SUPPLEMENTARY INFORMATION for "High-Density 'Windowpane' Coordination Patterns of Water Clusters and their NBO/NRT Characterization"

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This Supplementary Information (SI) consists of three sections:

(i) **NPA Charge Distributions** (pp. 2-7), displaying the natural atomic charge (Q_A) values for all monomer units of all windowpane clusters $^{q,t,d}W_n$, in tables similar to Table 1 of the main text;

(ii) **NRT Bond Order Distributions** (pp. 8-15), displaying the NRT bond orders $\{b_{O\cdots O}\}$ and associated $R_{O\cdots O}$ distances (Å) for all O–H···O hydrogen bonds of all windowpane clusters $^{q,t,d}W_n$, in tables similar to Table 2 of the main text;

(iii) **Optimized Cluster Geometries** (pp. 16-33), displaying ready-to-run *Gaussian-16* input files containing the optimized geometry, vibrational frequencies, and other thermochemical data for all windowpane clusters $^{q,t,d}W_n$, together with NBO keyword input to obtain the NRT bond orders and other NBO-based descriptors.

NPA Charge Distributions

cluster	O_i	Q_i	*q/t/d*
$^{0,2,4}W_6$	1	–0.00815	t_d
	4	+0.00247	*d*
	7	–0.00212	*d*
	10	+0.00797	t_a
	13	–0.00238	*d*
	16	+0.00222	*d*

cluster	O_i	Q_i	*q/t/d*
$^{1,0,6}W_7$	1	–0.00095	*d*
	4	+0.00108	*d*
	7	–0.00047	*d*
	10	+0.00396	*q*
	13	–0.00206	*d*
	16	–0.00262	*d*
	19	+0.00106	*d*

cluster	O_i	Q_i	*q/t/d*
$^{0,4,4}W_8$	1	–0.00710	t_d
	4	+0.00285	*d*
	7	–0.00240	*d*
	10	+0.00619	t_a
	13	+0.00247	t_a
	16	–0.00119	t_d
	19	–0.00347	*d*
	22	+0.00262	*d*

cluster	O_i	Q_i	*q/t/d*
$^{0,8,0}W_8$	1	–0.01797	t_d
	4	+0.01787	t_a
	7	–0.01799	t_d
	10	+0.01801	t_a
	13	–0.01796	t_d
	16	+0.01799	t_a
	19	–0.01806	t_d
	22	+0.01811	t_a

cluster	O_i	Q_i	*q/t/d*
$^{1,2,5}W_8$	1	–0.00580	t_d
	4	+0.00147	*d*
	7	+0.00276	*d*
	10	–0.00963	*q*
	13	+0.01800	t_a
	16	–0.00314	*d*
	19	–0.00293	*d*
	22	–0.00073	*d*

cluster	O_i	Q_i	*q/t/d*
$^{1,4,4}W_9$	1	+0.00799	t_d
	4	+0.00246	*d*
	7	–0.00818	*d*
	10	–0.01029	*q*
	13	+0.02714	t_d
	16	–0.00519	*d*
	19	–0.00536	t_d
	22	–0.00070	*d*
	25	–0.00786	*d*

cluster	O_i	Q_i	*q/t/d*
$^{0,6,4}W_{10}$	1	–0.00682	t_d
	4	+0.00278	*d*
	7	–0.00227	*d*
	10	+0.00526	t_a
	13	+0.00056	t_a
	16	+0.00093	t_d
	19	–0.00002	t_a
	22	+0.00036	t_d
	25	–0.00358	*d*
	28	+0.00278	*d*

cluster	O_i	Q_i	*q/t/d*
$^{1,4,5}W_{10}$	1	–0.00493	t_d
	4	+0.00107	*d*
	7	+0.00319	*d*
	10	–0.01207	*q*
	13	+0.02045	t_a

	16	+0.00393	t_a
	19	–0.00788	t_d
	22	–0.00152	*d*
	25	–0.00093	*d*
	28	–0.00132	*d*

cluster	**O$_i$**	***Q*$_i$**	***q/t/d***
^{3,2,7}**W$_{12}$**	1	–0.00067	t_d
	4	+0.00131	*d*
	7	+0.00160	*d*
	10	–0.00667	*q*
	13	+0.01490	t_a
	16	–0.00695	*q*
	19	–0.00017	*q*
	22	+0.00004	*d*
	25	+0.00352	*d*
	28	–0.00444	*d*
	31	+0.00131	*d*
	34	–0.00378	*d*

cluster	**O$_i$**	***Q*$_i$**	***q/t/d***
^{4,8,0}**W$_{12}$**	1	–0.01740	t_d
	4	+0.02204	t_a
	7	–0.01729	t_d
	10	+0.02202	t_a
	13	–0.00472	*q*
	16	–0.00457	*q*
	19	–0.00466	*q*
	22	–0.00494	*q*
	25	–0.01743	t_d
	28	+0.02210	t_a
	31	–0.01739	t_d
	34	+0.02222	t_a

cluster	**O$_i$**	***Q*$_i$**	***q/t/d***
^{3,8,3}**W$_{14}$**	1	+0.01895	t_a
	4	+0.00079	t_d
	7	–0.01597	t_d
	10	–0.01309	t_d

	13	+0.01075	*q*
	16	+0.00979	*q*
	19	–0.00828	*q*
	22	+0.00013	t_a
	25	+0.00566	t_a
	28	–0.00950	*d*
	31	–0.00404	*d*
	34	–0.00842	*d*
	37	+0.01367	t_a
	40	–0.00046	t_d

cluster	**O$_i$**	***Q*$_i$**	***q/t/d***
$^{4,4,6}\mathbf{W_{14}}$	1	–0.00662	t_d
	4	–0.00324	*d*
	7	+0.00963	t_a
	10	–0.00636	*q*
	13	–0.00107	*q*
	16	–0.00414	*q*
	19	+0.00264	*q*
	22	+0.01427	t_a
	25	+0.00079	*d*
	28	–0.00357	*d*
	31	+0.00465	*d*
	34	–0.00250	*d*
	37	+0.00087	*d*
	40	–0.00536	t_d

cluster	**O$_i$**	***Q*$_i$**	***q/t/d***
$^{4,12,0}\mathbf{W_{16}}$	1	+0.01923	t_a
	4	+0.00054	t_d
	7	–0.01434	t_d
	10	–0.01171	t_a
	13	+0.00938	*q*
	16	+0.00772	*q*
	19	+0.00288	*q*
	22	–0.01084	*q*
	25	+0.00423	t_a
	28	+0.00230	t_a
	31	–0.03123	t_d

	34	+0.01684	t_a
	37	+0.01538	t_a
	40	+0.00045	t_d
	43	–0.02058	t_d
	46	+0.00975	t_a

cluster	**O$_i$**	***Q*$_i$**	***q/t/d***
$^{8,0,8}W_{16}$	1	+0.00680	*q*
	4	–0.00077	*d*
	7	+0.00329	*d*
	10	–0.00751	*q*
	13	–0.00944	*q*
	16	–0.01028	*q*
	19	+0.00297	*q*
	22	+0.01152	*q*
	25	–0.00054	*d*
	28	+0.00240	*d*
	31	–0.00893	*q*
	34	+0.00774	*q*
	37	+0.00230	*d*
	40	–0.00207	*d*
	43	–0.00058	*d*
	46	+0.00311	*d*

cluster	**O$_i$**	***Q*$_i$**	***q/t/d***
$^{8,8,0}W_{16}$	1	–0.01708	t_d
	4	+0.02232	t_a
	7	–0.01718	t_d
	10	+0.02234	t_a
	13	+0.00000	*q*
	16	–0.00517	*q*
	19	–0.00005	*q*
	22	–0.00524	*q*
	25	–0.00530	*q*
	28	–0.00010	*q*
	31	–0.00530	*q*
	34	–0.00007	*q*
	37	–0.01706	t_d
	40	+0.02240	t_a

	43	–0.01700	t_d
	46	+0.02240	t_a

NRT Bond Order Distributions

$^{0,0,4}W_4$	i	j	b_{ij}	R_{ij}
	1	4	0.1068	2.7401
	1	10	0.1068	2.7401
	4	7	0.1068	2.7401
	7	10	0.1068	2.7401

$^{0,2,4}W_6$	i	j	b_{ij}	R_{ij}
	1	4	0.1365	2.6920
	1	10	0.0389	2.9572
	1	16	0.0813	2.7886
	4	7	0.1302	2.6957
	7	10	0.1351	2.6953
	10	13	0.0804	2.8021
	13	16	0.0873	2.7721

$^{1,0,6}W_7$	i	j	b_{ij}	R_{ij}
	1	4	0.1061	2.7412
	1	10	0.0766	2.7513
	4	7	0.1041	2.7377
	7	10	0.0706	2.7570
	10	13	0.0637	2.7513
	10	19	0.0695	2.7677
	13	16	0.0999	2.7469
	16	19	0.1082	2.7349

$^{0,4,4}W_8$	i	j	b_{ij}	R_{ij}
	1	4	0.1462	2.6785
	1	10	0.0280	3.0224
	1	16	0.1052	2.7426
	4	7	0.1387	2.6792
	7	10	0.1440	2.6812
	10	13	0.1063	2.7521
	13	16	0.0322	2.9885
	13	19	0.0724	2.8228
	16	22	0.0750	2.8075
	19	22	0.0822	2.7822

