Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Description of heteroaromaticity on the basis of π-electron density anisotropy

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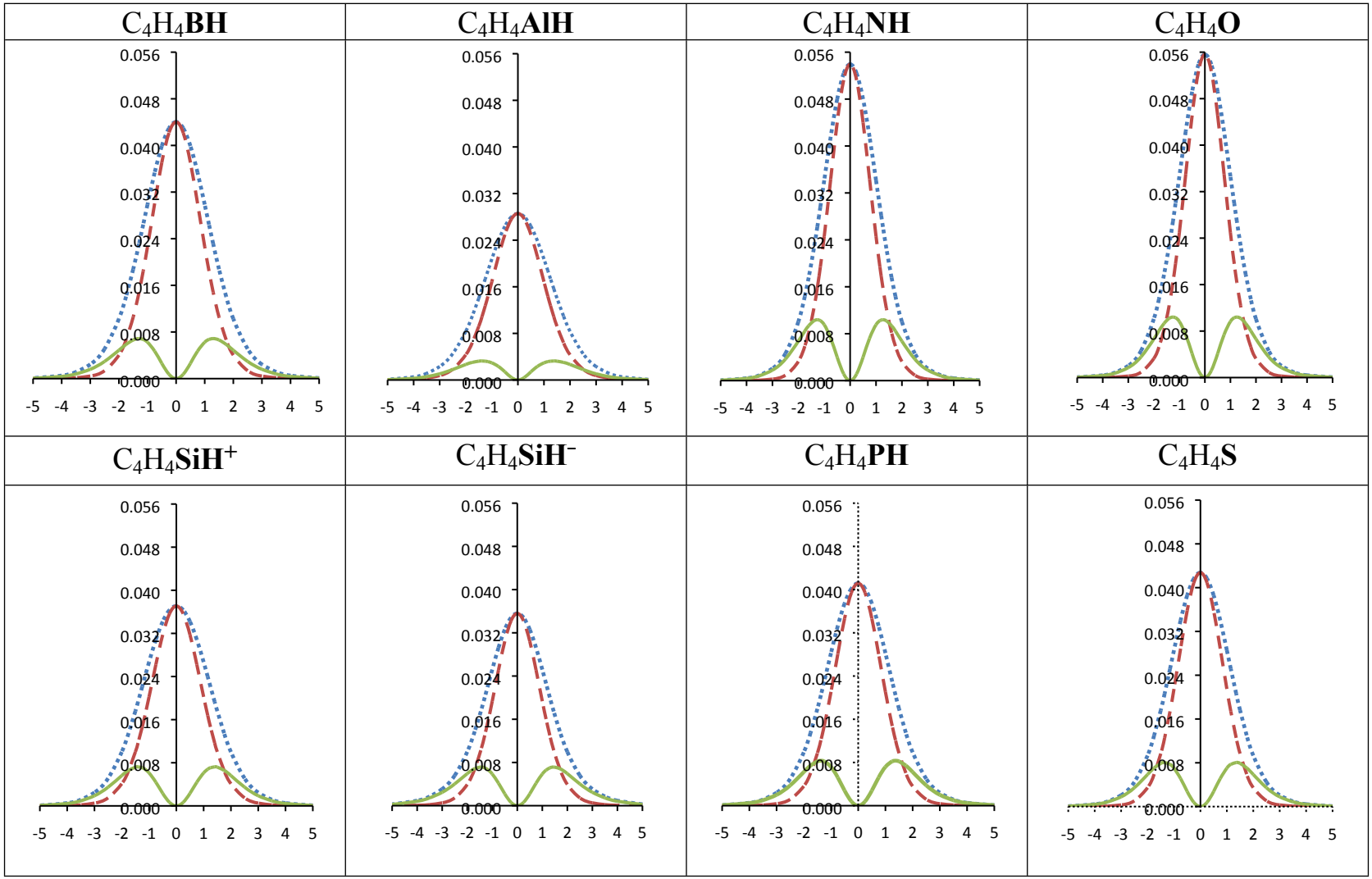
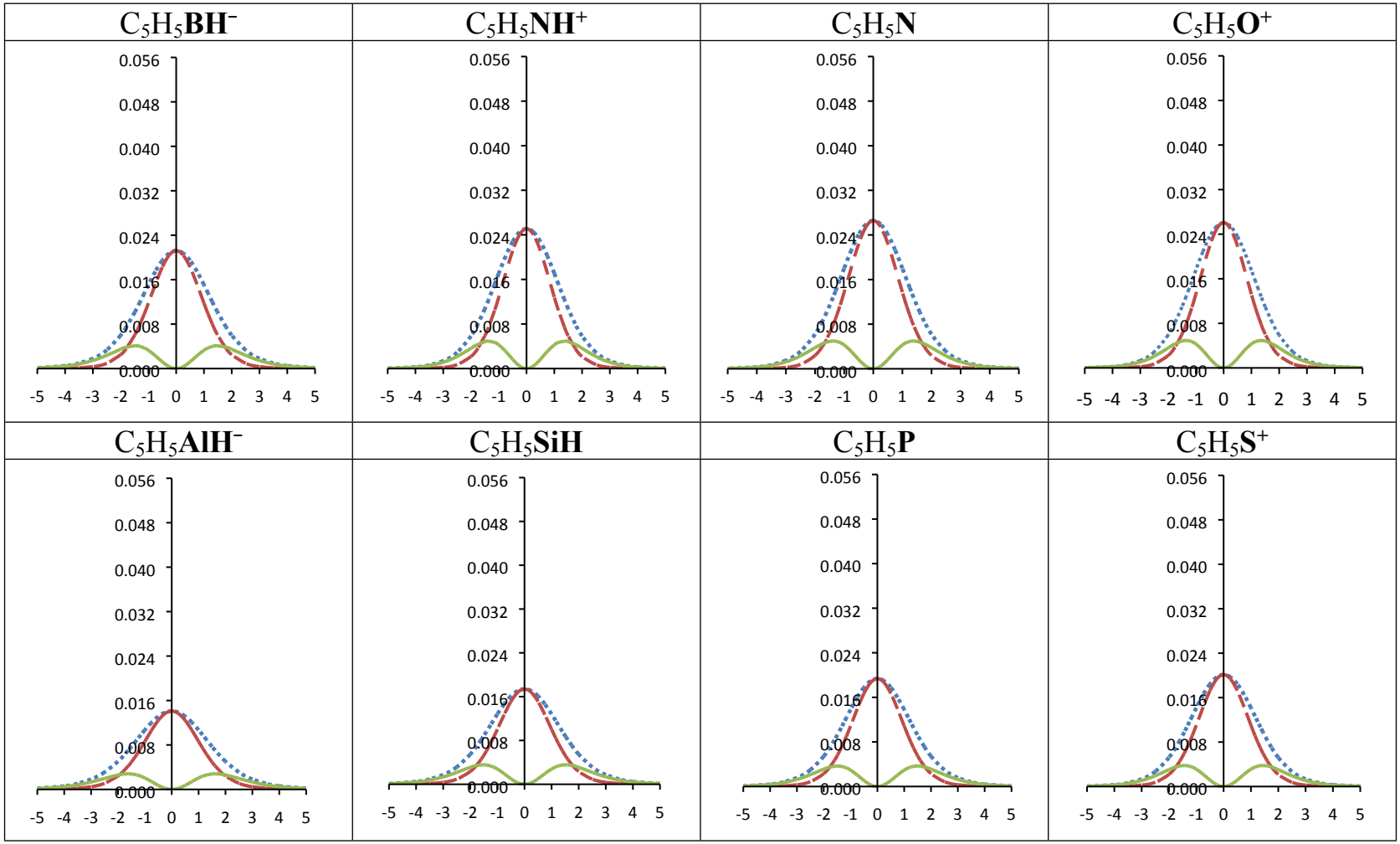
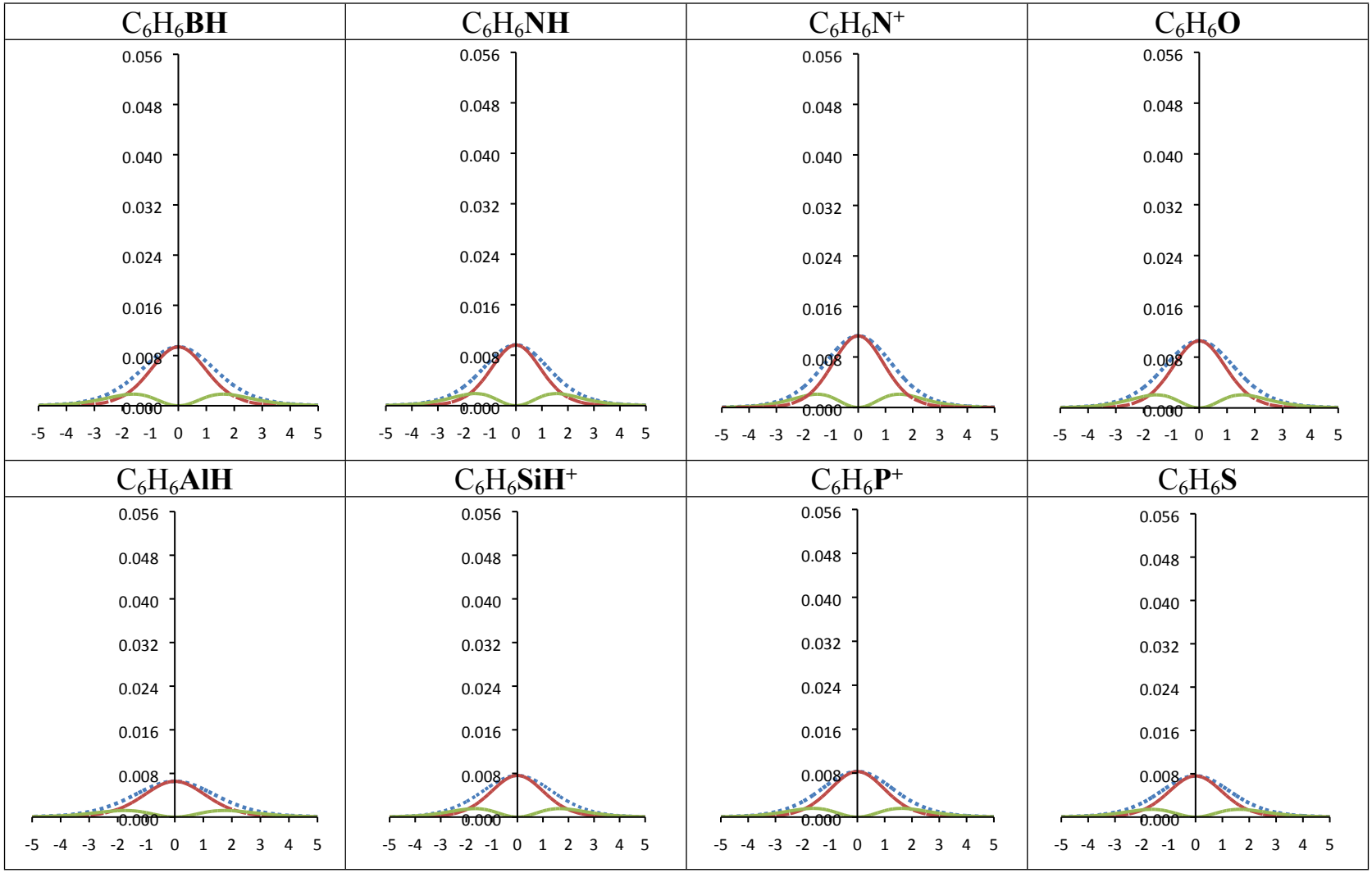
F1. The plot of ρ_{total} (*blue dotted line*) and its components, ρ_{σ} (*red dashed line*) and ρ_{π} (*green solid line*) versus distance (horizontal axis) from the ring center for five-membered ring systems (C_4H_4**X**), presented at the same scale for comparison purpose.



