Electronic Supplementary Information (ESI)

Localized Orbital Locator as Descriptor for Quantification and Digital Presentation of Lone Pairs: Benchmark Calculations of 4-Substituted Pyridines

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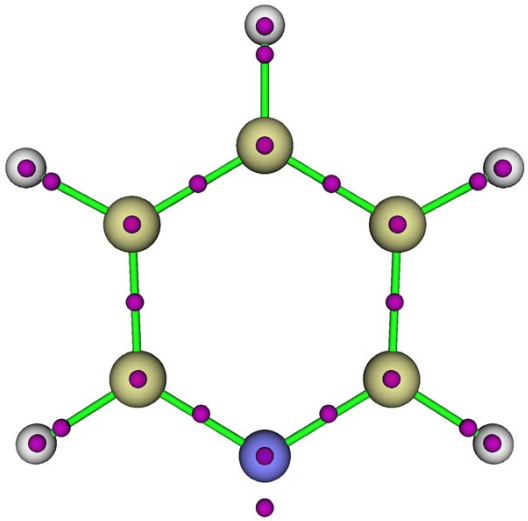

Fig. S1. Location of the (3,–3) critical points in the LOL topology of pyridine. The (3,–3) LOL critical points are indicated by purple circles inside the positions of nuclei, covalent bonds and near the nitrogen atom (bottom).

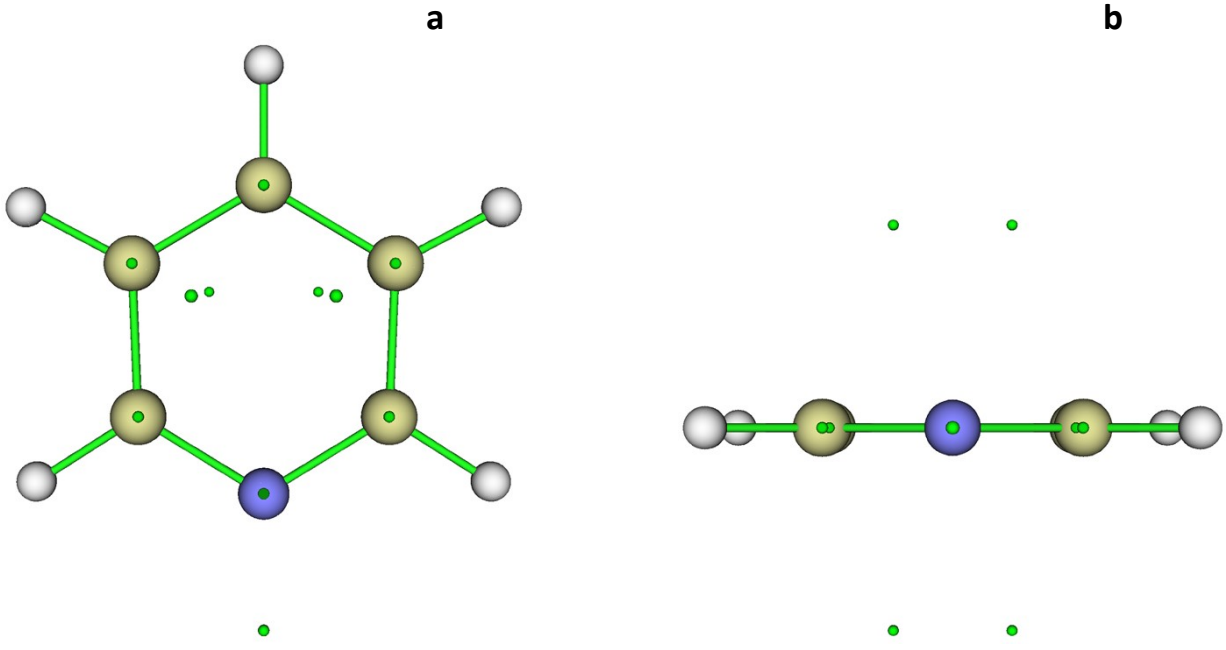

Fig. S2. Location of the (3,+3) critical points in the MESP topology of pyridine: (**a**) in the molecular plane, (**b**) in the plane orthogonal to the molecular plane. The (3,+3) MESP critical points are indicated by small green circles. The (3,+3) critical points in the MESP topology locate inside the position of carbons and nitrogen nuclei, inside the ring and near the nitrogen atom (bottom of part **a**). Part **b** shows that two (3,+3) MESP critical points are located "above" the plane of the pyridine ring and two symmetry-equivalent ones are located "below" the plane of the pyridine ring. Due to the "perspective" mode of the visualization, the symmetry-equivalent critical points in part **a** do not overlap.

Table S1. The *R* substituents and their Hammett constants for the studied 4-substituted pyridines **1a–44a** and benzenes **1b–44b**

N Comp	*R*	σ_p[a]	N Comp	*R*	σ_p[a]
1a,b	H	0	**23a,b**	N=NCN	1.03
2a,b	$N(C_3H_7)_2$	–0.93	**24a,b**	SO_2Cl	1.11
3a,b	$N(CH_3)_2$	–0.83	**25a,b**	SO_2CN	1.26
4a,b	$N(C_2H_5)_2$	–0.72	**26a,b**	$S(CF_3)=NSO_2CF_3$	1.28
5a,b	NH_2	–0.66	**27a,b**	$CH_2CH_2NH_3\oplus$[b]	0.17
6a,b	$NHNH_2$	–0.55	**28a,b**	$CH_2NH_3\oplus$	0.53
7a,b	OH	–0.37	**29a,b**	$NH_3\oplus$	0.60
8a,b	OCH_3	–0.27	**30a,b**	$P(CH_3)_3\oplus$	0.73
9a,b	CH_3	–0.17	**31a,b**	$N(CH_3)_3\oplus$	0.82
10a,b	$OCH=CH_2$	–0.09	**32a,b**	$S(CH_3)_2\oplus$	0.90
11a,b	F	0.06	**33a,b**	$P(C_2H_5)_3\oplus$	0.98
12a,b	SH	0.15	**34a,b**	$N\equiv N\oplus$	1.91
13a,b	Cl	0.23	**35a,b**	$CH_2\oplus$	[c]
14a,b	$CONH_2$	0.36	**36a,b**	$S\ominus$[d]	–1.21
15a,b	CHO	0.42	**37a,b**	$B(OH)\ominus_3$	–0.44
16a,b	CCl_3	0.46	**38a,b**	$NNO_2\ominus$	–0.43
17a,b	CF_3	0.54	**39a,b**	$CO_2\ominus$	0.00
18a,b	CN	0.66	**40a,b**	$OPO_3H\ominus$	0.00
19a,b	NO_2	0.78	**41a,b**	$PO_3H\ominus$	0.26
20a,b	NO	0.91	**42a,b**	$SO_3\ominus$	0.35
21a,b	SO_2F	0.91	**43a,b**	$CF_2OCF_2\ominus$	0.81
22a,b	$C(CN)=C(CN)_2$	0.98	**44a,b**	$CH_2\ominus$	[c]

[a]Taken from ref. 12; [b]symbol "$\oplus$" denotes positive charge; [c]not determined; [d]symbol "$\ominus$" denotes negative charge.

