.57157400	-0.17596200
6	4.11630600	-2.71989400	-1.41793600
6	3.45650700	-2.26336100	-2.56086700
6	2.19925400	-1.68409800	-2.44670300
6	1.57283400	-1.54669400	-1.19340500
7	0.31006700	-0.94300700	-1.12678800
6	1.62315000	-1.82111100	1.38733700
1	1.67818100	-1.33084800	-3.33370600
1	3.91600400	-2.36214900	-3.54009600
1	5.09532200	-3.18277100	-1.49118600
1	4.02428400	-2.92681900	0.70736200
1	5.23255700	1.71304200	0.66529200
1	5.17460100	2.41212100	-0.96394900
1	5.13371100	4.20455100	0.76921100
1	3.69292200	3.47959000	1.48771300
1	3.92945800	4.88727200	-1.21867500
1	2.84090500	5.24989000	0.10220900
1	1.42269200	3.95272900	-1.54332200
1	1.58277700	1.52356100	-1.34851700
1	3.53709900	0.55582400	-0.61315400
6	1.25517900	-3.20961400	1.95988400
1	2.13432400	-3.86075600	1.98225100
1	0.87943200	-3.12540700	2.98494400
1	0.49361900	-3.71484400	1.35788700
6	2.64901400	-1.14698400	2.32955800
1	2.21131300	-0.97394500	3.31810900
1	3.53337600	-1.77291900	2.47864900
1	2.97262700	-0.18487000	1.92077200
6	-1.43291800	0.45237200	2.36881100
1	-0.82858800	1.34024100	2.58548800
1	-2.24222400	0.42860000	3.10317100
6	-0.54375500	-0.79372200	2.50552000
1	-1.16490600	-1.69581100	2.57760800
1	0.02210800	-0.72737300	3.44009900
6	0.37946600	-0.88809400	1.28438700
1	0.77786400	0.11724300	1.09094700
6	-0.47856600	-1.25687800	0.06686400
1	-0.67706700	-2.34290500	0.10647100
6	-5.67739400	1.12235500	0.35447900
6	-5.09628400	-0.59837600	-1.77103100
6	-6.35025300	0.00419500	-1.69077300
6	-6.63778900	0.85930400	-0.62280800
1	-5.88350000	1.78052700	1.19198000
1	-4.86658200	-1.27751800	-2.58851900
1	-7.10033100	-0.19534800	-2.44946300
1	-7.61428200	1.32929000	-0.55082900
8	-3.51827700	0.74998200	1.25627100

6	−2.80640300	−0.98329400	−0.78048300
1	−2.64069900	−1.83085600	−1.44491100
6	−1.83359800	−0.56866900	0.04959900
6	−4.11532800	−0.34742000	−0.80267000
6	−4.41884800	0.52834900	0.25781700
6	−2.09008500	0.62587000	0.96601500
6	−1.63937800	1.93132000	0.28989100
1	−2.16088600	2.07009300	−0.66172200
1	−1.86713600	2.78069200	0.94214000
1	−0.56348600	1.92237000	0.09369300
1	−0.21604500	−1.00323100	−1.99017900

TS-5-tf
E(RB3LYP)= -1021.354302 a.u.

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7            1.64648100     0.02953300     1.80606000
6            2.15063600     0.95820000     0.87979900
6            3.16562200     0.19211600     0.19435400
6            2.03691400     2.33368100     0.74680600
6            3.13187500     2.98888700     0.15771200
6            4.26313600     2.29326100    -0.31492600
6            4.29609100     0.90524000    -0.31685800
1            1.25647600     2.90281200     1.24258300
1            3.14449500     4.07568000     0.14317100
1            5.11719100     2.85978400    -0.67347500
1            5.17371700     0.38229000    -0.68697500
1            3.02169800    -0.47592400     1.29620400
6            1.37633900    -1.73280400     0.11180100
1            1.92918800    -2.51003200     0.65553300
6            0.66739900    -0.90070300     1.30207700
1            0.51291200    -1.63868300     2.10205900
8           -2.54994100    -1.22071800    -0.53536800
6           -3.11927900     0.02195900    -0.47689000
6           -4.32155100     0.22995900    -1.15166900
1           -4.78128300    -0.60387500    -1.67200000
6           -4.90816100     1.49596200    -1.13797600
1           -5.85005800     1.65374300    -1.65520300
6           -4.29681700     2.55259600    -0.45715200
1           -4.75839600     3.53501600    -0.44450600
6           -3.08482700     2.34139100     0.19733700
1           -2.59139000     3.16216900     0.71207700
6           -2.47368200     1.07973000     0.19758100
6           -1.15855000     0.81233400     0.76823200
1           -0.54193300     1.65471000     1.05989600
6           -0.70726400    -0.44812000     0.87274800
6           -1.67168100    -1.59359500     0.56582100
6           -2.54223700    -1.92906700     1.78760500
1           -3.15869100    -1.07222000     2.07068100
1           -3.19889400    -2.77471200     1.55843800
1           -1.91663900    -2.19615300     2.64480300
6           -0.91123600    -2.83802300     0.06639300
1           -1.60845400    -3.43898200    -0.52551100
1           -0.61066400    -3.44975700     0.92531800
6            0.31091700    -2.43383000    -0.76148900
1           -0.04493500    -1.76807100    -1.55132400
1            0.74742100    -3.30860100    -1.25710800
6            2.45263800    -0.94807900    -0.71217900
6            3.53758500    -1.93946400    -1.17098800
1            4.27675900    -1.45079200    -1.81300400
1            4.06216400    -2.38272300    -0.31849200
1            3.09080600    -2.75163300    -1.75426500
6            1.87257300    -0.22752800    -1.95037000
1            2.63363700     0.41737700    -2.39769100
1            1.55728700    -0.94379800    -2.71520600
1            1.01311000     0.39676100    -1.69208700
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trans-**5**
E(RB3LYP)= -1021.525991 a.u.

6	-5.25205700	2.21034800	-0.34615300
6	-5.88269100	0.96630000	-0.42580200
6	-5.13811700	-0.21203900	-0.34911800
6	-3.75436300	-0.14057800	-0.19272700
6	-3.09961200	1.10159900	-0.11639400
6	-3.86717400	2.27032700	-0.19525400
8	-3.04831300	-1.30723500	-0.18844200
6	-1.70895000	-1.36432500	0.37991300
6	-0.97078400	-0.03453500	0.27938000
6	-1.64969500	1.09610400	0.02706000
6	-0.99058700	-2.40993600	-0.49592700
6	0.51765300	-2.47897400	-0.24157400
6	1.20453900	-1.11352900	-0.43867500
6	0.53358900	-0.09110000	0.50785500
6	-1.86655500	-1.82061000	1.84107400
6	2.76340400	-1.16058500	-0.28763600
6	3.33190700	0.26253100	-0.15454200
6	2.51113600	1.35568200	0.19126100
7	1.13041700	1.21929900	0.33676600
6	4.70437300	0.50386400	-0.31303900
6	5.26795600	1.76644500	-0.14822800
6	4.44053200	2.83944300	0.18914700
6	3.07824900	2.63400300	0.35502100
6	3.33847100	-1.84369600	-1.55145900
6	3.20114000	-1.97202000	0.95816400
1	-5.83391800	3.12469500	-0.40521100
1	-6.96057700	0.90895100	-0.54616500
1	-5.60899700	-1.18731900	-0.41448700
1	-3.36398100	3.23256000	-0.13927800
1	-1.12941800	2.04212100	-0.08487000
1	-1.17686700	-2.13158700	-1.53921000
1	-1.45749000	-3.38850500	-0.33707700
1	0.95350800	-3.22490100	-0.91320400
1	0.70202400	-2.84105600	0.77634100
1	0.99263100	-0.76554600	-1.45936700
1	0.69645800	-0.45937800	1.53992000
1	-0.89986100	-1.97781400	2.32739500
1	-2.42821500	-2.75900200	1.87350100
1	-2.41557300	-1.06643200	2.41221700
1	5.35846800	-0.32574500	-0.56385500
1	6.33588600	1.90928100	-0.27924500
1	4.85454600	3.83464400	0.32385600
1	2.42694500	3.46652800	0.61195400
1	4.42067200	-1.97929600	-1.48021200
1	3.13338400	-1.24769700	-2.44602800
1	2.90471600	-2.83774500	-1.69516000
1	4.28489200	-1.90078300	1.08643100
1	2.94842700	-3.03276700	0.86441000
1	2.74238700	-1.58852300	1.87557600
1	0.71934800	1.92977800	0.92786600

cis-**5**
E(RB3LYP)= -1021.522845 a.u.

8	-2.80938900	1.01129700	-0.97638500
6	-1.42426900	0.54995500	-1.01381600
6	-0.61992800	1.83016900	-1.29952400
6	0.88580700	1.68916300	-1.04430400
6	-1.31070200	-0.47542700	-2.15338000
1	-1.02419700	2.61310200	-0.64713300
1	-0.81126400	2.14671100	-2.33081300
1	1.35422100	2.65531500	-1.24954900
1	1.33345100	0.97043700	-1.73954700
1	-0.27803800	-0.81132000	-2.26887400
1	-1.65404400	-0.02404200	-3.08963400
1	-1.93401100	-1.34934200	-1.94064400
6	-3.36167400	-0.54927500	0.77635700
6	-4.35989400	-1.24327700	1.47265400
1	-4.07359800	-1.87286200	2.31166700
6	-5.69956900	-1.12905700	1.10616000
1	-6.46272000	-1.67401100	1.65267900
6	-6.05336900	-0.30178000	0.03641100
1	-7.09563100	-0.20328400	-0.25282100
6	-5.07687800	0.39902900	-0.67227600
1	-5.33297200	1.04746100	-1.50356400
6	-3.73651900	0.26890500	-0.30800200
6	-1.95000900	-0.57821000	1.13292500
1	-1.66814200	-1.02848200	2.08344900
6	-1.01333400	-0.04889500	0.32790700
6	0.45697500	-0.07998700	0.69506400
6	1.16505500	1.26435600	0.41050000
7	1.13334600	-1.12361300	-0.07690200
6	2.79979400	1.13454800	2.35036900
1	2.35870200	2.02772600	2.80947600
1	2.30775000	0.25499400	2.77333300
1	3.85291700	1.08689100	2.64392600
6	3.39747500	2.47903800	0.34063000
1	4.39276600	2.55623800	0.78718000
1	3.51791000	2.51777500	-0.74453900
1	2.83516000	3.36447900	0.65812300
1	0.51531300	-0.29239000	1.77420400
1	0.69841200	2.01220200	1.06674600
6	2.52558100	-1.18021800	-0.14229200
6	3.13768200	-2.35281700	-0.62216500
6	3.32153800	-0.06602600	0.20995300
6	4.51786100	-2.43480600	-0.75420800
1	2.51084800	-3.19864700	-0.89590300
6	4.70950500	-0.18024200	0.06062100
6	5.31654100	-1.34189400	-0.41352700
1	4.96776700	-3.35170600	-1.12435400
1	5.33846400	0.66265600	0.33000900
1	6.39614000	-1.39213500	-0.51372800
6	2.67640300	1.19342500	0.80484600
1	0.67205000	-2.02290300	-0.04571500

3-B
E(RMPWB1K)= -1345.460306 a.u.

8	-2.91704200	0.78153300	-1.53681800
6	-1.68755900	1.21288700	-0.93994500
6	-2.06079800	2.13363400	0.22363600
6	-0.94617900	3.01042400	0.77119300
6	-0.99604300	1.97946800	-2.04209600
6	2.49645600	1.73155100	2.03612800
6	2.06698100	3.76042800	0.59772700
1	-2.47160700	1.52109300	1.02598500
1	-2.86940300	2.76766200	-0.13841400
1	-1.38271900	3.61045900	1.57250100
1	-0.63014100	3.72530800	0.01434200
1	-0.05599200	2.40039400	-1.69528900
1	-1.63867300	2.79473000	-2.36095300
1	-0.80942300	1.33676600	-2.89818600
1	3.31118200	1.39713400	1.39563800
1	2.03661600	0.85444100	2.47831800
1	2.95165800	2.31989100	2.83395600
1	2.44174900	4.47711000	1.32872500
1	1.34843600	4.27742200	-0.03016700
1	2.92193200	3.48304000	-0.01940900
6	-3.05726300	-1.01780700	0.01243900
6	-3.85280800	-1.94996600	0.67456600
1	-3.37750700	-2.66819500	1.32539300
6	-5.21848700	-1.95133300	0.50321700
1	-5.83175700	-2.66552100	1.02813000
6	-5.79906500	-1.03529400	-0.36463700
1	-6.86816100	-1.04008300	-0.51084700
6	-5.02998200	-0.11221400	-1.04419300
1	-5.46754200	0.59990900	-1.72452600
6	-3.66184200	-0.09169900	-0.84072300
6	-1.62428900	-1.03593700	0.04789600
1	-1.12462700	-1.92301100	0.40336800
6	-0.91938900	-0.00736200	-0.45908200
6	3.29559300	-2.10557600	-0.70175800
1	2.78788400	-2.97335000	-0.31353900
6	4.54417300	-2.19763300	-1.28223200
1	5.02642000	-3.15988300	-1.35178100
6	5.17679300	-1.06754900	-1.77168700
1	6.15433400	-1.14578500	-2.22067000
6	4.55757500	0.16429300	-1.67083900
1	5.05280300	1.05253100	-2.03055900
6	3.30551000	0.26744400	-1.09327300
6	2.67342000	-0.87091300	-0.62171700
6	0.49178600	-0.10401600	-0.69016800
1	0.86335200	0.44301500	-1.54741200
6	0.20740600	2.24562500	1.32762100
1	-0.05906300	1.35328100	1.87965300
6	1.50227900	2.56121100	1.28854900
7	1.36471800	-0.81254100	-0.06450300
1	2.83199200	1.23168500	-0.97395000
5	1.15826500	-1.63981200	1.33924500
9	0.72513600	-2.89445700	0.97551000
9	2.38510000	-1.65037700	1.92254700
9	0.23027900	-0.96110500	2.08147900

TS-tf-B
E(RMPWB1K)= -1345.419862 a.u.

8	-3.17151900	1.37147900	0.34950500
6	-1.87804600	1.59007800	-0.20236000
6	-1.28297200	2.64720000	0.70457000
6	0.18033100	2.89327200	0.42930400
6	-2.04792100	2.07784700	-1.63302400
6	3.31541700	1.03560600	1.53701900
6	3.02774100	2.94179100	-0.09929700
1	-1.41629700	2.30883500	1.73050900
1	-1.85615700	3.56455000	0.58873600
1	0.52159400	3.74564500	1.01596100
1	0.32261500	3.17148000	-0.61573500
1	-1.08941700	2.26740700	-2.11048100
1	-2.63336100	2.99395300	-1.65005400
1	-2.56473400	1.31912500	-2.21524400
1	4.29025600	0.87159500	1.08646500
1	2.87208500	0.08949300	1.83218300
1	3.46413900	1.62135100	2.45058600
1	3.02743800	3.82557700	0.54617500
1	2.46439700	3.20973300	-0.98814200
1	4.05686400	2.73010100	-0.36941900
6	-3.14224300	-0.89268800	-0.36248700
6	-3.86024800	-2.03323500	-0.69769700
1	-3.31937700	-2.93415800	-0.94576000
6	-5.24062300	-2.02111700	-0.70158000
1	-5.78891700	-2.91179800	-0.96353400
6	-5.91692500	-0.86268600	-0.35401600
1	-6.99584100	-0.84946800	-0.34795500
6	-5.22207000	0.28399800	-0.01629300
1	-5.72889200	1.19402200	0.26122700
6	-3.84163000	0.26421900	-0.03057800
6	-1.70096700	-0.84754900	-0.28906400
1	-1.14853600	-1.77381400	-0.31749800
6	-1.06482100	0.31853300	-0.17389000
6	3.08469700	-2.06960800	-0.44448400
1	2.62382500	-2.88494300	0.08523100
6	4.36827300	-2.16754600	-0.90575500
1	4.92114300	-3.07765600	-0.73190800
6	4.96944100	-1.11413000	-1.59743700
1	5.98488500	-1.20298700	-1.94961400
6	4.23270600	0.01212200	-1.86611900
1	4.65670700	0.81291100	-2.45313100
6	2.92132100	0.12721900	-1.41275600
6	2.33910100	-0.89370300	-0.64814000
6	0.41860100	0.38576000	-0.28680300
1	0.65668100	0.84112000	-1.24450600
6	1.02193200	1.68085200	0.77355100
1	0.73166500	1.19430800	1.70229800
6	2.42513700	1.81745800	0.65633000
7	1.11035000	-0.77057600	-0.05071800
1	2.35483500	0.98222800	-1.73792000
5	0.81606800	-1.62651100	1.28207100
9	0.33899400	-2.85894500	0.90644400
9	2.00760300	-1.75796800	1.97378600
9	-0.07166700	-0.89375200	2.03268200

TS-cf-B
E(RMPWB1K)= -1345.418785 a.u.

6	4.83527900	-2.44478300	0.31896600
6	5.57051200	-1.39234300	-0.20322400
6	4.95649600	-0.19572800	-0.52697800
6	3.60227100	-0.04989500	-0.30166200
6	2.84604500	-1.09792000	0.21875100
6	3.47896500	-2.29638200	0.52273500
8	2.99991200	1.10486700	-0.65408500
6	1.85926500	1.51969400	0.09752300
6	0.92113000	0.35881300	0.31640700
6	1.43389600	-0.87176300	0.40049600
6	1.24502300	2.59168700	-0.78053700
6	-0.12549000	3.05938000	-0.33727600
6	-1.22800200	2.01816700	-0.26863900
6	-0.44965800	0.64118800	0.79325500
6	2.33471400	2.06556200	1.43424800
6	-1.85776600	1.52528500	-1.41636000
6	-1.18849000	-1.02509600	-1.34968700
6	-1.76329900	-1.12763100	-0.07572500
7	-1.37877200	-0.32261900	0.97222700
6	-1.73142900	-1.71010200	-2.43047100
6	-2.84557000	-2.49781300	-2.26998800
6	-3.39303100	-2.64297500	-0.99510700
6	-2.86533600	-1.98603700	0.08452500
6	-1.29248600	1.67205600	-2.78435100
6	-3.29584800	1.16276500	-1.33912900
1	5.32059700	-3.37535500	0.56549400
1	6.63121200	-1.50421000	-0.36541100
1	5.50969900	0.63229700	-0.93953800
1	2.89299100	-3.10933700	0.92473200
1	0.79560200	-1.70864000	0.64558100
1	1.22368700	2.19567300	-1.79117800
1	1.92632200	3.44011500	-0.80125500
1	-0.44544700	3.86744500	-0.99542000
1	-0.04453200	3.50515400	0.65322900
1	-1.95389900	2.22955500	0.50876200
1	-0.40706700	1.27756500	1.66782300
1	1.50714600	2.42378800	2.04071000
1	3.02827400	2.88648900	1.27118900
1	2.84120400	1.28230400	1.99231400
1	-1.26000000	-1.62096400	-3.39758900
1	-3.27253600	-3.02430700	-3.10898700
1	-4.25185800	-3.28012700	-0.85145500
1	-3.30125100	-2.09956100	1.06075900
1	-1.83531600	1.05529800	-3.49344600
1	-0.23897900	1.42720400	-2.84662300
1	-1.39850400	2.71477600	-3.09569100
1	-3.53956500	0.32764100	-1.99279700
1	-3.86877900	2.02752900	-1.68837700
1	-3.60579700	0.94310600	-0.32284200
5	-2.36499000	-0.12710100	2.22328700
9	-3.59745900	0.25485100	1.72124200
9	-1.82707800	0.88029400	2.99398200
9	-2.44109300	-1.31592900	2.89726500
1	-0.26864500	-0.48824600	-1.48836700

trans-**4**-**B**
E(RMPWB1K)= −1345.468388 a.u.

8	−3.10632000	1.42248700	0.51557200
6	−1.82468700	1.60846600	−0.07089600
6	−1.10848300	2.54224700	0.88496800
6	0.35401300	2.72593100	0.53766500
6	−2.01884600	2.23124400	−1.44573600
6	3.37879300	0.88213700	1.50537100
6	3.13208300	2.81761500	−0.02185300
1	−1.19829700	2.11339600	1.88182100
1	−1.62950300	3.49735800	0.89396700
1	0.79343500	3.44276700	1.22679200
1	0.45436900	3.15721800	−0.45958500
1	−1.06835800	2.40325500	−1.94551000
1	−2.54096700	3.18085100	−1.35587200
1	−2.60889100	1.56253300	−2.06764000
1	4.44690400	0.83305000	1.30046700
1	3.03114600	−0.11026900	1.78499700
1	3.22973700	1.53806200	2.36064500
1	2.92211800	3.50470300	0.79240800
1	2.68890200	3.22620700	−0.92788900
1	4.21108200	2.80214100	−0.14757700
6	−3.24230500	−0.76104800	−0.42105800
6	−4.04534800	−1.81738000	−0.82811500
1	−3.57354800	−2.71833000	−1.19124000
6	−5.42189100	−1.72847800	−0.75973900
1	−6.03420700	−2.55618500	−1.08037900
6	−6.00953300	−0.57616900	−0.26478900
1	−7.08415700	−0.50190600	−0.20148400
6	−5.22909200	0.48792500	0.14828300
1	−5.66514600	1.39234900	0.54090600
6	−3.85426900	0.39384400	0.06157000
6	−1.79552700	−0.81067700	−0.41423500
1	−1.31029000	−1.76504900	−0.55254400
6	−1.09298200	0.29487500	−0.19346400
6	3.13794900	−2.02315800	−0.60551500
1	2.68567400	−2.96226200	−0.33955600
6	4.41886100	−1.93467300	−0.99783400
1	5.01659900	−2.83201200	−1.04656600
6	5.02539800	−0.68575500	−1.37888600
1	6.05190300	−0.68530900	−1.70938900
6	4.31696500	0.44336800	−1.35986200
1	4.75675000	1.36770200	−1.70000500
6	2.89876700	0.48272400	−0.93546200
6	2.32394900	−0.84495100	−0.57359400
6	0.39763200	0.37659000	−0.28443100
1	0.58172200	0.72419000	−1.30870100
6	1.08812900	1.39889700	0.62360300
1	0.96251500	1.01465100	1.63651100
6	2.61545800	1.42572600	0.30486800
7	1.10536200	−0.87650400	−0.13420700
1	2.33449500	0.91620900	−1.76843800
5	0.70904800	−1.96738400	1.04667700
9	0.20879300	−3.08133800	0.43366700
9	1.88908100	−2.22998300	1.70170200
9	−0.15969600	−1.30296400	1.85354200

cis-**4**-**B**
E(RMPWB1K)= -1345.481828 a.u.

6	-4.76584700	-1.94549400	1.09335700
6	-5.34830800	-0.70577500	1.30021200
6	-4.65447000	0.45437100	1.00877000
6	-3.37200700	0.36547400	0.50528100
6	-2.76131800	-0.87026200	0.30680300
6	-3.47574700	-2.02219200	0.60649300
8	-2.68434000	1.50370500	0.26820800
6	-1.70109600	1.46861900	-0.76232300
6	-0.83520700	0.24194600	-0.62938400
6	-1.38895700	-0.87396800	-0.15362200
6	-0.88684600	2.72442100	-0.53459700
6	0.36786800	2.74796000	-1.37790300
6	1.32904500	1.59697200	-1.10208600
6	0.56165600	0.26161400	-1.21743500
6	-2.40295700	1.46752200	-2.10994500
6	2.17914100	1.67672700	0.19107800
6	1.59638700	0.63350400	1.20364300
6	1.76750400	-0.69342800	0.54783100
7	1.32836800	-0.83227100	-0.65877200
6	2.16202700	0.72927800	2.56802800
6	2.81994500	-0.27893000	3.13914900
6	2.99116600	-1.52443500	2.43553600
6	2.49237800	-1.74131000	1.20751200
6	2.21830100	3.06182900	0.81454400
6	3.61838500	1.28140600	-0.13873600
1	-5.31352400	-2.84675300	1.31787800
1	-6.35375400	-0.63954000	1.68608800
1	-5.08886300	1.42912400	1.16170600
1	-3.00412900	-2.98164700	0.45425100
1	-0.83411900	-1.80059100	-0.11388100
1	-0.64910700	2.76054900	0.52763400
1	-1.51011200	3.59116400	-0.74542200
1	0.88068500	3.69780000	-1.25529900
1	0.08819500	2.70274400	-2.43081100
1	2.04456600	1.59093000	-1.92275700
1	0.45984100	0.04079500	-2.27672500
1	-1.68713300	1.44454900	-2.92745100
1	-3.02292400	2.35515300	-2.20969600
1	-3.03152700	0.58519200	-2.19539700
1	1.99675500	1.64987500	3.10558800
1	3.21290900	-0.18727200	4.13914600
1	3.53539000	-2.31781700	2.92520400
1	2.61814300	-2.67926700	0.69771900
1	2.92742900	3.07963600	1.63821400
1	1.25329200	3.39041400	1.19161600
1	2.56083600	3.79165200	0.08542200
1	4.20798700	1.17728400	0.77116900
1	4.07903500	2.05433500	-0.75050000
1	3.67265300	0.34690400	-0.69259300
5	1.61377700	-2.15921300	-1.53304100
9	2.97871000	-2.29513600	-1.57030300
9	1.06455800	-1.93165500	-2.76228800
9	1.00979800	-3.19692900	-0.86014300
1	0.52086300	0.83546900	1.27119600

trans-**4**+**11** complex
E(RMPWB1K)= -1271.534301 a.u.