$^{0,8,0}W_8$	i	j	b_{ij}	R_{ij}
	1	4	0.1533	2.6849
	1	10	0.0271	2.8605
	1	16	0.0261	2.8601
	4	7	0.0283	2.8596
	4	19	0.0247	2.8603
	7	10	0.1534	2.6846
	7	22	0.0283	2.8600
	10	13	0.0267	2.8597
	13	16	0.0276	2.8599
	13	22	0.1535	2.6845
	16	19	0.1534	2.6845
	19	22	0.0247	2.8606

$^{1,2,5}W_8$	i	j	b_{ij}	R_{ij}
	1	4	0.1259	2.6991
	1	10	0.0499	2.8988
	1	22	0.0633	2.8435
	4	7	0.1225	2.7101
	7	10	0.1136	2.7477
	10	13	0.1765	2.6666
	10	19	0.0870	2.7837
	13	16	0.0761	2.7990
	13	22	0.0609	2.8239
	16	19	0.0865	2.7775

$^{1,4,4}W_9$	i	j	b_{ij}	R_{ij}
	1	4	0.0942	2.7519
	1	10	0.0775	2.8377
	1	22	0.0318	2.8918
	4	7	0.0797	2.8139
	7	10	0.1563	2.6300
	7	25	0.0401	2.9047
	10	13	0.1783	2.6516
	10	19	0.0722	2.8307
	13	16	0.0757	2.8002
	13	22	0.0377	2.8904
	16	19	0.0903	2.7557
	19	25	0.0228	2.9178

$^{0,6,4}W_{10}$	i	j	b_{ij}	R_{ij}
	1	4	0.1489	2.6746
	1	10	0.0257	3.0373
	1	16	0.1112	2.7333
	4	7	0.1417	2.6740
	7	10	0.1465	2.6755
	10	13	0.1137	2.7380
	13	16	0.0230	3.0541
	13	19	0.0948	2.7733
	16	22	0.0963	2.7642
	19	22	0.0303	2.9971
	19	25	0.0695	2.8306
	22	28	0.0720	2.8123
	25	28	0.0797	2.7870

$^{1,4,5}W_{10}$	i	j	b_{ij}	R_{ij}
	1	4	0.1238	2.6994
	1	10	0.0481	2.8857
	1	22	0.0552	2.8548
	4	7	0.1210	2.7156
	7	10	0.0998	2.7564
	10	13	0.2042	2.6307
	10	19	0.1275	2.7273
	13	16	0.1079	2.7462
	16	19	0.0308	2.9976
	16	25	0.0723	2.8257
	19	28	0.0792	2.7950
	25	28	0.0748	2.7913

$^{3,2,7}W_{12}$	i	j	b_{ij}	R_{ij}
	1	4	0.1219	2.7018
	1	10	0.0676	2.8712
	1	22	0.0526	2.8394
	4	7	0.1188	2.7178
	7	10	0.1155	2.7455
	10	13	0.1596	2.691
	10	19	0.0904	2.7886

	13	22	0.0649	2.8186
	13	16	0.0685	2.8446
	16	25	0.0720	2.7863
	16	34	0.1012	2.7519
	19	28	0.0728	2.7439
	19	31	0.0944	2.7560
	25	28	0.0791	2.7684
	31	34	0.0958	2.7531

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$^{3,4,5}W_{12}$	i	j	b_{ij}	R_{ij}
	1	4	0.0718	2.7944
	1	10	0.0877	2.7604
	4	7	0.1611	2.6749
	4	13	0.0718	2.8632
	7	16	0.0264	2.8826
	7	22	0.0561	2.8650
	10	13	0.0967	2.7489
	13	16	0.1108	2.7557
	13	19	0.0579	2.8272
	16	22	0.0436	2.8720
	19	22	0.1052	2.7520
	19	25	0.0498	2.8903
	19	31	0.1104	2.7418
	22	28	0.0772	2.8009
	25	28	0.0647	2.8362
	25	34	0.1348	2.7007
	31	34	0.1188	2.7178

$^{4,8,0}W_{12}$	i	j	b_{ij}	R_{ij}
	1	4	0.1475	2.6949
	1	10	0.0561	2.8813
	1	16	0.0538	2.8392
	4	7	0.0560	2.8820
	4	19	0.0394	2.8570
	7	10	0.1475	2.6947
	7	22	0.0541	2.8380
	10	13	0.0394	2.8575
	13	16	0.1082	2.7784

	13	22	0.1078	2.7795
	13	25	0.0542	2.8380
	16	19	0.1081	2.7785
	16	28	0.0395	2.8572
	19	22	0.1079	2.7789
	19	31	0.0538	2.8384
	22	34	0.0392	2.8585
	25	28	0.1478	2.6943
	25	34	0.0561	2.8831
	28	31	0.0560	2.8826

$^{3,8,3}W_{14}$	i	j	b_{ij}	R_{ij}
	1	4	0.0479	2.8915
	1	10	0.1394	2.6919
	1	40	0.0513	2.8748
	4	7	0.0832	2.7877
	4	13	0.0480	2.8933
	7	16	0.1956	2.6317
	7	40	0.0832	2.7941
	10	13	0.0652	2.8334
	10	37	0.0475	2.9123
	13	19	0.0456	2.8578
	16	22	0.0345	2.9366
	19	22	0.0674	2.8305
	19	25	0.0640	2.8759
	19	31	0.1063	2.7518
	22	28	0.1017	2.7621
	25	28	0.0752	2.8198
	25	34	0.1410	2.6906

$^{4,4,6}W_{14}$	i	j	b_{ij}	R_{ij}
	1	4	0.1223	2.6972
	1	10	0.0638	2.8562
	1	22	0.0495	2.9173
	4	7	0.1301	2.7127
	7	10	0.0655	2.8861
	7	40	0.0490	2.9332
	10	13	0.1148	2.7789
	13	16	0.0923	2.7808

	13	40	0.1148	2.6940
	16	19	0.0937	2.8005
	16	25	0.0901	2.7772
	16	34	0.0923	2.7725
	19	28	0.0997	2.7415
	19	31	0.0984	2.7440
	22	37	0.0666	2.8167
	25	28	0.0839	2.7599
	31	34	0.0900	2.7594
	37	40	0.0616	2.8367

$^{4,12,0}W_{16}$	i	j	b_{ij}	R_{ij}
	1	4	0.0460	2.8980
	1	10	0.1399	2.6902
	1	40	0.0501	2.8739
	4	7	0.0819	2.7894
	4	13	0.0492	2.8935
	7	16	0.1893	2.6394
	7	40	0.0819	2.7994
	10	13	0.0710	2.8210
	10	37	0.0461	2.9147
	13	19	0.0481	2.8574
	16	22	0.0379	2.9047
	16	37	0.1127	2.7430
	19	22	0.1045	2.7846
	19	25	0.0288	2.9592
	19	31	0.0768	2.7963
	22	28	0.0447	2.8969
	22	46	0.0739	2.8280
	25	28	0.0855	2.8269
	25	34	0.1175	2.7624
	28	43	0.0437	2.9257
	31	34	0.1998	2.6290
	31	46	0.0509	2.8990
	34	43	0.0484	2.8842
	37	40	0.0354	2.9494
	43	46	0.1407	2.7047

$^{8,0,8}W_{16}$	i	j	b_{ij}	R_{ij}
	1	4	0.0951	2.7445
	1	10	0.1161	2.7665
	1	22	0.0691	2.7757
	1	31	0.0819	2.7822
	4	7	0.0975	2.7630
	7	10	0.0690	2.7731
	10	13	0.0707	2.8545
	10	19	0.0846	2.8208
	13	16	0.0818	2.8054
	13	22	0.1076	2.7763
	13	40	0.0901	2.7615
	16	19	0.1005	2.8240
	16	25	0.0842	2.7734
	16	34	0.0789	2.7921
	19	28	0.0759	2.7644
	19	31	0.0890	2.7870
	22	34	0.0778	2.7782
	22	37	0.0942	2.7332
	25	28	0.0896	2.7629
	31	34	0.1009	2.8178
	31	43	0.0854	2.7708
	34	46	0.0780	2.7668
	37	40	0.0862	2.7714
	43	46	0.0911	2.7610

$^{8,8,0}W_{16}$	i	j	b_{ij}	R_{ij}
	1	4	0.1494	2.6919
	1	10	0.0347	2.8823
	1	16	0.0409	2.8353
	4	7	0.0429	2.8823
	4	19	0.0405	2.8562
	7	10	0.1494	2.6919
	7	22	0.0411	2.8354
	10	13	0.0405	2.8560
	13	16	0.0997	2.7928
	13	22	0.1050	2.7922
	13	25	0.0387	2.8358
	16	19	0.1050	2.7921

	16	28	0.0390	2.8358
	19	22	0.0997	2.7929
	19	31	0.0389	2.8354
	22	34	0.0387	2.8362
	25	28	0.1005	2.7929
	25	34	0.1053	2.7912
	25	37	0.0371	2.8353
	28	31	0.1049	2.7922
	28	46	0.0405	2.8578
	31	43	0.0367	2.8352
	34	40	0.0405	2.8561
	37	40	0.1495	2.6920
	37	46	0.0342	2.8825
	40	43	0.0336	2.8830
	43	46	0.1492	2.6925