Table S2. The values of the calculated parameters for the (3,–3) critical point in the LOL space topology related to the lone pair of the pyridine ring nitrogen atom for pyridines **1a–44a**: the distance between the (3,–3) LOL critical point and the nitrogen nucleus ($r_{LOL\text{-}LEP}$, in pm), the value of LOL at the (3,–3) LOL-LEP critical point, the value of ρ electron density at the (3,–3) LOL critical point ($\rho_{LOL\text{-}LEP}$, in a.u., 1 a.u. = 6.7483 eÅ^{-3}), the value of total H electron energy density at the (3,–3) LOL-LEP critical point ($H_{LOL-LEP}$, in a.u., 1 a.u. = 1 Hartree) and the complexation energy for pyridines **1a–44a**···HF complexes ($E_{complex}$, in kcal mol^{-1}).

N comp	$r_{LOL\text{-}LEP}$	LOL-LEP	$\rho_{LOL\text{-}LEP}$	$H_{LOL\text{-}LEP}$	$E_{complex}$
1a	46.4597	0.641585	0.459438	–0.867093	–14.29
2a	46.6646	0.636667	0.450923	–0.839884	–16.93
3a	46.6547	0.636808	0.451357	–0.841289	–16.75
4a	46.6587	0.636908	0.451260	–0.840879	–16.92
5a	46.6442	0.636726	0.451553	–0.842231	–16.28
6a	46.6302	0.637389	0.452368	–0.844535	–16.58
7a	46.5576	0.638564	0.454851	–0.852824	–14.85
8a	46.5669	0.638633	0.454709	–0.852101	–15.25
9a	46.5068	0.640456	0.457387	–0.860606	–14.82
10a	46.5350	0.639151	0.455778	–0.855619	–14.64
11a	46.4753	0.640265	0.458041	–0.863124	–13.63
12a	46.4753	0.640265	0.458041	–0.859521	–14.29
13a	46.4473	0.640999	0.459202	–0.866780	–13.42
14a	46.4056	0.642509	0.461214	–0.873012	–13.38
15a	46.3578	0.643459	0.463111	–0.879176	–12.81
16a	46.3965	0.642428	0.461288	–0.873408	–12.96
17a	46.3733	0.642906	0.462310	–0.876651	–12.59
18a	46.3464	0.643176	0.463126	–0.879521	–12.02
19a	46.3171	0.643845	0.464314	–0.883288	–11.59
20a	46.3206	0.644111	0.464485	–0.883688	–12.20
21a	46.2964	0.644131	0.465021	–0.885710	–11.31
22a	46.2897	0.644265	0.465057	–0.885870	–11.13
23a	46.3082	0.644128	0.464721	–0.884595	–11.79
24a	46.3015	0.643973	0.464757	–0.884916	–11.38
25a	46.2703	0.644543	0.465947	–0.888809	–10.81
26a	46.2941	0.643931	0.464886	–0.885425	–11.01
27a	46.2554	0.643710	0.465393	–0.887945	–8.74
28a	46.1459	0.645375	0.469140	–0.900669	–6.77
29a	46.0792	0.645623	0.470816	–0.907031	–5.04
30a	46.1151	0.646017	0.470342	–0.904566	–6.51
31a	46.1418	0.645032	0.468845	–0.899867	–6.23
32a	46.0769	0.646344	0.471496	–0.908701	–5.70
33a	46.1476	0.645563	0.469220	–0.900717	–7.08
34a	45.8562	0.649811	0.479303	–0.935474	–2.78
35a	45.6551	0.655139	0.488324	–0.965473	–1.81
36a	47.0098	0.631585	0.439799	–0.803970	–29.32
37a	46.8511	0.635949	0.446434	–0.824382	–25.97
38a	46.9167	0.633635	0.443303	–0.814673	–26.39
39a	46.7655	0.637707	0.449675	–0.834588	–23.95
40a	46.8289	0.635152	0.446419	–0.824609	–23.68
41a	46.7443	0.637782	0.450201	–0.836399	–22.99
42a	46.7115	0.638255	0.451303	–0.839979	–22.08
43a	46.6802	0.638762	0.452364	–0.843382	–20.22
44a	47.3274	0.623865	0.427575	–0.766651	–40.58

Table S3. The values of the calculated parameters for the (3,+3) critical point in the MESP space topology related to the lone pair of the pyridine ring nitrogen atom for 4-substituted pyridines **1a, 2a, 5a, 7a–9a, 13a, 15a, 18a, 19a, 25a, 27a, 29a, 31a, 32a, 34a–36a, 38a, 39a, 42a–44a**: the distance between the (3,+3) MESP critical point and the nitrogen nucleus (r_{MESP}, in pm) and the value of V_{min} electrostatic potential at the (3,+3) MESP critical point (V_{min}, in a.u.).

N comp	r_{MESP}	V_{min}
1a	124.6114	–0.095069
2a	123.5338	–0.111262
5a	123.5755	–0.110031
7a	124.3652	–0.098916
8a	124.2051	–0.101140
9a	124.3878	–0.098592
13a	125.3142	–0.086467
15a	125.5741	–0.082699
18a	126.1427	–0.075464
19a	126.3727	–0.073476
25a	127.1222	–0.064733
27a	128.7693	–0.002613
29a	133.1380	0.037554
31a	131.6760	0.026088
32a	132.2573	0.030940
34a	137.4626	0.064958
35a	139.2010	0.072679
36a	118.9386	–0.236733
38a	119.6215	–0.222653
39a	120.2031	–0.212224
42a	120.9980	–0.198354
43a	121.2470	–0.195825
44a	117.4219	–0.268136

Table S4. The values of the calculated parameters for the (3,–1) critical point in the ρ topology related to the *para*-C–H bond with respect to the *R* substituents for benzenes **1b–44b**: the distance between the (3,–1) ρ bond critical point and the carbon nucleus (r_{BCP}, in pm), the value of LOL at the (3,–1) ρ bond critical point (LOL-BCP), the value of ρ electron density at the (3,–1) ρ bond critical point (ρ_{BCP}, in a.u., 1 a.u. = 6.7483 eÅ^{-3}), the value of total *H* electron energy density at the (3,–1) ρ bond critical point (H_{BCP}, in a.u., 1 a.u. = 1 Hartree).

N comp	r_{BCP}	LOL-BCP	ρ_{BCP}	H_{BCP}
1b	67.6097	0.890873	0.294441	–0.343588
2b	67.2927	0.885759	0.293333	–0.342102
3b	67.2991	0.885661	0.293290	–0.341953
4b	67.2813	0.885675	0.293272	–0.341951
5b	67.3120	0.885807	0.293465	–0.342328
6b	67.3400	0.886528	0.293586	–0.342452
7b	67.4739	0.888398	0.294161	–0.343540
8b	67.4587	0.888145	0.293930	–0.343023
9b	67.5281	0.889727	0.294230	–0.343385
10b	67.5230	0.889357	0.294503	–0.344217
11b	67.6219	0.890681	0.294814	–0.344686
12b	67.5820	0.890214	0.294651	–0.344396
13b	67.6861	0.891813	0.295107	–0.345221
14b	67.7689	0.893199	0.295178	–0.345115
15b	67.8742	0.894649	0.295681	–0.346025
16b	67.8062	0.893722	0.295449	–0.345782
17b	67.8273	0.894054	0.295625	–0.346073
18b	67.9102	0.895046	0.296029	–0.346910
19b	67.9773	0.896054	0.296283	–0.347399
20b	67.9809	0.895994	0.296093	–0.346821
21b	68.0438	0.896749	0.296380	–0.347564
22b	68.1200	0.897890	0.296852	–0.348664
23b	68.0512	0.896858	0.296466	–0.347686
24b	68.0395	0.896721	0.296440	–0.347718
25b	68.1108	0.897782	0.296858	–0.348594
26b	68.0823	0.897271	0.296728	–0.348408
27b	68.2411	0.898678	0.297231	–0.349772
28b	68.5686	0.902425	0.298250	–0.352031
29b	68.7864	0.904692	0.299070	–0.354190
30b	68.6501	0.903558	0.298576	–0.352748
31b	68.5930	0.902800	0.298544	–0.352985
32b	68.7795	0.904841	0.298933	–0.353639
33b	68.5454	0.902500	0.298354	–0.352261
34b	69.4604	0.912122	0.301019	–0.358745
35b	69.9107	0.917397	0.302112	–0.360899
36b	66.5636	0.873372	0.288358	–0.332559
37b	66.7739	0.877867	0.289139	–0.333427
38b	66.7267	0.876575	0.289367	–0.334255
39b	66.8986	0.880312	0.290086	–0.335078
40b	66.8542	0.879116	0.290483	–0.336337
41b	66.9566	0.881356	0.290668	–0.336255
42b	67.0209	0.882318	0.291050	–0.336951
43b	67.1087	0.883875	0.291610	–0.338008
44b	66.1384	0.863504	0.285805	–0.328828