6	-1.24232400	4.14607500	-1.85842100
6	-0.32986500	3.14930100	-1.21868700
6	-0.71991100	2.38571000	-0.19909300
7	-1.98776000	2.43723700	0.35534100
6	-2.74088400	3.63304900	0.06814300
6	-2.67924700	3.91015200	-1.42013100
6	-2.81227400	-0.92552000	0.21617200
6	-4.24299100	-1.20024900	0.54568300
6	-4.77042300	-0.88768200	1.72635600
6	-3.93895100	-0.34703900	2.78310900
6	-2.61061300	-0.27839400	2.65208500
6	-1.94755900	-0.75388600	1.44378600
7	-0.69277900	-0.94447200	1.51009200
6	-2.17188300	-1.88147400	-0.79843200
1	-1.96813100	0.03577400	3.46004200
1	-4.40764600	-0.04263900	3.70702100
1	-5.82167200	-1.03831800	1.91694800
1	-4.87179800	-1.59725900	-0.23714800
1	-2.81127300	0.07782600	-0.23670200
1	-3.76870200	3.48675600	0.39155900
1	-2.33986000	4.49821100	0.60827500
1	-3.30723600	4.76349300	-1.66563600
1	-3.08409900	3.04498500	-1.94320700
1	-0.93445300	5.16360600	-1.60707700
1	-1.17440000	4.07839300	-2.94440400
1	0.66959100	3.02661900	-1.60395400
1	-0.06164600	1.64463200	0.23404100
1	-2.02948300	2.13808000	1.31184300
6	-2.25856200	-3.30597400	-0.27039300
1	-3.29876000	-3.62031100	-0.20905900
1	-1.74259900	-4.01028100	-0.91929300
1	-1.83443500	-3.38867500	0.72828100
6	-2.87603700	-1.78129300	-2.14246500
1	-2.41044700	-2.44117900	-2.87052800
1	-3.92192200	-2.07090500	-2.07701000
1	-2.82960300	-0.76482500	-2.53093700
6	1.56478100	-2.24137800	-1.74674500
1	2.13259300	-2.40719100	-2.65937600
1	1.75130000	-3.09794800	-1.10073800
6	0.07533600	-2.11253400	-2.05353500
1	-0.32388700	-3.11159900	-2.22082100
1	-0.06051300	-1.57588400	-2.99036200
6	-0.72176200	-1.39983200	-0.95291600
1	-0.79373300	-0.34038600	-1.21140200
6	0.01507300	-1.47258600	0.37688700
1	0.19568000	-2.53432900	0.59516500
6	5.45944000	-0.22939000	-0.08588800
6	4.07489300	1.00424900	1.96962300
6	5.42851800	1.23366400	1.81927000
6	6.11911400	0.60686900	0.79506700
1	5.97712100	-0.72599400	-0.89075500
1	3.53063400	1.46801800	2.77918000
1	5.94580800	1.88852000	2.50235100

1	7.17839400	0.77455800	0.67583900
8	3.48267800	−1.27908900	−0.79599500
6	1.99922500	−0.21108200	1.25931200
1	1.49878200	−0.04782300	2.20159000
6	1.37607700	−0.84639800	0.27095700
6	3.38954200	0.16919300	1.09751900
6	4.10103800	−0.43522300	0.05824600
6	2.10192000	−1.01770100	−1.03741000
6	2.00226900	0.23331200	−1.89401700
1	2.43075800	1.07760300	−1.35824200
1	2.55338500	0.08951700	−2.82090400
1	0.97096400	0.47868500	−2.12913700

TS-**6**
E(RMPWB1K)= -1271.497047 a.u.

6	-0.41328100	-2.80801700	2.45591900
6	0.01493500	-2.61220700	1.03952500
6	-0.80884700	-2.21721100	0.08391900
7	-2.19163900	-1.94104200	0.31980600
6	-2.71429100	-2.39513200	1.60693500
6	-1.72052800	-2.07869600	2.70081800
6	-2.83440900	0.55561700	-0.51161900
6	-4.21900300	0.22460100	-0.54497200
6	-4.73605800	-0.66733800	-1.43266200
6	-3.89445800	-1.14831300	-2.47274400
6	-2.60251500	-0.75880500	-2.57999600
6	-1.99316600	0.15603800	-1.63960000
7	-0.73934900	0.43120200	-1.79157200
6	-2.31829900	1.75686000	0.26261600
1	-1.97806800	-1.09331000	-3.39438500
1	-4.30213100	-1.83138400	-3.20486100
1	-5.77240800	-0.96003000	-1.38965300
1	-4.86245800	0.63180300	0.22218800
1	-2.41967200	-0.70954700	0.11479100
1	-3.66958500	-1.90075000	1.76587600
1	-2.88998600	-3.46957300	1.56184800
1	-2.14978200	-2.34045200	3.66423800
1	-1.53307600	-1.00478500	2.71409600
1	-0.51759900	-3.87119100	2.68037500
1	0.35753900	-2.43323800	3.12613100
1	1.05493100	-2.73462100	0.77866600
1	-0.48865800	-1.97337800	-0.91723200
1	-2.75344700	-2.28704200	-0.45151700
6	-2.53300200	2.99797000	-0.60014300
1	-3.59986700	3.17203800	-0.72614400
1	-2.10154600	3.89379100	-0.15589700
1	-2.10278900	2.86297000	-1.58982500
6	-3.02172500	1.94727000	1.59607000
1	-2.60000400	2.79439600	2.13280000
1	-4.08185500	2.15183700	1.46730300
1	-2.92347400	1.06500900	2.22853100
6	1.39612300	2.68113000	0.98187500
1	1.94287400	3.15463300	1.79426300
1	1.53210200	3.30820800	0.10304500
6	-0.08967800	2.55185200	1.32668300
1	-0.56082600	3.52105300	1.17470300
1	-0.20032000	2.33013100	2.38710700
6	-0.82444000	1.48309300	0.50379700
1	-0.78493800	0.53681800	1.05437200
6	-0.09234800	1.25468800	-0.81569500
1	0.06929800	2.24922800	-1.26024500
6	5.37220500	0.33332500	0.03861300
6	4.02031400	-1.52370600	-1.50398400
6	5.37705900	-1.66914500	-1.28921900
6	6.05109600	-0.73265900	-0.52383200
1	5.87897400	1.07382300	0.63645300
1	3.48848400	-2.23044000	-2.12445900
1	5.90941200	-2.49943600	-1.72590100

1	7.11264400	−0.83293100	−0.35766200
8	3.37354500	1.52739100	0.36701900
6	1.92208600	−0.18129400	−1.23057900
1	1.43223300	−0.62884500	−2.08232700
6	1.28126400	0.72981300	−0.50541500
6	3.31567100	−0.46340200	−0.94988100
6	4.01143200	0.46020100	−0.16481500
6	1.99656100	1.32598000	0.68132700
6	1.93535200	0.42565700	1.90520000
1	2.37146800	−0.54428500	1.68098200
1	2.49337900	0.88600400	2.71804800
1	0.90940900	0.29423200	2.23165900

IN1
E(RMPWB1K)= −1271.506761 a.u.

6	−1.26804700	3.63146500	−2.05356100
6	−0.41658000	2.87356600	−1.09240500
6	−0.88339200	2.06208600	−0.16286000
7	−2.31139900	1.87635000	0.01678600
6	−3.15917100	2.89694100	−0.62164500
6	−2.69629500	3.11795000	−2.04053200
6	−2.73944700	−1.07383500	0.51603900
6	−4.05765100	−0.67315100	0.39429000
6	−4.66345500	0.22465600	1.27272100
6	−3.91734900	0.65344400	2.37036600
6	−2.59510600	0.30178400	2.51974700
6	−1.91007800	−0.53383600	1.57178000
7	−0.61524500	−0.69189100	1.69462200
6	−2.09472600	−2.12413300	−0.35436900
1	−2.02094800	0.63764300	3.37008000
1	−4.37817800	1.28698000	3.11619100
1	−5.70058600	0.49450400	1.15859900
1	−4.64714600	−1.07821600	−0.41677200
1	−2.58037100	0.92182900	−0.28451300
1	−4.17953000	2.53603100	−0.55020300
1	−3.06445000	3.80682600	−0.03450500
1	−3.36784100	3.81429700	−2.53440400
1	−2.75819900	2.17629300	−2.58527500
1	−1.23882300	4.69322100	−1.80317500
1	−0.84528200	3.54985000	−3.05287300
1	0.65615300	2.97375500	−1.15874200
1	−0.29007700	1.45708900	0.50853600
1	−2.51920500	1.78517200	1.02745600
6	−2.07828000	−3.42957900	0.44081800
1	−3.09667600	−3.78342200	0.58321200
1	−1.51833800	−4.21491800	−0.06566500
1	−1.64267500	−3.27509900	1.42473300
6	−2.83163800	−2.33995000	−1.66398000
1	−2.32115900	−3.08124700	−2.27404000
1	−3.84223000	−2.70560400	−1.49831400
1	−2.89554600	−1.41625500	−2.24011700
6	1.64003000	−2.51518600	−1.31487900
1	2.19801100	−2.82941700	−2.19448700
1	1.87391100	−3.22369300	−0.52274700
6	0.14119300	−2.49988700	−1.60129700
1	−0.21949100	−3.52626300	−1.56459100
1	−0.03192000	−2.16158500	−2.62202500
6	−0.66657600	−1.62303400	−0.63565700
1	−0.79119000	−0.63463300	−1.09350300
6	0.08247200	−1.41361900	0.67820100
1	0.33769700	−2.42307500	1.04463100
6	5.45497700	−0.01970300	−0.19948500
6	4.05075600	1.49875900	1.63734200
6	5.38500200	1.76927800	1.40052100
6	6.08638900	1.00194300	0.48571500
1	5.98168600	−0.63148800	−0.91429500
1	3.50104800	2.07307900	2.36891800
1	5.87920200	2.56538800	1.93489500

1	7.13066700	1.20080700	0.29997900
8	3.53047900	−1.29451200	−0.62857600
6	2.02712300	0.07317000	1.23113300
1	1.52647500	0.38081600	2.13722400
6	1.41675400	−0.77042500	0.40226200
6	3.39280800	0.48067100	0.96031500
6	4.11582200	−0.27086000	0.02950500
6	2.13022400	−1.15818900	−0.86661200
6	1.94950400	−0.10433800	−1.94894300
1	2.36089700	0.84297900	−1.60706500
1	2.47521200	−0.40845500	−2.85169500
1	0.89998400	0.04577700	−2.18388700

trans-**5**+**11** complex
E(RMPWB1K)= -1271.580025 a.u.

6	3.09085200	4.23404200	-0.18176900
6	2.12508400	3.34117300	-0.89290400
6	2.30777700	2.02309400	-0.96514600
7	3.38369100	1.36104400	-0.40704700
6	4.51743100	2.18729800	-0.07969500
6	4.03628400	3.40947400	0.67799800
6	2.24214200	-1.83857100	-0.07233900
6	3.54415100	-2.28959600	-0.25029700
6	4.16676600	-2.30262300	-1.48269000
6	3.46957600	-1.84973000	-2.59042000
6	2.16967900	-1.41641600	-2.45203200
6	1.53803000	-1.41756400	-1.20836500
7	0.23896200	-0.94978400	-1.11693800
6	1.64906900	-1.75896200	1.32858200
1	1.61998800	-1.06460900	-3.31341600
1	3.93520900	-1.83888500	-3.56377400
1	5.18065200	-2.65725300	-1.57700800
1	4.09205500	-2.63462000	0.61401900
1	5.21278100	1.60844900	0.52384200
1	5.05015800	2.51430800	-0.98033900
1	4.88692000	4.00428500	1.00331000
1	3.51323600	3.06981600	1.57075400
1	3.65877100	4.83621900	-0.89498900
1	2.55562900	4.94765100	0.44516300
1	1.23706700	3.76679000	-1.33263500
1	1.58146900	1.38162800	-1.44082000
1	3.60539700	0.48705900	-0.84909500
6	1.37551700	-3.15848900	1.87065000
1	2.28720900	-3.75183500	1.85140500
1	1.03133900	-3.11407800	2.90266000
1	0.63062300	-3.69050100	1.28386800
6	2.63687300	-1.05718800	2.25880700
1	2.19270500	-0.90105100	3.23964800
1	3.53436600	-1.65161400	2.40996000
1	2.92734000	-0.09433100	1.84537500
6	-1.43889800	0.31394400	2.38655500
1	-0.87473700	1.21276300	2.63071800
1	-2.25067300	0.23678400	3.10375800
6	-0.51524100	-0.88750900	2.48158800
1	-1.09574400	-1.81118500	2.52334700
1	0.05575700	-0.83415800	3.40578700
6	0.37616700	-0.90855200	1.25815300
1	0.70992000	0.11469200	1.05879200
6	-0.48043200	-1.31914600	0.07604900
1	-0.62182900	-2.40759000	0.11857200
6	-5.56240900	1.15992300	0.33140100
6	-5.04244900	-0.58976300	-1.75085200
6	-6.24631000	0.08648500	-1.70734900
6	-6.50306900	0.95718600	-0.66117800
1	-5.74359800	1.83079500	1.15552500
1	-4.83468700	-1.28027300	-2.55540400
1	-6.98201800	-0.06722300	-2.48055600
1	-7.44201200	1.48707000	-0.61854000

8	−3.47666500	0.65315900	1.27871100
6	−2.80886200	−1.08300400	−0.72856600
1	−2.65360500	−1.91854700	−1.39972000
6	−1.84487300	−0.68852800	0.09955600
6	−4.08372600	−0.39791900	−0.76674700
6	−4.35577600	0.48966000	0.27244100
6	−2.08130800	0.49772200	1.00072600
6	−1.58897400	1.75469000	0.30381800
1	−2.12786600	1.89340200	−0.63108500
1	−1.75580500	2.62074700	0.94004000
1	−0.52756300	1.68188800	0.07828400
1	−0.29213200	−1.02746400	−1.96510600

trans-**4**
E(RMPWB1K)= -1021.164490 a.u.

8	-2.94051900	-1.24356600	-0.48004800
6	-1.66290100	-1.32694100	0.14745200
6	-0.90323000	-2.31322200	-0.71771400
6	0.55373500	-2.40996100	-0.33320500
6	-1.86455300	-1.82615900	1.56692600
6	3.51403100	-1.26148800	-1.45095800
6	3.12756900	-2.24164500	0.79526600
1	-0.99746600	-1.97200600	-1.74646400
1	-1.39306400	-3.28179100	-0.65203400
1	1.04953700	-3.14133700	-0.96893100
1	0.63712100	-2.78370700	0.68578600
1	-0.91917500	-1.90419600	2.09639800
1	-2.34386200	-2.80125600	1.55713400
1	-2.49679700	-1.12804800	2.10873600
1	4.57943300	-1.39870600	-1.28561300
1	3.38031600	-0.38723000	-2.08377800
1	3.14265500	-2.12921000	-1.99261700
1	2.95006700	-3.20970900	0.33695900
1	2.55919000	-2.19704800	1.72222800
1	4.18266200	-2.19481700	1.05198800
6	-3.11631700	1.07091500	0.01695200
6	-3.93386400	2.17780400	0.17637700
1	-3.47792500	3.13424400	0.37984800
6	-5.30534600	2.06712700	0.07417600
1	-5.92955800	2.93565200	0.20182100
6	-5.87103600	0.83656900	-0.20103200
1	-6.94113400	0.74088500	-0.28732700
6	-5.07376800	-0.27954500	-0.36426300
1	-5.49265100	-1.24662700	-0.58620600
6	-3.70508500	-0.15893600	-0.25190100
6	-1.67281800	1.12048600	0.09344600
1	-1.17074000	2.07357700	0.11611000
6	-0.96109200	0.00335100	0.16033200
6	2.98295900	2.61187600	-0.30432400
1	2.33983500	3.41087700	-0.63319700
6	4.31116000	2.72910400	-0.26715000
1	4.78127800	3.65150800	-0.56845600
6	5.15234700	1.63529200	0.16976900
1	6.22045000	1.77997100	0.18437600
6	4.62882200	0.47580500	0.55083700
1	5.27400600	-0.32361700	0.88089100
6	3.16417700	0.22546800	0.56260000
6	2.33457200	1.37797000	0.08262500
6	0.52845200	0.00850300	0.35877400
1	0.72610500	-0.21580500	1.42065900
6	1.24531700	-1.06645600	-0.46133900
1	1.13880400	-0.73929300	-1.49733700
6	2.75711500	-1.10360800	-0.14305300
7	1.06800400	1.29682500	0.03222300
1	2.86756400	0.08459700	1.61030100

TS-**5**-**tf**
E(RMPWB1K)= -1021.045397 a.u.

7	1.65315400	-0.01703700	1.80418500
6	2.14395300	0.90843400	0.90960600
6	3.15050900	0.16712500	0.21626800
6	1.99296900	2.27263300	0.74005000
6	3.05737400	2.92163400	0.13655400
6	4.19421000	2.24854300	-0.33907100
6	4.25461900	0.88004300	-0.32263400
1	1.20562000	2.83651900	1.21399200
1	3.04845300	4.00107800	0.09595900
1	5.02241300	2.82846600	-0.71475000
1	5.12522800	0.36533200	-0.70155500
1	2.99984200	-0.52060500	1.28635500
6	1.37016700	-1.71364900	0.12070100
1	1.94451300	-2.48416200	0.64019200
6	0.67129700	-0.91501400	1.29823100
1	0.48962500	-1.65793400	2.07964900
8	-2.45882300	-1.20004800	-0.56898300
6	-3.04630000	0.01444000	-0.49202100
6	-4.24294400	0.21408500	-1.15322500
1	-4.68391300	-0.61135300	-1.68858600
6	-4.84783200	1.45641700	-1.10857700
1	-5.78732700	1.60749600	-1.61726100
6	-4.26117400	2.49881200	-0.41031300
1	-4.73839900	3.46512900	-0.37364300
6	-3.05449300	2.29599700	0.22988400
1	-2.57710200	3.10719300	0.76003700
6	-2.42787000	1.05795200	0.19907400
6	-1.11816700	0.80215600	0.76355200
1	-0.51120000	1.63730900	1.07105400
6	-0.67360900	-0.44706100	0.85472600
6	-1.63439000	-1.56917200	0.53737100
6	-2.51598800	-1.86740900	1.73567900
1	-3.11702000	-0.99846200	1.98955100
1	-3.17613700	-2.70287500	1.51448800
1	-1.90455500	-2.12247000	2.59779500
6	-0.87872000	-2.80837700	0.08098600
1	-1.56995200	-3.42495200	-0.48828800
1	-0.56937900	-3.38709800	0.95098200
6	0.31807700	-2.39837800	-0.74928300
1	-0.05315100	-1.71500500	-1.50922000
1	0.75062400	-3.25166500	-1.26853100
6	2.39538100	-0.90334600	-0.69591400
6	3.43932800	-1.85620300	-1.25505800
1	4.13845200	-1.33062000	-1.90146100
1	4.00128300	-2.33960100	-0.45876500
1	2.96291700	-2.62903200	-1.85509000
6	1.75997000	-0.12349900	-1.84438900
1	2.47703200	0.58637400	-2.24964100
1	1.45765800	-0.78700300	-2.65150200
1	0.88476900	0.43062300	-1.51236200

trans-**5**
E(RMPWB1K)= -1021.238425 a.u.

6	-5.09027400	2.20643700	-0.10420300
6	-5.69059900	1.02760200	-0.51198800
6	-4.94390100	-0.12792900	-0.65327600
6	-3.58960800	-0.09895500	-0.38458100
6	-2.96568600	1.07838700	0.01887800
6	-3.73306700	2.22572900	0.15460600
8	-2.87021100	-1.21903800	-0.59422700
6	-1.65967800	-1.42365600	0.13324400
6	-0.90220400	-0.13573100	0.34332200
6	-1.53997800	1.02769800	0.27006700
6	-0.85743500	-2.35548500	-0.76454700
6	0.60049200	-2.49489000	-0.37073600
6	1.27662100	-1.13586400	-0.32097200
6	0.54064400	-0.30486200	0.72382100
6	-2.01808400	-2.06390800	1.46396700
6	2.79098900	-1.13475900	-0.03495400
6	3.23941400	0.30531100	-0.16322200
6	2.40525600	1.28803900	0.38426100
7	1.21922800	0.92844300	0.97429000
6	4.42630300	0.70356100	-0.75175900
6	4.81930300	2.03045600	-0.78044300
6	4.00045800	2.98701000	-0.21174100
6	2.79875500	2.62220600	0.35839200
6	3.51048300	-2.04503000	-1.01482300
6	3.08985900	-1.60762000	1.38826400
1	-5.67553400	3.10522400	0.00667500
1	-6.74906200	1.00371900	-0.72000400
1	-5.38991300	-1.05524600	-0.97479300
1	-3.25140600	3.14143700	0.46539400
1	-1.01687500	1.96245500	0.40816900
1	-0.91552200	-1.93926000	-1.76903400
1	-1.35202000	-3.32470300	-0.79197100
1	1.08863700	-3.13978100	-1.09614500
1	0.69245700	-2.98913600	0.59827100
1	1.13935400	-0.65122800	-1.29131300
1	0.54257000	-0.91395800	1.63955800
1	-1.13050600	-2.32156100	2.03558000
1	-2.59241800	-2.96951400	1.28703000
1	-2.61937100	-1.37815800	2.05571700
1	5.07113300	-0.03884000	-1.19427500
1	5.75366200	2.30970100	-1.24024900
1	4.28879800	4.02707200	-0.22110700
1	2.14788800	3.37222800	0.78491200
1	4.58469700	-2.01679400	-0.85316900
1	3.31400400	-1.75827700	-2.04635400
1	3.20269200	-3.07807100	-0.87851800
1	4.16529900	-1.65106900	1.54101500
1	2.68491600	-2.60222000	1.57105000
1	2.68236900	-0.92421900	2.12907700
1	0.71286500	1.64092400	1.45882500

11-B
E(RB3LYP)= -3917.171684 a.u.

8	-3.82209800	0.19688500	-1.89797900
6	-2.66700100	0.85844000	-1.28593000
6	-3.24480900	1.97540700	-0.37249900
6	-2.31155300	3.12048900	0.06636900
6	-1.92633600	1.43844800	-2.49130900
6	1.03532900	2.90848400	2.11326900
6	0.41585000	4.59530200	0.31404300
1	-3.67999800	1.50277200	0.51510600
1	-4.07682800	2.41404100	-0.93596500
1	-2.95197800	3.83341000	0.60765100
1	-1.96120200	3.66744000	-0.81555000
1	-1.06572100	2.03753800	-2.18730000
1	-2.60847700	2.08442000	-3.04958500
1	-1.59141400	0.64041200	-3.15972000
1	2.02764300	2.78704000	1.66041700
1	0.76181800	1.96055000	2.58100900
1	1.15078300	3.66183600	2.90459500
1	0.52025500	5.45537800	0.98890100
1	-0.30162400	4.87302500	-0.46097200
1	1.39685100	4.46139600	-0.16031000
6	-3.94911600	-1.37675300	-0.08004700
6	-4.71927900	-2.31614200	0.63131300
1	-4.25430200	-2.86142400	1.44774000
6	-6.04849900	-2.53743500	0.29825400
1	-6.64111800	-3.25261200	0.85881500
6	-6.61675300	-1.84071100	-0.77793100
1	-7.65333900	-2.01904300	-1.04845100
6	-5.87297800	-0.91625500	-1.50768500
1	-6.30006500	-0.37570800	-2.34533100
6	-4.54676000	-0.67010200	-1.14701800
6	-2.53996400	-1.18539900	0.13468700
1	-2.00494700	-1.92127800	0.72442800
6	-1.86346700	-0.17472800	-0.48105900
6	2.53120800	-1.73571700	0.38877300
1	2.03317500	-2.58323500	0.84506400
6	3.88234800	-1.79704800	0.06210100
1	4.45290000	-2.69677900	0.26077900
6	4.49790500	-0.69090900	-0.52352300
6	3.78441800	0.47735400	-0.77934100
1	4.28057100	1.33670500	-1.21529100
6	2.42970000	0.53362100	-0.45381300
6	1.79911900	-0.57452800	0.11857100
6	-0.42362900	-0.12457100	-0.47552100
1	0.04033700	0.27950200	-1.37393700
6	-1.16021400	2.72791700	0.96231100
1	-1.34037200	1.87376100	1.61186700
6	0.01812900	3.36366700	1.09245300
7	0.39845800	-0.56054400	0.43946900
1	1.87268500	1.45104700	-0.61387000
5	0.01664700	-1.02018200	2.00543600
9	-0.22330600	-2.38688200	1.94206700
9	1.12572000	-0.69356100	2.74349800
9	-1.09724600	-0.29720400	2.38167600
35	6.35229500	-0.77470600	-0.97153400

TS-tf-B-11
E(RB3LYP)= -3917.123859 a.u.