Optimized Cluster Geometries

```
%nproc=8
%chk=w2
%mem=2GB
#B3LYP/6-311++G** POP=NBO6Read

water dimer, E(RB3LYP) =  -152.926350055 (dE = -5.83 kcal/mol)
nu: 144,165,175,...
Vibrational temperatures:    206.49   237.01   251.99   283.88   534.25
         (Kelvin)            968.26  2320.93  2344.01  5331.39  5488.10
                            5600.08  5632.57
Zero-point correction=                           0.046234 (Hartree/Particle)
Thermal correction to Energy=                    0.051973
Thermal correction to Enthalpy=                  0.052917
Thermal correction to Gibbs Free Energy=         0.020146
Sum of electronic and zero-point Energies=           -152.880116
Sum of electronic and thermal Energies=              -152.874377
Sum of electronic and thermal Enthalpies=            -152.873433
Sum of electronic and thermal Free Energies=         -152.906204

  0  1
 H
 O     1   0.9681
 H     2   0.9775    1    105.8230
 O     3   1.9059    2    171.3648    1    180.0262
 H     4   0.9698    3    109.7952    2     57.8695
 H     4   0.9698    3    109.7952    2    302.0524

 $NBO file=water_dimer archive dipole nrt plot $END

********************************************************************************
%mem=2gb
%nprocshared=8
%chk=w4c
#b3lyp/6-311++G** pop=nbo7read

w4c, E(RB3LYP) =  -305.883182879
nu: 56,92,212,...
 Vibrational temperatures:     80.50   132.86   305.24   315.75   353.06
          (Kelvin)            353.07   373.97   377.79   377.80   447.25
                              594.34   642.43   674.69   674.71  1138.90
                             1214.13  1214.13  1461.70  2346.80  2371.02
                             2371.03  2418.89  4856.35  4991.12  4991.13
                             5045.49  5588.27  5589.36  5589.36  5590.89
 Zero-point correction=                           0.098934 (Hartree/Particle)
 Thermal correction to Energy=                    0.108534
 Thermal correction to Enthalpy=                  0.109478
 Thermal correction to Gibbs Free Energy=         0.065929
 Sum of electronic and zero-point Energies=           -305.784248
 Sum of electronic and thermal Energies=              -305.774649
 Sum of electronic and thermal Enthalpies=            -305.773704
 Sum of electronic and thermal Free Energies=         -305.817254

0 1
               8         -0.043224    1.936641    0.028239
               1         -0.824062    1.339305   -0.004245
               1         -0.196073    2.541087    0.760117
               8         -1.936652   -0.043224   -0.028238
               1         -1.339311   -0.824059    0.004247
               1         -2.541094   -0.196075   -0.760120
               8          0.043225   -1.936640    0.028239
               1          0.824061   -1.339300   -0.004243
               1          0.196076   -2.541087    0.760116
               8          1.936656    0.043224   -0.028235
```

```
               1          1.339308    0.824055    0.004252
               1          2.541050    0.196070   -0.760157

$nbo file=w4c archive nrt plot $end

********************************************************************************
%mem=2gb
%nprocshared=8
%chk=w6_q0_t2_d4
#b3lyp/6-311++G** pop=nbo7read

w6_q0_t2_d4 ("2-pane"), E(RB3LYP) =  -458.831339373
nu: 32,44,62,...
 Vibrational temperatures:     46.06    62.70    89.36   112.32   141.90
          (Kelvin)            212.21   262.12   284.37   300.12   336.45
                              356.55   366.68   380.12   416.18   422.01
                              435.32   462.58   574.56   599.63   663.11
                              679.58   714.43   804.39   902.73  1085.48
                             1128.82  1238.68  1266.92  1330.31  1507.48
                             2343.30  2360.76  2364.51  2393.65  2420.78
                             2471.52  4696.19  4809.84  4887.12  5042.15
                             5126.96  5152.88  5356.38  5576.31  5588.87
                             5591.25  5591.77  5593.75
 Zero-point correction=                           0.149713 (Hartree/Particle)
 Thermal correction to Energy=                    0.164610
 Thermal correction to Enthalpy=                  0.165554
 Thermal correction to Gibbs Free Energy=         0.108550
 Sum of electronic and zero-point Energies=           -458.681627
 Sum of electronic and thermal Energies=              -458.666730
 Sum of electronic and thermal Enthalpies=            -458.665786
 Sum of electronic and thermal Free Energies=         -458.722789

   0  1
               8         -0.102847    1.546527    0.865219
               1         -0.954782    1.531691    0.359698
               1         -0.244471    2.119056    1.625438
               8         -2.429522    1.232050   -0.451817
               1         -2.526997    0.248670   -0.487527
               1         -2.610745    1.555085   -1.338990
               8         -2.336467   -1.462044   -0.437681
               1         -1.462734   -1.586579    0.010730
               1         -2.954645   -2.053823    0.000041
               8          0.015314   -1.408329    0.878002
               1          0.057314   -0.465780    1.104985
               1          0.864936   -1.587018    0.427081
               8          2.498662   -1.404974   -0.419934
               1          2.585015   -0.432334   -0.497755
               1          3.313569   -1.714925   -0.014822
               8          2.360444    1.363630   -0.429104
               1          1.494977    1.540541   -0.007352
               1          2.393883    1.910541   -1.219010

$nbo file=w6_q0_t2_d4 archive nrt plot $end

********************************************************************************
%mem=2gb
%nprocshared=8
%chk=w8_q0_t4_d4
#b3lyp/6-311++G** pop=nbo7read

w8_q0_t4_d4 ("4-pane ladder"), E(RB3LYP) =  -611.777396076
nu: 20,29,44,...
 Vibrational temperatures:     28.53    41.47    63.82    70.85    73.77
          (Kelvin)            104.98   131.19   142.29   177.42   201.13
                              245.72   261.18   292.88   316.98   342.38
                              351.78   355.64   371.20   387.50   412.54
```

```
                          420.18   435.69   453.38   467.01   550.74
                          583.17   655.72   670.18   690.44   722.68
                          744.34   783.06   867.10   915.43  1040.48
                         1092.99  1210.04  1223.58  1241.15  1319.50
                         1370.98  1528.39  2341.44  2355.17  2361.50
                         2379.03  2401.28  2428.17  2448.10  2481.53
                         4627.88  4745.79  4835.93  4943.26  4990.94
                         5082.10  5163.22  5190.01  5399.34  5415.36
                         5574.19  5576.54  5588.85  5592.42  5592.47
                         5593.86
 Zero-point correction=                           0.200250 (Hartree/Particle)
 Thermal correction to Energy=                    0.220627
 Thermal correction to Enthalpy=                  0.221571
 Thermal correction to Gibbs Free Energy=         0.150633
 Sum of electronic and zero-point Energies=           -611.577146
 Sum of electronic and thermal Energies=              -611.556769
 Sum of electronic and thermal Enthalpies=            -611.555825
 Sum of electronic and thermal Free Energies=         -611.626764

  0  1
               8          1.215665    1.581900   -0.767618
               1          2.113017    1.506917   -0.348896
               1          1.317630    2.167450   -1.524278
               8          3.646856    1.172786    0.279516
               1          3.749541    0.187304    0.275238
               1          3.934382    1.472100    1.146682
               8          3.560690   -1.504197    0.212302
               1          2.642354   -1.619614   -0.144779
               1          4.127063   -2.096062   -0.290429
               8          1.095055   -1.437270   -0.838802
               1          1.017738   -0.503416   -1.082249
               1          0.303570   -1.606179   -0.279255
               8         -1.119606   -1.453350    0.794869
               1         -1.144067   -0.513638    1.028794
               1         -2.012160   -1.639640    0.444599
               8         -1.035024    1.533962    0.798895
               1         -0.221045    1.618999    0.251392
               1         -0.903556    2.090449    1.572856
               8         -3.758374   -1.467490   -0.207505
               1         -3.858477   -0.497125   -0.282184
               1         -4.515743   -1.777775    0.296793
               8         -3.618952    1.310353   -0.275865
               1         -2.713709    1.487740    0.047531
               1         -3.727018    1.828946   -1.078155

$nbo file=w8_q0_t4_d4 archive nrt plot $end

**************************************************************************
%mem=2gb
%nprocshared=8
%chk=w10_q0_t6_d4
#b3lyp/6-311++G** pop=nbo7read

w10_q0_t6_d4 ("4-pane ladder"), E(RB3LYP) =  -764.722600374
nu: 12,20,30,...
 Vibrational temperatures:     17.36    28.17    42.85    60.96    61.79
          (Kelvin)             68.50    69.05   104.55   122.05   129.59
                              141.86   157.77   177.62   198.23   240.99
                              253.12   287.70   290.47   312.33   330.94
                              353.83   361.44   365.00   385.19   395.34
                              399.78   405.11   418.46   436.32   459.70
                              473.72   539.96   574.63   634.91   650.85
                              668.78   694.33   712.31   726.98   748.86
                              761.91   860.06   878.46   886.12  1020.98
                             1080.59  1147.25  1209.55  1221.09  1249.20
                             1268.50  1338.10  1389.34  1535.08  2339.94
```

```
                          2352.90  2359.32  2370.62  2390.23  2410.26
                          2426.33  2438.64  2463.28  2483.89  4605.94
                          4725.20  4818.23  4895.19  4940.75  5005.39
                          5054.06  5099.77  5178.77  5204.54  5416.77
                          5427.47  5450.79  5573.47  5575.30  5577.34
                          5588.82  5592.31  5593.03  5594.45
 Zero-point correction=                           0.250654 (Hartree/Particle)
 Thermal correction to Energy=                    0.276622
 Thermal correction to Enthalpy=                  0.277566
 Thermal correction to Gibbs Free Energy=         0.192293
 Sum of electronic and zero-point Energies=           -764.471946
 Sum of electronic and thermal Energies=              -764.445978
 Sum of electronic and thermal Enthalpies=            -764.445034
 Sum of electronic and thermal Free Energies=         -764.530307

   0  1
                8         -2.471232    1.568119    0.747501