Figures S3 and S4

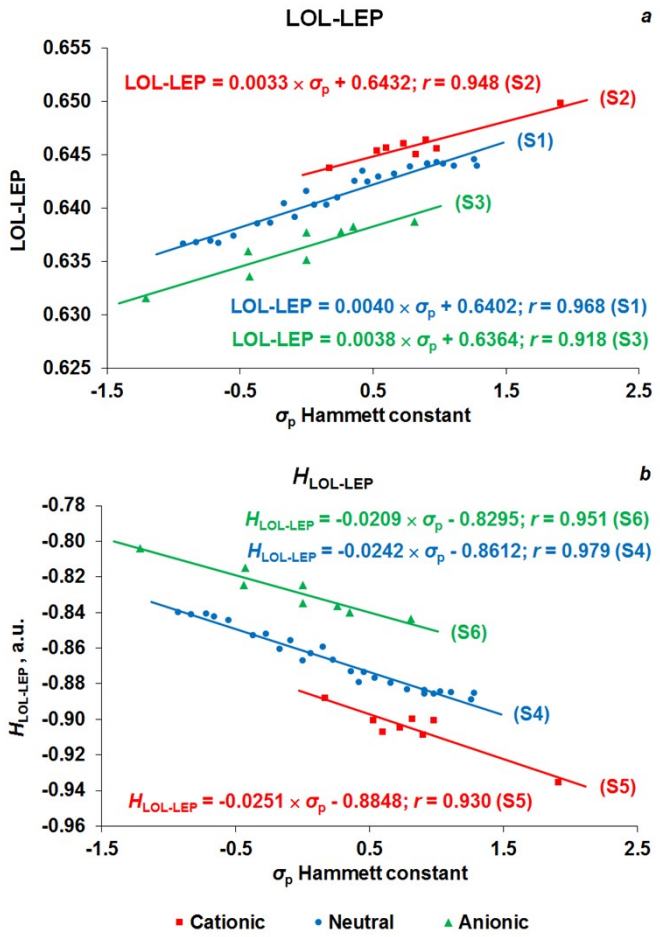

Fig. S3. Dependence of the (3,–3) LOL-LEP critical point parameters on the σ_p values: (**a**) the LOL-LEP values at the critical point; (**b**) the total $H_{LOL\text{-}LEP}$ electron energy density at the critical point.

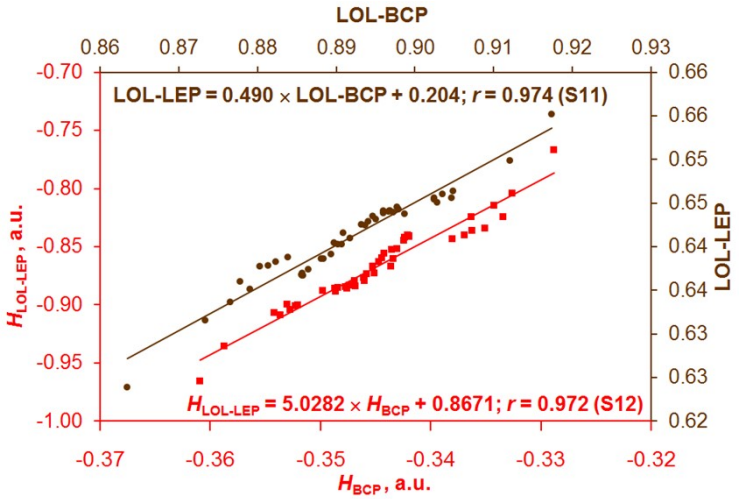

Fig. S4. Dependence of the (3,–3) LOL-LEP critical point parameters in pyridines **1a–44a** on the (3,–1) ρ bond critical point parameters in benzenes **1b–44b**: LOL-LEP values in the (3,–3) LOL critical point *vs* LOL-BCP values in the (3,–1) ρ bond critical point [brown circles, eqn (S11)]; $H_{LOL\text{-}LEP}$ total electron energy values in the (3,–3) LOL-LEP critical point *vs* H_{BCP} total electron energy values in the (3,–1) ρ bond critical point [red squares, eqn (S12)].

Equations (S7) – (S10)

Dependence of pyridines **1a**–**44a**···HF $E_{complex}$ complexation energy on the total $H_{LOL\text{-}LEP}$ electron energy density values at the (3,–3) LOL critical point:

$$\boldsymbol{E_{complex}} = -201.286 \times \boldsymbol{H_{LOL\text{-}LEP}} - 189.056;\ r=0.956 \quad \text{(S7)}$$

Dependence of pyridines **1a**–**44a**···HF $E_{complex}$ complexation energy on the LOL-LEP values at the (3,–3) LOL critical point:

$$\boldsymbol{E_{complex}} = 1355.076 \times \textbf{LOL-LEP} - 883.233;\ r=0.940 \quad \text{(S8)}$$

Dependence of pyridines **1a**–**44a**···HF $E_{complex}$ complexation energy on the $r_{LOL\text{-}LEP}$ distance between the (3,–3) LOL critical point and the nitrogen nucleus in pyridines **1a**–**44a**:

$$\boldsymbol{E_{complex}} = -23.47 \times \boldsymbol{r_{LOL\text{-}LEP}} + 1075.765;\ r=0.970 \quad \text{(S9)}$$

Dependence of pyridines **1a**–**44a**···HF $E_{complex}$ complexation energy on the $\rho_{LOL\text{-}LEP}$ electron density values at the (3,–3) LOL critical point:

$$\boldsymbol{E_{complex}} = 667.8527 \times \boldsymbol{\rho_{LOL\text{-}LEP}} - 321.216;\ r=0.959 \quad \text{(S10)}$$

Details of calculations

Geometry optimization of all compounds and complexes was performed with GAUSSIAN 09 program package[1] at the B3LYP/aug-cc-pVQZ level. All calculated structures are minima on the potential energy surfaces as proved by the absence of imaginary frequencies. Analysis of the electron density using the obtained wave functions were performed with the Multiwfn program[2] in order to locate the (3,–3) and (3,+3) critical points of the Localized Orbital Locator (LOL) and Molecular Electrostatic Potential (MESP) topological spaces, respectively, for 4-substituted pyridines **1a–44a** and (3,–1) bond critical points of the *ρ* electron density topological space for benzenes **1b–44b**. The search for the critical points was carried out from nuclear positions and the batch of points within a sphere with the gradient-norm convergence criterion equal to $1 \cdot 10^{-5}$ and the number of points in the sphere equal to 3000. The Counterpoise Correction approach was applied to estimate the Basis Set Superposition Error (BSSE)[3] for the complexes of pyridines **1a–44a** with HF.