8	-4.33689100	1.21530900	-0.12347700
6	-2.95826300	1.48409500	-0.48837800
6	-2.57961600	2.66128200	0.41946900
6	-1.09695400	3.01914200	0.35057200
6	-2.94130600	1.86734600	-1.98113900
6	2.00720600	1.64344400	2.08269600
6	1.80804500	3.32863400	0.18586400
1	-2.84768400	2.38609100	1.44528900
1	-3.19200600	3.52742100	0.14728500
1	-0.91578800	3.90875500	0.96531900
1	-0.82300100	3.29878600	-0.67335400
1	-1.93366900	2.11334800	-2.32978600
1	-3.58874700	2.73286500	-2.15301900
1	-3.30704800	1.03208500	-2.58406200
1	3.07901400	1.60945200	1.87069300
1	1.65947600	0.66558800	2.42214500
1	1.86434000	2.34530200	2.92238400
1	1.59886700	4.24802500	0.75663800
1	1.38127300	3.47779000	-0.80848100
1	2.89328200	3.24028100	0.10431800
6	-4.03562000	-1.13450500	-0.54428200
6	-4.62587900	-2.37759200	-0.81523800
1	-3.98869800	-3.25497000	-0.88583800
6	-6.00442000	-2.49211500	-0.97766200
6	-6.81219800	-1.35696000	-0.85772100
1	-7.88843000	-1.44088400	-0.97703400
6	-6.24819900	-0.10904000	-0.58903800
1	-6.85883300	0.78204700	-0.48846700
6	-4.86649100	-0.00310600	-0.44206700
6	-2.61332800	-0.95858400	-0.30532400
1	-2.00294300	-1.84462800	-0.17005200
6	-2.07006000	0.27067500	-0.22285900
6	2.34151600	-1.70995800	0.31550400
1	1.90451600	-2.55483700	0.82921300
6	3.68983500	-1.69069700	0.04770100
1	4.31760900	-2.51908000	0.35582700
6	4.26356600	-0.59709400	-0.63539900
6	3.47271900	0.43325700	-1.09628300
1	3.90383800	1.23406000	-1.68651900
6	2.09016400	0.42509000	-0.82932100
6	1.49477100	-0.63016700	-0.08003300
6	-0.58029400	0.48662300	-0.11744000
1	-0.24948800	0.83884800	-1.09853600
6	-0.20591300	1.87093900	0.85704400
1	-0.55835900	1.48745600	1.81828700
6	1.21805200	2.16553300	0.92506400
7	0.18412100	-0.60738500	0.31979000
1	1.48886400	1.14294600	-1.36733600
5	-0.22559600	-1.38797900	1.71295200
9	-0.54991200	-2.69328400	1.38429900
9	0.88973200	-1.33978400	2.55353400
9	-1.26900300	-0.67518500	2.27980100
1	-6.44947700	-3.45965500	-1.18661700
35	6.14074300	-0.59231900	-0.97751000

TS-cf-B-11
E(RB3LYP)= -3917.114742 a.u.

8	-4.13460700	-1.01094200	0.84772400
6	-2.87174000	-0.32401400	1.14117500
6	-2.18801200	-1.30060200	2.12305400
6	-0.65995500	-1.24693800	2.12008000
6	-3.22669300	0.99215100	1.84625500
1	-2.50901200	-2.31345800	1.85399600
1	-2.57155100	-1.10593800	3.12939600
1	-0.28297700	-1.92752900	2.89231300
1	-0.29757800	-0.24379200	2.36926300
1	-2.34207900	1.46241800	2.27384300
1	-3.93779000	0.75921500	2.64550200
1	-3.67923400	1.70306900	1.15443600
6	-4.25376400	-0.02365600	-1.33275900
6	-5.04223800	0.36858800	-2.42314000
1	-4.55712600	0.78414100	-3.30262700
6	-6.42752000	0.22863200	-2.38353200
1	-7.03089900	0.54146700	-3.22968600
6	-7.03547900	-0.32410700	-1.25151500
1	-8.11491900	-0.43937900	-1.21782900
6	-6.26983700	-0.72319300	-0.15537500
1	-6.72461100	-1.15440800	0.73014000
6	-4.88563500	-0.56007000	-0.19500900
6	-2.80236100	0.00147100	-1.31959400
1	-2.28918200	0.14158800	-2.26893700
6	-2.09474800	-0.14311400	-0.18211000
6	-0.59064500	-0.22770300	-0.31713200
6	-0.14957500	-1.68044600	0.74122300
7	0.24132800	0.83834400	-0.00317400
5	-0.26640700	2.26514000	0.63236800
9	0.60943700	3.23528800	0.18486400
9	-1.53993900	2.49087300	0.16100200
9	-0.21456700	2.13228800	2.02685800
6	1.46251600	-3.24905800	-0.39234300
1	1.30978400	-4.21383200	0.11487700
1	0.77738900	-3.22785600	-1.24497200
1	2.49371400	-3.23853000	-0.75364200
6	2.23960100	-1.90388300	1.62642300
1	3.23090500	-1.78018000	1.17881200
1	2.02241200	-1.04520600	2.26072400
1	2.29602200	-2.79480600	2.27209700
1	-0.36182300	-0.67964500	-1.28221700
1	-0.84276400	-2.36515300	0.24421200
6	1.59291700	0.66456300	-0.24365700
6	2.55308900	1.41633600	0.49611200
6	2.08773700	-0.31901900	-1.13400000
6	3.90362700	1.18836700	0.34499600
1	2.21307900	2.15664400	1.20463600
6	3.46460400	-0.52061500	-1.31398200
1	1.41779200	-0.83404800	-1.80971700
6	4.36132600	0.21362400	-0.56194400
1	4.61843800	1.75306100	0.93273400
1	3.81759500	-1.24898200	-2.03535500
6	1.18769300	-2.14308600	0.58899500
35	6.23543300	-0.08076800	-0.75203600

trans-**11**-**B**
E(RB3LYP)= -3917.166969 a.u.

6	5.60180100	-2.45969300	-1.68225300
6	6.43293700	-1.33873700	-1.75232400
6	5.96661300	-0.08478800	-1.35381900
6	4.65997100	0.04313100	-0.88571400
6	3.80293600	-1.07032400	-0.81889900
6	4.29421000	-2.31940800	-1.22008400
8	4.21407700	1.29500100	-0.56454800
6	3.07786400	1.45569100	0.32885700
6	2.06770900	0.32207500	0.16642200
6	2.43890900	-0.85532500	-0.35538300
6	2.48282600	2.81692900	-0.10603400
6	1.02959900	3.06513300	0.33264600
6	0.14979900	1.87475400	-0.08681900
6	0.68439600	0.65508400	0.69624900
6	3.61895700	1.49105700	1.76948700
6	-1.38890100	2.02252700	0.01563800
6	-1.92655800	0.67351500	-0.58466100
6	-1.37377600	-0.52761500	0.17001300
7	-0.20933800	-0.51208500	0.75321600
6	-3.41806100	0.62283100	-0.80349600
6	-4.12553200	-0.49319900	-0.58621000
6	-3.49586100	-1.70790800	-0.10399600
6	-2.19176800	-1.73052000	0.24854900
6	-1.85611700	3.20791600	-0.84874600
6	-1.88915000	2.21091100	1.46110600
1	5.96971500	-3.43414700	-1.98743900
1	7.45240900	-1.43831400	-2.11342400
1	6.59632200	0.79751100	-1.40120800
1	3.63597000	-3.18239200	-1.16351300
1	1.74656000	-1.69015200	-0.39464100
1	2.52429500	2.83522600	-1.20047400
1	3.13588600	3.62141300	0.24845700
1	0.68614300	3.99321300	-0.13373500
1	0.96648800	3.21730800	1.41756900
1	0.35815300	1.69598000	-1.15205200
1	0.80288300	0.94991000	1.74636900
1	2.83205700	1.72172900	2.49331900
1	4.39728300	2.25623000	1.84704800
1	4.04427100	0.52113600	2.03859500
1	-3.89099600	1.49948700	-1.22733100
1	-4.09805700	-2.60644000	-0.02559700
1	-1.73115700	-2.63617800	0.61661700
1	-2.94181700	3.33154300	-0.81891300
1	-1.55330600	3.09103800	-1.89564700
1	-1.42770500	4.14317100	-0.48012900
1	-2.98189400	2.27587000	1.48153900
1	-1.49663000	3.13935700	1.88687600
1	-1.59775600	1.38812700	2.12007200
5	0.18542500	-1.67515000	1.90799600
9	-0.91614700	-1.72964900	2.73717300
9	1.30348400	-1.19972900	2.54587500
9	0.39270500	-2.85649500	1.21337000
1	-1.49839700	0.61147800	-1.60269000
35	-5.99949400	-0.56209000	-0.94476300

cis-**11**-**B**
E(RB3LYP)=-3917.158362 a.u.

8	4.16785600	1.19632400	0.69248200
6	2.81750300	0.74166100	1.01811000
6	2.14790400	2.01640100	1.55991200
6	0.62086700	1.94098000	1.56824400
6	2.94570100	-0.32990800	2.10988400
1	2.46367800	2.84943400	0.92118800
1	2.53201800	2.22042900	2.56465600
1	0.23099500	2.87644900	1.97886600
1	0.27448200	1.13859900	2.23059100
1	1.97186400	-0.64658600	2.48783200
1	3.53401700	0.08409000	2.93493400
1	3.44347500	-1.21871500	1.72073400
6	4.29567800	-0.26857500	-1.20909100
6	5.10045500	-0.94239900	-2.13722200
1	4.62353800	-1.51685300	-2.92730400
6	6.48989000	-0.88178900	-2.05257500
1	7.10333400	-1.41258100	-2.77362000
6	7.08777300	-0.12885600	-1.03746900
1	8.17028400	-0.07407900	-0.96785300
6	6.30628700	0.55102200	-0.10251200
1	6.75267900	1.14112200	0.69089700
6	4.91656300	0.47197500	-0.18541100
6	2.84415900	-0.23378300	-1.26421200
1	2.36019300	-0.61524300	-2.16113200
6	2.10697700	0.23649900	-0.24424200
6	0.59795300	0.34417700	-0.39092900
6	0.09492700	1.72493900	0.13691200
7	-0.23127000	-0.74970900	0.19768200
6	-1.64941600	3.10314100	-1.07590400
1	-1.19479400	4.01679300	-0.67962700
1	-1.17734000	2.89080200	-2.04181600
1	-2.70758200	3.31884800	-1.25215500
6	-2.21998300	2.26288100	1.21594600
1	-3.28848300	2.35862600	1.00455000
1	-2.09842300	1.48670400	1.97595700
1	-1.88773300	3.21056500	1.64669200
1	0.40437700	0.31063700	-1.47342600
1	0.61074100	2.45724700	-0.49621300
6	-1.52540200	-0.57961400	0.07711800
6	-2.48303700	-1.47454400	0.69867800
6	-2.03162800	0.60676200	-0.70786900
6	-3.81071700	-1.31864600	0.48086900
1	-2.12185200	-2.25444800	1.35143300
6	-3.51222900	0.64097700	-0.93272300
1	-1.56731800	0.53426800	-1.70595100
6	-4.32374000	-0.27170100	-0.37841000
1	-4.52009400	-1.98473400	0.95966200
1	-3.90913900	1.42869300	-1.56203200
6	-1.44795400	1.94459500	-0.08021600
5	0.33122400	-2.21825100	0.81090400
9	1.64677400	-2.34905500	0.46415700
9	0.11440800	-2.13091400	2.17803800
9	-0.45498700	-3.18183400	0.21039600
35	-6.20999800	-0.22321100	-0.67084800

12-B
E(RB3LYP)=-1550.568076 a.u.

8	-3.53537000	0.33181000	-1.82953800
6	-2.34709200	0.94181300	-1.22765500
6	-2.87034300	2.03474700	-0.25457200
6	-1.89411600	3.13485900	0.20509500
6	-1.62718400	1.55100300	-2.43096700
6	1.49926700	2.74687400	2.14593700
6	0.89107400	4.50926700	0.41683700
1	-3.29515300	1.53710500	0.62430800
1	-3.70439800	2.51839600	-0.77666000
1	-2.49916000	3.83971800	0.79528000
1	-1.55373200	3.71078300	-0.66191700
1	-0.74539300	2.11964900	-2.12919800
1	-2.30962500	2.23258300	-2.94454700
1	-1.32915400	0.77244100	-3.13863300
1	2.47390400	2.59971100	1.66318900
1	1.20077700	1.79925900	2.59898000
1	1.66522800	3.47517100	2.95139400
1	1.03022400	5.34595900	1.11436900
1	0.16921300	4.82937400	-0.33749200
1	1.86014000	4.36297300	-0.07776200
6	-3.64994900	-1.30631400	-0.06816500
6	-4.42250800	-2.25628700	0.62814500
1	-3.94874100	-2.84181400	1.41088800
6	-5.76386000	-2.43561100	0.32274600
1	-6.35830400	-3.15831800	0.87141200
6	-6.34354200	-1.68601800	-0.71179600
1	-7.39048100	-1.83179800	-0.96096200
6	-5.59899800	-0.75116200	-1.42676200
1	-6.03565100	-0.17078000	-2.23211800
6	-4.25872200	-0.54646400	-1.09238400
6	-2.23319500	-1.15650000	0.11483600
1	-1.70170600	-1.92703700	0.66207100
6	-1.54727700	-0.14041700	-0.48582600
6	2.81313900	-1.87276500	0.16452100
1	2.29915800	-2.72354000	0.59539800
6	4.14780600	-1.95950300	-0.20898500
1	4.71194700	-2.87487600	-0.08424000
6	4.76986500	-0.83964800	-0.76008200
6	4.09528300	0.36542800	-0.93802400
1	4.62274700	1.21603300	-1.35025700
6	2.75780700	0.44609000	-0.56470500
6	2.11258100	-0.67388900	-0.02555300
6	-0.11039700	-0.12432500	-0.52086800
1	0.33677400	0.32004600	-1.40848900
6	-0.72988000	2.67432400	1.05023200
1	-0.91965500	1.80607500	1.67805100
6	0.47253800	3.26670200	1.16629200
7	0.72799300	-0.63435800	0.34309800
1	2.22268100	1.38481900	-0.65844200
5	0.38659600	-1.15594800	1.90347700
9	0.08946400	-2.50662200	1.78664700
9	1.53766600	-0.90733500	2.60577300
9	-0.67997500	-0.40515200	2.35110600

7	6.18198900	−0.92948000	−1.15919800
8	6.70374900	0.07538300	−1.64295200
8	6.75628800	−2.00426300	−0.98886300

TS-tf-B-12
E(RB3LYP)=-1550.521669 a.u.

8	-3.98589400	1.27593300	0.02397600
6	-2.61741400	1.53459400	-0.38065300
6	-2.17558500	2.65445600	0.57044500
6	-0.68581600	2.97346500	0.46729300
6	-2.64697500	1.99437000	-1.85129700
6	2.42178300	1.42892500	2.02408800
6	2.21419600	3.23219300	0.24036800
1	-2.41721400	2.33500900	1.58992900
1	-2.76999100	3.55052700	0.36370000
1	-0.45435300	3.81710800	1.12766900
1	-0.43950000	3.30554400	-0.54785200
1	-1.64815600	2.24142200	-2.22394100
1	-3.28372300	2.87848300	-1.95418100
1	-3.04990800	1.19821100	-2.48266100
1	3.49314800	1.41775400	1.81076700
1	2.07634600	0.43001600	2.29969900
1	2.27179100	2.07109900	2.90917100
1	2.01032900	4.11107100	0.87335500
1	1.77618200	3.44663700	-0.73671300
1	3.29812700	3.14852400	0.14444900
6	-3.75444000	-1.05295500	-0.53675300
6	-4.38229200	-2.26645700	-0.85421200
1	-3.76853100	-3.15166500	-0.99711900
6	-5.76779300	-2.34248300	-0.97158700
1	-6.24228600	-3.28702600	-1.21744200
6	-6.54445500	-1.19908300	-0.75858600
1	-7.62585300	-1.25368700	-0.84239300
6	-5.94297800	0.01967400	-0.44194600
1	-6.52912600	0.91614600	-0.26962500
6	-4.55491500	0.08821700	-0.34130900
6	-2.32119400	-0.92105500	-0.33955900
1	-1.72816600	-1.82640600	-0.27246700
6	-1.74826300	0.29054400	-0.21132600
6	2.62361300	-1.82769800	0.05640000
1	2.17552900	-2.69779100	0.51504200
6	3.96248700	-1.81177000	-0.23764100
1	4.59647000	-2.66056900	-0.01479000
6	4.53543400	-0.67180800	-0.84506700
6	3.75932500	0.40493800	-1.22006300
1	4.21604600	1.22808900	-1.75572600
6	2.38624000	0.40148600	-0.92855600
6	1.78930300	-0.70115500	-0.23713400
6	-0.25108700	0.47606400	-0.14257100
1	0.04991000	0.85575400	-1.12387100
6	0.18365800	1.76612400	0.86871200
1	-0.13642000	1.35476400	1.83070100
6	1.62604600	2.02927800	0.91197300
7	0.50355900	-0.67061900	0.20650900
1	1.78213700	1.14868600	-1.42130000
5	0.11854000	-1.52627600	1.57002500
9	-0.25703300	-2.79712600	1.17648500
9	1.26720700	-1.55620800	2.36354500
9	-0.87853500	-0.81336600	2.21207600

7	5.96820100	−0.65548400	−1.13603600
8	6.43930600	0.35896100	−1.65686100
8	6.62335900	−1.65520600	−0.83747600

TS-cf-B-12
E(RB3LYP)=-1550.510878 a.u.

8	-3.79829400	-0.94168900	0.93659300
6	-2.52911100	-0.24553200	1.17274600
6	-1.83921500	-1.16141600	2.20717000
6	-0.31177300	-1.11922100	2.17644000
6	-2.87241800	1.11309300	1.79950700
1	-2.17194400	-2.18722600	2.01175900
1	-2.20421600	-0.89710200	3.20431600
1	0.07452000	-1.75387900	2.98223000
1	0.06079200	-0.10520900	2.35629500
1	-1.98208400	1.60512100	2.18822800
1	-3.57557100	0.93134200	2.61867700
1	-3.33078400	1.78167700	1.07035700
6	-3.93542300	-0.08738900	-1.29847700
6	-4.73317600	0.24468500	-2.40236300
1	-4.25517400	0.60261800	-3.31054800
6	-6.11855300	0.11827800	-2.33895900
1	-6.72944600	0.38412700	-3.19561800
6	-6.71748300	-0.36053000	-1.16880000
1	-7.79722500	-0.46500400	-1.11661400
6	-5.94277500	-0.69896400	-0.05886400
1	-6.39072200	-1.07221000	0.85590900
6	-4.55812900	-0.54906500	-0.12339300
6	-2.48426900	-0.07402800	-1.30364700
1	-1.98181600	0.00256600	-2.26588800
6	-1.76460300	-0.15177900	-0.16647900
6	-0.26311500	-0.25432900	-0.31777400
6	0.17138000	-1.64258500	0.81722300
7	0.58454100	0.82596100	-0.08282000
5	0.08510400	2.28862700	0.49182700
9	0.95187400	3.23511700	-0.01618700
9	-1.19348100	2.48850400	0.02612100
9	0.15747400	2.21716800	1.88804000
6	1.75338900	-3.31091600	-0.21669900
1	1.59666800	-4.23171500	0.36582700
1	1.05699000	-3.34856800	-1.05935100
1	2.78027900	-3.33991300	-0.58774100
6	2.56378200	-1.81809900	1.68563000
1	3.56189500	-1.82257900	1.23945700
1	2.39670000	-0.87037200	2.19625300
1	2.55620800	-2.61238200	2.44962300
1	-0.05587300	-0.75846500	-1.26089100
1	-0.53527900	-2.34940500	0.37306800
6	1.92414100	0.63700900	-0.35800300
6	2.91172900	1.44616800	0.28411900
6	2.38617000	-0.41933000	-1.18753600
6	4.25434900	1.20593000	0.10215300
1	2.59577400	2.24409700	0.93800000
6	3.75101000	-0.63892400	-1.39669500
1	1.69298900	-0.98450300	-1.79520200
6	4.66965500	0.15534600	-0.73552700
1	5.00248900	1.80488900	0.60590700
1	4.09965000	-1.41812300	-2.06317600
6	1.50011200	-2.13566800	0.68359300

7	6.10123400	−0.09609400	−0.92394200
8	6.42753000	−1.04678900	−1.63778000
8	6.89231200	0.65404200	−0.35214300

trans-**12**-**B**
E(RB3LYP)=-1550.561402 a.u.

6	5.39435300	-2.30891700	-1.65524100
6	6.19993500	-1.16722900	-1.65953900
6	5.69149500	0.06084900	-1.23303200
6	4.36824300	0.14169300	-0.80299300
6	3.53678500	-0.99297600	-0.80234200
6	4.07000600	-2.21556100	-1.23088700
8	3.88147300	1.37091800	-0.45341100
6	2.71862800	1.47154700	0.41292000
6	1.74012300	0.32274200	0.17727100
6	2.15443400	-0.82612100	-0.37496700
6	2.10430200	2.83537300	0.01415900
6	0.63415500	3.03356800	0.41967900
6	-0.20519600	1.84256100	-0.07464800
6	0.33402200	0.60485500	0.67593900
6	3.21744900	1.46127400	1.86911000
6	-1.74897300	1.95502100	-0.01066600
6	-2.23877400	0.61655600	-0.67421600
6	-1.67752700	-0.60524300	0.04471400
7	-0.53271900	-0.58397800	0.66122900
6	-3.71452400	0.53959100	-0.93245900
6	-4.39301700	-0.60627300	-0.78074200
6	-3.76181000	-1.83124800	-0.33707700
6	-2.46851300	-1.83201200	0.05012100
6	-2.22067000	3.15951600	-0.84544100
6	-2.29286000	2.07686700	1.42635400
1	5.79523000	-3.26307100	-1.98212400
1	7.23227500	-1.23063200	-1.99087700
1	6.30094700	0.95845000	-1.22938900
1	3.43147000	-3.09503100	-1.22551600
1	1.48385500	-1.67450000	-0.46786800
1	2.17636200	2.89818700	-1.07702700
1	2.72755000	3.63954100	0.41903200
1	0.28268200	3.97269500	-0.01764700
1	0.53677000	3.13792000	1.50774100
1	0.03834700	1.71190700	-1.13956400
1	0.41309200	0.86012600	1.73996100
1	2.40417500	1.64063200	2.57813700
1	3.97215400	2.24238800	2.00135600
1	3.66124800	0.49238200	2.11064400
1	-4.22690900	1.40915700	-1.32344200
1	-4.35662300	-2.73571000	-0.31913200
1	-1.99179100	-2.73912700	0.39304400
1	-3.30944300	3.25792300	-0.84453800
1	-1.88405700	3.08936900	-1.88610300
1	-1.82616200	4.08976700	-0.42980500
1	-3.38649800	2.13182200	1.41939300
1	-1.92271400	2.99113800	1.89934700
1	-2.00988300	1.23145800	2.05979300
5	-0.14640000	-1.78285600	1.79327600
9	-1.27523500	-1.88330200	2.57853700
9	0.93767100	-1.30166000	2.48053200
9	0.10831800	-2.93151200	1.06406900
1	-1.79397900	0.61064500	-1.68727500

7	−5.83023900	−0.63834500	−1.11386000
8	−6.40571800	−1.71795800	−0.99128900
8	−6.35882600	0.40613500	−1.48910700

cis-**12-B**
E(RB3LYP)=−1550.552497 a.u.

8	−3.78199700	−1.12249400	0.90745700
6	−2.42641700	−0.61834100	1.11618200
6	−1.71174200	−1.81462000	1.76997500
6	−0.18614900	−1.74308200	1.67683900
6	−2.52308000	0.57127300	2.08200800
1	−2.05907700	−2.72045600	1.25998000
1	−2.03188900	−1.89365900	2.81390900
1	0.22874200	−2.62837900	2.16517100
1	0.19843200	−0.87372800	2.22357100
1	−1.53885200	0.93003300	2.38930200
1	−3.08021400	0.25283500	2.96879100
1	−3.03903300	1.40965300	1.61246700
6	−4.02135600	0.12025800	−1.13689800
6	−4.87867800	0.67859200	−2.09438900
1	−4.44808600	1.16721200	−2.96471000
6	−6.26137800	0.61264800	−1.93742400
1	−6.91590300	1.05377600	−2.68232000
6	−6.79955700	−0.03018500	−0.81848900
1	−7.87665000	−0.08882100	−0.69194200
6	−5.96513800	−0.59400500	0.14743200
1	−6.36508900	−1.09717900	1.02136600
6	−4.58221200	−0.50886700	−0.00944900
6	−2.57385500	0.09613500	−1.25721900
1	−2.13764900	0.38269700	−2.21206900
6	−1.78403900	−0.25155200	−0.22780900
6	−0.28230900	−0.36095000	−0.42696800
6	0.24400000	−1.69072800	0.19832300
7	0.55025800	0.77915200	0.06429000
6	1.86998400	−3.08884300	−1.14842100
1	1.45569500	−4.01291000	−0.73315400
1	1.30823200	−2.85423400	−2.05941800
1	2.90641500	−3.29798600	−1.43120500
6	2.58915000	−2.33314700	1.13357500
1	3.63466100	−2.50513400	0.86170000
1	2.56585600	−1.55530400	1.90155600
1	2.21755900	−3.25881500	1.58003100
1	−0.12159500	−0.40507500	−1.51508300
1	−0.32105400	−2.47793100	−0.31484000
6	1.84317300	0.60162900	−0.02648900
6	2.79154000	1.54468200	0.54154700
6	2.35725000	−0.62432300	−0.74644600
6	4.12153800	1.38843800	0.34733100
1	2.41413100	2.35739500	1.14369400
6	3.83470900	−0.66937100	−0.94306200
1	1.91680500	−0.57843800	−1.75735600
6	4.63021000	0.28506100	−0.43548300
1	4.83632000	2.07803200	0.77845700
1	4.27037400	−1.48583900	−1.50608800
6	1.76307000	−1.95412900	−0.11093400
5	−0.00659500	2.32858800	0.47781700
9	−1.31989700	2.41108800	0.11494200
9	0.21384600	2.42793900	1.84272900
9	0.79064600	3.18490100	−0.25253800

7	6.08733600	0.19778700	-0.65822900
8	6.78100600	1.08508900	-0.16548300
8	6.51325000	-0.74935000	-1.31596400

13-B
E(RB3LYP)=-1460.594675 a.u.