                1         -3.318946    1.482375    0.236016
                1         -2.661100    2.151721    1.488549
                8         -4.777481    1.150454   -0.541081
                1         -4.886152    0.164924   -0.545500
                1         -4.980676    1.450039   -1.431684
                8         -4.715089   -1.521855   -0.467714
                1         -3.837792   -1.641738   -0.018955
                1         -5.331434   -2.115431   -0.030031
                8         -2.372818   -1.466510    0.826545
                1         -2.317059   -0.537597    1.091368
                1         -1.528093   -1.629696    0.345702
                8         -0.019568   -1.487801   -0.572809
                1          0.040171   -0.562465   -0.846399
                1          0.833040   -1.659679   -0.117701
                8         -0.081844    1.565700   -0.579869
                1         -0.946886    1.612113   -0.108637
                1         -0.172661    2.113243   -1.365969
                8          2.405067   -1.496081    0.773392
                1          2.455412   -0.557616    1.005576
                1          3.250483   -1.679235    0.320995
                8          2.312164    1.499418    0.800456
                1          1.451278    1.576590    0.332830
                1          2.242621    2.038427    1.594563
                8          4.931225   -1.494584   -0.503730
                1          5.034977   -0.523679   -0.556177
                1          5.728384   -1.828032   -0.082304
                8          4.808463    1.289569   -0.477628
                1          3.931187    1.461529   -0.083731
                1          4.862147    1.832771   -1.269015

$nbo file=w10_q0_t6_d4 archive nrt plot $end

********************************************************************************
%mem=2gb
%nprocshared=8
%chk=w9_q1_t4_d4
#b3lyp/6-311++G** pop=nbo7read opt freq

w9_4_pane (w9_q1_t4_d4 "saddle"), E(RB3LYP) =  -688.246307864
nu: 12,25,37,...
 Vibrational temperatures:     17.43    36.33    53.52    64.71    76.51
          (Kelvin)             89.50    99.32   123.19   136.20   143.81
                              175.14   212.81   235.56   254.25   273.68
                              283.67   287.03   316.11   323.58   327.82
                              341.22   375.10   387.72   405.36   438.77
                              461.79   495.23   539.46   567.19   612.22
                              629.80   665.78   692.62   767.62   772.45
                              791.03   811.41   956.57  1008.13  1035.62
                             1073.07  1118.50  1153.30  1178.36  1221.82
```

```
                          1250.36  1407.33  1568.05  2315.21  2352.42
                          2360.46  2370.21  2381.74  2387.02  2402.71
                          2412.35  2492.27  4443.79  4777.17  4877.14
                          4954.01  5006.41  5125.07  5175.52  5207.92
                          5259.38  5316.47  5373.55  5495.09  5562.42
                          5568.98  5573.84  5591.00  5596.27  5597.96
 Zero-point correction=                           0.225212 (Hartree/Parti$
 Thermal correction to Energy=                    0.248483
 Thermal correction to Enthalpy=                  0.249427
 Thermal correction to Gibbs Free Energy=         0.171104
 Sum of electronic and zero-point Energies=           -688.021096
 Sum of electronic and thermal Energies=              -687.997825
 Sum of electronic and thermal Enthalpies=            -687.996881
 Sum of electronic and thermal Free Energies=         -688.075204

   0  1
              8          0.131053   -2.498922   -1.052882
              1          1.078473   -2.594556   -0.807112
              1          0.110244   -2.388383   -2.009173
              8          2.738637   -2.306524   -0.194697
              1          2.824623   -1.449619    0.272634
              1          3.566700   -2.452947   -0.660400
              8          2.511496    0.146091    1.165794
              1          1.521992    0.091597    1.057778
              1          2.684216    0.101866    2.111960
              8         -0.009101   -0.100293    0.456886
              1         -0.055396   -0.898067   -0.101622
              1         -0.908061   -0.019878    0.882922
              8         -2.542058    0.055159    1.225616
              1         -2.850282    0.817597    0.695451
              1         -2.852951   -0.756293    0.791284
              8         -2.853785    2.350301   -0.348011
              1         -1.934415    2.522623   -0.647545
              1         -3.214294    3.197920   -0.074785
              8         -0.194190    2.278638   -1.066041
              1         -0.074543    1.414737   -0.629839
              1          0.649058    2.730016   -0.904888
              8         -2.570862   -2.551145   -0.023578
              1         -1.658023   -2.729908   -0.305110
              1         -2.906322   -3.376444    0.337663
              8          2.569675    2.693908   -0.228034
              1          2.703105    1.875183    0.282204
              1          3.068956    3.376846    0.228153

$nbo file=w9_q1_t4_d4 archive nrt plot thresh=1.4 $end

**************************************************************************
%mem=2gb
%nprocshared=8
%chk=w8_t8
#b3lyp/6-311++G** pop=nbo7read

w8_t8 ("cube"), E(RB3LYP) =  -611.792369303
nu: 81,83,85,...
 Vibrational temperatures:    116.05   119.09   122.16   124.99   125.05
          (Kelvin)            182.83   230.44   241.33   250.51   250.63
                              272.63   296.27   296.41   298.01   384.08
                              393.58   393.67   418.81   421.40   437.91
                              501.50   501.59   644.41   663.34   663.46
                              752.98   757.78   792.28   801.16   801.29
                              887.53  1008.12  1008.53  1014.50  1065.17
                             1065.27  1109.30  1284.20  1346.12  1516.02
                             1516.49  1616.43  2355.35  2356.90  2356.91
                             2374.79  2411.59  2411.71  2449.30  2480.70
                             4622.93  4657.52  4658.30  4744.90  5199.81
                             5199.92  5222.88  5227.18  5248.45  5248.70
```

```
                          5312.94  5312.97  5579.80  5579.96  5580.04
                          5580.50
 Zero-point correction=                           0.204049 (Hartree/Particle)
 Thermal correction to Energy=                    0.222157
 Thermal correction to Enthalpy=                  0.223101
 Thermal correction to Gibbs Free Energy=         0.161017
 Sum of electronic and zero-point Energies=           -611.588320
 Sum of electronic and thermal Energies=              -611.570213
 Sum of electronic and thermal Enthalpies=            -611.569268
 Sum of electronic and thermal Free Energies=         -611.631352

  0  1
               8          2.082972    0.137875   -1.345066
               1          2.178068    0.140096   -0.355425
               1          2.968129    0.194557   -1.717317
               8          1.952156    0.119848    1.336558
               1          1.346677    0.853935    1.546015
               1          1.446927   -0.687727    1.541240
               8         -0.137979    2.071318    1.359495
               1         -0.140516    2.174413    0.370574
               1         -0.193407    2.953527    1.738862
               8         -0.119835    1.962628   -1.322889
               1          0.687908    1.459142   -1.531057
               1         -0.853817    1.358315   -1.536110
               8         -2.071050   -0.127565   -1.361248
               1         -2.174732   -0.138096   -0.372445
               1         -2.952894   -0.181221   -1.741711
               8          0.130806   -1.952417   -1.334686
               1         -0.674714   -1.446603   -1.545973
               1          0.867076   -1.347821   -1.538817
               8          0.126437   -2.081968    1.346666
               1          0.137754   -2.177313    0.357046
               1          0.182379   -2.966759    1.719867
               8         -1.964035   -0.129493    1.321120
               1         -1.459143    0.675789    1.535493
               1         -1.361471   -0.866040    1.530151

$nbo file=w8_t8 archive nrt plot $end

************************************************************************
%mem=2gb
%nprocshared=8
%chk=w12_q4_t8
#b3lyp/6-311++G** pop=nbo7read

w12_q4_t8 ("2-cube"), E(RB3LYP) = -917.699234818
 nu: 59,61(2),78(2),...
 Vibrational temperatures:     84.29    87.48    87.49   112.07   112.09
          (Kelvin)            124.64   129.42   133.17   156.70   170.63
                              176.95   189.18   189.37   227.98   244.75
                              245.78   250.95   251.42   294.23   297.54
                              306.91   307.17   353.70   370.02   370.32
                              371.89   379.43   384.70   401.04   401.32
                              461.12   480.89   488.98   489.24   637.00
                              665.15   673.70   673.80   732.44   751.09
                              760.87   761.34   761.71   791.61   824.49
                              824.67   843.91   953.05   982.89   988.96
                              989.23   995.04  1039.46  1040.15  1041.82
                             1066.14  1066.64  1215.10  1232.98  1233.28
                             1289.40  1436.87  1437.42  1518.20  1553.55
                             1577.44  2359.08  2359.11  2365.07  2367.94
                             2396.68  2399.88  2399.92  2425.21  2459.96
                             2461.35  2461.48  2496.16  4661.82  4665.26
                             4718.75  4719.83  4858.27  4990.26  4990.61
                             5047.93  5216.46  5221.54  5221.94  5223.23
                             5256.65  5263.12  5263.58  5267.93  5332.12
```

```
                          5333.64  5334.11  5342.74  5576.89  5577.08
                          5577.26  5577.59
 Zero-point correction=                           0.308262 (Hartree/Particle)
 Thermal correction to Energy=                    0.335615
 Thermal correction to Enthalpy=                  0.336560
 Thermal correction to Gibbs Free Energy=         0.254260
 Sum of electronic and zero-point Energies=           -917.390973
 Sum of electronic and thermal Energies=              -917.363619
 Sum of electronic and thermal Enthalpies=            -917.362675
 Sum of electronic and thermal Free Energies=         -917.444975

  0  1
               8         -2.887376   -1.734013   -1.034863
               1         -2.939569   -0.804219   -1.381025