For the detailed consideration of the mathematical apparatus to calculate the localized orbital locator function see ref. 4.

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Cartesian coordinates (Å) and absolute energies (E_0, Hartree) for B3LYP/aug-cc-pVQZ optimized geometries of studied 4-substituted pyridines 1a–44a

1a

E_0=-248.3930965 Hartree

1	6	0.000000	1.139406	0.720019
2	6	0.000000	1.193322	-0.669674
3	6	0.000000	0.000000	-1.378708
4	6	0.000000	-1.193322	-0.669674
5	6	0.000000	-1.139406	0.720019
6	7	0.000000	0.000000	1.411176
7	1	0.000000	2.053325	1.302608
8	1	0.000000	2.147307	-1.177600
9	1	0.000000	0.000000	-2.460136
10	1	0.000000	-2.147307	-1.177600
11	1	0.000000	-2.053325	1.302608

2a

E_0=-539.7395389 Hartree

1	6	-0.342349	1.072532	2.987306
2	6	-0.362464	1.130755	1.604568
3	6	0.000000	0.000000	0.840898
4	6	0.362464	-1.130755	1.604568
5	6	0.342349	-1.072532	2.987306
6	7	0.000000	0.000000	3.702084
7	7	0.000000	0.000000	-0.542440
8	6	0.000000	1.298602	-1.246014
9	6	0.000000	-1.298602	-1.246014
10	1	-0.633428	1.950911	3.552941
11	1	-0.693543	2.046165	1.142505
12	1	0.693543	-2.046165	1.142505
13	6	0.997761	1.385339	-2.406697
14	6	-1.397182	1.782354	-1.665053
15	1	0.371721	2.007769	-0.510401
16	6	1.397182	-1.782354	-1.665053
17	1	-0.371721	-2.007769	-0.510401
18	6	-0.997761	-1.385339	-2.406697
19	1	1.024336	2.414908	-2.764169
20	1	2.002164	1.118769	-2.083272
21	1	0.728654	0.758143	-3.253268
22	1	-1.352343	2.832837	-1.956886
23	1	-1.788331	1.221357	-2.510967
24	1	-2.104979	1.690551	-0.842590
25	1	1.352343	-2.832837	-1.956886
26	1	1.788331	-1.221357	-2.510967
27	1	2.104979	-1.690551	-0.842590
28	1	-1.024336	-2.414908	-2.764169
29	1	-2.002164	-1.118769	-2.083272
30	1	-0.728654	-0.758143	-3.253268
31	1	0.633428	-1.950911	3.552941

3a

E_0=-382.4244943 Hartree

1	6	1.129504	-1.952292	0.000000
2	6	1.193549	-0.569823	0.000000
3	6	0.000000	0.179078	0.000000
4	6	-1.193659	-0.569653	0.000000
5	6	-1.129780	-1.952160	0.000000
6	7	-0.000152	-2.662491	0.000000
7	1	2.051708	-2.522741	0.000000
8	1	2.159508	-0.090811	0.000000
9	7	0.000096	1.548497	0.000000
10	1	-2.159551	-0.090550	0.000000
11	1	-2.051941	-2.522644	0.000000
12	6	1.254068	2.276990	0.000000
13	6	-1.253771	2.277287	0.000000
14	1	1.047682	3.342742	0.000000
15	1	1.855879	2.050413	0.884522
16	1	1.855879	2.050413	-0.884522
17	1	-1.047113	3.342986	0.000000
18	1	-1.855563	2.050796	-0.884531
19	1	-1.855563	2.050796	0.884531

4a

E_0=-461.0701289 Hartree

1	6	0.000000	1.125483	2.697040
2	6	0.000000	1.189538	1.313887
3	6	0.000000	-0.000000	0.551114
4	6	-0.000000	-1.189538	1.313887
5	6	-0.000000	-1.125483	2.697040
6	7	0.000000	-0.000000	3.411229
7	7	-0.000000	0.000000	-0.829730
8	6	0.000000	1.329106	-1.461119
9	6	-0.000000	-1.329106	-1.461119
10	1	0.000000	2.050852	3.262653
11	1	0.000000	2.162874	0.855155
12	1	-0.000000	-2.162874	0.855155
13	6	0.000000	1.477665	-2.975675
14	1	-0.873382	1.871515	-1.086739
15	1	-0.873382	-1.871515	-1.086739
16	6	-0.000000	-1.477665	-2.975675
17	1	0.000000	2.548326	-3.181472
18	1	0.884040	1.059022	-3.448123
19	1	-0.884040	1.059022	-3.448123
20	1	-0.000000	-2.548326	-3.181472
21	1	-0.884040	-1.059022	-3.448123
22	1	0.884040	-1.059022	-3.448123
23	1	0.873382	1.871515	-1.086739
24	1	0.873382	-1.871515	-1.086739
25	1	-0.000000	-2.050852	3.262653

5a

E_0=-303.7832072 Hartree

1	6	0.000000	1.132321	-1.187611
2	6	0.000000	1.193388	0.195504
3	6	0.000000	0.000000	0.929743
4	6	0.000000	-1.193388	0.195504
5	6	0.000000	-1.132321	-1.187611
6	7	0.000000	0.000000	-1.893727
7	7	0.000000	0.000000	2.297022
8	1	0.000000	2.053076	-1.760059
9	1	0.000000	2.151432	0.698426
10	1	0.000000	-2.151432	0.698426
11	1	0.000000	-2.053076	-1.760059
12	1	0.000000	0.858041	2.813516
13	1	0.000000	-0.858041	2.813516

6a

E_0=-359.1240289 Hartree

1	6	1.857142	-0.933161	0.042885
2	6	0.516138	-1.269778	-0.000103
3	6	-0.440277	-0.247528	-0.055128
4	6	0.028396	1.068703	-0.056510
5	6	1.397295	1.284117	-0.009652
6	7	2.318036	0.320107	0.039474
7	7	-1.782305	-0.569150	-0.147450
8	1	2.603725	-1.718069	0.084979
9	1	0.216242	-2.309962	0.004260
10	1	-0.663638	1.894318	-0.093735
11	1	1.773144	2.301120	-0.010558
12	1	-2.021758	-1.512244	0.118931
13	7	-2.742608	0.423390	0.095378
14	1	-3.490972	0.348056	-0.578634
15	1	-3.120770	0.362230	1.033994

7a

E_0=-323.6564319 Hartree

1	6	1.152030	-1.156558	0.000000
2	6	1.202153	0.228377	0.000000
3	6	0.000000	0.928565	0.000000
4	6	-1.189717	0.207060	0.000000
5	6	-1.118489	-1.179642	0.000000
6	7	0.021805	-1.867541	0.000000
7	8	0.047497	2.284852	0.000000
8	1	2.074137	-1.725532	0.000000
9	1	2.142668	0.759241	0.000000
10	1	-2.149407	0.708220	0.000000
11	1	-2.032226	-1.762358	0.000000
12	1	-0.843646	2.647589	0.000000