8	-3.43097100	0.29198000	-1.76591600
6	-2.22866600	0.91202900	-1.20325000
6	-2.72957400	2.00027300	-0.21224100
6	-1.75590000	3.11991800	0.20443000
6	-1.55596500	1.52871700	-2.42974100
6	1.72663600	2.78784000	1.99365800
6	1.01114600	4.54136700	0.29798800
1	-3.10940500	1.49792400	0.68437500
1	-3.59241100	2.46758000	-0.70162400
1	-2.35012500	3.81665900	0.81521200
1	-1.46039900	3.69725500	-0.67824200
1	-0.66617400	2.09967900	-2.15754100
1	-2.25984200	2.20792500	-2.91718900
1	-1.27930100	0.75309100	-3.14922400
1	2.67409900	2.64456100	1.45855000
1	1.46219000	1.83929400	2.46525700
1	1.92919400	3.52193300	2.78567600
1	1.18683100	5.37716500	0.98849100
1	0.24314800	4.85851200	-0.41063700
1	1.94949900	4.40172900	-0.25459700
6	-3.47035800	-1.34810500	-0.00419000
6	-4.21100600	-2.29936600	0.72122800
1	-3.70470200	-2.88369400	1.48438100
6	-5.56403700	-2.48466700	0.46925800
1	-6.13222000	-3.21055200	1.04140600
6	-6.18813500	-1.73749000	-0.53933000
1	-7.24378700	-1.88651500	-0.74659000
6	-5.47473400	-0.79862900	-1.28150500
1	-5.94477800	-0.21782400	-2.06771200
6	-4.12283800	-0.59103800	-1.00147900
6	-2.04544900	-1.18736400	0.12495000
1	-1.48650700	-1.95337000	0.65079500
6	-1.39307200	-0.16347600	-0.49190400
6	3.04152800	-1.79285200	0.06187100
1	2.57007600	-2.64349100	0.54012800
6	4.36970100	-1.86608500	-0.35348400
1	4.92177000	-2.78305000	-0.18846600
6	4.97112200	-0.76227200	-0.97225900
6	4.22932000	0.41248900	-1.16375900
1	4.71691900	1.26590600	-1.62238700
6	2.90513200	0.47824800	-0.75226500
6	2.29875600	-0.62979000	-0.14635900
6	0.04732400	-0.13558700	-0.58019200
1	0.45759700	0.28368200	-1.49741700
6	-0.55084900	2.68280000	1.00349500
1	-0.69900000	1.80996100	1.63582900
6	0.64572800	3.29369700	1.06659400
7	0.92074500	-0.60842200	0.26456000
1	2.34872100	1.40291000	-0.86835400
5	0.62700000	-1.10911600	1.83371800
9	0.36140100	-2.47085000	1.74556900
9	1.77960300	-0.82272100	2.52085600
9	-0.45182900	-0.38404000	2.30157100

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8              6.26020200   -0.72584200   -1.41234700
6              7.07046100   -1.87674300   -1.22065900
1              8.04906800   -1.62625500   -1.63194000
1              7.17748200   -2.12273700   -0.15692600
1              6.66779000   -2.74782100   -1.75274800
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TS-tf-B-13
E(RB3LYP)=-1460.547062 a.u.

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8              -3.76703700      1.37614200      0.03962500
6              -2.38010800      1.58052700     -0.33830400
6              -1.90535100      2.65746600      0.64585600
6              -0.40626700      2.93558800      0.56028800
6              -2.37136400      2.07651500     -1.79756400
6               2.67518500      1.23162700      2.05092400
6               2.51424100      3.07537200      0.30530700
1              -2.16215200      2.31632400      1.65457200
1              -2.47329300      3.57578200      0.46195200
1              -0.16018100      3.76714800      1.23169300
1              -0.14345400      3.27676800     -0.44780400
1              -1.35857800      2.28927200     -2.15265900
1              -2.96869800      2.98935700     -1.88569000
1              -2.80058300      1.31338200     -2.45215400
1               3.72016100      1.10424300      1.75311600
1               2.25597300      0.26902500      2.34908100
1               2.67028100      1.88238700      2.94204800
1               2.43103300      3.95856200      0.95948300
1               2.04395800      3.34500000     -0.64318700
1               3.57951000      2.89804300      0.13914100
6              -3.63375900     -0.95512200     -0.54027100
6              -4.31289200     -2.13564500     -0.87490500
1              -3.73805200     -3.04619600     -1.02079500
6              -5.69964900     -2.14852700     -1.00602300
1              -6.21339400     -3.06892500     -1.26478400
6              -6.42614200     -0.97338100     -0.79084800
1              -7.50810100     -0.97805800     -0.88566700
6              -5.77273300      0.21400300     -0.45756300
1              -6.31910100      1.13494200     -0.28302500
6              -4.38398400      0.21883900     -0.34174000
6              -2.19661100     -0.88764200     -0.33740000
1              -1.64192700     -1.81802600     -0.28752600
6              -1.56924200      0.29487200     -0.19092600
6               2.74175600     -1.96456000      0.00993600
1               2.27746000     -2.81682100      0.48543600
6               4.07107600     -2.00211100     -0.32083500
1               4.67224100     -2.87976300     -0.10744400
6               4.70022400     -0.90222600     -0.95875600
6               3.94010700      0.20420600     -1.30659900
1               4.36841600      1.02740300     -1.86571000
6               2.57220100      0.25031100     -0.97244800
6               1.94344200     -0.81233400     -0.27164900
6              -0.06757300      0.40495900     -0.13331000
1               0.25414200      0.83475900     -1.08496700
6               0.43470000      1.71139500      0.95612600
1               0.08118400      1.26034900      1.88630600
6               1.86842800      1.90364500      0.98420900
7               0.64651700     -0.75063600      0.18379300
1               1.99477400      1.04995200     -1.41229700
5               0.24267200     -1.62308300      1.52231100
9              -0.17025800     -2.87632500      1.09823000
9               1.38625300     -1.71153000      2.31988900
9              -0.73806500     -0.90904600      2.19067700
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8                 6.02602400   -1.06272000   -1.21786600
6                 6.71389600   -0.00142600   -1.86251600
1                 7.75283500   -0.32173600   -1.94728900
1                 6.31065700    0.18944400   -2.86509100
1                 6.66513800    0.92387400   -1.27403600
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TS-cf-B-13
E(RB3LYP)=-1460.539029 a.u.

8	-3.61417700	-0.94820300	0.96441000
6	-2.34742800	-0.23578000	1.17210200
6	-1.64483700	-1.11583300	2.22880000
6	-0.11747400	-1.04802500	2.20484000
6	-2.69949100	1.13634900	1.76477400
1	-1.95772900	-2.15158100	2.05329200
1	-2.02213200	-0.83689500	3.21755700
1	0.27344400	-1.65014900	3.03352200
1	0.23493300	-0.02215500	2.35695400
1	-1.81063200	1.64751100	2.13185600
1	-3.39452000	0.97078300	2.59443000
1	-3.16952800	1.78042400	1.02099900
6	-3.76984500	-0.16078800	-1.29442900
6	-4.57743700	0.12840100	-2.40270700
1	-4.10805800	0.46668600	-3.32298000
6	-5.96125100	-0.01497000	-2.33018200
1	-6.57885600	0.21809900	-3.19174800
6	-6.54890600	-0.46788900	-1.14454700
1	-7.62697100	-0.58556200	-1.08411000
6	-5.76412000	-0.76328600	-0.02924000
1	-6.20260800	-1.11583900	0.89834900
6	-4.38153900	-0.59722200	-0.10390500
6	-2.31818400	-0.12392200	-1.30653600
1	-1.82066300	-0.06130400	-2.27234100
6	-1.59201400	-0.16524800	-0.17265800
6	-0.08857000	-0.24908500	-0.31802700
6	0.38830900	-1.60057100	0.86889400
7	0.73867900	0.84252800	-0.11178100
5	0.23875600	2.31225200	0.41342100
9	1.09930400	3.24728200	-0.12979500
9	-1.04650000	2.49880600	-0.04510700
9	0.31927400	2.29742700	1.81462500
6	2.03027700	-3.21966800	-0.14728400
1	1.93825300	-4.14287700	0.44501500
1	1.32470300	-3.30369200	-0.97939500
1	3.05036000	-3.19370700	-0.54026000
6	2.79677900	-1.68510900	1.73005300
1	3.76566400	-1.53030400	1.24196900
1	2.55207000	-0.80115400	2.31791900
1	2.92906900	-2.52998700	2.42462200
1	0.13489100	-0.79106700	-1.23662900
1	-0.29822000	-2.33763800	0.44240100
6	2.08978500	0.65835900	-0.35875500
6	3.05515900	1.46994300	0.31361800
6	2.58749300	-0.37091400	-1.18840500
6	4.40004700	1.25976900	0.13944000
1	2.71625200	2.24331100	0.98652200
6	3.96342400	-0.56099000	-1.39523500
1	1.91061200	-0.94851000	-1.80442800
6	4.87770300	0.24307300	-0.72405700
1	5.12945300	1.86686700	0.66532600
1	4.28889300	-1.33020500	-2.08505800
6	1.73356400	-2.04042800	0.73843400

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8              6.22845900     0.15666200    -0.83043400
6              6.77394500    -0.83193000    -1.69367400
1              6.45711400    -0.67600500    -2.73204700
1              7.85695100    -0.72575100    -1.62638700
1              6.48743000    -1.84295600    -1.37717500
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trans-**13-B**
E(RB3LYP)=-1460.586942 a.u.

6	5.24214700	-2.41218600	-1.50094600
6	6.07650700	-1.29196300	-1.47234300
6	5.58123100	-0.05005500	-1.07075400
6	4.24273300	0.06681700	-0.69965700
6	3.38296800	-1.04632700	-0.73198700
6	3.90329000	-2.28304800	-1.13439400
8	3.77491400	1.30918300	-0.37364900
6	2.57278000	1.44665300	0.43368700
6	1.58093800	0.31672600	0.17040100
6	1.98894500	-0.84409600	-0.36061600
6	2.00480000	2.81465600	-0.01524500
6	0.52394600	3.05193200	0.32800500
6	-0.32387400	1.86948100	-0.17303500
6	0.16473300	0.63401300	0.61535100
6	3.00345800	1.45025400	1.91154700
6	-1.86660200	2.01074000	-0.16071400
6	-2.36961200	0.67693700	-0.82346600
6	-1.85359800	-0.53682500	-0.06713900
7	-0.72548600	-0.53575400	0.58852500
6	-3.84379300	0.62800200	-1.12083200
6	-4.58079500	-0.49250600	-0.98430900
6	-3.95194500	-1.71088900	-0.50004300
6	-2.66871800	-1.74033400	-0.07306400
6	-2.28561200	3.21606000	-1.02182900
6	-2.45080300	2.16582300	1.25668100
1	5.63177500	-3.37760800	-1.80809300
1	7.12047100	-1.38269100	-1.75803300
1	6.21277000	0.83176600	-1.04181300
1	3.24265900	-3.14587400	-1.15407600
1	1.30173500	-1.67669200	-0.47249600
1	2.12016500	2.85278700	-1.10389700
1	2.63019500	3.61344600	0.39755700
1	0.21059000	3.98864200	-0.14235300
1	0.38759100	3.18288800	1.40908800
1	-0.04869600	1.71552200	-1.22697000
1	0.21592000	0.90792700	1.67639700
1	2.16236500	1.65748000	2.57927100
1	3.76807500	2.21757000	2.06637100
1	3.41426600	0.47610600	2.18786700
1	-4.30531100	1.50157000	-1.56455200
1	-4.52475300	-2.63133300	-0.48020100
1	-2.22620200	-2.65612800	0.29185800
1	-3.37179900	3.33231500	-1.05297500
1	-1.92201000	3.12469000	-2.05182300
1	-1.88393600	4.14382000	-0.60655100
1	-3.54298900	2.22214800	1.21143600
1	-2.09005700	3.08708900	1.72422800
1	-2.19237600	1.33035300	1.91353500
5	-0.40395700	-1.71969700	1.73340700
9	-1.55543900	-1.80153900	2.49234000
9	0.66925800	-1.25997500	2.45733600
9	-0.14601800	-2.88785400	1.03047800
1	-1.87297700	0.63781600	-1.81190600

8	−5.89193700	−0.45859400	−1.37106800
6	−6.75633800	−1.52340900	−0.99216700
1	−6.52579600	−2.45241000	−1.52852600
1	−6.72765800	−1.71059200	0.08807000
1	−7.76055200	−1.20098500	−1.27056800

cis-**13**-**B**
E(RB3LYP)= -1460.578494 a.u.

8	3.66329800	1.15158000	0.78535000
6	2.29118700	0.71960700	1.04805800
6	1.62021000	2.00430900	1.56464500
6	0.09306200	1.95701100	1.50319600
6	2.35266900	-0.35753600	2.14010400
1	1.97967600	2.83364500	0.94446200
1	1.96235600	2.19780400	2.58663200
1	-0.29771900	2.89854800	1.89895100
1	-0.29727800	1.15962600	2.14687600
1	1.35779700	-0.65959700	2.47210000
1	2.91014800	0.04396400	2.99237600
1	2.85269700	-1.25320300	1.76986400
6	3.84914400	-0.30348000	-1.11887600
6	4.68271600	-0.98509700	-2.01519600
1	4.23143900	-1.54648600	-2.82941100
6	6.06809700	-0.94891000	-1.86947100
1	6.70343700	-1.48580600	-2.56672400
6	6.63358200	-0.21270100	-0.82413600
1	7.71278900	-0.17687300	-0.70670600
6	5.82303500	0.47462100	0.08022100
1	6.24380800	1.05215700	0.89659200
6	4.43706200	0.42020800	-0.06409400
6	2.40189800	-0.24479000	-1.23614800
1	1.95041000	-0.61403600	-2.15479700
6	1.62873000	0.23100100	-0.24597900
6	0.12892700	0.36295700	-0.45665100
6	-0.37256100	1.75282100	0.04935600
7	-0.74146300	-0.71419500	0.09629500
6	-2.03873800	3.15479700	-1.24338700
1	-1.59362500	4.06545900	-0.82914700
1	-1.52299300	2.93265300	-2.18454100
1	-3.08524000	3.37822500	-1.47131600
6	-2.72074500	2.33602400	1.02378600
1	-3.77746600	2.44227800	0.76501700
1	-2.64130200	1.56393500	1.79360400
1	-2.39371100	3.28261400	1.46154000
1	-0.01957200	0.33431800	-1.54664600
1	0.18407500	2.47654900	-0.55878100
6	-2.02821900	-0.51949600	-0.08090000
6	-3.02666100	-1.38888300	0.50295600
6	-2.48451500	0.66868100	-0.88881500
6	-4.34230300	-1.21399600	0.22343300
1	-2.70967200	-2.16502200	1.18254800
6	-3.94810300	0.71924500	-1.18195800
1	-1.96659600	0.58686500	-1.86001700
6	-4.82141700	-0.17528300	-0.67054600
1	-5.05918100	-1.87498400	0.69741900
1	-4.31781500	1.50365500	-1.83250300
6	-1.90024000	1.99724700	-0.23627000
5	-0.23548300	-2.18664700	0.72453500
9	1.09058800	-2.34738000	0.42759500
9	-0.49831400	-2.10279600	2.08576900
9	-1.01634600	-3.13962100	0.09719400

6	−7.06215000	−1.05932700	−0.60921400
1	−6.76076900	−2.04677600	−0.97941800
1	−7.19711700	−1.10434600	0.47872700
1	−8.01263600	−0.78374300	−1.06787500
8	−6.14325100	−0.04343300	−0.99225900

14-B
E(RB3LYP)=-1421.289533 a.u.

8	-3.21195600	0.58176800	-1.64515200
6	-1.94325200	1.06640500	-1.09600700
6	-2.31552800	2.11457900	-0.00912900
6	-1.24339300	3.13369400	0.42509800
6	-1.27287200	1.71916500	-2.30468900
6	2.30620000	2.44839000	1.96474100
6	1.61829000	4.35715500	0.43496400
1	-2.68599600	1.57915000	0.87213800
1	-3.16511900	2.67320700	-0.41930600
1	-1.75202000	3.82024500	1.11903700
1	-0.95983600	3.75423000	-0.43158500
1	-0.33288400	2.20181000	-2.03025700
1	-1.94047500	2.48226900	-2.71259200
1	-1.08371400	0.98017200	-3.08827100
1	3.21277600	2.29203300	1.36620600
1	2.00980500	1.48371400	2.38153100
1	2.59710600	3.10692400	2.79481900
1	1.89960400	5.12662300	1.16636800
1	0.83329200	4.77799400	-0.19679400
1	2.50677800	4.19205600	-0.18849800
6	-3.30812500	-1.17734000	-0.00392500
6	-4.09075600	-2.12266900	0.68429800
1	-3.60135800	-2.79654300	1.38181500
6	-5.46253100	-2.18948300	0.47904400
1	-6.06221600	-2.91207300	1.02246300
6	-6.06584900	-1.32604700	-0.44598200
1	-7.13692800	-1.38173100	-0.61706000
6	-5.31210300	-0.38963600	-1.15026000
1	-5.76636000	0.28033800	-1.87218300
6	-3.93854900	-0.30260300	-0.91562200
6	-1.87109800	-1.13202700	0.07361500
1	-1.35325400	-1.97355300	0.52047000
6	-1.16629800	-0.11785300	-0.49974800
6	3.14864400	-2.10915700	-0.19877200
1	2.63275700	-2.93927600	0.26897900
6	4.44840200	-2.25772100	-0.66978700
1	4.95337500	-3.21526300	-0.56490500
6	5.10743200	-1.18066400	-1.27450900
6	4.45492300	0.05009500	-1.40128800
1	4.98475000	0.88297000	-1.85037400
6	3.15320300	0.19498500	-0.93313100
6	2.48856900	-0.88459700	-0.34019300
6	0.26709400	-0.19343400	-0.65142300
1	0.67122400	0.24541800	-1.56226800
6	-0.02767400	2.56167200	1.11467700
1	-0.20116600	1.65975000	1.69793500
6	1.21070500	3.08620400	1.14199400
7	1.13317500	-0.77800800	0.12831100
1	2.66394300	1.16163500	-0.99717800
5	0.85978400	-1.34183900	1.68009300
9	0.50391900	-2.67735800	1.53168600
9	2.05239400	-1.16576200	2.33643300
9	-0.15229000	-0.57668400	2.22490700

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8                    6.38295700   -1.26800100   -1.75047200
1                    6.72794600   -2.15343100   -1.57517300
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TS-tf-B-14
E(RB3LYP)=-1421.241573 a.u.

8	-3.51939800	1.36364200	0.16931100
6	-2.15914100	1.57617000	-0.29067800
6	-1.62954400	2.65289000	0.66511100
6	-0.13840900	2.93212000	0.49002700
6	-2.23882700	2.07409000	-1.74717100
6	3.02848400	1.25505200	1.79863400
6	2.75602800	3.08534600	0.05583600
1	-1.82578400	2.31049800	1.68692400
1	-2.20782100	3.57110000	0.51627100
1	0.14962000	3.75720000	1.15232700
1	0.06284200	3.28054900	-0.52955900
1	-1.24930100	2.28856400	-2.16198900
1	-2.84147100	2.98625900	-1.79868000
1	-2.70524000	1.31102400	-2.37587300
1	4.06035400	1.14325100	1.45283000
1	2.63850400	0.28928200	2.12490900
1	3.05422000	1.91463600	2.68306600
1	2.69130500	3.96689200	0.71441800
1	2.23638200	3.34854400	-0.86834500
1	3.81412700	2.92344700	-0.16185100
6	-3.40813300	-0.96332200	-0.43350700
6	-4.09956600	-2.14491000	-0.73722200
1	-3.52959500	-3.05133900	-0.92266500
6	-5.49154000	-2.16451900	-0.78849400
1	-6.01459400	-3.08584200	-1.02438200
6	-6.21042100	-0.99512100	-0.52281100
1	-7.29600400	-1.00504000	-0.55518300
6	-5.54477400	0.19337800	-0.21894400
1	-6.08476500	1.11011900	-0.00654700
6	-4.15170200	0.20519800	-0.18371500
6	-1.96175800	-0.88983900	-0.31101100
1	-1.40066600	-1.81767400	-0.29447000
6	-1.33410500	0.29512200	-0.19369600
6	2.99129200	-1.94085800	-0.21600000
1	2.55720500	-2.79698000	0.28055400
6	4.30709200	-1.96555000	-0.60870700
1	4.90778900	-2.85118500	-0.41127400
6	4.89231600	-0.86110800	-1.27502800
6	4.10576300	0.23293200	-1.59160100
1	4.53271100	1.04048200	-2.17663400
6	2.75797900	0.27241800	-1.19588500
6	2.17145200	-0.79772600	-0.46041000
6	0.16995700	0.41759500	-0.21407600
1	0.42970300	0.83180700	-1.19202800
6	0.72287200	1.70132200	0.82308600
1	0.43505700	1.26492000	1.78296300
6	2.16192200	1.90580400	0.76668400
7	0.90252900	-0.74446700	0.06183600
1	2.14984500	1.05661700	-1.62212200
5	0.57949600	-1.61522300	1.42048500
9	0.16221200	-2.87596300	1.02235500
9	1.76504700	-1.68877500	2.15895600
9	-0.37289900	-0.91186900	2.13814700

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8                    6.19948700    -0.85978600    -1.66315600
1                    6.60702400    -1.70003000    -1.41482200
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TS-cf-B-14
E(RB3LYP)= -1421.233508 a.u.

8	3.34098000	1.02954400	0.93032600
6	2.04563800	0.38332400	1.17195000
6	1.31723800	1.42508200	2.04797500
6	-0.20830300	1.38291100	1.95563000
6	2.32439800	-0.89700100	1.97137300
1	1.66557600	2.41638200	1.73605200
1	1.63906300	1.29070500	3.08548200
1	-0.62356000	2.10857300	2.66470000
1	-0.59595900	0.39795300	2.23734900
1	1.40402100	-1.32960600	2.36163200
1	2.98362800	-0.63142900	2.80437900
1	2.80922400	-1.65235600	1.35231500
6	3.58129000	-0.07028300	-1.18554000
6	4.43147300	-0.53020000	-2.20023700
1	3.99654400	-0.98299200	-3.08760400
6	5.81393300	-0.40954600	-2.07752300
1	6.46459300	-0.77476800	-2.86574600
6	6.35776100	0.19142300	-0.93769800
1	7.43474800	0.29199900	-0.83916800
6	5.53007000	0.65779300	0.08434700
1	5.93434500	1.12693000	0.97510900
6	4.14833200	0.51426900	-0.03744800
6	2.13150200	-0.07318300	-1.26677000
1	1.67903200	-0.25645400	-2.23932000
6	1.35391500	0.14336700	-0.18847900
6	-0.13910100	0.24494000	-0.42222200
6	-0.63226100	1.73963700	0.52678700
7	-1.00243000	-0.79857000	-0.11575800
5	-0.56540500	-2.19384900	0.61853400
9	-1.42430000	-3.17636100	0.16034000
9	0.73474900	-2.46501700	0.25367000
9	-0.71319200	-1.99613400	2.00070500
6	-2.17449500	3.23910900	-0.78775900
1	-2.07199800	4.23430100	-0.32852100
1	-1.43067200	3.18006100	-1.58790300
1	-3.17712900	3.18873400	-1.22041300
6	-3.07619700	2.00843300	1.24721600
1	-4.02586500	1.81216100	0.73659800
1	-2.88606000	1.21132000	1.96513000
1	-3.21273500	2.94699400	1.80782300
1	-0.29595400	0.64816100	-1.42307600
1	0.09003400	2.40322100	0.04191800
6	-2.33416800	-0.62473600	-0.45410100
6	-3.34778400	-1.31804000	0.27117200
6	-2.76640200	0.28831200	-1.44671500
6	-4.68100200	-1.11026000	0.00016400
1	-3.06063900	-1.99665800	1.06045600
6	-4.12206300	0.47157600	-1.74126400
1	-2.04522200	0.76197200	-2.10002500
6	-5.08671000	-0.21439300	-1.01511600
1	-5.43392000	-1.63814700	0.58187800
1	-4.43183500	1.13677400	-2.54007400
6	-1.95827900	2.19231000	0.26988800

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8                     -6.39652900   -0.00693200   -1.32125400
1                     -6.94885100   -0.58693800   -0.78011000
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trans-**14-B**
E(RB3LYP)= -1421.283596 a.u.