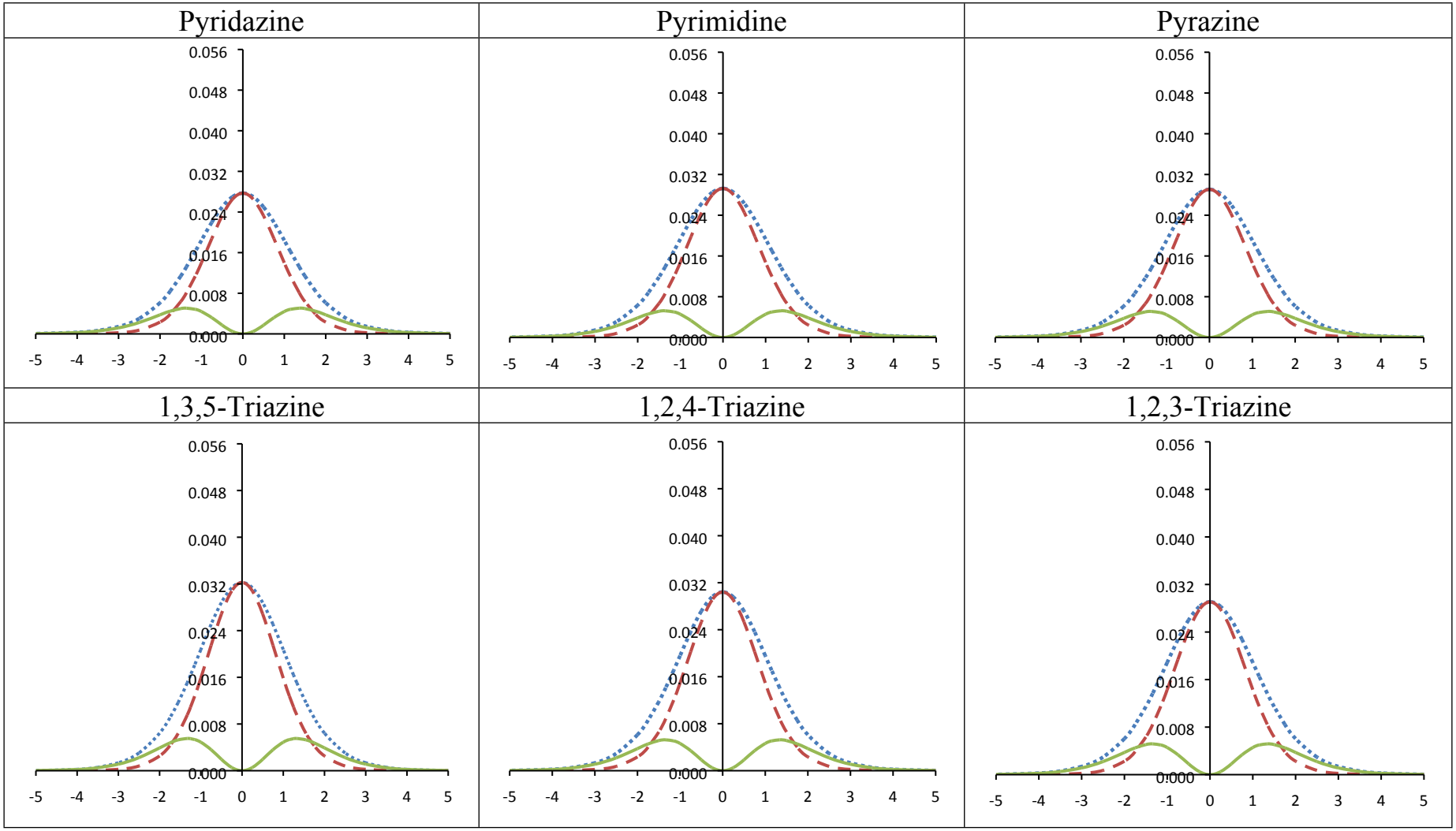
F1(continued). The plot of ρ_{total} (*blue dotted line*) and its components, ρ_{σ} (*red dashed line*) and ρ_{π} (*green solid line*) versus distance (horizontal axis) from the ring center for six-membered ring systems ($C_5H_5\mathbf{X}$), presented at the same scale for comparison purpose.



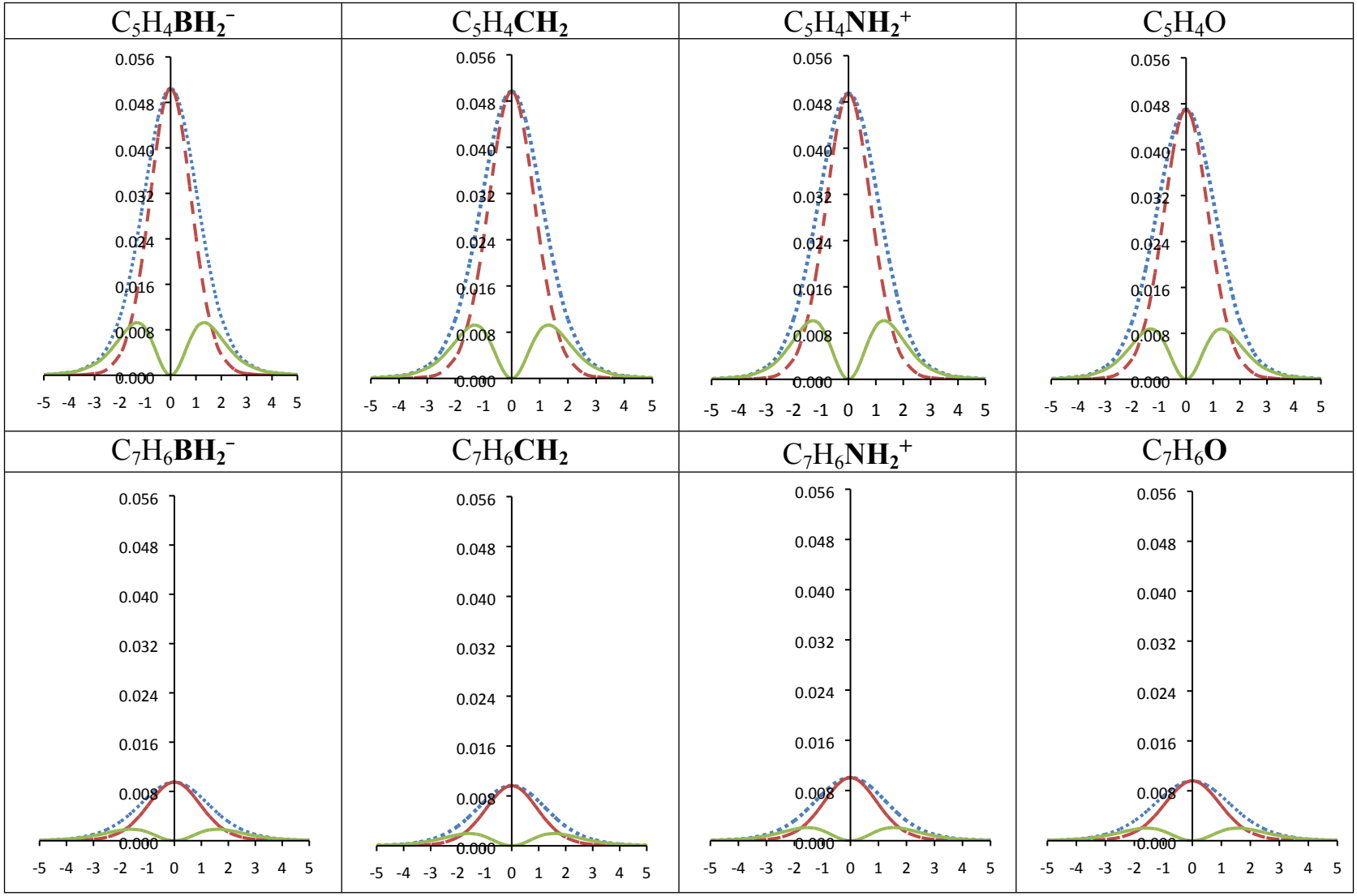
F1(continued). The plot of ρ_{total} (*blue dotted line*) and its components, ρ_{σ} (*red dashed line*) and ρ_{π} (*green solid line*) versus distance (horizontal axis) from the ring center for seven-membered ring systems (C_6H_6**X**), presented at the same scale for comparison purpose.