8a

E_0=-362.9727368 Hartree

1	6	-1.759879	-1.092259	0.000000
2	6	-1.365568	0.232507	0.000000
3	6	0.000000	0.523401	0.000000
4	6	0.899147	-0.540809	0.000000
5	6	0.383655	-1.833722	0.000000
6	7	-0.912480	-2.127640	0.000000
7	8	0.344319	1.830875	0.000000
8	1	-2.814986	-1.338701	0.000000
9	1	-2.087597	1.035824	0.000000
10	1	1.967124	-0.391612	0.000000
11	1	1.066736	-2.675522	0.000000
12	6	1.723894	2.173160	0.000000
13	1	1.761880	3.257980	0.000000
14	1	2.226079	1.792424	0.891391
15	1	2.226079	1.792424	-0.891391

9a

E_0=-287.7289135 Hartree

1	6	-1.130268	-1.220331	0.000000
2	6	-1.185347	0.165691	0.000000
3	6	0.000000	0.900966	0.000000
4	6	1.186884	0.174601	0.000000
5	6	1.140599	-1.215092	0.000000
6	7	0.008675	-1.915809	0.000000
7	6	-0.012563	2.404514	0.000000
8	1	-2.045183	-1.801337	0.000000
9	1	-2.144982	0.666015	0.000000
10	1	2.142885	0.681112	0.000000
11	1	2.060215	-1.788942	0.000000
12	1	-0.533128	2.790245	0.877710
13	1	0.996759	2.811236	0.000000
14	1	-0.533128	2.790245	-0.877710

10a

E_0=-401.0712275 Hartree

1	6	-0.301993	-1.150808	0.000000
2	6	-1.643902	-1.518462	0.000000
3	7	-2.661410	-0.662632	0.000000
4	6	-2.349178	0.636280	0.000000
5	6	-1.052847	1.120209	0.000000
6	6	0.000000	0.207887	-0.000000
7	8	1.249300	0.752387	-0.000000
8	6	2.385585	-0.008751	-0.000000
9	6	3.579407	0.563179	-0.000000
10	1	0.451858	-1.920755	-0.000000
11	1	-1.901969	-2.571105	0.000000
12	1	-3.181452	1.329852	0.000000
13	1	-0.846686	2.180200	0.000000
14	1	2.252694	-1.079164	-0.000000
15	1	4.463408	-0.053593	-0.000000
16	1	3.695190	1.636695	-0.000000

11a

E_0=-347.6785915 Hartree

1	6	0.000000	1.138712	-1.152548
2	6	0.000000	1.201968	0.236021
3	6	0.000000	0.000000	0.917212
4	6	0.000000	-1.201968	0.236021
5	6	0.000000	-1.138712	-1.152548
6	7	0.000000	0.000000	-1.845105
7	1	0.000000	2.053969	-1.731902
8	1	0.000000	2.142695	0.765659
9	9	0.000000	0.000000	2.260364
10	1	0.000000	-2.142695	0.765659
11	1	0.000000	-2.053969	-1.731902

12a

E_0=-646.6222967 Hartree

1	6	-1.133651	-1.605384	0.000000
2	6	-1.193274	-0.219074	0.000000
3	6	0.000000	0.501618	0.000000
4	6	1.194063	-0.216758	0.000000
5	6	1.136270	-1.603291	0.000000
6	7	0.002017	-2.303312	0.000000
7	1	-2.051518	-2.181316	0.000000
8	1	-2.150619	0.282844	0.000000
9	16	-0.080171	2.267578	0.000000
10	1	2.151901	0.283658	0.000000
11	1	2.055185	-2.177868	0.000000
12	1	1.243223	2.491941	0.000000

13a

E_0=-708.0290161 Hartree

1	6	0.000000	1.137200	-1.587254
2	6	0.000000	1.198638	-0.198050
3	6	0.000000	0.000000	0.497877
4	6	0.000000	-1.198638	-0.198050
5	6	0.000000	-1.137200	-1.587254
6	7	0.000000	0.000000	-2.280299
7	1	0.000000	2.054260	-2.164193
8	1	0.000000	2.146025	0.318868
9	17	0.000000	0.000000	2.240537
10	1	0.000000	-2.146025	0.318868
11	1	0.000000	-2.054260	-2.164193

14a

E_0=-417.1769019 Hartree

1	6	-1.222807	-1.849194	0.000000
2	6	-1.218553	-0.461553	0.000000
3	6	0.000000	0.210518	0.000000
4	6	1.160886	-0.559294	0.000000
5	6	1.050869	-1.944654	0.000000
6	7	-0.113553	-2.589738	0.000000
7	1	-2.160354	-2.391728	0.000000
8	1	-2.136911	0.105658	0.000000
9	6	-0.035262	1.718415	0.000000
10	1	2.149260	-0.121992	0.000000
11	1	1.942314	-2.560448	0.000000
12	8	-1.091063	2.323418	0.000000
13	7	1.160812	2.365550	0.000000
14	1	1.148164	3.370082	0.000000
15	1	2.044416	1.894969	0.000000

15a

E_0=-361.7649722 Hartree

1	6	-0.677899	-1.728014	0.000000
2	6	-1.023022	-0.385529	0.000000
3	6	0.000000	0.560632	0.000000
4	6	1.317315	0.114646	0.000000
5	6	1.557577	-1.255041	0.000000
6	7	0.585389	-2.164169	0.000000
7	1	-1.445614	-2.491947	0.000000
8	1	-2.055419	-0.067437	0.000000
9	6	-0.292270	2.016618	0.000000
10	1	2.140495	0.817163	0.000000
11	1	2.571906	-1.635244	0.000000
12	8	-1.400437	2.489936	0.000000
13	1	0.604196	2.667286	0.000000

16a

E_0=-1666.6075331 Hartree

1	6	-1.572586	2.463285	0.000000
2	6	-1.365396	1.094107	0.000000
3	6	-0.056853	0.611452	0.000000
4	6	0.975986	1.537042	0.000000
5	6	0.657521	2.893198	0.000000
6	7	-0.584981	3.361543	0.000000
7	1	-2.581168	2.857610	0.000000
8	1	-2.208410	0.420002	0.000000
9	6	0.176044	-0.889877	0.000000
10	1	2.008212	1.228281	0.000000
11	1	1.451776	3.629868	0.000000
12	17	-0.584981	-1.620731	1.462633
13	17	1.907383	-1.342173	0.000000
14	17	-0.584981	-1.620731	-1.462633

17a

E_0=-585.5959478 Hartree

1	6	-1.752092	1.679875	0.000000
2	6	-1.361085	0.348577	0.000000
3	6	-0.000511	0.063489	0.000000
4	6	0.905918	1.112005	0.000000
5	6	0.406347	2.410754	0.000000
6	7	-0.892194	2.699259	0.000000
7	1	-2.803733	1.938437	0.000000
8	1	-2.098903	-0.440402	0.000000
9	6	0.457094	-1.373722	0.000000
10	1	1.969656	0.931780	0.000000
11	1	1.086977	3.253341	0.000000
12	9	-0.000511	-2.036123	1.082902
13	9	1.796282	-1.485958	0.000000
14	9	-0.000511	-2.036123	-1.082902

18a

E_0=-340.6697145 Hartree

1	6	0.000000	1.140659	-1.499569
2	6	0.000000	1.200303	-0.112891
3	6	0.000000	0.000000	0.598273
4	6	0.000000	-1.200303	-0.112891
5	6	0.000000	-1.140659	-1.499569
6	7	0.000000	0.000000	-2.188298
7	1	0.000000	2.054036	-2.081443
8	1	0.000000	2.149126	0.402004
9	6	0.000000	0.000000	2.029262
10	1	0.000000	-2.149126	0.402004
11	1	0.000000	-2.054036	-2.081443
12	7	0.000000	0.000000	3.180183