               1         -3.566769   -2.242276   -1.488415
               8         -2.804543    0.872889   -1.712763
               1         -2.935032    1.342788   -0.869352
               1         -1.889967    1.072107   -1.977073
               8         -2.885812    1.733393    1.036614
               1         -2.937688    0.803415    1.382355
               1         -3.563155    2.241996    1.492849
               8         -2.802254   -0.873537    1.713671
               1         -2.932814   -1.343217    0.870096
               1         -1.887877   -1.073168    1.978263
               8          0.054756   -0.861769    1.763770
               1          0.058007    0.100220    1.561214
               1          0.965392   -1.065423    2.042908
               8         -0.053610   -1.763313   -0.862103
               1         -0.059484   -1.559371    0.099651
               1         -0.962762   -2.046173   -1.066767
               8          0.052027    0.862683   -1.763940
               1          0.056107   -0.099119   -1.560289
               1          0.961733    1.066012   -2.046104
               8         -0.053340    1.765199    0.862247
               1         -0.964259    2.044534    1.064280
               1         -0.055018    1.561992   -0.099606
               8          2.887164   -1.036857    1.732713
               1          2.939375   -1.382675    0.802734
               1          3.565337   -1.491758    2.241367
               8          2.803154   -1.714061   -0.873768
               1          1.887899   -1.977228   -1.071515
               1          2.933630   -0.870213   -1.342890
               8          2.884998    1.035861   -1.734290
               1          2.937552    1.381800   -0.804378
               1          3.564161    1.489593   -2.242690
               8          2.804696    1.713645    0.872502
               1          1.891011    1.979230    1.073855
               1          2.935308    0.870192    1.342224

$nbo file=w12_q4_t8 archive nrt plot memory=10gb nrtres=50000 $end

*********************************************************************
%mem=2gb
%nprocshared=8
%chk=w16_q8_t8
#b3lyp/6-311++G** pop=nbo7read

w16_q8_t8 ("3-cube"), E(RB3LYP) = -1223.60719747
nu: 44,45(2),64,...
 Vibrational temperatures:     63.87    64.59    65.27    92.21   100.60
          (Kelvin)            114.32   116.40   116.98   123.36   129.54
                              130.40   143.12   151.59   159.80   159.86
                              162.63   179.98   205.99   230.17   232.50
                              241.82   248.72   256.11   263.91   277.97
                              281.88   286.77   288.09   293.97   305.07
                              310.63   351.71   354.68   356.51   374.32
```

```
                          377.91   379.31   380.43   385.07   387.95
                          402.89   407.21   468.73   474.44   487.54
                          495.10   641.53   659.12   663.56   676.76
                          718.81   731.51   735.93   739.84   742.54
                          756.78   762.72   771.66   783.11   817.05
                          823.79   841.74   877.20   897.78   946.34
                          961.20   972.02   991.37   994.09  1000.31
                         1020.10  1032.79  1044.20  1045.51  1047.98
                         1062.15  1093.57  1193.02  1205.59  1206.44
                         1242.10  1257.71  1305.50  1306.85  1439.48
                         1446.61  1477.24  1534.98  1558.91  1576.76
                         2358.86  2360.10  2365.63  2367.82  2387.30
                         2388.87  2396.03  2412.34  2418.35  2420.09
                         2451.97  2453.55  2461.92  2470.49  2473.36
                         2503.03  4656.24  4657.02  4710.84  4714.56
                         4879.79  4881.88  4982.08  4982.14  5018.53
                         5035.45  5046.40  5076.41  5215.88  5216.45
                         5220.83  5221.21  5248.23  5248.64  5249.02
                         5254.59  5297.20  5301.35  5316.70  5317.44
                         5338.37  5340.61  5340.94  5347.65  5576.24
                         5576.30  5576.63  5576.80
Zero-point correction=                           0.412633 (Hartree/Particle)
Thermal correction to Energy=                    0.449176
Thermal correction to Enthalpy=                  0.450120
Thermal correction to Gibbs Free Energy=         0.347911
Sum of electronic and zero-point Energies=          -1223.194565
Sum of electronic and thermal Energies=             -1223.158021
Sum of electronic and thermal Enthalpies=           -1223.157077
Sum of electronic and thermal Free Energies=        -1223.259287

  0  1
               8         -4.296553   -1.496620    1.356834
               1         -4.353644   -1.556024    0.366439
               1         -4.971037   -2.082308    1.714205
               8         -4.222145   -1.384905   -1.331755
               1         -4.352233   -0.441586   -1.537476
               1         -3.308467   -1.581324   -1.601637
               8         -4.297111    1.496303   -1.356558
               1         -4.354373    1.555716   -0.366168
               1         -4.971867    2.081593   -1.714067
               8         -4.222868    1.384645    1.331974
               1         -4.352523    0.441272    1.537716
               1         -3.309236    1.581442    1.601744
               8         -1.367410    1.437911    1.350343
               1         -1.352839    1.527342    0.371776
               1         -0.480711    1.706230    1.646193
               8         -1.466110   -1.351715    1.438337
               1         -1.455839   -0.373819    1.532210
               1         -2.383022   -1.613979    1.638857
               8         -1.366503   -1.437532   -1.350674
               1         -1.352211   -1.526879   -0.372106
               1         -0.479717   -1.705963   -1.646209
               8         -1.466569    1.352195   -1.438803
               1         -2.383729    1.613692   -1.639185
               1         -1.455525    0.374319   -1.532662
               8          1.465818    1.352323    1.436612
               1          1.455085    0.374547    1.531818
               1          2.383163    1.614133    1.636021
               8          1.367087   -1.437507    1.352170
               1          0.479275   -1.702771    1.647510
               1          1.352674   -1.527852    0.373736
               8          1.466316   -1.353865   -1.436994
               1          1.455089   -0.376076   -1.531728
               1          2.383760   -1.615054   -1.636689
               8          1.367036    1.436347   -1.351579
               1          0.480616    1.703608   -1.649098
```

```
                1          1.350446    1.525641   -0.373004
                8          4.296134    1.499195    1.355131
                1          4.353719    1.557065    0.364654
                1          4.967639    2.088639    1.711905
                8          4.222607    1.383683   -1.333357
                1          3.308292    1.578646   -1.602204
                1          4.353632    0.440402   -1.538414
                8          4.296641   -1.498239   -1.355295
                1          4.354503   -1.556090   -0.364908
                1          4.969082   -2.086526   -1.712251
                8          4.224267   -1.382293    1.333712
                1          3.310640   -1.578630    1.603617
                1          4.354261   -0.438816    1.538622

$nbo file=w16_q8_t8 archive nrt plot memory=10gb nrtres=50000 $end

*********************************************************************
%mem=2gb
%nprocshared=8
%chk=w7_q1_d6
#b3lyp/6-311++G** pop=nbo7read

w7_2_pane (w7_q1_d6), E(RB3LYP) =  -535.304096032
nu: 20,21,35,...
 Vibrational temperatures:     28.89    30.70    50.56    79.55    84.01
          (Kelvin)             96.63   132.97   228.58   245.02   300.16
                              311.94   319.09   322.82   341.51   351.71
                              366.24   372.45   386.20   399.74   411.90
                              437.52   588.58   610.41   639.04   648.12
                              704.38   808.98   954.33  1015.07  1059.35
                             1115.19  1170.67  1216.83  1255.71  1417.00
                             1444.86  2355.29  2363.88  2376.25  2388.92
                             2408.61  2419.36  2432.94  4849.98  4877.72
                             4960.04  4982.73  5021.29  5025.23  5063.16
                             5087.47  5587.36  5587.93  5592.73  5593.48
                             5595.90  5605.01
 Zero-point correction=                           0.174368 (Hartree/Particle)
 Thermal correction to Energy=                    0.192388
 Thermal correction to Enthalpy=                  0.193332
 Thermal correction to Gibbs Free Energy=         0.127129
 Sum of electronic and zero-point Energies=           -535.129728
 Sum of electronic and thermal Energies=              -535.111708
 Sum of electronic and thermal Enthalpies=            -535.110764
 Sum of electronic and thermal Free Energies=         -535.176967

0 1
            8          1.911789   -1.248910   -1.448148
            1          2.730968   -0.874115   -1.053877
            1          2.063596   -2.192978   -1.547023
            8          3.930843    0.002077   -0.079789
            1          3.371962    0.485958    0.568633
            1          4.503985    0.660651   -0.482686
            8          2.046666    1.210961    1.496046
            1          1.224217    0.826568    1.116936
            1          1.962962    1.151094    2.451621
            8          0.006390   -0.030527    0.118645
            1          0.578420   -0.570841   -0.471110
            1         -0.631277   -0.642439    0.546151
            8         -2.074540   -1.538603    1.101115
            1         -2.857052   -1.048888    0.763997
            1         -2.301052   -1.860377    1.977454
            8         -3.936683    0.078122   -0.108849
            1         -3.298534    0.670240   -0.567566
            1         -4.592173    0.652842    0.296011
            8         -1.878703    1.534815   -1.168342
            1         -1.110445    1.062163   -0.776027
```

```
            1         -1.691678    1.616641   -2.107949

$nbo file=w7_q1_d6 archive nrt plot $end

--------------------------------------------------------------------
%mem=2gb
%nprocshared=8
%chk=w8_q1_t2_d5
#b3lyp/6-311++G** pop=nbo7read

w8_3_pane (w8_q1_t2_d5) (from w2@w6c start), -611.778975556
nu: 23,34,38,...
 Vibrational temperatures:     33.41    49.59    54.46    62.84    89.63
          (Kelvin)             98.15   122.43   136.63   207.89   245.66