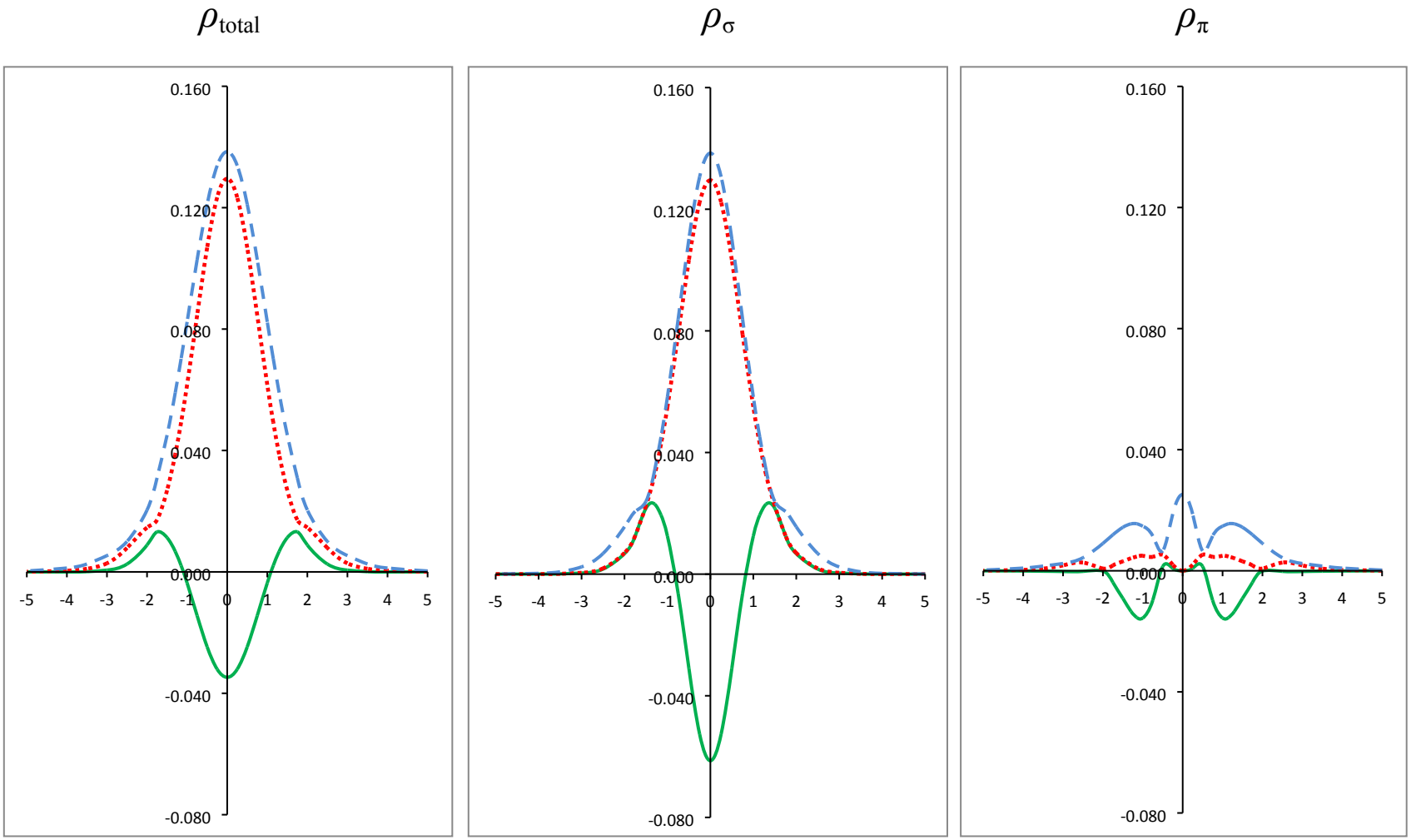
F1(continued). The plot of ρ_{total} (*blue dotted line*) and its components, ρ_{σ} (*red dashed line*) and ρ_{π} (*green solid line*) versus distance (horizontal axis) from the ring center for studied azines, presented at the same scale for comparison purpose.



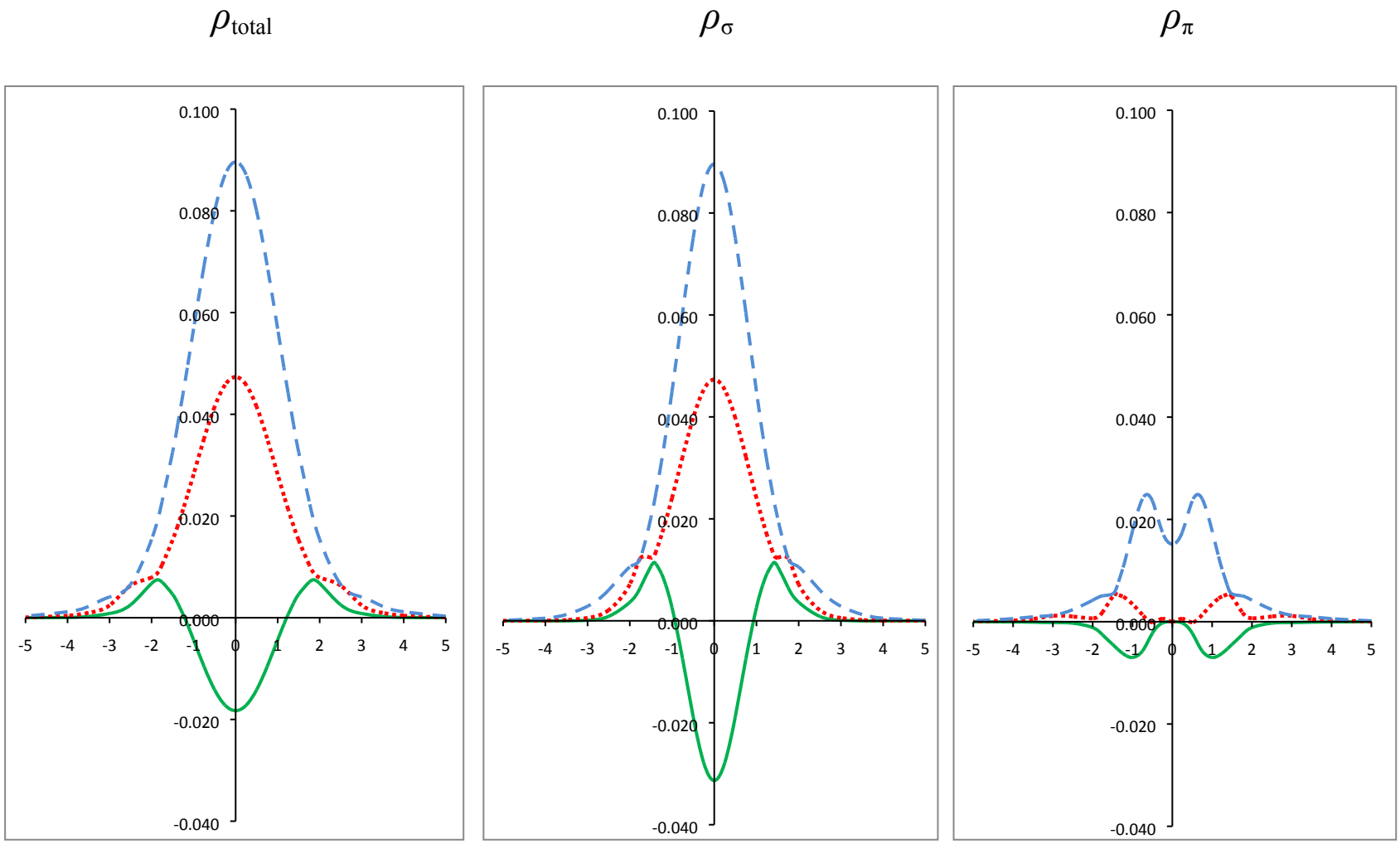
F1(continued). The plot of ρ_{total} (*blue dotted line*) and its components, ρ_{σ} (*red dashed line*) and ρ_{π} (*green solid line*) versus distance (horizontal axis) from the ring center for substituted fulvene systems ($C_nH_{n-1}\mathbf{X}$), presented at the same scale for comparison purpose.