6	5.17524800	-2.10246600	-1.47480600
6	5.93741900	-0.93574900	-1.37595300
6	5.35410800	0.25655400	-0.94360900
6	4.00042200	0.27639200	-0.61217900
6	3.21246300	-0.88455900	-0.71491000
6	3.82046400	-2.07016100	-1.14746600
8	3.44609400	1.47384300	-0.25480100
6	2.21934000	1.50255400	0.52532800
6	1.30464500	0.32836500	0.18452300
6	1.79816600	-0.78225200	-0.38054500
6	1.58148100	2.85468600	0.12448400
6	0.08031000	2.98616300	0.43256700
6	-0.67902300	1.78118700	-0.15005900
6	-0.13997000	0.54185700	0.59833000
6	2.61194000	1.46101500	2.01314900
6	-2.22699500	1.82938100	-0.18280300
6	-2.62894500	0.49943200	-0.91795400
6	-2.06514800	-0.71388900	-0.19346800
7	-0.95876900	-0.67513400	0.49561000
6	-4.08896900	0.38023100	-1.26848500
6	-4.75455300	-0.78669400	-1.19499800
6	-4.07342700	-1.98481400	-0.73544100
6	-2.80665000	-1.96466500	-0.26745500
6	-2.69072500	3.04415500	-1.00692800
6	-2.86191200	1.88887700	1.22002100
1	5.63322900	-3.02919300	-1.80587900
1	6.99320000	-0.95146100	-1.63044800
1	5.92836300	1.17337400	-0.86032200
1	3.21581000	-2.97026000	-1.22180400
1	1.16719900	-1.64908300	-0.54914400
1	1.72471400	2.95318900	-0.95702600
1	2.14531600	3.66794200	0.59384200
1	-0.27625100	3.92484500	-0.00181000
1	-0.09435000	3.05516700	1.51383800
1	-0.36352900	1.69390200	-1.20013700
1	-0.13548700	0.77051800	1.67119700
1	1.74400100	1.59092200	2.66601300
1	3.32801000	2.26121500	2.22359600
1	3.06948600	0.49902200	2.25665300
1	-4.58674300	1.24345800	-1.69219900
1	-4.60803900	-2.93250200	-0.77455300
1	-2.32259600	-2.86664400	0.07831700
1	-3.78044400	3.10024300	-1.06669500
1	-2.29330900	3.01632500	-2.02812900
1	-2.35482800	3.97503500	-0.54310000
1	-3.95373300	1.88407900	1.14242500
1	-2.56992600	2.80840500	1.73644000
1	-2.57418000	1.04265600	1.85043200
5	-0.60009800	-1.88641000	1.60340400
9	-1.76643700	-2.06326800	2.32213400
9	0.42406500	-1.39677800	2.37606500
9	-0.25704900	-3.00743700	0.86188800
1	-2.09793200	0.53102900	-1.88843100

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8                    -6.05807600   -0.86429300   -1.60007400
1                    -6.41360300   -1.73684600   -1.38921500
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cis-**14-B**
E(RB3LYP)= -1421.275109 a.u.

8	3.35329700	1.23500900	0.80542400
6	1.99283400	0.76128800	1.05514700
6	1.27555700	2.02595000	1.55814200
6	-0.24831200	1.92117000	1.49092300
6	2.07576100	-0.30863500	2.15305400
1	1.60774600	2.86273800	0.93268000
1	1.60595800	2.23941200	2.57999000
1	-0.67746900	2.84852700	1.88088000
1	-0.61009500	1.11213100	2.13652300
1	1.08726300	-0.64362700	2.47253300
1	2.60709200	0.11496600	3.01130100
1	2.61131400	-1.18800400	1.79377300
6	3.60550900	-0.22071200	-1.09045700
6	4.46952600	-0.88022200	-1.97443600
1	4.04500200	-1.45801900	-2.79154800
6	5.85134600	-0.80175000	-1.81275800
1	6.51068100	-1.32188500	-2.50035200
6	6.38217600	-0.04494800	-0.76396400
1	7.45836500	0.02379000	-0.63423000
6	5.54087400	0.62108400	0.12818400
1	5.93453600	1.21408500	0.94697700
6	4.15899000	0.52424500	-0.03195000
6	2.15868600	-0.20659600	-1.22400700
1	1.72899300	-0.59234100	-2.14636800
6	1.36009000	0.24758500	-0.24377500
6	-0.14052600	0.32809700	-0.47224700
6	-0.70340400	1.69308500	0.03764000
7	-0.98043000	-0.78970000	0.04926300
6	-2.43960700	3.06561000	-1.19413300
1	-2.03215200	3.97482500	-0.73985600
1	-1.92271500	2.91194200	-2.14818600
1	-3.49701700	3.25235600	-1.40370800
6	-3.08254700	2.10744500	1.02744600
1	-4.14283700	2.16207300	0.76718600
1	-2.95986700	1.31135100	1.76652500
1	-2.81383500	3.05305400	1.50501800
1	-0.27092900	0.30650600	-1.56435300
1	-0.18056500	2.44027800	-0.57231500
6	-2.26800400	-0.64567500	-0.16136400
6	-3.24412500	-1.57002200	0.38114200
6	-2.75208900	0.54296800	-0.95485400
6	-4.55434900	-1.43548900	0.06735900
1	-2.91339900	-2.35006300	1.04913600
6	-4.20963800	0.54401200	-1.28883300
1	-2.20389100	0.51220300	-1.91188500
6	-5.05029100	-0.39706800	-0.81573000
1	-5.27229200	-2.13001700	0.50093000
1	-4.59106700	1.32442400	-1.93700700
6	-2.24121900	1.87052000	-0.24277700
5	-0.42749700	-2.23837300	0.69841300
9	0.91071900	-2.34392100	0.43591700
9	-0.72938000	-2.15661300	2.05080800
9	-1.15061100	-3.22709900	0.05693500

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8              -6.37678500    -0.36239400    -1.14272000
1              -6.82041800    -1.14482400    -0.79162200
```

15-B
E(RB3LYP)=-3917.167284 a.u.

8	-3.34231400	-0.09529600	-1.75029100
6	-2.15993600	0.71761200	-1.44855100
6	-2.70538100	2.02757600	-0.81695800
6	-1.74321300	3.21370500	-0.61979000
6	-1.56544100	0.96550500	-2.83675100
6	1.11187700	3.69472500	2.03277000
6	0.54439100	5.16813000	0.02812400
1	-3.16289600	1.77664400	0.14703900
1	-3.52094500	2.34792100	-1.47573700
1	-2.37879800	4.08959800	-0.42611700
1	-1.23499200	3.44311300	-1.56511300
1	-0.73190300	1.66985700	-2.80890700
1	-2.34119200	1.38837200	-3.47964600
1	-1.22488400	0.02814300	-3.28489200
1	2.17756300	3.69362700	1.76666500
1	0.88327600	2.74734700	2.52443500
1	0.98027200	4.50783900	2.75969400
1	0.40090800	6.06077800	0.65149200
1	-0.08208500	5.27966300	-0.85961900
1	1.59426100	5.18641400	-0.29284300
6	-3.23282000	-1.15041000	0.40916200
6	-3.89346400	-1.88646000	1.41179500
1	-3.33025200	-2.19742600	2.28701300
6	-5.23800500	-2.20482800	1.28353200
1	-5.74583000	-2.76071900	2.06452100
6	-5.93312000	-1.81672700	0.12853800
1	-6.98260000	-2.07422700	0.01961300
6	-5.30053200	-1.10081900	-0.88489500
1	-5.82673900	-0.80080400	-1.78449400
6	-3.95695500	-0.75063500	-0.73567400
6	-1.81877600	-0.89461500	0.42365800
1	-1.20364200	-1.45092600	1.12108200
6	-1.24098000	-0.06315000	-0.49181300
6	3.27482600	-1.13956100	-0.58890100
6	4.58003100	-0.96378600	-1.04483600
1	5.17931500	-1.83340100	-1.28890400
6	5.09573400	0.32381600	-1.18771900
6	4.30547000	1.43196100	-0.88258600
1	4.70262000	2.43586500	-0.99364600
6	3.00183100	1.25137500	-0.42386100
6	2.47924200	-0.03469400	-0.26987300
6	0.18691900	0.05739800	-0.63706100
1	0.53251900	0.40456100	-1.60923800
6	-0.75004300	3.06384900	0.51464900
1	-0.89049600	2.20883000	1.17073100
6	0.24216200	3.91784800	0.81820300
7	1.13524700	-0.20243000	0.22166300
1	2.37330800	2.09761400	-0.16667600
5	1.00045300	-0.51426100	1.86724500
9	0.55751200	-1.81767000	2.00977100
9	2.26070000	-0.31352700	2.35719200
9	0.07535200	0.40532000	2.34144000
1	6.11391100	0.45569100	-1.54019100
35	2.56468200	-2.89679100	-0.43669700

TS-tf-B-15
E(RB3LYP)=-3917.118631 a.u.

8	-3.89378000	1.19131100	0.12849200
6	-2.59351500	1.58590200	-0.38347200
6	-2.25659200	2.82646100	0.45311800
6	-0.83090200	3.33098000	0.24203800
6	-2.77201300	1.92445200	-1.87704100
6	2.52175500	2.19349700	1.73405200
6	2.00339400	4.00490400	0.02874900
1	-2.40160500	2.56243900	1.50631000
1	-2.97906600	3.61486700	0.21705000
1	-0.69362500	4.25488300	0.81657500
1	-0.67778200	3.60640900	-0.80898900
1	-1.84086700	2.27426200	-2.33326700
1	-3.52907400	2.70606500	-1.99425100
1	-3.09841600	1.03654000	-2.42469400
1	3.56771400	2.30764000	1.43850200
1	2.32250700	1.15442800	2.00010600
1	2.37207700	2.79200900	2.64817300
1	1.75419700	4.84111000	0.70132900
1	1.48597200	4.19913900	-0.91338100
1	3.08179200	4.03567200	-0.13802700
6	-3.40131700	-1.12751900	-0.27410000
6	-3.88691300	-2.43126600	-0.45413200
1	-3.17438500	-3.24218200	-0.57803400
6	-5.25576100	-2.68738500	-0.46078600
1	-5.61955000	-3.70035700	-0.60017800
6	-6.15779500	-1.63486800	-0.27495300
1	-7.22637900	-1.82913400	-0.27321300
6	-5.69898600	-0.32932000	-0.09503400
1	-6.38316300	0.49941800	0.05377100
6	-4.32741300	-0.08230400	-0.10361800
6	-1.98680200	-0.80599700	-0.20322500
1	-1.28044200	-1.62371700	-0.13627000
6	-1.56126000	0.47262700	-0.19768800
6	3.10280200	-0.98908100	-0.58119800
6	4.39652000	-0.69108400	-0.96767900
1	5.14098500	-1.47777400	-0.92465900
6	4.74318400	0.57776800	-1.46263900
6	3.74523500	1.51414900	-1.64685500
1	3.95756800	2.45982200	-2.13649000
6	2.43218500	1.23959900	-1.23102700
6	2.07430100	0.00926900	-0.59531400
6	-0.10462000	0.84113600	-0.29128600
1	0.05010400	1.27288900	-1.28329000
6	0.20788600	2.29566200	0.69245200
1	-0.04437600	1.83924100	1.65117800
6	1.58698400	2.72582400	0.69423500
7	0.83404000	-0.16265900	-0.01312600
1	1.66467500	1.91764500	-1.57107600
5	0.69251700	-0.94714400	1.47032000
9	0.17111100	-2.20793500	1.29460400
9	1.96779900	-0.95377200	2.01873800
9	-0.15345800	-0.14557200	2.23314800
1	5.76594800	0.77802700	-1.76480700
35	2.73952400	-2.82144100	-0.22360000

TS-cf-B-15
E(RB3LYP)=-3917.109317 a.u.

8	3.51316700	0.28839000	1.44863400
6	2.16364700	-0.24563500	1.21659700
6	1.37635700	0.30794500	2.42879700
6	-0.09949900	0.62267100	2.16424800
6	2.26731300	-1.77434800	1.25513500
1	1.88067200	1.22993900	2.73972300
1	1.46629200	-0.39645700	3.26162100
1	-0.53537500	1.04658700	3.07575300
1	-0.66781100	-0.28089700	1.92042500
1	1.28115800	-2.23461600	1.25196300
1	2.80793600	-2.06152500	2.16305100
1	2.80703700	-2.14847600	0.38243400
6	3.97485000	0.26372500	-0.90556500
6	4.92867100	0.22446000	-1.93203500
1	4.59320400	0.27742300	-2.96459400
6	6.28619300	0.12114400	-1.63769800
1	7.01621700	0.08421500	-2.44002500
6	6.70346700	0.07411600	-0.30344800
1	7.76117000	-0.00140000	-0.06832100
6	5.77228900	0.11269100	0.73480400
1	6.07806600	0.07597600	1.77510200
6	4.41345300	0.19262000	0.43122600
6	2.55394500	0.47828900	-1.11528100
1	2.23116300	0.82389000	-2.09503500
6	1.65264500	0.28179200	-0.13490900
6	0.22196300	0.72460600	-0.37531800
6	-0.19416500	1.62474000	0.99988300
7	-0.81064500	-0.22411100	-0.61180000
5	-0.53490100	-1.83651300	-0.89860400
9	-1.57911700	-2.24031300	-1.70610200
9	0.68268300	-1.90276200	-1.54537800
9	-0.50874400	-2.52160200	0.31306000
6	-1.24928600	3.83331100	0.36019700
1	-1.00241500	4.48075800	1.21647600
1	-0.43110600	3.93529300	-0.35852500
1	-2.17339000	4.21686800	-0.07783100
6	-2.65874600	2.11730100	1.59921400
1	-3.54035300	2.45588000	1.04479600
1	-2.76922600	1.06141200	1.84593500
1	-2.64599600	2.68690800	2.54335100
1	0.27631300	1.48984600	-1.15325600
1	0.65722200	2.31617600	1.01655200
6	-2.03655400	0.32073400	-0.91764300
6	-3.28391700	-0.27567700	-0.52469000
6	-2.15148000	1.58236900	-1.56240500
6	-4.49538400	0.28391100	-0.88051800
6	-3.38507500	2.14951700	-1.91413300
6	-4.55970500	1.49476300	-1.59513200
1	-5.40745800	-0.19832300	-0.54784000
1	-3.40256800	3.09315200	-2.45094800
6	-1.39806800	2.42618700	0.86082100
1	-5.52560800	1.90926100	-1.86561800
35	-3.35499800	-1.68952800	0.73877700
1	-1.25743500	2.05048700	-1.95295800

trans-**15-B**
E(RB3LYP)=-3917.150760 a.u.

6	4.93094800	-2.53905300	-0.94384100
6	5.85305500	-1.48987900	-0.97478500
6	5.43914900	-0.17591700	-0.74907800
6	4.09373600	0.08426500	-0.49377100
6	3.14762800	-0.95609200	-0.46803700
6	3.58678900	-2.26693800	-0.69355200
8	3.71219700	1.38775400	-0.34088300
6	2.47426500	1.71288900	0.34932500
6	1.41323500	0.63085200	0.16051900
6	1.75505800	-0.60890300	-0.21878900
6	2.03756600	3.03725100	-0.32070700
6	0.57049900	3.42871000	-0.08424800
6	-0.36018200	2.26394100	-0.46459200
6	0.00144400	1.09775500	0.47491800
6	2.81159900	1.89301900	1.84006600
6	-1.88514900	2.52992000	-0.47224100
6	-2.50175800	1.20102200	-1.01923700
6	-1.99221200	-0.03485400	-0.28027900
7	-0.94905300	-0.03074900	0.49111300
6	-4.01070800	1.21129700	-1.13707700
6	-4.74608600	0.09485900	-1.02794500
6	-4.09143300	-1.18463700	-0.82590600
6	-2.78168000	-1.25848200	-0.50162200
6	-2.21020900	3.68278200	-1.44118000
6	-2.44067200	2.85833800	0.92842300
1	5.25723800	-3.56013000	-1.11432800
1	6.90213500	-1.69233800	-1.17010200
1	6.13942400	0.65258000	-0.76946400
1	2.85854100	-3.07317700	-0.66709300
1	1.00754100	-1.38873900	-0.30869500
1	2.19791900	2.90629100	-1.39647300
1	2.70847800	3.83973900	0.00416900
1	0.35159500	4.31687300	-0.68461800
1	0.40797800	3.71029600	0.96368100
1	-0.09568700	1.96558700	-1.49043200
1	0.00183700	1.47909500	1.49901200
1	1.94294400	2.21986000	2.41887200
1	3.60428200	2.63943700	1.94915600
1	3.15718500	0.94651400	2.26387300
1	-4.47712600	2.15199900	-1.40588300
1	-4.65655800	-2.09860700	-0.97338700
1	-3.28638600	3.85356400	-1.53296400
1	-1.81170100	3.48972700	-2.44389800
1	-1.77683300	4.61987200	-1.08314400
1	-3.52303900	3.01613900	0.88618800
1	-1.99129100	3.77810100	1.31495800
1	-2.25219900	2.06237500	1.65348000
5	-0.86137600	-1.00070300	1.96555900
9	-2.14577600	-1.43598700	2.15701400
9	-0.49062900	-0.03772500	2.87956700
9	0.06280300	-1.98732400	1.79894700
1	-2.14191900	1.10034200	-2.06218100
35	-1.91018100	-2.94447400	-0.47317000
1	-5.82224400	0.11436000	-1.16625100

cis-**15-B**
E(RB3LYP)=-3917.146640 a.u.

8	-3.26121500	0.71850400	-1.51946700
6	-1.84428600	0.46605100	-1.26846600
6	-1.14729200	1.54629600	-2.11202200
6	0.32474600	1.75330500	-1.74750700
6	-1.52935500	-0.94614200	-1.78368800
1	-1.69141400	2.48477100	-1.95402900
1	-1.25096000	1.29296100	-3.17240400
1	0.72325200	2.54902500	-2.38136900
1	0.90976100	0.85411500	-1.97344200
1	-0.46555900	-1.18039000	-1.70284400
1	-1.83589500	-1.01732700	-2.83246900
1	-2.06454800	-1.69462500	-1.19798000
6	-3.85037700	0.14681300	0.74384300
6	-4.84936400	-0.23634800	1.64841200
1	-4.59001200	-0.34999800	2.69781800
6	-6.15295700	-0.47084500	1.21567500
1	-6.91701500	-0.77238400	1.92512600
6	-6.47023500	-0.31049100	-0.13631500
1	-7.48486900	-0.48793000	-0.48112100
6	-5.49155700	0.06937100	-1.05572500
1	-5.71953700	0.19825500	-2.10859600
6	-4.18630200	0.28818700	-0.61585400
6	-2.48301300	0.45264900	1.13243600
1	-2.24923700	0.50552400	2.19139800
6	-1.51665300	0.63117500	0.21725700
6	-0.09435800	0.98456100	0.62552900
6	0.45471800	2.14030900	-0.25953800
7	0.80301100	-0.20413700	0.52882300
6	1.69730600	3.72007400	1.27818300
1	1.26993600	4.62172900	0.82821800
1	1.02941400	3.40011800	2.08500800
1	2.65660700	3.99885700	1.72792800
6	2.71254200	3.18342600	-0.94586100
1	3.64711600	3.61056000	-0.57202000
1	2.96851100	2.42148800	-1.68675800
1	2.17293500	3.98649400	-1.45716100
1	-0.11527400	1.30374100	1.67519700
1	-0.23047000	2.98230400	-0.09747900
6	2.08107500	0.04115600	0.42121100
6	3.03512200	-0.93371600	-0.07437300
6	2.60531800	1.38823000	0.89026200
6	4.37197100	-0.70934900	0.02036100
6	4.09232300	1.50713000	0.96130400
1	2.25893900	1.39918800	1.93818500
6	4.90941900	0.50004100	0.60188000
1	5.05811200	-1.43860300	-0.39694700
1	4.49853900	2.44270700	1.33338200
6	1.86754600	2.61849200	0.21247100
5	0.28558000	-1.61738100	1.42307100
9	-0.28010000	-1.00187800	2.52341200
9	-0.58881600	-2.33893900	0.67115300
9	1.44332200	-2.27799400	1.74571400
1	5.98718500	0.59672400	0.68481800
35	2.40250100	-2.41006900	-1.08609100

16-B
E(RB3LYP)=-1460.590149 a.u.

8	-3.29177700	0.32192000	-1.67677400
6	-2.03503700	0.95558900	-1.26482700
6	-2.44604100	2.13914600	-0.34663100
6	-1.39158700	3.20191500	0.01172300
6	-1.46173400	1.44716000	-2.59552900
6	1.81380100	2.84418800	2.25187000
6	1.26921700	4.67946300	0.56771500
1	-2.86295500	1.72347500	0.57793200
1	-3.27327800	2.63637000	-0.86677200
1	-1.94643500	4.02662500	0.48342400
1	-0.97301700	3.63520300	-0.90468100
1	-0.55910600	2.04607700	-2.46035500
1	-2.20945600	2.07171900	-3.09050800
1	-1.23387100	0.60375300	-3.25306300
1	2.81871000	2.71134300	1.83026000
1	1.48291600	1.88226000	2.64773400
1	1.92033200	3.55004100	3.08700300
1	1.33119200	5.48064100	1.31635300
1	0.58308400	5.01199000	-0.21445000
1	2.27199100	4.59514600	0.12859300
6	-3.22377200	-1.15259600	0.22198200
6	-3.92292300	-2.01616400	1.08624500
1	-3.36782400	-2.54412700	1.85639400
6	-5.29454300	-2.18762500	0.95698700
1	-5.82993000	-2.84511300	1.63383800
6	-5.98174900	-1.51707000	-0.06502300
1	-7.05305500	-1.65702100	-0.17625900
6	-5.31215100	-0.66724500	-0.94246900
1	-5.83177700	-0.14750900	-1.74009700
6	-3.93853100	-0.47055100	-0.78660700
6	-1.79008800	-1.02812400	0.22218600
1	-1.21205000	-1.76735600	0.76400700
6	-1.16236600	-0.08229100	-0.53325600
6	3.37519200	-1.52049400	-0.72474800
6	4.68386400	-1.34585600	-1.18426900
1	5.32286100	-2.20617900	-1.34350600
6	5.16940200	-0.06287000	-1.45128700
6	4.36091300	1.05479600	-1.26631600
1	4.74073300	2.05142600	-1.46539400
6	3.05612300	0.88588700	-0.79638200
6	2.56113100	-0.38673100	-0.52271300
6	0.26622500	-0.06458000	-0.74018300
1	0.59546300	0.42146500	-1.65605100
6	-0.29948500	2.74311900	0.95299400
1	-0.49898500	1.82965500	1.50797900
6	0.85342600	3.38178500	1.21771100
7	1.22750100	-0.56256000	-0.01106900
1	2.41809200	1.74194700	-0.59979600
5	1.11196200	-1.17427700	1.54780800
9	0.53793700	-2.43232800	1.47214300
9	2.39573200	-1.19213800	2.02299900
9	0.30138700	-0.27425900	2.22837900
1	6.18888200	0.05344900	-1.80671300

6	3.60715500	−3.87691300	−0.42165900
1	4.03330400	−4.12791400	−1.40151100
1	4.41629200	−3.74942700	0.30662300
1	2.95021200	−4.68384600	−0.09671500
8	2.78817700	−2.71815500	−0.48854900

TS-tf-B-16
E(RB3LYP)= -1460.539740 a.u.

8	-3.59136900	1.29384600	0.27986300
6	-2.27922500	1.61478600	-0.25484400
6	-1.79462500	2.73300700	0.67699300
6	-0.33762600	3.12706500	0.44794200
6	-2.47921100	2.10676800	-1.70163700
6	2.96210400	1.60967200	1.68576400
6	2.53510500	3.54805500	0.09979400
1	-1.92385700	2.38134400	1.70624900
1	-2.44902300	3.60200600	0.54972400
1	-0.09808900	3.98279000	1.09096700
1	-0.19718700	3.47912400	-0.58158900
1	-1.53543500	2.40780600	-2.16652000
1	-3.16008900	2.96355400	-1.71425300
1	-2.91075600	1.30836200	-2.31105000
1	3.99144500	1.60119200	1.31619100
1	2.65384300	0.59481000	1.94126300
1	2.95613900	2.19842300	2.61835900
1	2.41247600	4.36550200	0.82825700
1	1.98766500	3.84536300	-0.79743600
1	3.59984500	3.48270100	-0.13446700
6	-3.33766000	-1.01272100	-0.35028200
6	-3.95193300	-2.24320300	-0.62535300
1	-3.32484000	-3.10124000	-0.85177900
6	-5.33870300	-2.37033300	-0.59659400
1	-5.80234600	-3.32802200	-0.81089200
6	-6.12892400	-1.26126700	-0.27877800
1	-7.21057200	-1.35533200	-0.24892000
6	-5.54092500	-0.02618300	-0.00221900
1	-6.13697800	0.84471500	0.24953800
6	-4.15306100	0.09321200	-0.04716400
6	-1.89710200	-0.82921800	-0.31081000
1	-1.26780800	-1.71071300	-0.34006500
6	-1.35281200	0.39935900	-0.21380500
6	3.11962900	-1.48271300	-0.71098600
6	4.45440000	-1.30886800	-1.03797300
1	5.13371300	-2.15114600	-0.97555800
6	4.92509900	-0.06925500	-1.51321300
6	4.04111900	0.97366400	-1.71087500
1	4.37098200	1.89816400	-2.17417800
6	2.69353800	0.83545000	-1.32791600
6	2.21335600	-0.36465500	-0.73415100
6	0.13003000	0.63190600	-0.32652400
1	0.31116200	1.12792500	-1.28342600
6	0.62282800	1.97417700	0.76668400
1	0.36546200	1.46104600	1.69471900
6	2.03172300	2.27661900	0.72004900
7	0.97067700	-0.46637300	-0.14412900
1	2.00478700	1.60609300	-1.64059500
5	0.78814000	-1.36857400	1.25703800
9	0.22535100	-2.59233400	0.97249000
9	2.05435000	-1.47393500	1.83596200
9	-0.03095700	-0.60057200	2.08206300
1	5.97102400	0.03324100	-1.78596700

6	3.35446700	−3.69941200	0.14919600
1	4.04162200	−4.14213900	−0.58316400
1	3.91632800	−3.31245300	1.00512100
1	2.64948500	−4.45742000	0.49057400
8	2.55728500	−2.67536000	−0.43008800

TS-cf-B-16
E(RB3LYP)=-1460.529814 a.u.

8	3.34195200	0.55007100	1.31205700
6	1.99573600	-0.03510900	1.24865800
6	1.25579300	0.71458100	2.38124700
6	-0.24789100	0.90265200	2.16025400
6	2.13656600	-1.52944700	1.56326400
1	1.72479400	1.70113700	2.47261600
1	1.43621000	0.19115700	3.32549000
1	-0.66390900	1.44341100	3.01793400
1	-0.76385900	-0.06143200	2.09864500
1	1.16236700	-1.99523500	1.70065000
1	2.72743700	-1.63015100	2.47972700
1	2.64135000	-2.05293700	0.74928900
6	3.68640900	0.14418100	-1.02655300
6	4.58826800	-0.04853800	-2.08188200
1	4.20060800	-0.16947400	-3.09022600
6	5.96098900	-0.08378000	-1.84690600
1	6.65062600	-0.24084800	-2.67023700
6	6.44530900	0.09266700	-0.54675900
1	7.51485400	0.07069800	-0.35866700
6	5.56622500	0.28751900	0.51917200
1	5.92398600	0.42503000	1.53414500
6	4.19256500	0.29947800	0.27863700
6	2.25094900	0.29260100	-1.19182000
1	1.87003300	0.46382300	-2.19654900
6	1.40478900	0.23709500	-0.14628500
6	-0.05251600	0.57666600	-0.39120400
6	-0.46537000	1.69861300	0.86359400
7	-1.04572900	-0.42355300	-0.43323000
5	-0.75657700	-2.03709300	-0.28346600
9	-1.74501000	-2.67615800	-1.01747300
9	0.49328500	-2.25565500	-0.83514400
9	-0.78220800	-2.39782800	1.06594000
6	-1.69484600	3.69787200	-0.07599300
1	-1.50012100	4.50341100	0.64970000
1	-0.89639200	3.74419100	-0.82235000
1	-2.65300900	3.91880300	-0.55247400
6	-2.93389800	2.11071900	1.47818700
1	-3.85091500	2.27163600	0.90153700
1	-2.94328800	1.10702100	1.90269700
1	-2.95785100	2.83111400	2.31299000
1	-0.07249600	1.22493900	-1.26919500
1	0.34987000	2.41327100	0.70179100
6	-2.30212000	0.01657800	-0.79617900
6	-3.48193200	-0.61913400	-0.26356300
6	-4.74357400	-0.23930300	-0.69580000
6	-3.79886100	1.54183700	-2.02817600
6	-4.90675400	0.84112600	-1.57991800
1	-5.61618200	-0.73987100	-0.29097600
1	-3.91085300	2.38181500	-2.70646700
6	-1.71624000	2.38719300	0.65592100
1	-5.90593500	1.12885900	-1.89310100
6	-2.51588200	1.14097500	-1.62954100
1	-1.66775000	1.61784800	-2.10381000

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8              -3.28309600   -1.47824700    0.75585000
6              -4.11523100   -2.62925100    0.87484500
1              -5.11350100   -2.37415200    1.25211000
1              -4.19046800   -3.14131100   -0.08802400
1              -3.60897600   -3.27699600    1.59033800
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trans-**16-B**
E(RB3LYP)= -1460.580656 a.u.

6	5.03085000	-2.32086500	-1.15822900
6	5.88888500	-1.21537000	-1.05498700
6	5.36983500	0.03828800	-0.71121100
6	4.00372900	0.18117300	-0.47329100
6	3.13121700	-0.91644800	-0.58227800
6	3.66519500	-2.16536500	-0.92422800
8	3.52761500	1.43265300	-0.20114900
6	2.25664000	1.59690900	0.48760200
6	1.27446700	0.47712200	0.15146800
6	1.71197100	-0.68983800	-0.34304800
6	1.74822000	2.95706900	-0.04189700
6	0.25479200	3.22361900	0.19877800
6	-0.59216600	2.05427500	-0.33513000
6	-0.17351500	0.80982400	0.47276500
6	2.55151900	1.62562300	1.99757800
6	-2.12924400	2.23937400	-0.35219600
6	-2.67246700	0.94432900	-1.03924000
6	-2.11537900	-0.32690200	-0.41150500
7	-1.05194500	-0.36952200	0.33632700
6	-4.17671600	0.90138500	-1.19330900
6	-4.86789800	-0.24731000	-1.13883200
6	-4.19479200	-1.51703000	-0.95144400
6	-2.86651000	-1.57128500	-0.67085600
6	-2.49649000	3.46945900	-1.20421000
6	-2.72829600	2.39494700	1.05980500
1	5.43102100	-3.29535900	-1.41992400
1	6.94391200	-1.32684800	-1.23687100
1	6.01159600	0.90900000	-0.62579200
1	2.99364300	-3.01637800	-1.00109000
1	1.02566100	-1.50930500	-0.52052300
1	1.93618600	2.95779500	-1.12120200
1	2.35869900	3.75895100	0.38719000
1	-0.01158800	4.15850400	-0.30304900
1	0.05461000	3.37378800	1.26713500
1	-0.29030000	1.89295100	-1.38122400
1	-0.21856600	1.06717700	1.53511600
1	1.65284700	1.83192600	2.58566000
1	3.29437100	2.40022700	2.21121000
1	2.94420600	0.65834900	2.32124200
1	-4.67473400	1.83226600	-1.43678000
1	-4.76135100	-2.43316700	-1.07169500
1	-3.57844000	3.59082500	-1.30257500
1	-2.07001900	3.40299900	-2.21173900
1	-2.12177100	4.38587600	-0.74149000
1	-3.81446300	2.51482300	1.00235300
1	-2.32409800	3.28177400	1.55696900
1	-2.52950600	1.52968900	1.69804800
5	-0.84232200	-1.55003700	1.60308600
9	-2.12861300	-1.89974300	1.95599700
9	-0.22175900	-0.80808600	2.58588400
9	-0.07840700	-2.59419700	1.15740200
1	-2.27996100	0.95583600	-2.07533800
1	-5.94215500	-0.25288800	-1.29651200

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8              -2.11010700    -2.68000500    -0.60003200
6              -2.74484900    -3.92582200    -0.33203100
1              -3.33252300    -4.27036100    -1.19206400
1              -1.93513700    -4.62750800    -0.13489900
1              -3.38196000    -3.84004100     0.55358300
```