                              266.05   282.36   301.27   309.23   317.89
                              328.69   333.90   349.26   376.18   382.50
                              403.70   410.08   446.01   467.49   541.36
                              591.88   624.79   646.07   671.69   816.46
                              832.40   930.74   987.51  1041.06  1090.43
                             1110.15  1167.78  1177.64  1220.82  1249.38
                             1406.41  1574.06  2349.62  2357.04  2364.19
                             2373.97  2402.05  2407.74  2428.16  2507.23
                             4523.50  4768.16  4885.30  4947.49  5015.66
                             5087.37  5142.69  5182.50  5262.52  5275.94
                             5577.48  5584.87  5592.64  5593.70  5594.54
                             5596.56
 Zero-point correction=                           0.200422 (Hartree/Parti$
 Thermal correction to Energy=                    0.220678
 Thermal correction to Enthalpy=                  0.221622
 Thermal correction to Gibbs Free Energy=         0.151112
 Sum of electronic and zero-point Energies=           -611.578553
 Sum of electronic and thermal Energies=              -611.558298
 Sum of electronic and thermal Enthalpies=            -611.557354
 Sum of electronic and thermal Free Energies=         -611.627863

0 1
           8          1.736329    0.965622    1.369414
           1          2.550428    0.577434    0.963085
           1          1.933799    1.122497    2.297875
           8          3.713564   -0.265693    0.005766
           1          3.212105   -0.959323   -0.485992
           1          4.517371   -0.683729    0.326705
           8          2.033750   -2.065766   -1.126656
           1          1.180829   -1.760564   -0.738011
           1          1.880574   -2.160982   -2.071267
           8         -0.106594   -0.913149    0.154090
           1          0.410610   -0.352203    0.759382
           1         -0.558947   -0.257487   -0.449895
           8         -1.366770    0.943616   -1.286463
           1         -2.294772    0.909985   -0.981687
           1         -0.975716    1.775703   -0.963161
           8         -3.853848    0.291825   -0.180135
           1         -3.537569   -0.495155    0.310554
           1         -4.595800   -0.007543   -0.713023
           8         -2.573126   -1.846744    1.044839
           1         -1.637116   -1.638483    0.835273
           1         -2.597876   -2.090790    1.974098
           8          0.268210    2.912680   -0.093139
           1          0.861026    2.331396    0.419032
           1          0.838946    3.510110   -0.584689

$nbo file=w8_q1_t2_d5 archive nrt $end

--------------------------------------------------------------------
%mem=2gb
%nprocshared=8
```

```
%chk=w10_q1_t4_d5
#b3lyp/6-311++G** pop=nbo7read

w10_4_pane (w10_q1_t4_d5), E(RB3LYP) =  -764.725313538
nu: 14,24,30,...
 Vibrational temperatures:     20.51    34.08    43.22    47.38    52.33
          (Kelvin)             71.03    80.41    89.20   119.00   125.94
                              144.27   190.55   211.41   243.38   250.20
                              263.94   284.94   292.90   303.76   307.31
                              313.92   328.61   330.48   356.73   382.67
                              395.25   403.20   418.99   427.08   461.40
                              482.43   535.44   540.33   631.38   654.77
                              673.49   735.09   759.65   819.63   841.53
                              858.09   960.30   991.41  1008.08  1043.13
                             1066.77  1159.51  1183.32  1199.60  1207.70
                             1251.04  1282.16  1415.73  1651.53  2349.11
                             2356.28  2370.50  2371.78  2381.68  2406.14
                             2410.57  2425.53  2471.09  2515.93  4322.20
                             4776.94  4818.58  4910.22  4966.69  4973.54
                             5082.98  5149.20  5186.91  5193.87  5259.35
                             5273.08  5397.59  5576.76  5579.56  5581.21
                             5594.85  5596.18  5597.08  5601.77
 Zero-point correction=                           0.250880 (Hartree/Particle)
 Thermal correction to Energy=                    0.276654
 Thermal correction to Enthalpy=                  0.277598
 Thermal correction to Gibbs Free Energy=         0.192841
 Sum of electronic and zero-point Energies=           -764.474433
 Sum of electronic and thermal Energies=              -764.448660
 Sum of electronic and thermal Enthalpies=            -764.447716
 Sum of electronic and thermal Free Energies=         -764.532473

  0  1
               8          3.150771    0.618464    1.202148
               1          3.763650   -0.001187    0.735041
               1          3.501820    0.746178    2.088833
               8          4.497432   -1.168370   -0.308007
               1          3.753461   -1.657903   -0.732651
               1          5.157846   -1.823917   -0.067316
               8          2.215460   -2.302714   -1.246407
               1          1.557204   -1.774071   -0.738595
               1          1.953088   -2.239339   -2.169693
               8          0.696993   -0.617300    0.319313
               1          1.438373   -0.234282    0.823029
               1          0.378056    0.143499   -0.258433
               8         -0.144492    1.456287   -1.063732
               1         -0.999676    1.698569   -0.642356
               1          0.500910    2.156284   -0.859721
               8         -2.486173    1.665999    0.355398
               1         -2.338889    0.929768    0.967874
               1         -3.320661    1.438063   -0.098520
               8         -1.690436   -0.943842    1.596774
               1         -0.777854   -0.911112    1.218034
               1         -1.600958   -1.170159    2.527422
               8          2.146322    2.887482   -0.209372
               1          2.608436    2.170622    0.262610
               1          2.802701    3.303904   -0.775028
               8         -4.795468    0.524901   -0.806370
               1         -4.586168   -0.405157   -0.587871
               1         -4.992693    0.543226   -1.746850
               8         -3.853287   -1.931097    0.127359
               1         -3.058965   -1.679418    0.639979
               1         -3.636658   -2.752050   -0.322618

$nbo file=w10_q1_t4_d5 archive nrt plot $end

****************************************************************
```

```
%mem=2gb
%nprocshared=8
%chk=w12_q3_t2_d7
#b3lyp/6-311++G** pop=nbo7read

w12_5_pane (w12_q3_t2_d7), E(RB3LYP) =  -917.678777032
nu: 9,19,25,...
 Vibrational temperatures:     13.33    27.82    36.39    44.29    47.12
          (Kelvin)              53.85    61.36    77.69    80.69    89.58
                               109.06   114.91   128.51   134.66   175.72
                               194.72   221.67   245.29   263.00   271.08
                               279.47   295.59   304.63   309.68   324.54
                               330.87   332.66   336.85   346.06   354.28
                               367.77   376.55   399.38   401.78   408.24
                               429.46   445.23   484.11   544.95   584.86
                               603.34   640.40   667.11   704.19   769.75
                               787.25   817.59   838.45   890.41   934.04
                               955.54  1005.11  1028.31  1056.13  1108.64
                              1121.03  1140.10  1159.56  1185.41  1197.25
                              1212.95  1239.63  1283.00  1416.14  1456.15
                              1583.68  2352.91  2358.33  2371.33  2377.11
                              2384.96  2396.03  2400.90  2405.29  2423.22
                              2437.09  2482.06  2504.38  4622.48  4789.29
                              4876.37  4899.69  4953.38  4970.10  4990.08
                              5014.19  5060.29  5081.22  5117.83  5133.96
                              5156.47  5193.88  5235.73  5266.32  5574.08
                              5586.10  5590.50  5592.52  5593.48  5597.15
                              5600.62  5612.38
 Zero-point correction=                           0.302194 (Hartree/Particle)
 Thermal correction to Energy=                    0.333166
 Thermal correction to Enthalpy=                  0.334110
 Thermal correction to Gibbs Free Energy=         0.236318
 Sum of electronic and zero-point Energies=           -917.376583
 Sum of electronic and thermal Energies=              -917.345611
 Sum of electronic and thermal Enthalpies=            -917.344667
 Sum of electronic and thermal Free Energies=         -917.442459

  0  1
               8         -3.075179   -1.265748    0.622555
               1         -3.893211   -0.720308    0.721684
               1         -3.027105   -1.853565    1.383043
               8         -5.083186    0.541513    0.661123
               1         -4.587503    1.362208    0.428911
               1         -5.691692    0.779223    1.366206
               8         -3.402097    2.589294    0.055451
               1         -2.542763    2.106599    0.035095
               1         -3.443189    3.101830   -0.757120
               8         -1.246828    0.889642    0.117494
               1         -1.756721    0.118236    0.429248
               1         -0.916778    0.605188   -0.778069
               8         -0.327931   -0.136649   -2.194657
               1          0.581179   -0.434800   -2.003870
               1         -0.881176   -0.934906   -2.283062
               8          2.227839   -0.612006   -1.039798
               1          1.930608   -0.070145   -0.277342
               1          3.004230   -0.123895   -1.386744
               8          1.319663    0.824380    1.206153
               1          0.372891    0.942730    0.978663
               1          1.374279    0.115289    1.883087
               8         -2.242518   -2.188265   -1.930427
               1         -2.632843   -1.956550   -1.066964
               1         -2.980109   -2.374485   -2.518097
               8          4.337803    1.125249   -1.581749
               1          4.151857    1.720608   -0.826029
               1          4.354196    1.684742   -2.363447
               8          3.455755    2.462992    0.675817
```

```
               1          2.645954    1.989104    0.963306
               1          3.388209    3.362802    1.004387
               8          1.598628   -1.441297    2.750294
               1          1.967661   -2.048903    2.071563
               1          2.169231   -1.516380    3.520204
               8          2.514284   -2.833589    0.558785