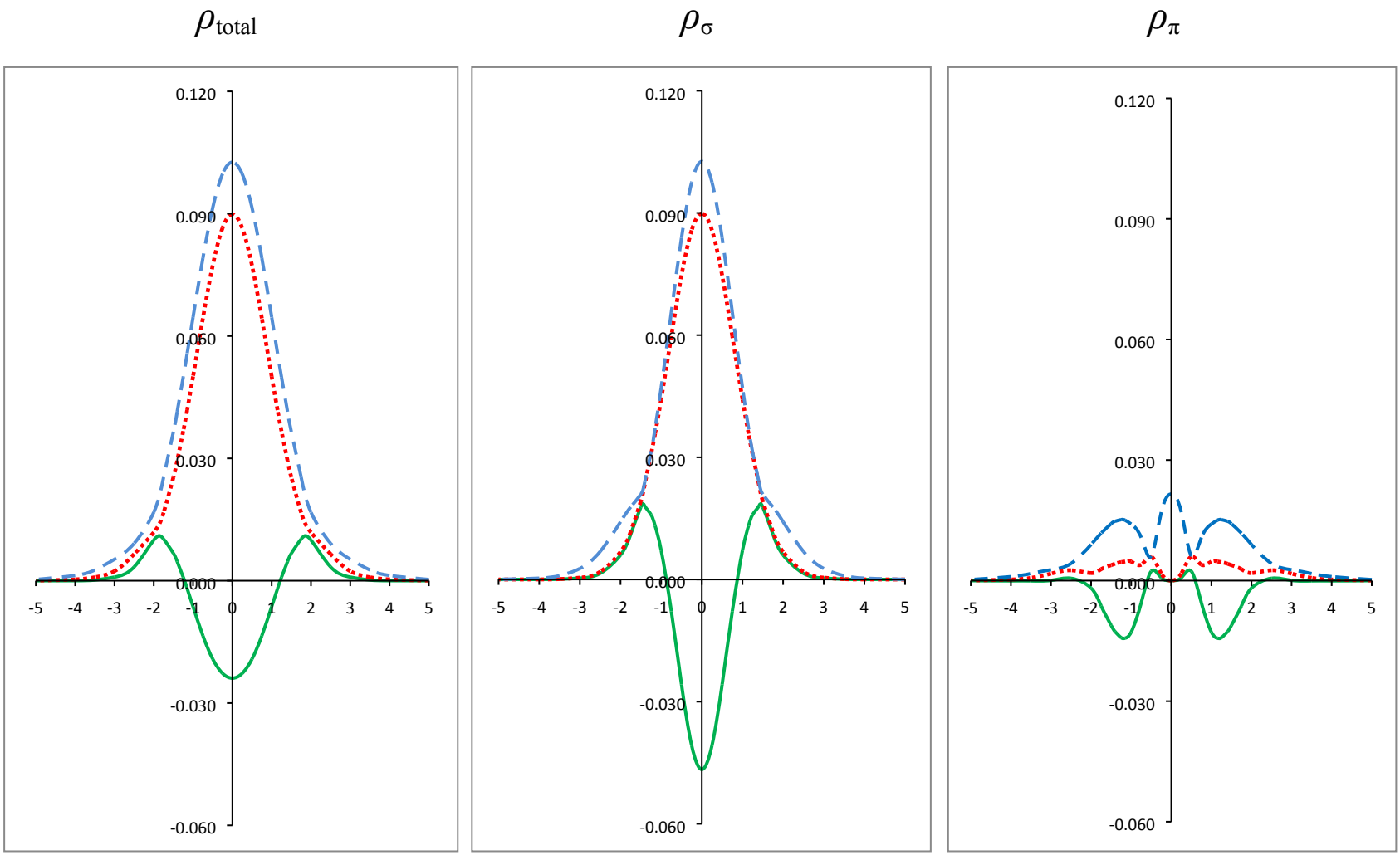
F2. The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_4H_4**BH**. The two in-plane eigenvalues have been depicted by red dotted line and blue dashed line while the eigenvalue normal to the ring plane have shown by green solid line.The plots have been presented at the same scale for comparison purpose.



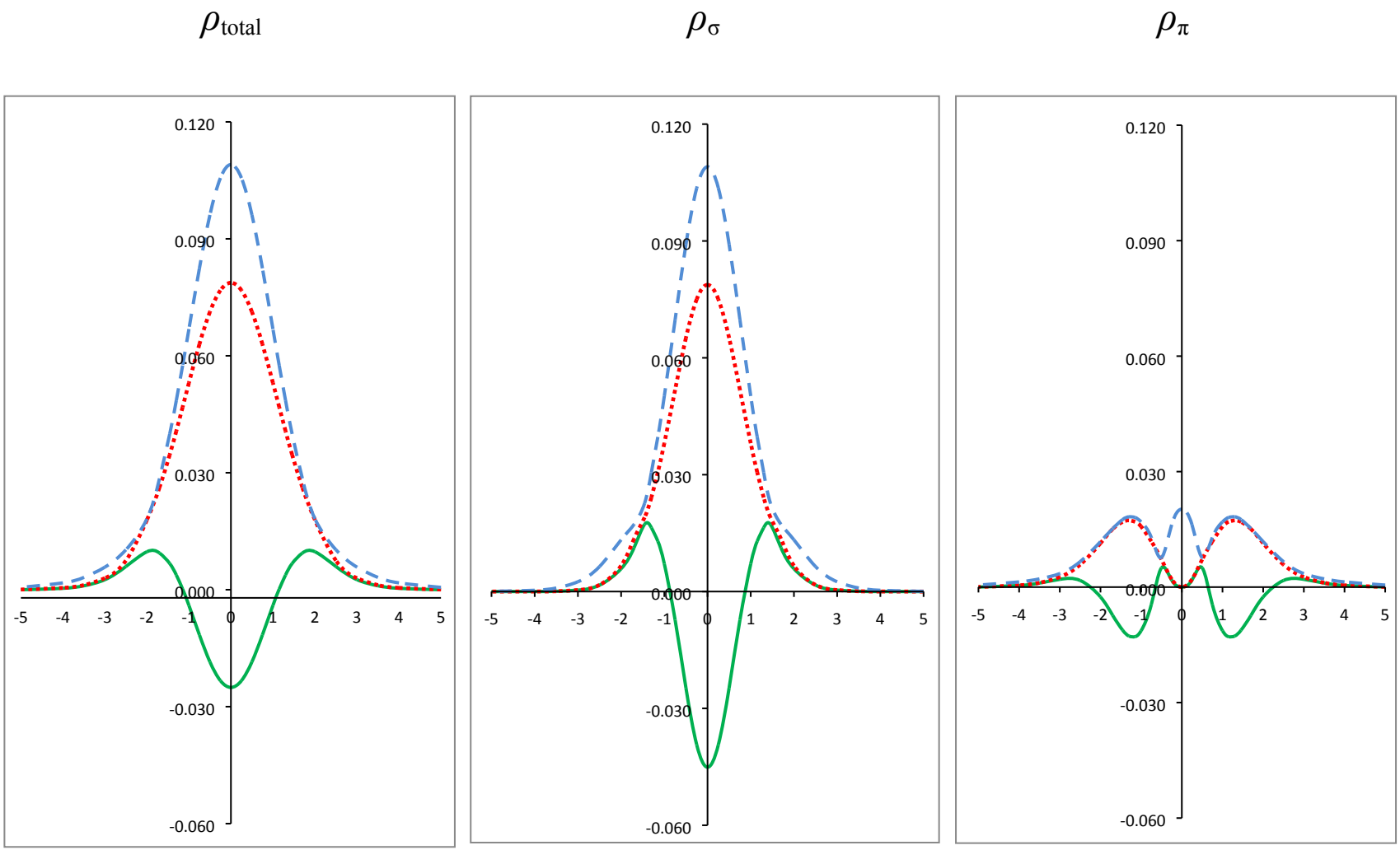
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_4H_4**AlH**.