cis-**16-B**
E(RB3LYP)=−1460.572111 a.u.

8	3.16215500	0.96826000	1.34585000
6	1.74940300	0.61224700	1.23063100
6	1.04071900	1.81221400	1.87986400
6	−0.45124200	1.89391100	1.55256300
6	1.53361200	−0.67764000	2.03461100
1	1.53712600	2.71919800	1.51570200
1	1.19848400	1.77628300	2.96307800
1	−0.85713000	2.78334800	2.04016300
1	−0.98748700	1.03592800	1.97394300
1	0.48141000	−0.96873000	2.05226200
1	1.88695700	−0.52173300	3.05923500
1	2.08247600	−1.50590700	1.58403900
6	3.67426100	−0.03320700	−0.78139100
6	4.64945400	−0.55061100	−1.64413100
1	4.34832000	−0.88840800	−2.63240300
6	5.98262400	−0.63454800	−1.24708100
1	6.72799400	−1.04172300	−1.92293600
6	6.35361900	−0.18646300	0.02406000
1	7.39135400	−0.24527600	0.33957800
6	5.39963500	0.33175000	0.90078100
1	5.66865700	0.68497600	1.89073600
6	4.06559400	0.39964900	0.49948700
6	2.27663200	0.13178200	−1.14723900
1	1.99397300	−0.03995500	−2.18109900
6	1.34331900	0.45547700	−0.23731900
6	−0.10848200	0.68188400	−0.64089600
6	−0.65505200	1.97938500	0.02567700
7	−0.97896700	−0.47864600	−0.28956100
6	−1.99754300	3.24257100	−1.70728700
1	−1.57290000	4.21464500	−1.43660300
1	−1.35533400	2.80025800	−2.47659900
1	−2.98012500	3.42505500	−2.15607300
6	−2.92155800	3.07145700	0.61126100
1	−3.88553400	3.39089500	0.20692400
1	−3.11982400	2.44485100	1.48472600
1	−2.39661900	3.97060600	0.94812500
1	−0.13400900	0.79361200	−1.73293000
1	0.00252000	2.78461100	−0.32633300
6	−2.25994100	−0.23166000	−0.20642600
6	−3.16170800	−1.16830900	0.45272300
6	−2.82470700	0.99415600	−0.89011900
6	−4.51124100	−1.02702400	0.30475200
6	−4.31786500	1.05535700	−0.94686000
1	−2.49852000	0.82482600	−1.93172000
6	−5.08524500	0.07701800	−0.43207500
1	−5.18244000	−1.72506200	0.79193500
1	−4.76574700	1.90563500	−1.45093900
6	−2.09972700	2.33566200	−0.46414300
5	−0.46340400	−2.04027200	−0.81628200
9	0.18468100	−1.70934300	−1.99316500
9	0.34302200	−2.60615900	0.12795000
9	−1.61172900	−2.75841200	−1.07558300
8	−2.53944600	−2.05615600	1.25404400

1	-6.16666200	0.12216500	-0.51901400
6	-3.22853200	-3.25270400	1.59802300
1	-2.49580100	-3.87949000	2.10557400
1	-4.06918000	-3.05532800	2.27535300
1	-3.58376700	-3.75913900	0.69481100

17-B
E(RB3LYP)= -1421.284620 a.u.

8	-3.12518200	0.51651300	-1.67072400
6	-1.81101200	1.01560100	-1.25353800
6	-2.09952800	2.21809100	-0.31327400
6	-0.94228200	3.16145800	0.06297700
6	-1.19345000	1.47229700	-2.57677000
6	2.21343900	2.45532400	2.29051900
6	1.83424100	4.38107300	0.66344300
1	-2.55689100	1.83134900	0.60456600
1	-2.87129900	2.80686300	-0.82288300
1	-1.41082900	4.02698900	0.55471500
1	-0.48549400	3.57117000	-0.84607600
1	-0.23843100	1.98087900	-2.43176500
1	-1.87843400	2.17334400	-3.06000800
1	-1.04650100	0.62257700	-3.24903200
1	3.20271300	2.24275500	1.86430500
1	1.79663700	1.51803900	2.66343400
1	2.38307300	3.12752400	3.14277800
1	1.95366700	5.15287200	1.43564300
1	1.18646000	4.79123400	-0.11461000
1	2.83139000	4.22695800	0.23056700
6	-3.20140900	-0.97876300	0.21194500
6	-3.98237300	-1.77739900	1.06885400
1	-3.48203100	-2.36687200	1.83186900
6	-5.36427400	-1.80978300	0.94085700
1	-5.96181100	-2.41763800	1.61204400
6	-5.98243000	-1.06372900	-0.07303900
1	-7.06247300	-1.09506100	-0.18336100
6	-5.23256100	-0.27591400	-0.94326000
1	-5.69850600	0.30173800	-1.73417000
6	-3.84606500	-0.21830200	-0.78804700
6	-1.76273800	-1.00062700	0.20779800
1	-1.26073600	-1.80049700	0.73935900
6	-1.04531000	-0.11581900	-0.54255400
6	3.30993400	-2.00314800	-0.82231200
6	4.62097800	-1.95342100	-1.30208700
1	5.14542000	-2.88354000	-1.50865200
6	5.24683200	-0.72694400	-1.52589800
6	4.56586100	0.46425000	-1.28131400
1	5.04971400	1.42091200	-1.44774700
6	3.25726400	0.41938300	-0.79800200
6	2.62540000	-0.80224200	-0.56491700
6	0.37550500	-0.24274800	-0.75971700
1	0.74814000	0.22237100	-1.66988900
6	0.10286000	2.57654700	0.98796400
1	-0.17656400	1.66704400	1.51407300
6	1.30625200	3.10422500	1.27208000
7	1.28430400	-0.84901900	-0.04510000
1	2.71808500	1.33172700	-0.56207600
5	1.11794400	-1.47166200	1.50503400
9	0.41107500	-2.65783700	1.41394300
9	2.39746700	-1.63595700	1.96204900
9	0.41551200	-0.50113800	2.20904800
1	6.26772900	-0.70891900	-1.89492100

| 8 | 2.62968500 | -3.16353900 | -0.63449200 |
| 1 | 3.24379500 | -3.90822100 | -0.67152500 |

TS-tf-B-17
E(RB3LYP)=-1421.235729 a.u.

8	-3.37673500	1.39426900	0.26830100
6	-2.04500600	1.63131300	-0.25863800
6	-1.49156000	2.71880600	0.67006900
6	-0.01411400	3.01832000	0.43050500
6	-2.20258000	2.12629300	-1.70969700
6	3.22012500	1.38664700	1.64288100
6	2.86237500	3.20934000	-0.08772300
1	-1.63937300	2.37897400	1.70083800
1	-2.08908500	3.62757100	0.54187300
1	0.28765400	3.85545500	1.07110600
1	0.14057300	3.35767900	-0.60031000
1	-1.23758800	2.35770000	-2.17084600
1	-2.82248400	3.02795600	-1.73238300
1	-2.68469400	1.35532400	-2.31640200
1	4.24088600	1.30353600	1.26041200
1	2.86576000	0.40917300	1.97213400
1	3.25826000	2.03822000	2.53289900
1	2.81788900	4.08999900	0.57343200
1	2.30340900	3.46823500	-0.98967600
1	3.91152600	3.05271200	-0.34685700
6	-3.26345100	-0.92236000	-0.36842300
6	-3.95143400	-2.11059400	-0.65456800
1	-3.37863800	-3.00598400	-0.88060800
6	-5.34349000	-2.15032700	-0.63757300
1	-5.86445700	-3.07597200	-0.86038600
6	-6.06505400	-0.99518100	-0.32041400
1	-7.15058900	-1.02133300	-0.29940800
6	-5.40306600	0.19939800	-0.03366700
1	-5.94533100	1.10492600	0.21726100
6	-4.01028100	0.23184500	-0.06755700
6	-1.81481800	-0.82895300	-0.30988100
1	-1.24255100	-1.74922100	-0.33176000
6	-1.19600600	0.36252000	-0.20430300
6	3.10628900	-1.92311700	-0.58079000
6	4.42387300	-1.88156500	-1.02440200
1	5.00303800	-2.79370600	-0.92820000
6	4.97387500	-0.73534600	-1.61081700
6	4.18085600	0.38336300	-1.80908800
1	4.55729900	1.24532700	-2.35057600
6	2.85824800	0.38247700	-1.34352700
6	2.29939200	-0.72940500	-0.64916300
6	0.30519300	0.49767000	-0.28630900
1	0.52703600	0.91956200	-1.26893600
6	0.87595800	1.80386500	0.74417800
1	0.61933300	1.36054100	1.70882300
6	2.30468600	2.03080100	0.65217800
7	1.05064700	-0.66508900	-0.04682000
1	2.22317300	1.19325300	-1.66680700
5	0.80430100	-1.44632700	1.36192200
9	0.33827300	-2.74508500	1.03920600
9	2.02370600	-1.53244000	2.02173900
9	-0.11356900	-0.74235000	2.10943900
1	6.00270200	-0.75297100	-1.95743300

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8              2.66102700   -3.12194600   -0.16602300
1              1.75013900   -3.09426200    0.18863400
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TS-cf-B-17
E(RB3LYP)=-1421.228901 a.u.

8	3.18106400	0.92092300	1.14572000
6	1.84938000	0.31407000	1.22673700
6	1.09236200	1.29430500	2.14930600
6	-0.42512400	1.30697500	1.95040100
6	2.01625800	-1.05582800	1.89851800
1	1.48382200	2.29838500	1.94826700
1	1.34047700	1.06154000	3.18959600
1	-0.87085400	2.01261300	2.65999200
1	-0.86117000	0.32350000	2.15515600
1	1.05322100	-1.49037400	2.16416200
1	2.61348400	-0.91775100	2.80557100
1	2.52203600	-1.75912000	1.23576600
6	3.52374800	0.03436600	-1.05788900
6	4.42526100	-0.35101200	-2.05936600
1	4.03618900	-0.69545900	-3.01410300
6	5.79960600	-0.29473300	-1.83896900
1	6.48927300	-0.60175200	-2.61874700
6	6.28508900	0.16620500	-0.61104200
1	7.35571200	0.21609000	-0.43520600
6	5.40622300	0.55625600	0.40009600
1	5.76490900	0.91637100	1.35855400
6	4.03188800	0.47780100	0.17807400
6	2.08272600	0.08959000	-1.23127600
1	1.68876900	0.01125100	-2.24254600
6	1.24551700	0.23572100	-0.18810500
6	-0.23490300	0.41626600	-0.47003600
6	-0.73142900	1.72564700	0.50557600
7	-1.12958700	-0.66781500	-0.28085800
5	-0.72846200	-2.17047100	0.10765900
9	-1.63097600	-3.00147400	-0.52001100
9	0.57146400	-2.42825600	-0.23947000
9	-0.90041100	-2.29336300	1.53797500
6	-2.15984900	3.28193800	-0.88121900
1	-2.02914800	4.27116400	-0.41435500
1	-1.38202800	3.18482600	-1.64385200
1	-3.14314400	3.27730900	-1.35723300
6	-3.21594500	2.11603200	1.10759700
1	-4.15210800	2.02240400	0.54622000
1	-3.13150700	1.28749000	1.81014000
1	-3.29519300	3.05065500	1.68797900
1	-0.31371200	0.84652600	-1.47221500
1	0.00219700	2.46428000	0.15939100
6	-2.45121900	-0.42455500	-0.64303700
6	-3.54124100	-0.94938900	0.14385600
6	-2.79194400	0.36961000	-1.76563800
6	-4.85469600	-0.69381900	-0.24966900
6	-4.11180300	0.62236500	-2.13668300
6	-5.14468300	0.08414700	-1.37243000
1	-5.64612700	-1.09714000	0.37292400
1	-4.32212700	1.21277700	-3.02251400
6	-2.04746100	2.23698300	0.18823000
1	-6.18057400	0.25972000	-1.64762500
1	-1.99609600	0.71296800	-2.41627500

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8                     -3.38897000   -1.58574200    1.31293400
1                     -2.46089300   -1.86846200    1.48479600
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trans-**17-B**
E(RB3LYP)= -1421.281259 a.u.

6	5.09455700	-2.04002400	-1.30004200
6	5.85777000	-0.88069000	-1.14032500
6	5.25828400	0.31121400	-0.72976100
6	3.88698400	0.33818100	-0.48147900
6	3.09889200	-0.81503200	-0.64540700
6	3.72278900	-2.00050600	-1.05481000
8	3.32049800	1.53521100	-0.14480900
6	2.04384600	1.57138300	0.55068900
6	1.14667700	0.39887000	0.15995300
6	1.66845100	-0.70599900	-0.39104500
6	1.43436200	2.91575200	0.08901500
6	-0.07792500	3.05734700	0.32321400
6	-0.82422400	1.84968200	-0.27292900
6	-0.31810900	0.61685100	0.49936600
6	2.33997500	1.54705200	2.06079100
6	-2.36902300	1.90144100	-0.32135400
6	-2.77646900	0.57924100	-1.05825400
6	-2.20457200	-0.66444000	-0.38033200
7	-1.12550200	-0.61536300	0.36706200
6	-4.23800900	0.48908600	-1.40788000
6	-4.89515700	-0.68182800	-1.39575500
6	-4.20984700	-1.89791000	-1.05233400
6	-2.91320700	-1.93365500	-0.62198000
6	-2.81616900	3.12352000	-1.14651400
6	-3.01966900	1.96255700	1.07494700
1	5.56488500	-2.96634300	-1.61425500
1	6.92688600	-0.90194500	-1.33040700
1	5.83319000	1.22223800	-0.60056400
1	3.11755900	-2.89505200	-1.17675200
1	1.04621400	-1.56687200	-0.60803500
1	1.63090600	2.98935900	-0.98613900
1	1.97802700	3.73737700	0.56749700
1	-0.40875800	3.99087200	-0.14099700
1	-0.30045200	3.14395700	1.39427900
1	-0.49021000	1.75552900	-1.31674500
1	-0.36541200	0.85833200	1.56610300
1	1.43287800	1.67721700	2.65747800
1	3.03778900	2.35287100	2.30737800
1	2.78710400	0.59028200	2.34163300
1	-4.71467000	1.38960500	-1.77390100
1	-4.71333700	-2.85271400	-1.16290800
1	-3.90419700	3.20094800	-1.20681500
1	-2.41832100	3.09139800	-2.16741400
1	-2.46535900	4.04764800	-0.68096200
1	-4.11029600	1.97389600	0.98374700
1	-2.72193100	2.87410700	1.60190100
1	-2.75466000	1.10729600	1.70258900
5	-0.80202600	-1.72446800	1.57339400
9	-2.01764300	-2.02710600	2.13280300
9	0.06589600	-1.12458800	2.44407100
9	-0.21705700	-2.85253000	0.95159600
1	-2.26845300	0.61651700	-2.04267600
1	-5.93625900	-0.73921500	-1.69779300

8	-2.35005300	-3.14277800	-0.47197200
1	-1.48003500	-3.12142700	-0.02128900

cis-**17-B**
E(RB3LYP)=-1421.264563 a.u.

8	-3.01593500	-1.23110800	1.15288600
6	-1.62478800	-0.78300800	1.14097000
6	-0.85978000	-2.03285200	1.60688500
6	0.64134500	-1.97678100	1.31600100
6	-1.50404600	0.36750400	2.14992400
1	-1.29393000	-2.89307400	1.08409100
1	-1.04163100	-2.18531100	2.67609500
1	1.08981800	-2.91099700	1.66189900
1	1.11603400	-1.17253900	1.88990000
1	-0.46990000	0.70056800	2.25810600
1	-1.88155600	0.03041900	3.12084600
1	-2.08071000	1.23132700	1.81616000
6	-3.54105900	0.07476300	-0.79852500
6	-4.52567600	0.67387700	-1.59513900
1	-4.22312100	1.18504400	-2.50542700
6	-5.86957300	0.62013600	-1.23060300
1	-6.62274200	1.09239800	-1.85335300
6	-6.24077200	-0.04988700	-0.06115500
1	-7.28665800	-0.09941100	0.22796900
6	-5.27742300	-0.65307200	0.74851400
1	-5.54714800	-1.17763900	1.65914100
6	-3.93334100	-0.58200700	0.38292000
6	-2.12869100	0.04862600	-1.14305900
1	-1.83531700	0.40213000	-2.12637000
6	-1.19729900	-0.36545300	-0.26857200
6	0.27353800	-0.43742700	-0.65654500
6	0.88415600	-1.79469100	-0.19707600
7	1.06303600	0.69602200	-0.09090000
6	2.34033100	-2.67443700	-2.07108300
1	1.97683000	-3.70274400	-1.97671300
1	1.68488200	-2.15193200	-2.77610600
1	3.34137300	-2.71715400	-2.51390800
6	3.19957800	-2.83673600	0.27321400
1	4.19206300	-3.02705900	-0.14355300
1	3.33476900	-2.35453500	1.24487700
1	2.72506300	-3.80889800	0.43850900
1	0.33097700	-0.36331100	-1.75070300
1	0.28485300	-2.56536800	-0.69871300
6	2.35514500	0.51407900	-0.01418600
6	3.18697000	1.36812600	0.82160200
6	3.00850500	-0.54820900	-0.87149400
6	4.54438900	1.30158200	0.71998500
6	4.50371300	-0.52093100	-0.88906700
1	2.69624700	-0.22821700	-1.88138300
6	5.20435600	0.38266300	-0.17919000
1	5.15369100	1.92351100	1.37136200
1	5.00971400	-1.24360400	-1.52105300
6	2.35790300	-1.98177500	-0.69346800
5	0.46484900	2.29800600	-0.37571700
9	-0.14764600	2.12152800	-1.60357300
9	-0.38361600	2.65953800	0.62812200
9	1.57921300	3.09739000	-0.49184800
8	2.51798400	2.08727600	1.75309000

| 1 | 3.05951900 | 2.82799900 | 2.05572500 |
| 1 | 6.28854600 | 0.40623100 | −0.22974900 |

18-B
E(RB3LYP)=-3917.170524 a.u.