19a

E_0=-452.9858707 Hartree

1	6	0.000000	1.141880	1.838025
2	6	0.000000	1.203618	0.449107
3	6	0.000000	0.000000	-0.231195
4	6	0.000000	-1.203618	0.449107
5	6	0.000000	-1.141880	1.838025
6	7	0.000000	0.000000	2.524383
7	7	0.000000	0.000000	-1.714632
8	8	0.000000	1.082302	-2.275236
9	8	0.000000	-1.082302	-2.275236
10	1	0.000000	2.054296	2.420770
11	1	0.000000	2.141380	-0.082220
12	1	0.000000	-2.141380	-0.082220
13	1	0.000000	-2.054296	2.420770

20a

E_0=-377.7361916 Hartree

1	6	1.556487	-1.216299	0.000000
2	6	1.318641	0.154659	0.000000
3	6	0.000000	0.583301	0.000000
4	6	-1.033144	-0.348224	0.000000
5	6	-0.683555	-1.688826	0.000000
6	7	0.581918	-2.122384	0.000000
7	1	2.569614	-1.598833	0.000000
8	1	2.123744	0.875526	0.000000
9	7	-0.199348	2.020953	0.000000
10	1	-2.063579	-0.025711	0.000000
11	1	-1.448691	-2.455214	0.000000
12	8	-1.351207	2.375823	0.000000

21a

E_0=-896.4042951 Hartree

1	6	2.381608	-1.142573	-0.005742
2	6	0.993295	-1.204265	0.043262
3	6	0.307032	0.000115	0.063097
4	6	0.993277	1.204280	0.043377
5	6	2.381825	1.142385	-0.005590
6	7	3.065507	0.000008	-0.031463
7	16	-1.469669	0.000050	0.135147
8	1	2.964840	-2.054629	-0.021721
9	1	0.471653	-2.148425	0.074919
10	1	0.471982	2.148629	0.075131
11	1	2.964894	2.054574	-0.021576
12	8	-1.946815	-1.252932	0.625234
13	8	-1.946904	1.252196	0.626069
14	9	-1.778854	0.000581	-1.432191

22a

E_0=-602.6376973 Hartree

1	6	-2.645133	-1.913430	0.000000
2	6	-2.035223	-0.667663	0.000000
3	6	-0.636048	-0.585933	0.000000
4	6	0.069372	-1.796212	0.000000
5	6	-0.641460	-2.987392	0.000000
6	7	-1.971964	-3.061572	0.000000
7	6	0.000000	0.744260	0.000000
8	6	-0.896198	1.863527	0.000000
9	1	-3.725424	-1.985874	0.000000
10	1	-2.646013	0.222168	0.000000
11	1	1.143957	-1.838799	0.000000
12	7	-1.637348	2.743573	0.000000
13	6	1.333592	1.056086	0.000000
14	6	1.771054	2.416234	0.000000
15	6	2.402473	0.113210	0.000000
16	7	3.306808	-0.599462	0.000000
17	7	2.159651	3.499659	0.000000
18	1	-0.107129	-3.929006	0.000000

23a

E_0=-450.1497919 Hartree

1	6	0.711792	2.643595	0.000000
2	6	-0.325068	1.717543	0.000000
3	6	0.000000	0.364594	0.000000
4	6	1.344940	-0.012438	0.000000
5	6	2.295248	0.994310	0.000000
6	7	1.996470	2.298089	0.000000
7	7	-1.097721	-0.525421	0.000000
8	7	-0.784948	-1.740358	0.000000
9	1	0.497495	3.704988	0.000000
10	1	-1.360877	2.023182	0.000000
11	1	1.630091	-1.052873	0.000000
12	6	-1.822341	-2.605011	0.000000
13	1	3.349547	0.747525	0.000000
14	7	-2.591471	-3.466364	0.000000

24a

E_0=-1256.7454968 Hartree

1	6	-0.281349	2.565272	1.142514
2	6	-0.281349	1.175866	1.204905
3	6	-0.279145	0.492656	0.000000
4	6	-0.281349	1.175866	-1.204905
5	6	-0.281349	2.565272	-1.142514
6	7	-0.278753	3.250005	0.000000
7	16	-0.309231	-1.296153	0.000000
8	8	-0.821857	-1.764817	1.254638
9	1	-0.285672	3.148431	2.054772
10	1	-0.292514	0.653619	2.149114
11	1	-0.292514	0.653619	-2.149114
12	8	-0.821857	-1.764817	-1.254638
13	17	1.743077	-1.719306	0.000000
14	1	-0.285672	3.148431	-2.054772

25a

E_0=-889.3493411 Hartree

1	6	-0.250673	2.494222	1.143120
2	6	-0.250673	1.104437	1.205538
3	6	-0.248495	0.418774	0.000000
4	6	-0.250673	1.104437	-1.205538
5	6	-0.250673	2.494222	-1.143120
6	7	-0.248500	3.176601	0.000000
7	1	-0.255690	3.078056	2.054797
8	1	-0.264818	0.581857	2.149823
9	16	-0.270481	-1.362679	0.000000
10	1	-0.264818	0.581857	-2.149823
11	1	-0.255690	3.078056	-2.054797
12	8	-0.771146	-1.837325	1.258341
13	8	-0.771146	-1.837325	-1.258341
14	6	1.467337	-1.721444	0.000000
15	7	2.592806	-1.960550	0.000000

26a

E_0=-1925.0293196 Hartree

1	6	-4.415748	-0.636211	-0.805356
2	6	-3.178093	-0.066201	-1.084303
3	6	-2.135894	-0.363361	-0.218426
4	6	-2.328773	-1.211963	0.856985
5	6	-3.610293	-1.725279	1.033543
6	7	-4.633393	-1.446445	0.228184
7	16	-0.494191	0.304781	-0.567066
8	1	-5.262066	-0.435360	-1.450161
9	1	-3.047024	0.572956	-1.945276
10	1	-1.514550	-1.469210	1.517691
11	6	-0.748066	2.010828	0.222194
12	9	-1.675478	2.662501	-0.481720
13	9	0.402447	2.660425	0.149991
14	9	-1.133151	1.924365	1.484273
15	7	0.484454	-0.387583	0.501206
16	16	1.740860	-1.220396	-0.136080
17	8	2.052363	-2.295946	0.759342
18	8	1.597956	-1.440072	-1.556586
19	6	3.162856	-0.004475	0.037715
20	9	4.278272	-0.568922	-0.415378
21	9	2.910979	1.096054	-0.681842
22	9	3.334311	0.345554	1.309638
23	1	-3.815402	-2.392022	1.861532

27a

E_0=-382.7884699 Hartree

1	6	-0.410536	-2.187744	1.139379
2	6	-0.410536	-0.797843	1.192506
3	6	-0.407893	-0.081622	0.000000
4	6	-0.410536	-0.797843	-1.192506
5	6	-0.410536	-2.187744	-1.139379
6	7	-0.407335	-2.875280	0.000000
7	1	-0.418658	-2.768756	2.053165
8	1	-0.429605	-0.296498	2.151517
9	6	-0.374405	1.431717	0.000000
10	1	-0.429605	-0.296498	-2.151517
11	1	-0.418658	-2.768756	-2.053165
12	6	1.068744	1.923842	0.000000
13	7	1.122115	3.450194	0.000000
14	1	2.083928	3.794397	0.000000
15	1	0.653468	3.832928	-0.823344
16	1	0.653468	3.832928	0.823344
17	1	-0.894128	1.813246	-0.881895
18	1	-0.894128	1.813246	0.881895
19	1	1.612326	1.601392	0.884489
20	1	1.612326	1.601392	-0.884489