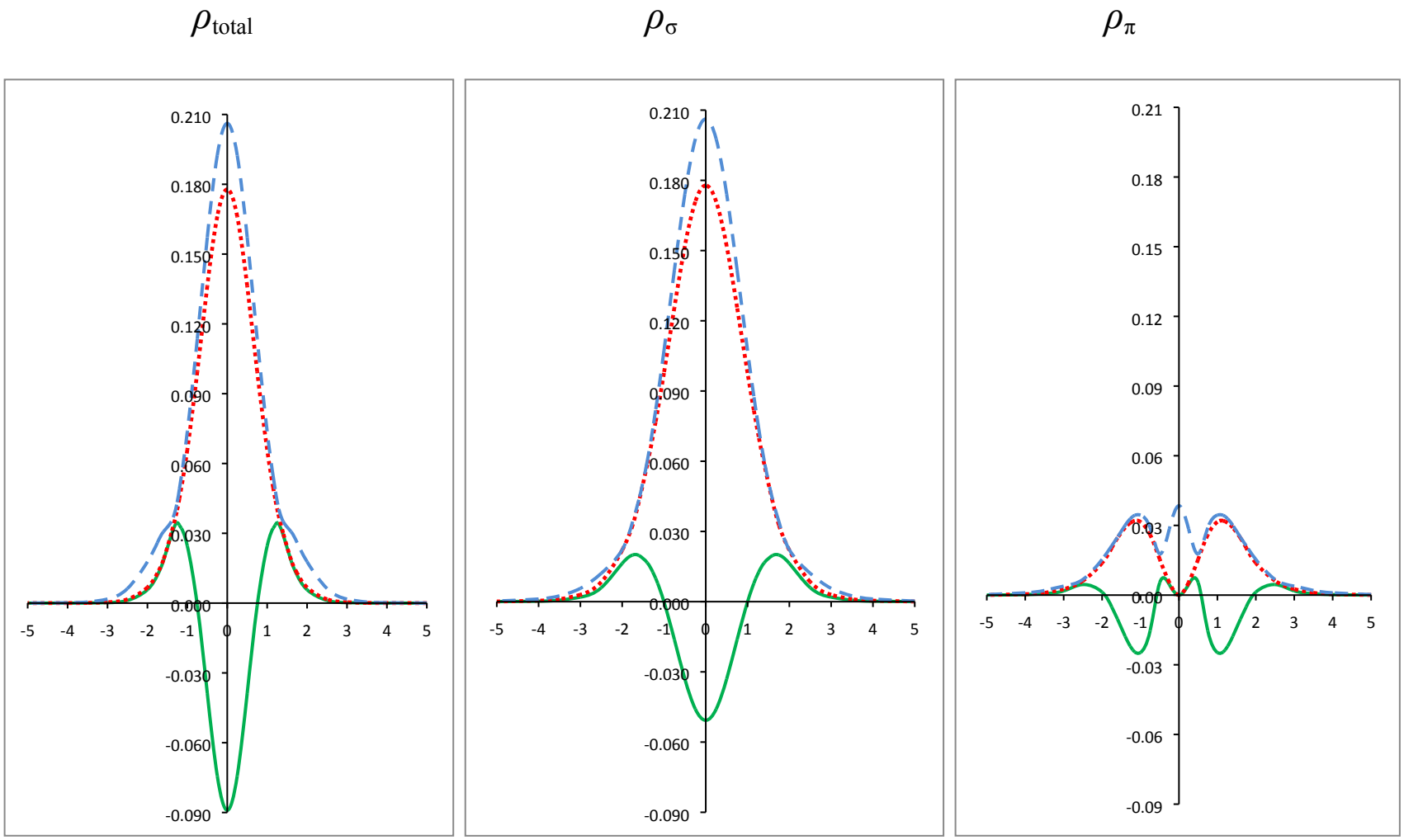
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_4H_4**SiH**$^+$.