8	-1.53427600	1.95740600	-1.69802500
6	-0.21172800	1.90586500	-1.06655100
6	-0.29799000	2.82106900	0.18623200
6	1.01336800	3.32930500	0.81623300
6	0.69963200	2.49891700	-2.14176900
6	3.96246200	1.24564800	2.36470700
6	4.09523300	3.49909300	1.19460100
1	-0.89040000	2.30390400	0.94939800
1	-0.88186000	3.69377800	-0.12931700
1	0.70863000	4.04205100	1.59752600
1	1.56396300	3.93002000	0.08396500
1	1.72778500	2.60214500	-1.78972000
1	0.33190100	3.49253100	-2.40960300
1	0.68887300	1.87860500	-3.04225200
1	4.82229900	0.88423400	1.78645500
1	3.32244200	0.38889000	2.58462400
1	4.36729400	1.62532900	3.31284800
1	4.52325000	4.00291900	2.07151800
1	3.55962000	4.25255800	0.61332300
1	4.94844700	3.14977800	0.59869800
6	-2.28233200	0.06477100	-0.41481600
6	-3.35964000	-0.68896900	0.08423200
1	-3.16485400	-1.59606200	0.64583600
6	-4.65944400	-0.26443100	-0.14533000
6	-4.91657500	0.89004300	-0.89348700
1	-5.93966900	1.20139200	-1.07096600
6	-3.85931300	1.63850900	-1.40287900
1	-4.03763900	2.53330400	-1.98895000
6	-2.54494500	1.24018100	-1.14992900
6	-0.91126000	-0.36983300	-0.32382200
1	-0.71512800	-1.39816000	-0.04157500
6	0.11035200	0.45028800	-0.69211700
6	3.54883200	-2.81955400	-0.82703900
1	2.75440200	-3.51616200	-0.58597400
6	4.77790500	-3.26173500	-1.30927200
1	4.94497000	-4.32564400	-1.44649300
6	5.79060700	-2.34848000	-1.61270300
1	6.74884500	-2.70023200	-1.98234500
6	5.57079600	-0.98360100	-1.42662800
1	6.35922200	-0.26866800	-1.64159100
6	4.34174900	-0.52874800	-0.94800100
6	3.32937300	-1.44842100	-0.65910400
6	1.45809600	-0.04919800	-0.84115500
1	2.04595700	0.40481700	-1.63723400
6	1.89742000	2.27524500	1.44064500
1	1.38181100	1.40123800	1.83321800
6	3.22797400	2.34077800	1.62684500
7	2.03800500	-1.01682500	-0.19060100
1	4.17794300	0.52854000	-0.76515600
5	1.48907300	-1.76603000	1.20607500
9	0.72457800	-2.84077200	0.77098100
9	2.62601500	-2.13703800	1.87488600
9	0.75017100	-0.83009600	1.90208300
35	-6.12501800	-1.27347800	0.55019700

TS-tf-B-18
E(RB3LYP)=-3917.123514 a.u.

8	-1.68823600	2.54085000	0.32759000
6	-0.38178600	2.29238300	-0.25837400
6	0.54510500	3.19857500	0.56165400
6	2.02335300	2.99383900	0.23950800
6	-0.45797300	2.71469600	-1.73838700
6	4.63319700	0.46759300	1.41181700
6	4.76606600	2.21805700	-0.43263300
1	0.36193600	2.98578200	1.62033500
1	0.25966700	4.24161200	0.38845700
1	2.61468300	3.72451900	0.80416900
1	2.21178400	3.20793800	-0.81886000
1	0.50078100	2.59406200	-2.25148800
1	-0.75960300	3.76412700	-1.81184900
1	-1.19532900	2.10183200	-2.26358100
1	5.55542300	0.04628300	1.00365700
1	4.00293800	-0.32810100	1.81436800
1	4.91735200	1.11489100	2.25939000
1	5.02314500	3.11605800	0.15268100
1	4.26329500	2.57010400	-1.33613300
1	5.70432300	1.73276100	-0.70851200
6	-2.35311900	0.26464400	-0.07401300
6	-3.39369100	-0.66386900	-0.21523700
1	-3.16158500	-1.71223300	-0.36741200
6	-4.71515100	-0.23694000	-0.14646700
6	-5.02941400	1.10426500	0.07421100
1	-6.06509600	1.41858300	0.13068800
6	-4.00117400	2.03634600	0.21514000
1	-4.21691100	3.08475700	0.39070900
6	-2.67412900	1.61909200	0.13265500
6	-0.94909700	-0.11136900	-0.08150900
1	-0.69900800	-1.16505500	-0.03032400
6	0.01711900	0.82478800	-0.12321000
6	3.38875800	-2.67294800	-0.36101000
1	2.75962800	-3.31660400	0.23778900
6	4.57825800	-3.13774700	-0.87523000
1	4.88022600	-4.16021700	-0.66851900
6	5.40528300	-2.31347800	-1.66957200
1	6.34063100	-2.69731700	-2.06467100
6	4.98037500	-1.03639700	-1.98217500
1	5.56643800	-0.41173600	-2.65042000
6	3.76622800	-0.53809500	-1.47264600
6	2.95973200	-1.33653600	-0.61223700
6	1.47430300	0.46566000	-0.28480300
1	1.74627800	0.73227200	-1.30924300
6	2.50048100	1.57832700	0.60204300
1	2.18697000	1.29438200	1.60986900
6	3.91580700	1.32156000	0.41680600
7	1.84039500	-0.84860400	0.02242200
1	3.39883300	0.38808200	-1.88983900
5	1.41455900	-1.49740300	1.47508600
9	0.57756000	-2.57310500	1.22717100
9	2.59057100	-1.90436700	2.10884800
9	0.81634800	-0.48340700	2.20769100
35	-6.12851300	-1.51123200	-0.34987800

TS-cf-B-18
E(RB3LYP)= -3917.114683 a.u.

8	1.63814500	2.23286700	0.38913000
6	0.38259900	1.63645100	0.86726000
6	-0.62530300	2.78943200	0.66285200
6	-2.06635800	2.34505400	0.40912000
6	0.56826500	1.34469500	2.36302500
1	-0.27961900	3.37720800	-0.19528400
1	-0.58016700	3.44917600	1.53474600
1	-2.69863800	3.23697400	0.33009600
1	-2.44989300	1.74908000	1.24404900
1	-0.38024800	1.09365500	2.83534300
1	0.97942000	2.24684900	2.82741100
1	1.25080700	0.50986400	2.52462100
6	2.49275300	0.08700300	-0.24648800
6	3.60124600	-0.72585700	-0.51627100
1	3.45579900	-1.74727100	-0.85147600
6	4.88432300	-0.21429900	-0.35678700
6	5.09002600	1.10331200	0.05447900
1	6.09775900	1.48588200	0.16901500
6	3.99180400	1.91919500	0.32524600
1	4.12427600	2.94689500	0.64575000
6	2.70094500	1.41003000	0.18714600
6	1.11628700	-0.31657500	-0.47654700
1	0.94304200	-1.21095500	-1.07100400
6	0.07734500	0.38585000	0.01463500
6	-1.30907800	-0.04902500	-0.41171000
6	-2.11837800	1.54337600	-0.89582300
7	-2.15303600	-0.75918100	0.42762600
5	-1.83054600	-1.10226800	1.99832800
9	-2.47702900	-2.28513100	2.29558400
9	-0.46436500	-1.24170800	2.11314500
9	-2.33166400	-0.03683600	2.76162100
6	-3.33609600	1.36506900	-3.09407400
1	-3.40124800	2.39979700	-3.46363700
1	-2.40925800	0.94298800	-3.49353600
1	-4.18959200	0.82254400	-3.50756900
6	-4.67181200	1.67309700	-0.94713500
1	-5.45659000	1.00911200	-1.32412400
1	-4.63715100	1.60366900	0.13935900
1	-4.97309800	2.69920200	-1.21239500
1	-1.23632200	-0.47708000	-1.41064300
1	-1.32811100	1.83820200	-1.59264200
6	-3.36300100	-1.17065800	-0.11203000
6	-4.48380400	-1.39687200	0.73892100
6	-3.57232100	-1.28042400	-1.50877200
6	-5.71659400	-1.71368000	0.20760900
1	-4.36306000	-1.29508700	1.80678700
6	-4.82542500	-1.63980600	-2.02915900
1	-2.73424900	-1.23637900	-2.19228200
6	-5.90376600	-1.83803700	-1.18401100
1	-6.55785900	-1.86207600	0.87804400
1	-4.93838400	-1.75893000	-3.10290800
6	-3.35078500	1.38993100	-1.59050800
1	-6.87760300	-2.10440700	-1.58319400
35	6.39540300	-1.33047900	-0.72376100

trans-**18-B**
E(RB3LYP)= -3917.168977 a.u.

6	4.56786400	-0.19791800	-0.42586400
6	4.89876200	1.15585000	-0.44228600
6	3.89020800	2.10901400	-0.29536200
6	2.56679900	1.70133700	-0.13765200
6	2.22946800	0.33541800	-0.13110400
6	3.24880500	-0.61387700	-0.27390800
8	1.60334100	2.66469600	-0.06267000
6	0.31450400	2.36001400	0.54234700
6	-0.09251400	0.90853000	0.30414000
6	0.82417200	-0.02272200	0.00690500
6	-0.64587200	3.34291200	-0.16875000
6	-2.13769700	2.98132500	-0.06993800
6	-2.35095300	1.52422100	-0.51592200
6	-1.57634200	0.65114900	0.49656000
6	0.43106300	2.64387200	2.05039800
6	-3.80045400	1.02441300	-0.74064200
6	-3.60866200	-0.43950200	-1.27640300
6	-2.81135300	-1.28963500	-0.29593500
7	-1.91764200	-0.77842600	0.50601100
6	-4.85723300	-1.11271200	-1.78518300
6	-5.10305800	-2.42004700	-1.60275900
6	-4.16217600	-3.23964600	-0.86374700
6	-3.07385700	-2.71888200	-0.25021300
6	-4.48835800	1.89402500	-1.80870200
6	-4.64836400	1.02346200	0.54639900
1	5.93068200	1.46436900	-0.56263000
1	4.11827300	3.16947400	-0.30467000
1	3.00384900	-1.67038900	-0.26372700
1	0.54924800	-1.06888400	-0.07741100
1	-0.35682500	3.34648900	-1.22534000
1	-0.46683200	4.35413200	0.21169400
1	-2.69899000	3.67444800	-0.70340100
1	-2.50736100	3.12194400	0.95357300
1	-1.84950000	1.42211400	-1.48976700
1	-1.83290500	0.99668500	1.50555800
1	-0.53244400	2.54362900	2.55807600
1	0.79892300	3.66316000	2.20181100
1	1.12559400	1.94039000	2.51603400
1	-5.52287000	-0.51233900	-2.39521200
1	-5.98670400	-2.88457600	-2.02880700
1	-4.34460100	-4.30843200	-0.79736800
1	-2.39105700	-3.34194400	0.30919400
1	-5.51002200	1.56116800	-2.00935100
1	-3.93457200	1.88845500	-2.75470000
1	-4.56040300	2.93077200	-1.47067900
1	-5.65097400	0.63410100	0.34178600
1	-4.76271700	2.04026000	0.93408600
1	-4.21258400	0.40697500	1.33762000
5	-1.36961800	-1.64168500	1.84085400
9	-2.51110800	-2.13623400	2.43771400
9	-0.71739200	-0.72574800	2.63198600
9	-0.54564400	-2.64241100	1.34864400
1	-2.96982500	-0.34282100	-2.17472100
35	5.95109300	-1.50724000	-0.62274300

cis-**18-B**
E(RB3LYP)=-3917.161627 a.u.

8	1.67946900	2.36351100	0.18519900
6	0.39929500	1.83179900	0.66131200
6	-0.59303800	2.95703400	0.32312700
6	-2.04628300	2.48032100	0.31978700
6	0.52543500	1.63218000	2.17815500
1	-0.33114500	3.34498300	-0.66841400
1	-0.45256300	3.77679400	1.03490600
1	-2.70165900	3.33579300	0.12184300
1	-2.32266400	2.08251800	1.30075500
1	-0.43068100	1.36202400	2.62577200
1	0.88413000	2.56701100	2.62073600
1	1.22878000	0.83025400	2.40740400
6	2.47259000	0.15580400	-0.31880400
6	3.55977000	-0.70163400	-0.52976600
1	3.38717800	-1.73673900	-0.80462100
6	4.85624300	-0.21902000	-0.38805900
6	5.09736600	1.11365900	-0.05337200
1	6.11474200	1.47363800	0.04812800
6	4.02061800	1.97475600	0.15791300
1	4.18016400	3.01546600	0.41861700
6	2.71611200	1.49657100	0.03750200
6	1.08658400	-0.22757500	-0.52831000
1	0.89038400	-1.15834100	-1.05646400
6	0.06905400	0.53859000	-0.09786600
6	-1.35507900	0.16078700	-0.48864600
6	-2.24618800	1.40914400	-0.76284700
7	-2.08409700	-0.85151200	0.34334400
1	-1.23289500	-0.34385900	-1.45512100
1	-1.83983300	1.82315400	-1.69667000
6	-3.21465300	-1.25649400	-0.19933900
6	-4.04160000	-2.29770200	0.36889900
6	-3.71734800	-0.52752600	-1.43140800
6	-5.21197700	-2.65053800	-0.22395300
1	-3.70210000	-2.78974400	1.26549400
6	-5.00153200	-1.03299400	-2.00308300
1	-2.96597300	-0.61837500	-2.23437600
6	-5.70430600	-2.02728300	-1.43142700
1	-5.80126600	-3.44624900	0.22344800
1	-5.33860000	-0.57675400	-2.92825900
1	-6.63002300	-2.38361500	-1.87229600
6	-3.73141000	1.02150500	-1.05510900
5	-1.63682600	-1.15267600	1.91888800
9	-0.26712400	-1.18533200	1.96921700
9	-2.19060500	-0.06461300	2.59742700
9	-2.17150000	-2.35263700	2.34533800
6	-4.67009300	1.23798800	0.15169700
1	-4.79917300	2.30556200	0.34886400
1	-5.65973700	0.82256400	-0.06279500
1	-4.29233400	0.77558600	1.06616500
6	-4.24390500	1.85665500	-2.24187300
1	-3.70616400	1.62215300	-3.16774500
1	-5.31317000	1.70482300	-2.41580500
1	-4.09590700	2.92176400	-2.03572800
35	6.33647700	-1.40078500	-0.66966600

19-B
E(RB3LYP)=-1267.428057 a.u.

8	-2.83191700	1.05318500	-1.31423000
6	-1.59082900	1.45401600	-0.64824700
6	-2.01851400	2.14645500	0.67608600
6	-0.99901700	3.06144300	1.38390000
6	-0.97424200	2.44594900	-1.63366900
1	-2.35445500	1.37158200	1.37363600
1	-2.89856500	2.75135800	0.42833700
1	-1.50617900	3.43281900	2.28657700
1	-0.79321500	3.94950800	0.77437600
1	-0.05909400	2.88958500	-1.23665500
1	-1.68941800	3.25016000	-1.82386600
1	-0.75330000	1.95690500	-2.58648800
6	-2.81587900	-1.05888400	-0.15974800
6	-3.53885600	-2.18716900	0.27065800
1	-3.00626900	-2.98435600	0.78144800
6	-4.90643700	-2.27737600	0.04893600
1	-5.46048200	-3.14366200	0.39474400
6	-5.56495400	-1.24819900	-0.63900800
1	-6.63270200	-1.32028300	-0.82406200
6	-4.87092700	-0.12695100	-1.08793400
1	-5.36797200	0.67332400	-1.62540000
6	-3.50249400	-0.02339500	-0.83093300
6	-1.38228700	-0.95840200	-0.07502000
1	-0.81584400	-1.85692500	0.14300300
6	-0.73788100	0.20308300	-0.37872500
6	3.63023100	-1.58657300	-0.78273400
1	3.13841300	-2.53535000	-0.60203300
6	4.91969300	-1.52769800	-1.30387700
1	5.44461300	-2.44985300	-1.53382500
6	5.53768800	-0.29475000	-1.52833700
1	6.54589300	-0.25558200	-1.92919800
6	4.85941000	0.88512000	-1.22360800
1	5.33973500	1.84686400	-1.37667300
6	3.56468400	0.83828600	-0.70495100
6	2.94908400	-0.39885700	-0.49610900
6	0.69366300	0.24195100	-0.56497300
1	1.05455600	0.93610900	-1.32256400
6	0.29753600	2.42068100	1.80263600
1	0.23138700	1.43837500	2.26752000
6	1.49627700	2.99296700	1.66099800
7	1.60443600	-0.49205700	0.00993100
1	3.04645800	1.75149000	-0.43010200
5	1.40378500	-1.47256600	1.35355200
9	1.00803100	-2.71062200	0.85777700
9	2.63046000	-1.50415600	1.95852500
9	0.43410400	-0.87580100	2.13711900
1	1.61263900	3.97487900	1.20532700
1	2.40011000	2.50983900	2.01963400

TS-tf-B-19
E(RB3LYP)=-1267.379887 a.u.

6	-4.60213400	2.19142000	1.33209000
6	-5.37136000	1.46518500	0.41642400
6	-4.80283300	0.43626800	-0.33468400
6	-3.45104200	0.13927300	-0.17053300
6	-2.65296900	0.87185700	0.73003100
6	-3.24969600	1.89675100	1.48072900
8	-2.89503500	-0.82433000	-0.95968900
6	-1.70996100	-1.52349400	-0.48170200
6	-0.73644200	-0.54046700	0.17082900
6	-1.23931100	0.55396400	0.78281200
6	-1.14678800	-2.15396400	-1.76582200
6	0.23801300	-2.78117600	-1.59899700
6	1.35149200	-1.77243400	-1.30823700
6	0.68142100	-0.95482800	0.36898100
6	-2.16454200	-2.58733400	0.53384500
6	1.65035600	-0.76154800	-2.23164700
6	1.22791900	1.33737700	-1.20295400
6	1.97076800	1.01364100	-0.02665000
7	1.67565900	-0.09340700	0.74033700
6	1.64843200	2.39481900	-2.04206200
6	2.79644600	3.10249900	-1.75924800
6	3.53357900	2.78887700	-0.59506300
6	3.13827500	1.78028000	0.25552700
1	-5.05442600	2.98527000	1.91745300
1	-6.42551000	1.69467700	0.29224100
1	-5.38551600	-0.13714700	-1.04769400
1	-2.63672000	2.46234100	2.17746800
1	-0.58113500	1.22020700	1.33375000
1	-1.12158700	-1.37299400	-2.53413900
1	-1.86074800	-2.90635700	-2.11636800
1	0.49213000	-3.33366100	-2.51093100
1	0.22150100	-3.52613200	-0.79602400
1	2.22774500	-2.18845900	-0.81623900
1	0.75128500	-1.87725200	0.94145400
1	-1.32204600	-3.17525400	0.90799300
1	-2.88208200	-3.26643500	0.06367000
1	-2.64448300	-2.10952600	1.39179700
1	1.04022000	2.65050700	-2.90480200
1	3.11867300	3.91370700	-2.40483400
1	4.43098700	3.35394600	-0.36129600
1	3.70911500	1.55246800	1.14392200
5	2.85447000	-0.78903800	1.66999600
9	3.85383200	-1.15618800	0.77746400
9	2.27056700	-1.89352200	2.27077800
9	3.27243300	0.14126600	2.60147700
1	0.21511100	0.97982900	-1.31403400
1	2.66690800	-0.40970700	-2.34537400
1	0.96966300	-0.52214400	-3.04232100

TS-cf-B-19
E(RB3LYP)=-1267.369909 a.u.

8	2.86882300	1.07156200	0.96228400
6	1.51840800	0.52428700	1.14438800
6	0.81544400	1.66423800	1.91613800
6	-0.70209500	1.74643600	1.74764600
6	1.65911800	-0.72431800	2.02514400
1	1.25798300	2.60660300	1.57396400
1	1.07199800	1.56558000	2.97542800
1	-1.08372100	2.52517600	2.41877000
1	-1.19275500	0.81040700	2.03814900
1	0.68977200	-1.07602700	2.37588200
1	2.27939000	-0.45415500	2.88589200
1	2.13285900	-1.54153300	1.48023000
6	3.17700700	-0.11005100	-1.09837000
6	4.05989900	-0.65509000	-2.04098700
1	3.65582200	-1.10630900	-2.94355400
6	5.43551700	-0.62082300	-1.82618100
1	6.11202800	-1.05087400	-2.55776800
6	5.94024600	-0.02271500	-0.66662800
1	7.01248000	0.01034500	-0.49684800
6	5.07969200	0.52775600	0.28380400
1	5.45412500	0.99669400	1.18751300
6	3.70284800	0.47168500	0.07028200
6	1.73924700	-0.03316100	-1.27197700
1	1.33765000	-0.23047600	-2.26390200
6	0.90607100	0.25440300	-0.25012500
6	-0.54826200	0.39056900	-0.58571400
6	-1.05246000	2.10858700	0.30712900
7	-1.51205500	-0.51217000	-0.22374200
5	-1.20772300	-1.93363400	0.57778000
9	-2.10375500	-2.85321900	0.07564700
9	0.08856700	-2.28361300	0.28462400
9	-1.42277300	-1.67987300	1.93369300
1	-0.67004100	0.80415200	-1.58444700
1	-0.28595500	2.68903400	-0.20819600
6	-2.81749100	-0.22385000	-0.56632900
6	-3.89415900	-0.82252200	0.15446600
6	-3.14144300	0.78807700	-1.51361500
6	-5.19661500	-0.46746500	-0.11430800
1	-3.67473200	-1.54272600	0.92779600
6	-4.49248300	1.08938900	-1.81256400
1	-2.38820000	1.13193900	-2.21212800
6	-5.51081100	0.48391300	-1.11248900
1	-5.99701600	-0.92734500	0.45737500
1	-4.70848300	1.81562500	-2.59030200
1	-6.54742100	0.72662800	-1.32463600
6	-2.36152300	2.44150700	-0.05306400
1	-3.19134800	2.25804000	0.62108300
1	-2.54727900	3.15532800	-0.84684300

trans-**19-B**
E(RB3LYP)=-1267.436371 a.u.

6	4.66057100	-2.22020200	-1.26989100
6	5.48715700	-1.10640900	-1.10217900
6	4.95312000	0.11676500	-0.69275800
6	3.58383500	0.22095800	-0.45398400
6	2.73261400	-0.88533400	-0.62663700
6	3.29143600	-2.10341700	-1.03427800
8	3.08467400	1.44808100	-0.11644200
6	1.80715400	1.55598600	0.57007100
6	0.84883800	0.43473100	0.16754600
6	1.30919200	-0.69805200	-0.38060800
6	1.28898200	2.94582300	0.11862700
6	-0.21877300	3.17342200	0.31741100
6	-1.00394800	2.00476100	-0.28878000
6	-0.60222200	0.73528700	0.49227600
6	2.08877100	1.50290300	2.08248800
6	-2.51963000	2.14551900	-0.35209600
6	-3.05581100	0.89987300	-1.08058400
6	-2.59816100	-0.36955900	-0.37871500
7	-1.50534500	-0.42256500	0.33223600
6	-4.52843300	0.93821700	-1.38974800
6	-5.29228800	-0.16471300	-1.35681500
6	-4.70484900	-1.43889300	-0.97754300
6	-3.43588700	-1.55138700	-0.51871900
1	5.07993800	-3.17131700	-1.58239600
1	6.55478600	-1.18782700	-1.28448400
1	5.57799100	0.99326900	-0.55662600
1	2.63680600	-2.96167400	-1.16093500
1	0.63873300	-1.52356200	-0.59610900
1	1.51508600	3.02424600	-0.95029200
1	1.87138700	3.72386400	0.62331400
1	-0.50595500	4.11543300	-0.16434300
1	-0.46937900	3.27662400	1.38167200
1	-0.65279700	1.88206600	-1.32416300
1	-0.65719500	0.97007500	1.56339500
1	1.18723400	1.69398800	2.67173400
1	2.83810300	2.25745800	2.34013900
1	2.46501900	0.51569300	2.36169600
1	-4.92734600	1.89428800	-1.71853100
1	-6.34157000	-0.12835900	-1.63174900
1	-5.31856600	-2.33224300	-1.05121600
1	-3.02943300	-2.50467600	-0.21264200
5	-1.25175500	-1.70249000	1.39819800
9	-2.45218200	-1.87204200	2.05517600
9	-0.24690400	-1.28845500	2.23799200
9	-0.91874400	-2.79659000	0.61332000
1	-2.56501000	0.88160500	-2.07315700
1	-2.80709700	3.05055500	-0.89912000
1	-2.96148900	2.21236500	0.64982900

cis-**19-B**
E(RB3LYP)= –1267.431164 a.u.

8	−2.89389000	−1.28695600	0.80036600
6	−1.47791900	−0.96053800	0.96092500
6	−0.84618700	−2.33431000	1.25931900
6	0.66904700	−2.34940500	1.07106700
6	−1.36278800	−0.01597700	2.16551700
1	−1.30101900	−3.05851400	0.57360400
1	−1.12072300	−2.63892400	2.27454100
1	1.05489800	−3.35466000	1.27812000
1	1.16360300	−1.67457800	1.78182300
1	−0.32312500	0.20058500	2.41937900
1	−1.85169200	−0.48545000	3.02507500
1	−1.84417600	0.93865800	1.95126400
6	−3.17131500	0.31241200	−0.97467200
6	−4.04625700	1.08483800	−1.74957200
1	−3.63914600	1.68902900	−2.55639700
6	−5.41595500	1.08450900	−1.49336400
1	−6.08353400	1.69101800	−2.09709000
6	−5.92371400	0.29514300	−0.45733500
1	−6.99050900	0.28727400	−0.25328400
6	−5.07099900	−0.48261600	0.32710400
1	−5.44752800	−1.10282000	1.13368500
6	−3.70011300	−0.46659700	0.07123700
6	−1.74049500	0.22503100	−1.20941000
1	−1.34695800	0.67173500	−2.12028100
6	−0.90919200	−0.35772800	−0.33036300
6	0.56791100	−0.49307700	−0.66368500
6	1.04347100	−1.94893200	−0.36325100
7	1.50419200	0.49809800	−0.04572100
1	0.64752600	−0.33573600	−1.74958900
1	0.46369200	−2.57923800	−1.04856600
6	2.78084800	0.29194600	−0.27702000
6	3.82029900	1.08483200	0.34686700
6	3.18436700	−0.84011400	−1.19421200
6	5.12588100	0.83940900	0.06942700
1	3.53807600	1.84560700	1.05819600
6	4.65135000	−0.99022400	−1.44014100
1	2.70399700	−0.63914800	−2.16783900
6	5.55919000	−0.19537200	−0.84838500
1	5.88568200	1.43466600	0.56805700
1	4.95261600	−1.78941600	−2.11240800
1	6.62099700	−0.32430700	−1.03296600
6	2.54490000	−2.14923900	−0.65286800
5	1.06651400	1.95493800	0.68590900
9	−0.27557700	2.14400300	0.50030200
9	1.42936200	1.81097400	2.01717200
9	1.81575200	2.91596800	0.03548300
1	3.07878900	−2.43149500	0.26045600
1	2.70792400	−2.95245400	−1.37792300

20-B
E(RB3LYP)= -1192.408212 a.u.