28a

E_0=-343.4554193 Hartree

1	6	-0.264024	-1.659666	1.142504
2	6	-0.264024	-0.269266	1.197397
3	6	-0.257262	0.441725	0.000000
4	6	-0.264024	-0.269266	-1.197397
5	6	-0.264024	-1.659666	-1.142504
6	7	-0.259650	-2.342117	0.000000
7	1	-0.275255	-2.243568	2.054037
8	1	-0.292306	0.233544	2.155628
9	6	-0.216891	1.940068	0.000000
10	1	-0.292306	0.233544	-2.155628
11	1	-0.275255	-2.243568	-2.054037
12	7	1.242337	2.421334	0.000000
13	1	1.311043	3.441260	0.000000
14	1	-0.671191	2.373712	-0.886933
15	1	-0.671191	2.373712	0.886933
16	1	1.734571	2.066632	0.822382
17	1	1.734571	2.066632	-0.822382

29a

E_0=-304.1138383 Hartree

1	6	-1.144259	-1.246858	0.000000
2	6	-1.208105	0.145782	0.000000
3	6	0.000000	0.812668	0.000000
4	6	1.206256	0.145057	0.000000
5	6	1.143866	-1.248804	0.000000
6	7	0.000150	-1.924163	0.000000
7	1	-2.056111	-1.829576	0.000000
8	1	-2.161578	0.656056	0.000000
9	7	0.000700	2.305866	0.000000
10	1	2.159857	0.655854	0.000000
11	1	2.055777	-1.831612	0.000000
12	1	-0.473384	2.680675	0.826223
13	1	0.956327	2.668946	0.000000
14	1	-0.473384	2.680675	-0.826223

30a

E_0=-708.7705021 Hartree

1	6	0.033524	2.518367	1.141291
2	6	0.033524	1.128177	1.199233
3	6	0.034591	0.416109	0.000000
4	6	0.033524	1.128177	-1.199233
5	6	0.033524	2.518367	-1.141291
6	7	0.033598	3.200884	0.000000
7	1	0.035933	3.100442	2.054155
8	1	0.037435	0.639926	2.162717
9	15	-0.018969	-1.387134	0.000000
10	1	0.037435	0.639926	-2.162717
11	1	0.035933	3.100442	-2.054155
12	6	-1.736816	-1.947106	0.000000
13	6	0.809070	-2.035400	-1.466321
14	6	0.809070	-2.035400	1.466321
15	1	-1.772316	-3.035789	0.000000
16	1	-2.244991	-1.569691	0.885651
17	1	-2.244991	-1.569691	-0.885651
18	1	0.799296	-3.123735	-1.426452
19	1	0.293644	-1.716059	-2.369511
20	1	1.839484	-1.686442	-1.497136
21	1	0.799296	-3.123735	1.426452
22	1	1.839484	-1.686442	1.497136
23	1	0.293644	-1.716059	2.369511

31a

E_0=-422.0998214 Hartree

1	6	1.444721	1.993406	0.000000
2	6	1.282188	0.612647	0.000000
3	6	-0.011465	0.110601	0.000000
4	6	-1.082311	0.985923	0.000000
5	6	-0.800231	2.353439	0.000000
6	7	0.428373	2.851652	0.000000
7	1	2.440414	2.417802	0.000000
8	1	2.158287	-0.017411	0.000000
9	7	-0.210077	-1.383714	0.000000
10	1	-2.111371	0.669564	0.000000
11	1	-1.615535	3.065670	0.000000
12	6	0.428373	-1.978614	1.235908
13	6	-1.663234	-1.776814	0.000000
14	6	0.428373	-1.978614	-1.235908
15	1	0.266380	-3.052097	1.221097
16	1	1.489864	-1.763652	1.231936
17	1	-0.036913	-1.535953	2.110637
18	1	-1.711166	-2.860774	0.000000
19	1	-2.142927	-1.389428	0.891989
20	1	-2.142927	-1.389428	-0.891989
21	1	0.266380	-3.052097	-1.221097
22	1	-0.036913	-1.535953	-2.110637
23	1	1.489864	-1.763652	-1.231936

32a

E_0=-725.6175609 Hartree

1	6	0.811682	2.291531	0.000000
2	6	0.949630	0.907570	0.000000
3	6	-0.219157	0.157217	0.000000
4	6	-1.459673	0.776765	0.000000
5	6	-1.472784	2.172434	0.000000
6	7	-0.368577	2.909207	0.000000
7	1	1.690039	2.924135	0.000000
8	1	1.934167	0.463527	0.000000
9	16	-0.223863	-1.636025	0.000000
10	1	-2.382604	0.215461	0.000000
11	1	-2.415103	2.705087	0.000000
12	6	0.811682	-2.096726	1.414092
13	6	0.811682	-2.096726	-1.414092
14	1	0.887939	-3.181504	1.406925
15	1	1.791583	-1.635218	1.341392
16	1	0.288959	-1.767602	2.307967
17	1	0.887939	-3.181504	-1.406925
18	1	0.288959	-1.767602	-2.307967
19	1	1.791583	-1.635218	-1.341392

33a

E_0=-826.753753 Hartree

1	6	-0.021574	-3.295981	1.139051
2	6	-0.036053	-1.906060	1.195833
3	6	-0.046489	-1.187314	0.000000
4	6	-0.036053	-1.906060	-1.195833
5	6	-0.021574	-3.295981	-1.139051
6	7	-0.014978	-3.981704	0.000000
7	1	-0.016347	-3.875984	2.053331
8	1	-0.041834	-1.424694	2.161975
9	15	-0.002614	0.630662	0.000000
10	1	-0.041834	-1.424694	-2.161975
11	1	-0.016347	-3.875984	-2.053331
12	6	1.776079	1.059465	0.000000
13	6	-0.843584	1.174996	-1.528414
14	6	2.204128	2.530084	0.000000
15	1	2.182271	0.541084	0.871471
16	1	2.182271	0.541084	-0.871471
17	6	-1.078754	2.671867	-1.765284
18	1	-0.240076	0.765787	-2.340163
19	1	-1.790822	0.632756	-1.545285
20	6	-0.843584	1.174996	1.528414
21	6	-1.078754	2.671867	1.765284
22	1	3.291901	2.571954	0.000000
23	1	1.858953	3.061784	-0.882602
24	1	1.858953	3.061784	0.882602
25	1	-1.495228	2.798272	-2.762891
26	1	-1.789911	3.092128	-1.061107
27	1	-0.162299	3.253247	-1.718077
28	1	-1.790822	0.632756	1.545285
29	1	-0.240076	0.765787	2.340163
30	1	-1.495228	2.798272	2.762891
31	1	-0.162299	3.253247	1.718077
32	1	-1.789911	3.092128	1.061107

34a

E_0=-357.0096577 Hartree

1	6	-0.000000	1.152957	-1.504875
2	6	-0.000000	1.228092	-0.117028
3	6	0.000000	-0.000000	0.543558
4	6	-0.000000	-1.228092	-0.117028
5	6	-0.000000	-1.152957	-1.504875
6	7	0.000000	0.000000	-2.171864
7	1	-0.000000	2.059422	-2.095829
8	1	-0.000000	2.169889	0.410505
9	7	0.000000	-0.000000	1.935019
10	1	-0.000000	-2.169889	0.410505
11	1	-0.000000	-2.059422	-2.095829
12	7	0.000000	-0.000000	3.032865