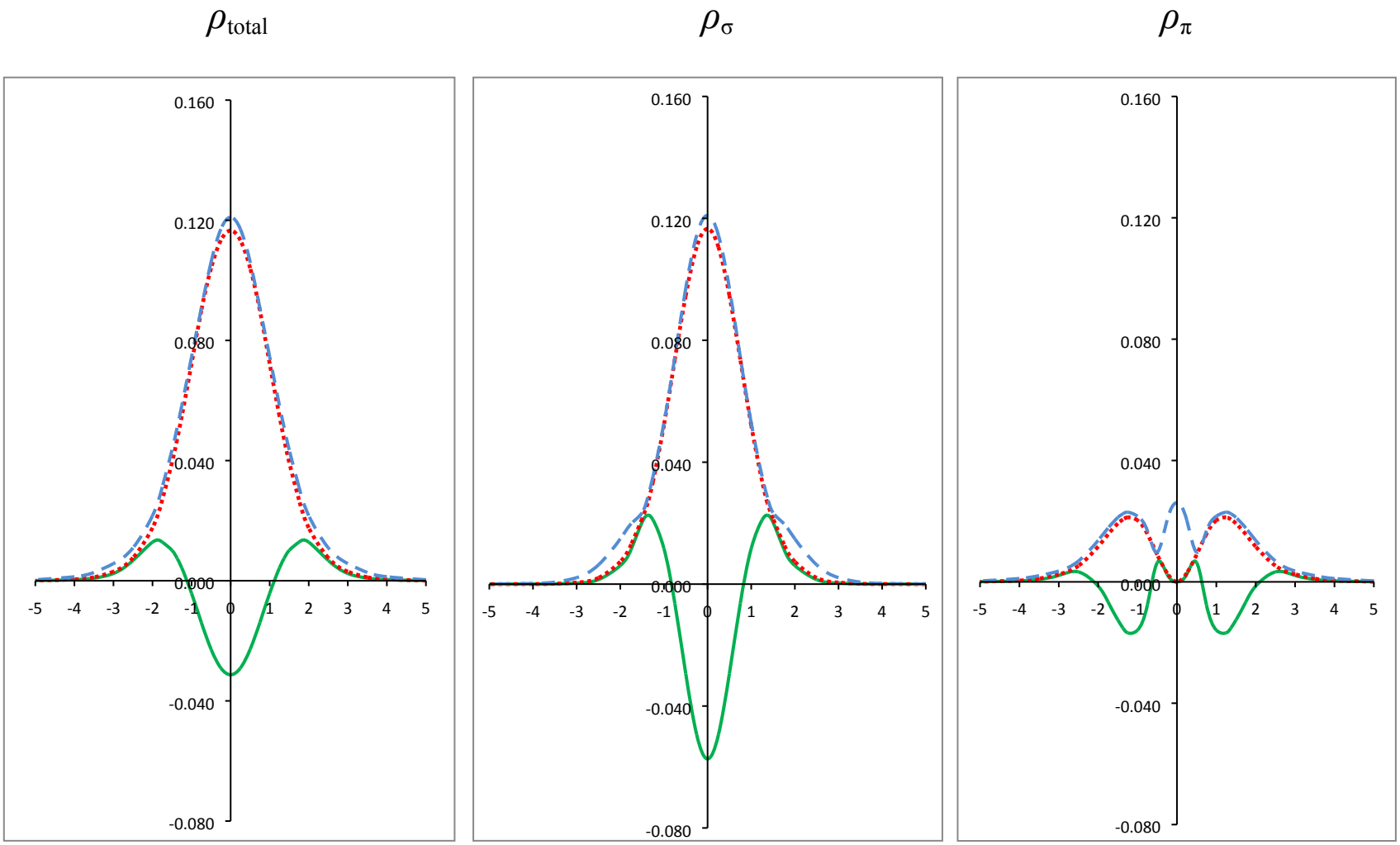
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_4H_4**SiH**$^-$.



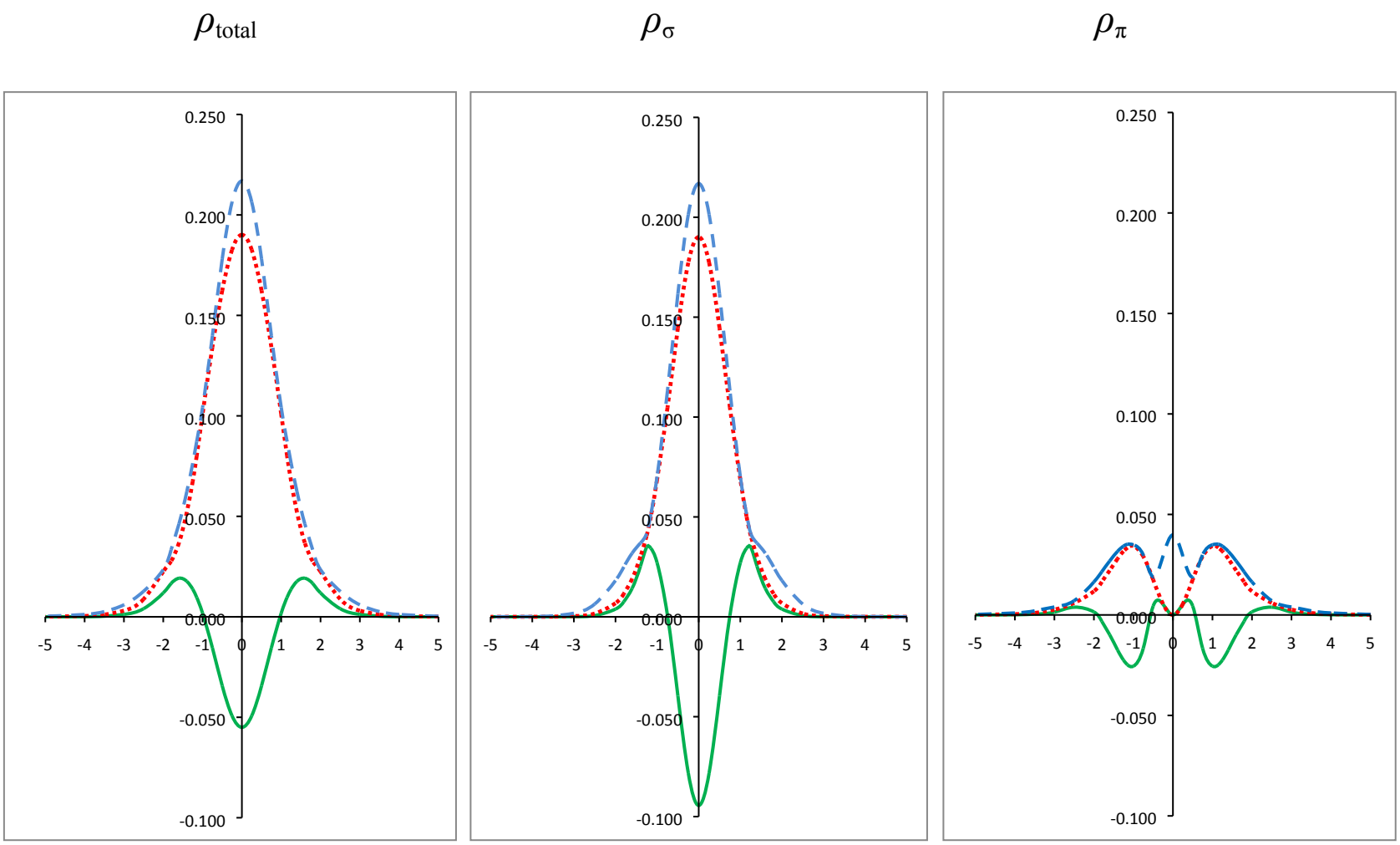
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_4H_4**NH**.