               1          2.500504   -2.137787   -0.136919
               1          3.302423   -3.360946    0.403933

$nbo file=w12_q3_t2_d7 archive nrt $end

****************************************************************
%mem=2gb
%nprocshared=8
%chk=w14_q3_t8_d3
#b3lyp/6-311++G** pop=nbo7read

w14_6p (w14_q3_t8_d3), E(RB3LYP) =  -1070.63164768
nu: 9,15,27,....
 Vibrational temperatures:     13.61    21.20    39.21    48.96    54.32
          (Kelvin)             71.89    77.74    88.89   102.06   114.28
                              116.13   124.70   130.26   136.00   160.42
                              180.54   197.07   205.01   230.08   239.29
                              244.87   256.65   267.41   277.17   289.13
                              297.48   303.41   305.23   322.23   342.32
                              349.50   361.15   368.96   390.06   393.04
                              400.81   411.05   424.09   438.55   448.69
                              457.43   501.57   510.46   611.78   628.01
                              634.42   657.96   683.12   697.04   714.87
                              728.88   765.24   784.24   825.09   830.82
                              859.56   874.04   880.10   913.47   946.16
                              956.93   984.84  1001.97  1032.13  1054.82
                             1067.23  1095.21  1136.82  1145.88  1165.68
                             1171.78  1201.93  1231.67  1302.38  1398.32
                             1438.98  1507.38  1657.74  2347.83  2361.36
                             2364.22  2375.92  2376.24  2393.38  2398.53
                             2412.91  2427.33  2440.94  2454.39  2474.55
                             2483.01  2511.33  4351.35  4718.55  4758.49
                             4891.84  4938.42  4965.03  4995.16  5010.39
                             5027.14  5096.99  5150.94  5157.19  5173.51
                             5254.94  5262.76  5272.78  5291.82  5337.03
                             5342.83  5382.68  5388.58  5559.61  5573.77
                             5574.16  5578.46  5584.00  5592.74  5595.44
 Zero-point correction=                           0.356184 (Hartree/Particle)
 Thermal correction to Energy=                    0.390613
 Thermal correction to Enthalpy=                  0.391557
 Thermal correction to Gibbs Free Energy=         0.288126
 Sum of electronic and zero-point Energies=          -1070.275464
 Sum of electronic and thermal Energies=             -1070.241034
 Sum of electronic and thermal Enthalpies=           -1070.240090
 Sum of electronic and thermal Free Energies=        -1070.343522

  0  1
               8         -4.376155   -1.658535   -0.769855
               1         -3.908854   -1.988313    0.016363
               1         -4.772469   -0.818721   -0.478702
               8         -2.626073   -1.992290    1.507595
               1         -2.733221   -1.115370    1.934573
               1         -2.589576   -2.647464    2.211787
               8         -2.897795    0.704252    2.160522
               1         -2.142377    1.045399    1.590457
               1         -2.802761    1.117862    3.024925
               8         -2.421644   -0.978518   -2.491401
               1         -3.201434   -1.316868   -1.981977
               1         -2.452758   -1.381261   -3.364856
               8         -0.558634   -1.244679   -0.373328
```

```
                1          -1.140083   -1.709925    0.252799
                1          -1.029767   -1.262273   -1.228858
                8          -1.026777    1.397476    0.444488
                1          -0.727394    0.509482    0.151061
                1          -1.549191    1.727402   -0.323526
                8           2.172432   -0.681883    0.252529
                1           1.336053   -1.087365   -0.029021
                1           2.751757   -1.388824    0.614292
                8           1.731065    1.903244    1.317517
                1           0.806941    2.020251    1.048136
                1           1.926864    0.974696    1.082571
                8           4.216823    0.584195   -1.324876
                1           3.404662    0.190920   -0.958411
                1           4.224347    1.496830   -0.974515
                8           3.834372    3.066656   -0.043313
                1           3.052297    2.797949    0.488515
                1           3.586540    3.879865   -0.491409
                8           4.088264   -2.477994    1.074668
                1           4.835348   -2.154361    0.517118
                1           4.414666   -2.460667    1.978999
                8           5.962185   -1.289627   -0.499175
                1           5.430426   -0.526574   -0.842722
                1           6.387409   -1.686427   -1.264300
                8          -2.781334    1.783497   -1.640935
                1          -3.631914    1.656787   -1.191922
                1          -2.643701    0.965813   -2.149708
                8          -4.910548    0.978639    0.242086
                1          -4.347198    0.985375    1.044077
                1          -5.734053    1.420323    0.472078

$nbo file=w14_q3_t8_d3 archive $end

****************************************************************
%mem=2gb
%nprocshared=8
%chk=w14_q4_t4_d6
#b3lyp/6-311++G** pop=nbo7read

w14_6_pane (w14_q4_t4_d6), E(RB3LYP) =  -1070.63220856
nu: 16,18,29,...
 Vibrational temperatures:     22.96    26.34    41.39    48.62    53.58
          (Kelvin)             59.27    60.92    71.49    78.82    90.96
                              100.06   106.47   111.36   128.62   134.54
                              136.03   182.71   195.81   214.87   222.45
                              229.05   240.59   260.36   269.78   278.77
                              286.84   293.30   304.78   306.67   313.05
                              318.32   322.74   332.94   341.77   349.92
                              361.82   377.00   384.32   402.31   412.36
                              427.03   434.73   444.43   471.27   592.30
                              594.85   596.00   620.87   701.59   730.00
                              735.60   760.40   777.03   792.25   829.41
                              888.82   904.22   911.60   915.08   929.61
                              998.10  1008.28  1029.39  1037.99  1102.64
                             1112.15  1118.27  1151.44  1163.07  1187.16
                             1209.45  1251.20  1265.96  1299.00  1416.44
                             1438.84  1501.23  1546.31  2353.09  2361.88
                             2363.96  2372.78  2384.44  2391.76  2392.96
                             2397.40  2403.41  2422.34  2423.74  2463.48
                             2480.69  2488.27  4701.40  4772.62  4823.88
                             4870.39  4887.48  4938.16  4941.86  5002.40
                             5036.61  5049.08  5083.45  5094.75  5111.34
                             5144.86  5170.32  5184.26  5212.33  5233.05
                             5309.68  5320.92  5579.74  5580.19  5595.00
                             5598.54  5598.72  5601.48  5602.82  5609.01
 Zero-point correction=                           0.354244 (Hartree/Particle)
 Thermal correction to Energy=                    0.389778
```

```
 Thermal correction to Enthalpy=                  0.390723
 Thermal correction to Gibbs Free Energy=         0.284144
 Sum of electronic and zero-point Energies=          -1070.277965
 Sum of electronic and thermal Energies=             -1070.242430
 Sum of electronic and thermal Enthalpies=           -1070.241486
 Sum of electronic and thermal Free Energies=        -1070.348064

  0  1
               8          2.416491   -2.434217   -0.151069
               1          3.206778   -2.186202   -0.691190
               1          2.420495   -3.392673   -0.068481
               8          4.378606   -1.345355   -1.647472
               1          3.936484   -0.495442   -1.891180
               1          4.838825   -1.652068   -2.433233
               8          2.833601    0.819231   -2.182533
               1          1.962804    0.387494   -2.099444
               1          2.829748    1.503418   -1.491561
               8          0.508695   -0.638253   -1.288117
               1          1.021892   -1.412561   -0.987963
               1          0.470562   -0.058475   -0.494114
               8          0.445683    0.953246    0.988991
               1         -0.499272    0.981372    1.246232
               1          0.941650    0.338295    1.588498
               8         -2.323306    0.729192    1.113925
               1         -2.309012    0.248590    0.255877
               1         -2.905221    1.499632    0.942713
               8         -2.265581   -0.731207   -1.275004
               1         -1.305909   -0.844558   -1.444829
               1         -2.623915   -1.593636   -0.969085
               8          2.182360   -0.703464    2.185652
               1          2.355459   -1.379122    1.507664
               1          2.983040   -0.146766    2.221780
               8         -4.072143    2.641571    0.115232
               1         -4.128095    2.264648   -0.788490
               1         -3.951434    3.588871    0.007700
               8         -3.964733    1.195249   -2.232939
               1         -3.341700    0.461042   -2.040549
               1         -3.904063    1.374937   -3.174504
               8         -3.314153   -2.924122   -0.001718
               1         -3.421884   -2.551329    0.900018
               1         -4.148153   -3.347432   -0.223336
               8         -3.367699   -1.511898    2.368287
               1         -3.041454   -0.629712    2.086579
               1         -4.036409   -1.358121    3.040846
               8          4.182255    1.264794    1.939789
               1          3.717512    1.870312    1.332755
               1          4.586026    1.812135    2.618798
               8          2.424749    2.569482    0.135429
               1          1.599227    2.137863    0.467308
               1          2.227442    3.505503    0.033559

$nbo file=w14_q4_t4_d6 archive nrt plot $end

****************************************************************
%mem=4GB
 %nprocshared=8
 %chk=w16_q8_d8
 #N B3LYP/6-311++G** POP=NBO6Read

 w16_7_pane (w16_q8_d8), E(RB3LYP) =  -1223.5921758
 nu: 20,25,29,...
 Vibrational temperatures:     28.19    35.44    42.25    44.58    47.35
          (Kelvin)             50.72    55.81    60.90    61.91    92.05
                               97.10   102.51   111.57   114.14   118.62
                              135.05   148.16   154.97   164.71   186.55
                              198.38   209.43   217.59   247.40   253.21