8	-3.68396500	-0.96437500	-1.46489600
6	-2.58802500	-0.04854100	-1.06417200
6	-3.24515000	0.95088600	-0.07582600
6	-2.48551600	2.25107600	0.25190600
6	-2.20942300	0.62490500	-2.38248600
6	1.05372600	2.63241800	1.90956000
6	-0.05785900	4.20166300	0.24171700
1	-3.46387100	0.41742300	0.85541500
1	-4.21036700	1.22168200	-0.52053900
1	-3.17617100	2.84974800	0.86514800
1	-2.33984400	2.83680500	-0.66234700
1	-1.46540500	1.40966600	-2.23444700
1	-3.10135100	1.08274100	-2.81767100
1	-1.81922900	-0.10666200	-3.09531600
1	1.98566000	2.62453300	1.32971900
1	0.96675600	1.67089200	2.41915000
1	1.16906300	3.41870300	2.66818300
1	-0.03635700	5.06352600	0.92205200
1	-0.89425300	4.34795600	-0.44539900
1	0.87305500	4.24961500	-0.33829400
6	-3.19011200	-2.42741000	0.33793500
6	-4.01169400	-1.95663300	-0.63420500
6	-1.84039800	-1.95727000	0.34552400
1	-1.08506700	-2.55136700	0.84587700
6	-1.47106200	-0.87131500	-0.40489900
6	3.23170500	-1.50093200	-0.55601900
1	3.02141200	-2.45312200	-0.08286900
6	4.46139700	-1.24899200	-1.15838000
1	5.22560000	-2.02025500	-1.15346300
6	4.71480200	-0.01559000	-1.76400800
1	5.67753700	0.17675400	-2.22754200
6	3.73015100	0.97213100	-1.75940900
1	3.92511300	1.94041000	-2.21067900
6	2.49355200	0.72909100	-1.15999000
6	2.24190900	-0.51253500	-0.56865800
6	-0.09902500	-0.54977600	-0.67675100
1	0.08651000	-0.05170900	-1.62658100
6	-1.18942800	2.07518100	1.00736600
1	-1.12993700	1.19313200	1.64115500
6	-0.13911800	2.91416200	1.02650400
7	0.96880900	-0.80966400	0.03228200
1	1.73696900	1.50659400	-1.12132200
5	1.01760900	-1.36924100	1.60025600
9	0.92816700	-2.75496200	1.51565900
9	2.21603500	-0.93818700	2.10582000
9	-0.06378800	-0.80786300	2.25853300
1	-4.97172100	-2.39994800	-0.88372000
1	-3.49841600	-3.26428000	0.95103200

TS-tf-B-20
E(RB3LYP)= -1192.356364 a.u.

8	4.15597500	-0.21443100	0.06911300
6	2.88134400	-0.80311700	-0.33944400
6	2.59357900	-1.82442500	0.76810200
6	1.19510800	-2.43096600	0.67607800
6	3.11504200	-1.47160300	-1.70690600
1	2.70988400	-1.31071700	1.72848900
1	3.35287400	-2.61284600	0.72951800
1	1.09140000	-3.20422400	1.44668300
1	1.06797600	-2.94447300	-0.28436700
1	2.21220000	-1.97249000	-2.06942300
1	3.91753100	-2.21266600	-1.63413200
1	3.39850100	-0.71731800	-2.44531600
6	3.55647300	1.87027100	-0.89058500
6	4.47627300	1.00392400	-0.42899700
6	2.15666600	1.52042400	-0.75959900
1	1.40794700	2.29462700	-0.88012500
6	1.79241500	0.26473800	-0.42431700
6	-2.90383000	1.52046700	-0.62258300
1	-2.65123200	2.51949100	-0.29579500
6	-4.19976500	1.19784000	-0.95363700
1	-4.96983200	1.96024100	-0.88101800
6	-4.54437000	-0.10146900	-1.39111300
1	-5.57314900	-0.33626200	-1.64589100
6	-3.54816800	-1.04460100	-1.54598400
1	-3.77984900	-2.02534200	-1.95201500
6	-2.21129500	-0.74073500	-1.21792600
6	-1.86604100	0.54487000	-0.70674000
6	0.35239400	-0.17137400	-0.36778600
1	0.17294600	-0.78360900	-1.25573900
6	0.09706300	-1.37262600	0.87376900
1	0.30025800	-0.73967200	1.74140200
6	-1.26677500	-1.87235800	0.91895700
7	-0.61021600	0.83878900	-0.23600000
1	-1.45283200	-1.43543000	-1.54864600
5	-0.46059700	1.96061500	0.96114400
9	-0.30546500	3.20032200	0.36278500
9	-1.63018100	1.91050100	1.72459300
9	0.61921400	1.57786900	1.74087200
1	5.53897900	1.20987600	-0.34864100
1	3.85768100	2.84414700	-1.25552300
6	-2.23258800	-1.24652300	1.87549300
1	-3.27108600	-1.42384400	1.58374000
1	-2.08336700	-1.72224100	2.85981300
1	-2.05992900	-0.17619500	2.00482900
6	-1.60276400	-3.25510800	0.44329400
1	-1.30943300	-3.97661800	1.22308900
1	-2.67662300	-3.37103600	0.28305200
1	-1.07081200	-3.54655600	-0.46532700

TS-cf-B-20
E(RB3LYP)= -1192.347797 a.u.

8	-3.89544500	-1.04538400	0.21926400
6	-2.65416100	-0.32900800	0.58576500
6	-2.04224200	-1.26158400	1.65387200
6	-0.51747400	-1.20947000	1.75253300
6	-3.08755700	1.00357400	1.20742700
1	-2.34708400	-2.28546000	1.40841600
1	-2.49133200	-1.02365800	2.62333300
1	-0.19675300	-1.86286400	2.57241000
1	-0.17226300	-0.19801900	1.99197200
1	-2.24343600	1.50323100	1.68160100
1	-3.85451100	0.79117000	1.95988600
1	-3.49364700	1.67804800	0.45323000
6	-3.86023900	-0.15939400	-1.97266900
6	-4.51677100	-0.69392600	-0.92591500
6	-2.41988500	-0.07348000	-1.86919800
1	-1.84203800	0.04987800	-2.78239900
6	-1.78463100	-0.18432400	-0.68242300
6	-0.27761000	-0.26590100	-0.70529600
6	0.08785500	-1.68912600	0.42905600
7	0.53068500	0.80773100	-0.35529500
5	-0.02715500	2.24776400	0.19980300
9	0.88166800	3.21135500	-0.19412500
9	-1.25732000	2.46475900	-0.38036100
9	-0.09631400	2.15044000	1.59760600
6	1.77709700	-3.29018000	-0.53374000
1	1.58460800	-4.23770900	-0.00781000
1	1.15853600	-3.29695100	-1.43608400
1	2.83216600	-3.29038700	-0.81805800
6	2.40322800	-1.88566700	1.49601400
1	3.42634800	-1.77329700	1.12307100
1	2.14243700	-1.00845000	2.08700100
1	2.40552800	-2.75837800	2.16859600
1	0.02767600	-0.74460800	-1.63552700
1	-0.56920800	-2.38863300	-0.09488400
6	1.89789800	0.62524500	-0.48279200
6	2.80042800	1.39981300	0.30446200
6	2.45400200	-0.39122300	-1.29938600
6	4.15798600	1.16390300	0.25338400
1	2.40605400	2.16136300	0.96000300
6	3.84288900	-0.59008300	-1.36701100
1	1.83211000	-0.92105700	-2.00885800
6	4.69733600	0.16463900	-0.58319200
1	4.82049900	1.75662500	0.87721900
1	4.23694000	-1.34568400	-2.04066900
1	5.77055600	0.00516600	-0.62257500
6	1.43330600	-2.15037900	0.38633100
1	-5.56882900	-0.96401100	-0.92745200
1	-4.38084700	0.08425100	-2.88989200

trans-**20-B**
E(RB3LYP)= -1192.400372 a.u.

6	4.20684500	-0.52685000	-1.53173500
6	3.26346600	-1.46673600	-1.69988000
8	4.00526700	0.62190300	-0.83496100
6	2.90720900	0.67988000	0.13179300
6	1.73670400	-0.20538500	-0.29985500
6	1.94389500	-1.23820400	-1.13201000
6	2.52724800	2.17936500	0.14683100
6	1.12753900	2.48882000	0.70603000
6	0.07768600	1.61848900	-0.00689100
6	0.42018900	0.15710600	0.36056200
6	3.46653200	0.20696400	1.48450900
6	-1.42146300	1.94704800	0.20363300
6	-2.15708500	0.93159200	-0.74367200
6	-1.79451000	-0.50706700	-0.39860300
7	-0.64117000	-0.83191300	0.11735300
6	-3.63674600	1.15901400	-0.91591300
6	-4.52042500	0.15275600	-1.01226600
6	-4.06833500	-1.22246600	-0.92006600
6	-2.78461200	-1.54507900	-0.63895900
6	-1.70803500	3.39123000	-0.24707600
6	-1.88348800	1.76178700	1.66223900
1	1.13895400	-1.92512600	-1.37010700
1	2.56909500	2.52001300	-0.89348700
1	3.29325700	2.73904500	0.69448300
1	0.92787400	3.55392600	0.55520100
1	1.09096200	2.31249200	1.78843600
1	0.25826600	1.73692900	-1.08543800
1	0.57994100	0.11288300	1.44571400
1	2.73183800	0.32521200	2.28633300
1	4.35707200	0.78999900	1.73999200
1	3.73357500	-0.85127500	1.43197200
1	-3.96066700	2.18476800	-1.05250000
1	-5.57270300	0.35187400	-1.18939800
1	-4.79075100	-2.01838500	-1.07722600
1	-2.46676300	-2.57473600	-0.56054700
1	-2.76110800	3.65577400	-0.11977100
1	-1.44015300	3.54853400	-1.29841900
1	-1.13492200	4.10240200	0.35300700
1	-2.95434900	1.97160500	1.75310500
1	-1.35450100	2.45341300	2.32515400
1	-1.71500500	0.74605800	2.02997400
5	-0.44145200	-2.31285500	0.88754800
9	-1.54128300	-2.42863500	1.71540900
9	0.73442200	-2.21608100	1.59105900
9	-0.41835700	-3.27750000	-0.10850400
1	-1.73666900	1.11426000	-1.75053800
1	3.47443200	-2.35375200	-2.28376800
1	5.19691600	-0.55711000	-1.97540400

cis-**20-B**
E(RB3LYP)= -1192.392673 a.u.

8	-3.91904000	-1.07122900	0.31187300
6	-2.60067800	-0.50181000	0.64497600
6	-1.94363200	-1.61279900	1.48421100
6	-0.41584100	-1.52495900	1.52428800
6	-2.86300100	0.75257400	1.48764200
1	-2.23259000	-2.57325200	1.04189200
1	-2.35851100	-1.59023700	2.49735200
1	-0.04057900	-2.34831700	2.13760200
1	-0.09193800	-0.59627200	2.00946800
1	-1.93632200	1.16405500	1.89168200
1	-3.52822200	0.48432500	2.31517300
1	-3.32818400	1.53338400	0.88502600
6	-3.95484400	0.02547900	-1.78984000
6	-4.57675300	-0.57804100	-0.76069300
6	-2.50676700	0.06553500	-1.76501400
1	-1.97557700	0.30022400	-2.68471500
6	-1.81649500	-0.21612800	-0.64386200
6	-0.30562900	-0.34028000	-0.68968000
6	0.15105900	-1.60942100	0.09328900
7	0.50195200	0.83126300	-0.22761600
6	1.88513100	-3.15587900	-0.90980600
1	1.42287200	-4.01757400	-0.41734100
1	1.41703200	-3.04758800	-1.89468700
1	2.94213400	-3.39673100	-1.06013000
6	2.40753000	-2.09763500	1.30065900
1	3.47544700	-2.26832200	1.14024700
1	2.30338900	-1.23349600	1.96219100
1	2.01204100	-2.97253000	1.82331900
1	-0.04726200	-0.48150900	-1.74981300
1	-0.36997600	-2.43924400	-0.39949300
6	1.80022900	0.63812800	-0.22500300
6	2.72699200	1.60413900	0.32921300
6	2.34037700	-0.65149700	-0.79869800
6	4.06454700	1.40619500	0.22057800
1	2.33257500	2.47037700	0.83738800
6	3.83139700	-0.71984100	-0.91150800
1	1.94600000	-0.70893200	-1.82748700
6	4.63398300	0.25274200	-0.44485700
1	4.74011300	2.13871900	0.65331000
1	4.24995500	-1.59736700	-1.39430100
1	5.71266400	0.18079200	-0.54366000
6	1.69131700	-1.89247900	-0.04826600
5	-0.08797800	2.35749000	0.13387100
9	-1.36453800	2.45014400	-0.35083800
9	-0.00644000	2.45056500	1.51872900
9	0.75980500	3.24492600	-0.50275000
1	-4.51839700	0.37932000	-2.64378600
1	-5.64107900	-0.79112600	-0.72231000

21-B
E(RB3LYP)= -1113.767045 a.u.

8	-3.57229200	-0.10460800	-1.60255200
6	-2.53248500	0.57855700	-0.79779700
6	-3.24559600	0.98768500	0.51876600
6	-2.58240000	2.07706600	1.38602900
6	-2.17295600	1.79262700	-1.65173900
1	-3.39389700	0.08548800	1.12070300
1	-4.24109600	1.34628100	0.23092400
1	-3.23414700	2.19754300	2.26378300
1	-2.60250900	3.04329700	0.86802700
1	-1.46182300	2.44211400	-1.13785400
1	-3.07848400	2.37049300	-1.85356500
1	-1.74718200	1.48225800	-2.60989900
6	-3.03412000	-2.19205000	-0.60796500
6	-3.86305200	-1.37385100	-1.30402700
6	-1.70858700	-1.72236400	-0.34911400
1	-0.93113200	-2.44508100	-0.13007800
6	-1.38244900	-0.40506300	-0.53723700
6	3.32915800	-0.84439000	-0.74298700
1	3.12347800	-1.90723700	-0.68889000
6	4.57219100	-0.36765700	-1.14999800
1	5.35256700	-1.07334800	-1.41816300
6	4.81801000	1.00639600	-1.21282300
1	5.79091100	1.37232800	-1.52643000
6	3.81261100	1.90572700	-0.85876000
1	4.00158800	2.97475900	-0.88557400
6	2.56205300	1.43868200	-0.45167000
6	2.31927600	0.06303100	-0.40580700
6	-0.01879600	0.04233300	-0.60669000
1	0.17023100	0.88762300	-1.26664100
6	-1.18580400	1.78893600	1.87073400
1	-0.99199200	0.78474400	2.24385800
6	-0.20051800	2.69069000	1.89053100
7	1.03538900	-0.45957600	-0.01978900
1	1.78901100	2.13293700	-0.13727700
5	1.04743000	-1.58274000	1.21328300
9	1.01824000	-2.83003100	0.59510700
9	2.20871900	-1.35559600	1.90152300
9	-0.08244600	-1.34316500	1.97606900
1	-4.79546300	-1.69816000	-1.75756500
1	-3.31003600	-3.22407600	-0.43436600
1	-0.34569900	3.70754100	1.52952400
1	0.77929400	2.44909300	2.29105400

TS-tf-B-21
E(RB3LYP)= -1113.711778 a.u.

8	4.02175300	-0.20852400	0.04209300
6	2.73283300	-0.86242100	-0.20777500
6	2.52843200	-1.70716300	1.06234100
6	1.14917900	-2.35771200	1.19832800
6	2.91747400	-1.72981600	-1.46559400
1	2.69594900	-1.04495500	1.91889100
1	3.31081200	-2.47295500	1.09593300
1	1.15147600	-2.97848300	2.10221500
1	0.95102600	-3.04571700	0.36468100
1	2.01932900	-2.31376500	-1.68854400
1	3.75225400	-2.42334200	-1.32424400
1	3.12966500	-1.09503700	-2.32999100
6	3.32979700	1.77079300	-1.07478000
6	4.28569200	0.96320300	-0.57726100
6	1.94789700	1.40057000	-0.87163500
1	1.16774500	2.12469600	-1.07896400
6	1.62562000	0.17391700	-0.40316800
6	-3.20382300	0.89591500	-0.60442900
1	-3.05434800	1.96428600	-0.52626700
6	-4.46416000	0.36652800	-0.74537400
1	-5.31998300	1.03401500	-0.77635300
6	-4.66526500	-1.03135300	-0.85625300
1	-5.66986500	-1.42636400	-0.97162700
6	-3.57880300	-1.87443900	-0.86725200
1	-3.71049400	-2.94236600	-1.01461700
6	-2.26356800	-1.36277600	-0.71837800
6	-2.05926800	0.04710300	-0.57641700
6	0.22780400	-0.30319900	-0.29248700
1	0.08470200	-1.15784200	-0.95375000
6	0.02294600	-1.33177900	1.30420400
1	0.23855500	-0.48565000	1.95639000
6	-1.31151600	-1.79211100	1.36899800
7	-0.82515300	0.57819900	-0.29657800
1	-1.45788100	-2.01516800	-1.03063300
5	-0.81683600	1.89230700	0.74903400
9	-0.96649700	3.02331600	-0.03082600
9	-1.88231600	1.68023200	1.61032800
9	0.37453900	1.84922400	1.44381100
1	5.34622300	1.19503500	-0.56832100
1	3.59670100	2.71127900	-1.53958700
1	-1.53853100	-2.84714900	1.25411100
1	-2.06626900	-1.18776700	1.85658300

TS-cf-B-21
E(RB3LYP)= -1113.711778 a.u.

8	-3.81972700	-0.84553800	0.21966400
6	-2.52202400	-0.26583100	0.58506000
6	-2.05597500	-1.19787600	1.72445200
6	-0.53951900	-1.29901500	1.88946000
6	-2.79278600	1.14796900	1.11763200
1	-2.45872100	-2.19570400	1.51647700
1	-2.51741300	-0.86084200	2.65794500
1	-0.32194500	-1.92351100	2.76379500
1	-0.09403700	-0.31605400	2.07621200
1	-1.90758500	1.56851700	1.59308500
1	-3.60156300	1.07662000	1.85233800
1	-3.09080800	1.82328300	0.31514100
6	-3.60538500	-0.09403100	-2.04533700
6	-4.40564400	-0.43431600	-0.93860100
6	-2.16933100	-0.21957800	-1.87256100
1	-1.55115400	-0.23765600	-2.76789300
6	-1.60032600	-0.31156700	-0.65473500
6	-0.10886300	-0.56569100	-0.61287400
6	0.05732900	-1.93234100	0.62802600
7	0.80342700	0.43595200	-0.31780300
5	0.40037300	1.96591800	0.11272900
9	1.41750800	2.78969800	-0.32887400
9	-0.78767100	2.26785800	-0.51600600
9	0.29640500	1.98477200	1.51124100
1	0.16066000	-1.14645600	-1.49454200
1	-0.65269600	-2.59547900	0.12555000
6	2.14583300	0.09692700	-0.38952200
6	3.10602300	0.81999600	0.37713800
6	2.60744600	-1.02371700	-1.12287900
6	4.43004300	0.43426200	0.38898000
1	2.78057600	1.66186000	0.96951100
6	3.96610900	-1.37812400	-1.12838200
1	1.94848600	-1.53290900	-1.81409500
6	4.87746400	-0.67093600	-0.36343200
1	5.13667900	0.99133300	0.99699600
1	4.29216800	-2.21515400	-1.73912200
1	5.92676800	-0.94951900	-0.35506300
6	1.34443100	-2.53673700	0.67389700
1	-4.03962200	0.15051700	-2.88183300
1	-5.37685200	-0.44250900	-1.00773400
1	2.03168700	-2.35651600	1.47395900
1	1.52220400	-3.41409300	0.08777200

trans-**B-21**
E(RB3LYP)= −1113.770929 a.u.

6	3.99041700	−0.66270300	−1.51278700
6	2.94076000	−1.46546400	−1.74612200
8	3.92776300	0.45133700	−0.73814200
6	2.82840200	0.60005600	0.21761300
6	1.56781200	−0.13108000	−0.25558700
6	1.65608500	−1.12191200	−1.15665900
6	2.62631900	2.13519400	0.28207200
6	1.26800200	2.58605500	0.84422300
6	0.13603700	1.84958700	0.11902700
6	0.30066100	0.34567300	0.42809700
6	3.31527200	0.02113600	1.55704900
6	−1.28703100	2.31116000	0.40515600
6	−2.21364200	1.49409900	−0.51336800
6	−2.00992700	0.00369500	−0.28689400
7	−0.88481400	−0.49187900	0.14930000
6	−3.65402300	1.93051000	−0.49937700
6	−4.66518800	1.05524100	−0.61040300
6	−4.38132000	−0.36662900	−0.71389000
6	−3.13541600	−0.87601200	−0.56775200
1	0.77782200	−1.69462600	−1.43315200
1	2.71441400	2.50002300	−0.74700600
1	3.45046300	2.58198800	0.84849000
1	1.16540400	3.66940100	0.70966400
1	1.20132900	2.39750700	1.92403200
1	0.30156900	1.98488900	−0.96013300
1	0.44856000	0.24149100	1.51155200
1	2.59393200	0.20074900	2.35960700
1	4.26619600	0.48658400	1.83464600
1	3.45649900	−1.05895000	1.47111900
1	−3.83246900	3.00229200	−0.47184900
1	−5.69640900	1.39161700	−0.64825900
1	−5.20864400	−1.04567400	−0.89992000
1	−2.95172400	−1.93969800	−0.61840400
5	−0.83721600	−2.05949300	0.76521000
9	−1.94624900	−2.16331300	1.57907400
9	0.33873300	−2.14505600	1.46878200
9	−0.90454100	−2.90716900	−0.33048300
1	−1.87533700	1.68536800	−1.55020500
1	3.04656000	−2.32910400	−2.39048900
1	4.97373900	−0.78466400	−1.95595100
1	−1.40312100	3.38083600	0.19687700
1	−1.56189400	2.14810000	1.45462500

cis-**B-21**
E(RB3LYP)= -1113.767741 a.u.

8	-3.84781500	-0.91246800	0.14963600
6	-2.51608000	-0.44510800	0.58065600
6	-2.02457400	-1.59303500	1.48432400
6	-0.50197800	-1.65422600	1.60307000
6	-2.74194100	0.84055900	1.38546800
1	-2.38490100	-2.53117000	1.04668500
1	-2.49222000	-1.49906700	2.46977000
1	-0.21800400	-2.49534400	2.24679300
1	-0.10251000	-0.74537600	2.07126300
1	-1.82139700	1.16983600	1.86826100
1	-3.50139200	0.64353500	2.14955000
1	-3.07994900	1.65024100	0.73742300
6	-3.65928600	0.22970000	-1.91706800
6	-4.39485500	-0.34114100	-0.94486500
6	-2.21929900	0.12302300	-1.80923700
1	-1.61755200	0.30275900	-2.69750600
6	-1.62329700	-0.24057900	-0.65653500
6	-0.13818200	-0.55781600	-0.64491600
6	0.12820000	-1.82823600	0.21425600
7	0.83923000	0.52437600	-0.26420200
5	0.35985000	2.03200800	0.27397600
9	1.31541700	2.95380100	-0.11906700
9	-0.84877300	2.31822500	-0.30466500
9	0.29860500	1.89007100	1.65592900
1	0.11597000	-0.80207200	-1.68534900
1	-0.40222200	-2.63792300	-0.30283100
6	2.10354400	0.16253000	-0.31253400
6	3.19984000	1.02972400	0.07210600
6	2.43040700	-1.26457200	-0.70335000
6	4.48025900	0.57893600	0.03749600
1	2.97665800	2.03565000	0.38889600
6	3.87956400	-1.62583600	-0.73877700
1	2.02014500	-1.44540500	-1.71124500
6	4.84211400	-0.75830400	-0.38359900
1	5.27497000	1.25361000	0.34386600
1	4.11874100	-2.63855600	-1.05297500
1	5.88964500	-1.04178200	-0.40364000
6	1.62672400	-2.17861700	0.26883600
1	-4.13434200	0.64947900	-2.79458900
1	-5.47338700	-0.46474300	-0.97888000
1	2.02671000	-2.02833100	1.27699400
1	1.79951800	-3.22715400	0.00820100