35a

E_0=-286.7837174 Hartree

1	6	-1.164311	-1.145636	0.000000
2	6	-1.228710	0.232807	0.000000
3	6	0.000000	0.963844	0.000000
4	6	1.228533	0.233253	0.000000
5	6	1.164770	-1.145107	0.000000
6	7	0.000313	-1.807156	0.000000
7	1	-2.060700	-1.750890	0.000000
8	1	-2.176506	0.752780	0.000000
9	1	2.061433	-1.749927	0.000000
10	6	-0.000499	2.335182	0.000000
11	1	2.176289	0.753374	0.000000
12	1	-0.925714	2.898994	0.000000
13	1	0.924307	2.899695	0.000000

36a

E_0=-646.0856235 Hartree

1	6	0.000000	1.129599	-1.565306
2	6	0.000000	1.185255	-0.184619
3	6	0.000000	0.000000	0.593046
4	6	0.000000	-1.185255	-0.184619
5	6	0.000000	-1.129599	-1.565306
6	7	0.000000	0.000000	-2.290462
7	16	0.000000	0.000000	2.319249
8	1	0.000000	2.055734	-2.135188
9	1	0.000000	2.143169	0.318226
10	1	0.000000	-2.143169	0.318226
11	1	0.000000	-2.055734	-2.135188

37a

E_0=-500.435344 Hartree

1	6	-1.721448	1.802626	0.000000
2	6	-1.352051	0.464964	0.000000
3	6	-0.004190	0.081272	0.000000
4	6	0.895642	1.153830	0.000000
5	6	0.442489	2.466429	0.000000
6	7	-0.848933	2.815273	0.000000
7	5	0.486317	-1.499079	0.000000
8	1	-2.772456	2.080977	0.000000
9	1	-2.139536	-0.283802	0.000000
10	1	1.958021	0.948486	0.000000
11	1	1.152774	3.289411	0.000000
12	8	-0.004190	-2.187124	1.233888
13	8	1.940295	-1.527561	0.000000
14	8	-0.004190	-2.187124	-1.233888
15	1	-0.961136	-2.200669	1.273458
16	1	2.216439	-2.445501	0.000000
17	1	-0.961136	-2.200669	-1.273458

38a

E_0=-507.8241954 Hartree

1	6	-2.356118	-0.212645	0.000000
2	6	-1.032076	-0.625483	0.000000
3	6	0.000000	0.345829	0.000000
4	6	-0.460859	1.687602	0.000000
5	6	-1.807274	1.976349	0.000000
6	7	-2.782786	1.053900	0.000000
7	1	-3.135136	-0.970339	0.000000
8	1	-0.792554	-1.672283	0.000000
9	1	0.273842	2.480826	0.000000
10	1	-2.132740	3.012675	0.000000
11	7	1.365429	0.232715	0.000000
12	7	1.947647	-0.967818	0.000000
13	8	3.193535	-0.967645	0.000000
14	8	1.308031	-2.046401	0.000000

39a

E_0=-436.514664 Hartree

1	6	0.000000	1.135867	1.846405
2	6	0.000000	1.185655	0.458745
3	6	0.000000	0.000000	-0.271330
4	6	0.000000	-1.185655	0.458745
5	6	0.000000	-1.135867	1.846405
6	7	0.000000	0.000000	2.552309
7	1	0.000000	2.053646	2.427075
8	1	0.000000	2.123997	-0.078074
9	1	0.000000	-2.123997	-0.078074
10	1	0.000000	-2.053646	2.427075
11	6	0.000000	0.000000	-1.824270
12	8	0.000000	1.131721	-2.353273
13	8	0.000000	-1.131721	-2.353273

40a

E_0=-891.0362532 Hartree

1	6	-0.507226	3.205607	0.000000
2	6	0.442973	2.200590	0.000000
3	6	0.025621	0.862861	0.000000
4	6	-1.354978	0.626398	0.000000
5	6	-2.211860	1.714856	0.000000
6	7	-1.827834	2.996059	0.000000
7	1	-0.188565	4.243351	0.000000
8	1	1.499747	2.427241	0.000000
9	1	-1.737004	-0.382368	0.000000
10	1	-3.283042	1.542041	0.000000
11	8	0.964869	-0.081381	0.000000
12	15	0.644353	-1.746732	0.000000
13	8	2.249702	-2.102404	0.000000
14	8	0.025621	-2.108476	1.301626
15	8	0.025621	-2.108476	-1.301626
16	1	2.344724	-3.057671	0.000000

41a

E_0=-815.7433568 Hartree

1	15	0.085541	-1.543471	0.000000
2	8	1.749207	-1.625229	0.000000
3	8	-0.433097	-2.053864	1.304595
4	8	-0.433097	-2.053864	-1.304595
5	1	2.004601	-2.551374	0.000000
6	6	0.782647	2.551066	0.000000
7	6	1.019008	1.181384	0.000000
8	6	-0.057265	0.294441	0.000000
9	6	-1.330614	0.869680	0.000000
10	6	-1.464882	2.249158	0.000000
11	7	-0.433097	3.100344	0.000000
12	1	1.618119	3.244858	0.000000
13	1	2.031288	0.805226	0.000000
14	1	-2.210386	0.240696	0.000000
15	1	-2.452528	2.699541	0.000000

42a

E_0=-871.8714521 Hartree

1	16	0.223215	-1.533848	0.000000
2	8	-0.441538	-1.972806	1.229930
3	8	1.678275	-1.699521	0.000000
4	8	-0.441538	-1.972806	-1.229930
5	6	-1.463600	2.183496	0.000000
6	6	-1.312634	0.805503	0.000000
7	6	-0.027817	0.270445	0.000000
8	6	1.042115	1.153504	0.000000
9	6	0.783544	2.520353	0.000000
10	7	-0.441538	3.047580	0.000000
11	1	-2.456093	2.622035	0.000000
12	1	-2.173635	0.152562	0.000000
13	1	2.051004	0.767416	0.000000
14	1	1.606806	3.227753	0.000000

43a

E_0=-798.8715202 Hartree

1	6	-0.576175	0.975238	0.364487
2	6	2.927498	0.212996	-0.926407
3	6	1.694755	0.840006	-0.791939
4	6	0.753911	0.292318	0.069472
5	6	1.107004	-0.858816	0.766500
6	6	2.364969	-1.403064	0.566173
7	7	3.278673	-0.888860	-0.264526
8	1	3.670878	0.622017	-1.602785
9	1	1.466788	1.729021	-1.359106
10	1	0.397631	-1.333133	1.427422
11	1	2.654854	-2.304951	1.093785
12	8	-1.639447	0.209150	0.516198
13	9	-0.400692	1.685362	1.550695
14	9	-0.779395	1.979583	-0.582667
15	6	-1.787475	-0.845594	-0.581023
16	9	-2.076075	-1.967734	0.234335
17	9	-3.069638	-0.524171	-1.051340

44a

E_0=-287.1275832 Hartree

1	6	-1.129408	-1.153967	0.000000
2	6	-1.194738	0.217350	0.000000
3	6	0.000000	1.029936	0.000000
4	6	1.194174	0.217108	0.000000
5	6	1.129166	-1.153902	0.000000
6	7	-0.000204	-1.897286	0.000000
7	1	-2.059471	-1.720752	0.000000
8	1	-2.166013	0.700763	0.000000
9	1	2.059201	-1.720682	0.000000
10	6	0.000756	2.407272	0.000000
11	1	2.165321	0.700890	0.000000
12	1	-0.923839	2.969922	0.000000
13	1	0.926524	2.968081	0.000000