```

```
                          270.42   271.56   280.63   282.58   288.97
                          290.76   303.93   307.12   311.47   313.66
                          338.77   340.87   345.09   356.63   361.21
                          372.78   375.25   378.27   383.11   392.72
                          401.57   418.66   435.74   445.53   458.01
                          593.48   615.70   619.83   622.04   635.03
                          637.36   652.05   768.09   776.27   800.14
                          826.39   845.03   883.26   892.22   898.21
                          930.15   952.36   991.87  1002.00  1031.51
                         1038.29  1062.07  1080.48  1092.31  1102.61
                         1112.14  1135.85  1147.48  1168.05  1209.38
                         1221.96  1230.76  1240.96  1252.51  1291.87
                         1352.67  1379.42  1466.12  1487.82  1501.52
                         2353.75  2358.74  2359.43  2363.81  2381.82
                         2384.42  2386.39  2393.79  2400.12  2403.48
                         2425.88  2463.31  2472.89  2473.30  2487.12
                         2500.89  4846.66  4882.88  4926.88  4970.69
                         4977.96  4983.97  4985.47  5005.45  5018.38
                         5028.30  5034.54  5062.80  5079.44  5081.96
                         5098.55  5103.56  5111.67  5127.09  5150.87
                         5153.52  5171.01  5185.24  5190.45  5208.68
                         5588.57  5591.07  5591.38  5596.84  5597.67
                         5598.74  5601.38  5606.55
Zero-point correction=                           0.406965 (Hartree/Particle)
Thermal correction to Energy=                    0.446898
Thermal correction to Enthalpy=                  0.447842
Thermal correction to Gibbs Free Energy=         0.332048
Sum of electronic and zero-point Energies=          -1223.185211
Sum of electronic and thermal Energies=             -1223.145278
Sum of electronic and thermal Enthalpies=           -1223.144334
Sum of electronic and thermal Free Energies=        -1223.260128

  0  1
               8         -1.380573   -1.959443   -0.092851
               1         -1.927699   -2.681500    0.284925
               1         -0.445719   -2.247670   -0.114047
               8         -3.066345   -3.557316    1.369066
               1         -3.227002   -2.946263    2.121017
               1         -2.932670   -4.429768    1.749451
               8         -3.270915   -1.597528    3.305975
               1         -2.660887   -0.911281    2.960528
               1         -4.094773   -1.146158    3.511204
               8         -1.410777   -0.070526    1.928136
               1         -1.433249   -0.724967    1.191050
               1         -1.536977    0.790277    1.481694
               8         -1.347454    2.073678    0.044910
               1         -0.403359    2.326123    0.094299
               1         -1.373418    1.398228   -0.670651
               8          1.456824    2.010462    0.092332
               1          1.484168    1.302456    0.770673
               1          2.155184    2.638358    0.374548
               8          1.409492   -0.119501    1.945933
               1          0.456729   -0.125480    2.174869
               1          1.535141   -0.883155    1.343089
               8         -1.458804    0.122519   -1.926979
               1         -1.660333   -0.710386   -1.456000
               1         -2.244307    0.396597   -2.447271
               8          3.512182    3.361492    1.373638
               1          3.591423    2.702999    2.096510
               1          3.455240    4.220837    1.800839
               8          3.380523    1.325929    3.237248
               1          2.701912    0.706802    2.895292
               1          4.086282    0.784695    3.601441
               8          1.400547   -1.938380   -0.165651
               1          1.414060   -1.229347   -0.844094
               1          2.066866   -2.584170   -0.483504
```

```
               8          1.317283    0.185215   -2.015936
               1          1.497021    0.954171   -1.434819
               1          0.356532    0.212449   -2.204150
               8         -3.659046    1.342174   -2.995638
               1         -3.709232    2.145925   -2.435850
               1         -3.911228    1.602173   -3.885391
               8         -3.473184    3.385464   -1.132581
               1         -2.693293    3.098422   -0.610221
               1         -3.416182    4.341429   -1.210889
               8          3.320858   -3.368334   -1.560275
               1          3.376914   -2.716774   -2.291863
               1          4.226182   -3.540274   -1.286297
               8          3.223542   -1.289522   -3.374715
               1          2.559575   -0.665196   -3.014064
               1          3.073871   -1.330626   -4.323224

 $NBO file=w16_q8_d8 archive nrt memory=10gb nrtres=30000 plot $END

**********************************************************************
%mem=10gb
%nprocshared=20
%chk=w16_q4_t12
#b3lyp/6-311++G** pop=nbo7read

w16_q4_t12 ("dicubane"), E(RB3LYP) =  -1223.58854441
nu: 9,20,33,...
 Vibrational temperatures:     12.23    28.51    47.91    58.20    69.38
          (Kelvin)             72.59   109.32   110.58   111.22   115.93
                              120.46   123.87   131.84   136.89   141.98
                              165.78   174.93   192.54   205.37   219.40
                              222.19   235.58   238.08   241.53   251.27
                              261.48   270.63   284.34   292.49   295.86
                              300.59   312.55   319.11   320.35   347.35
                              358.58   377.53   383.36   392.84   401.53
                              410.79   435.91   437.03   452.14   457.23
                              497.09   506.01   508.04   626.33   632.24
                              655.07   679.72   687.10   702.82   722.06
                              733.57   758.61   770.43   782.09   809.05
                              825.92   842.35   862.26   874.01   876.49
                              907.18   918.83   935.62   958.01   983.36
                              996.38  1006.43  1020.02  1035.89  1055.04
                             1063.23  1084.41  1108.74  1148.17  1149.70
                             1171.59  1175.58  1215.90  1287.59  1321.22
                             1406.65  1439.35  1440.74  1645.64  1652.47
                             2346.56  2360.89  2361.67  2375.68  2378.08
                             2396.20  2401.46  2425.88  2429.06  2440.01
                             2440.84  2452.41  2473.55  2484.00  2492.71
                             2509.69  4349.06  4392.36  4753.72  4756.39
                             4907.78  4912.42  4963.07  5014.26  5032.15
                             5085.50  5105.06  5123.51  5147.33  5156.90
                             5256.05  5268.26  5273.59  5276.05  5282.65
                             5291.61  5322.19  5342.71  5344.90  5369.64
                             5388.98  5392.32  5558.24  5572.02  5573.09
                             5577.31  5579.14  5585.51
 Zero-point correction=                           0.409866 (Hartree/Particle)
 Thermal correction to Energy=                    0.447916
 Thermal correction to Enthalpy=                  0.448860
 Thermal correction to Gibbs Free Energy=         0.339527
 Sum of electronic and zero-point Energies=          -1223.178679
 Sum of electronic and thermal Energies=             -1223.140628
 Sum of electronic and thermal Enthalpies=           -1223.139684
 Sum of electronic and thermal Free Energies=        -1223.249017

  0  1
               8          5.312777    0.993429    0.891361
               1          4.747172    0.646344    1.601650
```

```
                1          5.546172    0.208897    0.364885
                8          3.206968   -0.259911    2.438355
                1          3.130629   -1.109850    1.954029
                1          3.143397   -0.463567    3.376995
                8          3.030001   -2.333862    0.581418
                1          2.359743   -1.899148   -0.027311
                1          2.730383   -3.237523    0.726622
                8          3.648228    2.441736   -0.647746
                1          4.357959    2.045360   -0.080851
                1          3.888663    3.359172   -0.811410
                8          1.468921    1.321412    0.749913
                1          1.965455    0.939207    1.494330
                1          2.104327    1.900753    0.283965
                8          1.441585   -0.907226   -0.970384
                1          1.326711   -0.117413   -0.398878
                1          2.063551   -0.592613   -1.669049
                8         -1.376542    1.328838    0.489138
                1         -0.450846    1.510980    0.723839
                1         -1.850651    1.072952    1.305631
                8         -1.460810   -0.988811   -1.052161
                1         -0.535881   -1.190416   -1.267950
                1         -1.416279   -0.134545   -0.568365
                8         -3.746691    2.287297   -1.000944
                1         -2.855227    2.230637   -0.624301
                1         -3.777630    1.566553   -1.664052
                8         -3.830162   -0.122640   -2.476220
                1         -2.981321   -0.531388   -2.237244
                1         -4.488559   -0.618371   -1.961271
                8         -3.144218    0.292959    2.392111
                1         -3.983202    0.614016    1.939032
                1         -3.256511    0.463368    3.331997
                8         -5.226796    1.065476    0.985791
                1         -4.817802    1.622846    0.282502
                1         -5.542654    0.272545    0.518382
                8          3.501760    0.149044   -2.441533
                1          4.265510   -0.329704   -2.082742
                1          3.566520    1.042989   -2.063885
                8          5.327260   -1.391841   -0.711685
                1          4.627548   -1.916809   -0.270588
                1          6.033051   -2.002610   -0.946447
                8         -5.431536   -1.446527   -0.416450
                1         -4.667305   -1.847853    0.070467
                1         -6.108568   -2.125510   -0.489285
                8         -3.165272   -2.173323    0.868538
                1         -2.485161   -1.945918    0.204469
                1         -3.082981   -1.481771    1.548828

$nbo file=w16_q4_t12 archive nrt plot memory=30gb nrtres=50000 $end

*********************************************************************
```