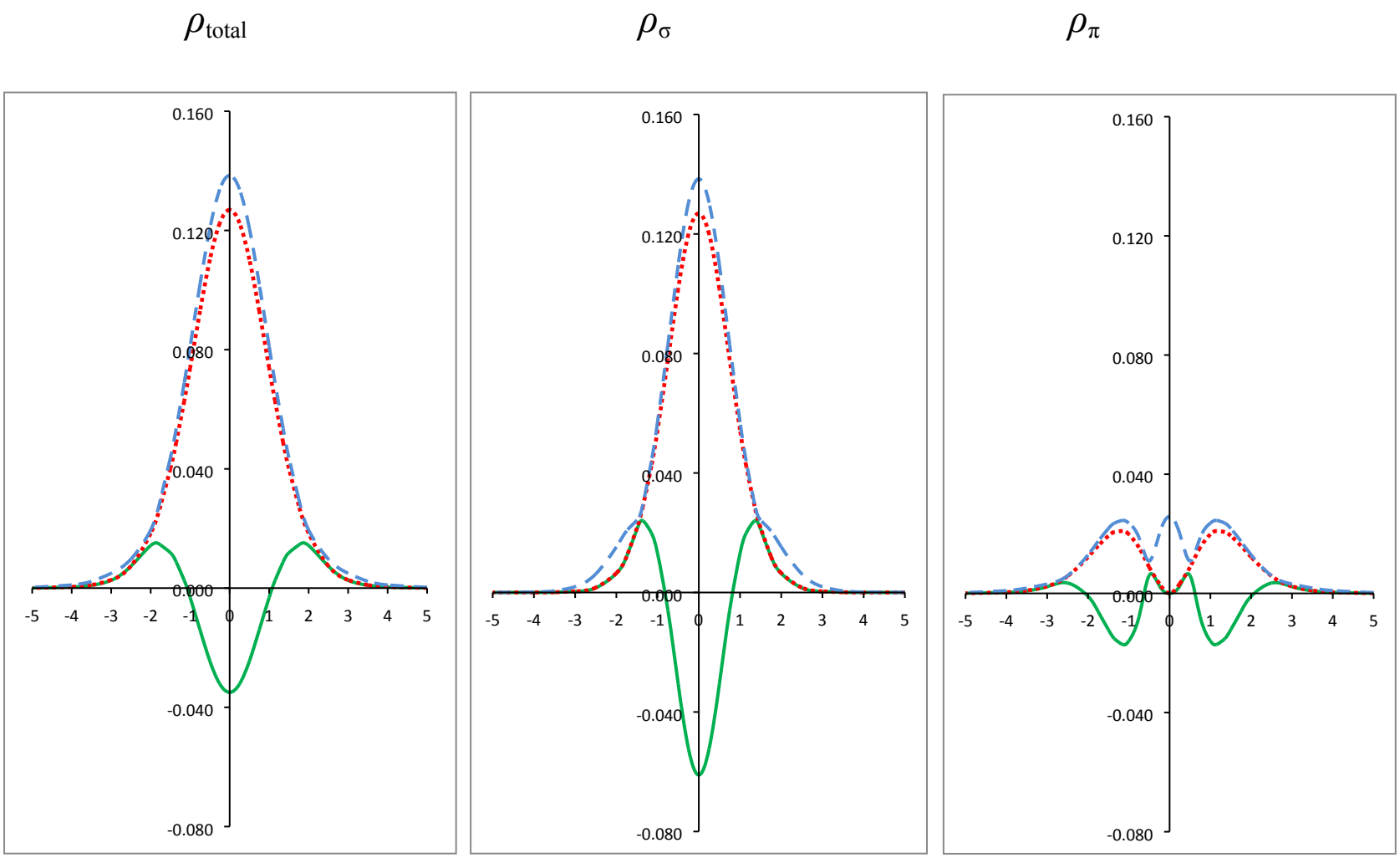
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_4H_4**PH**.



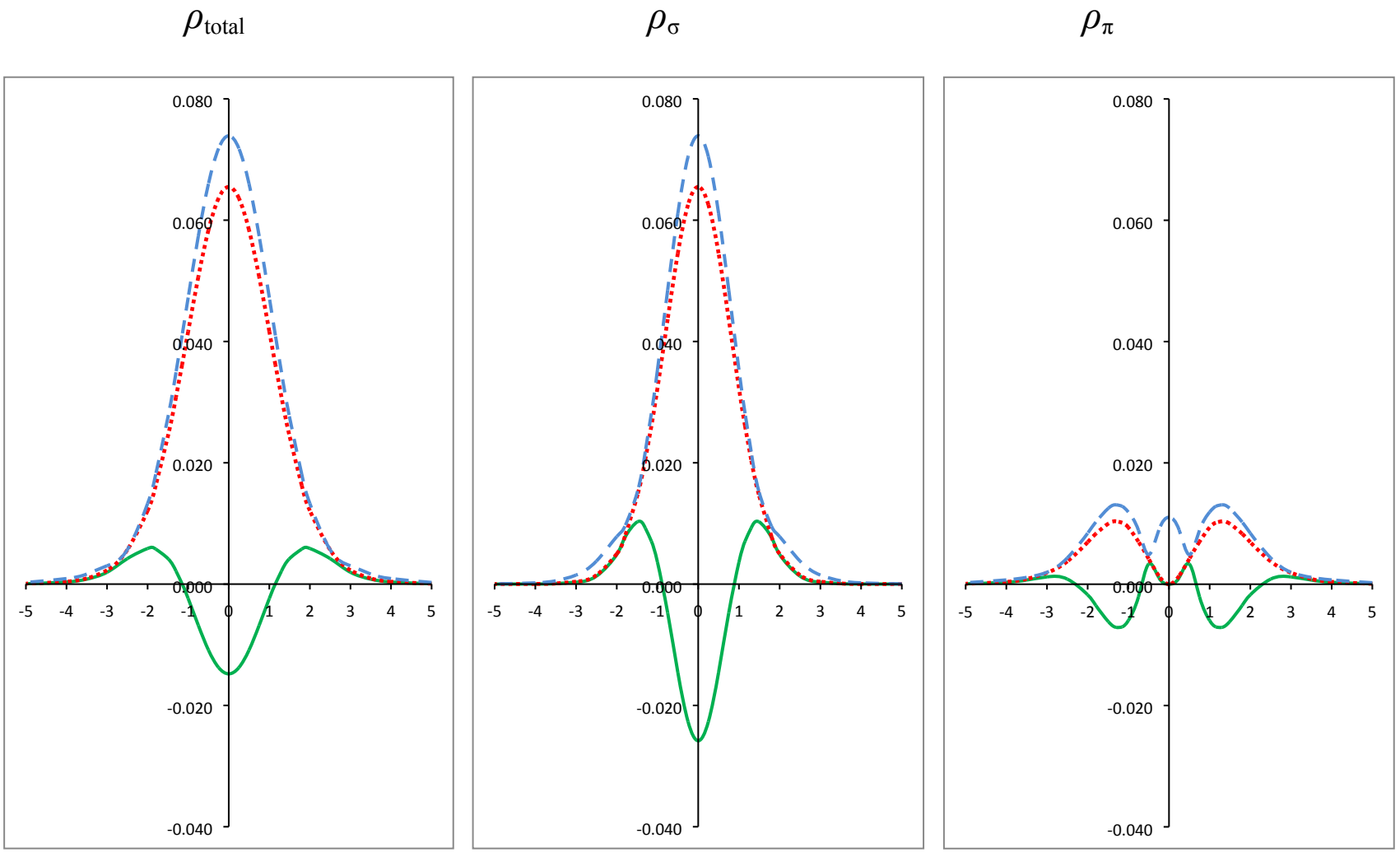
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_4H_4\mathbf{O}$.



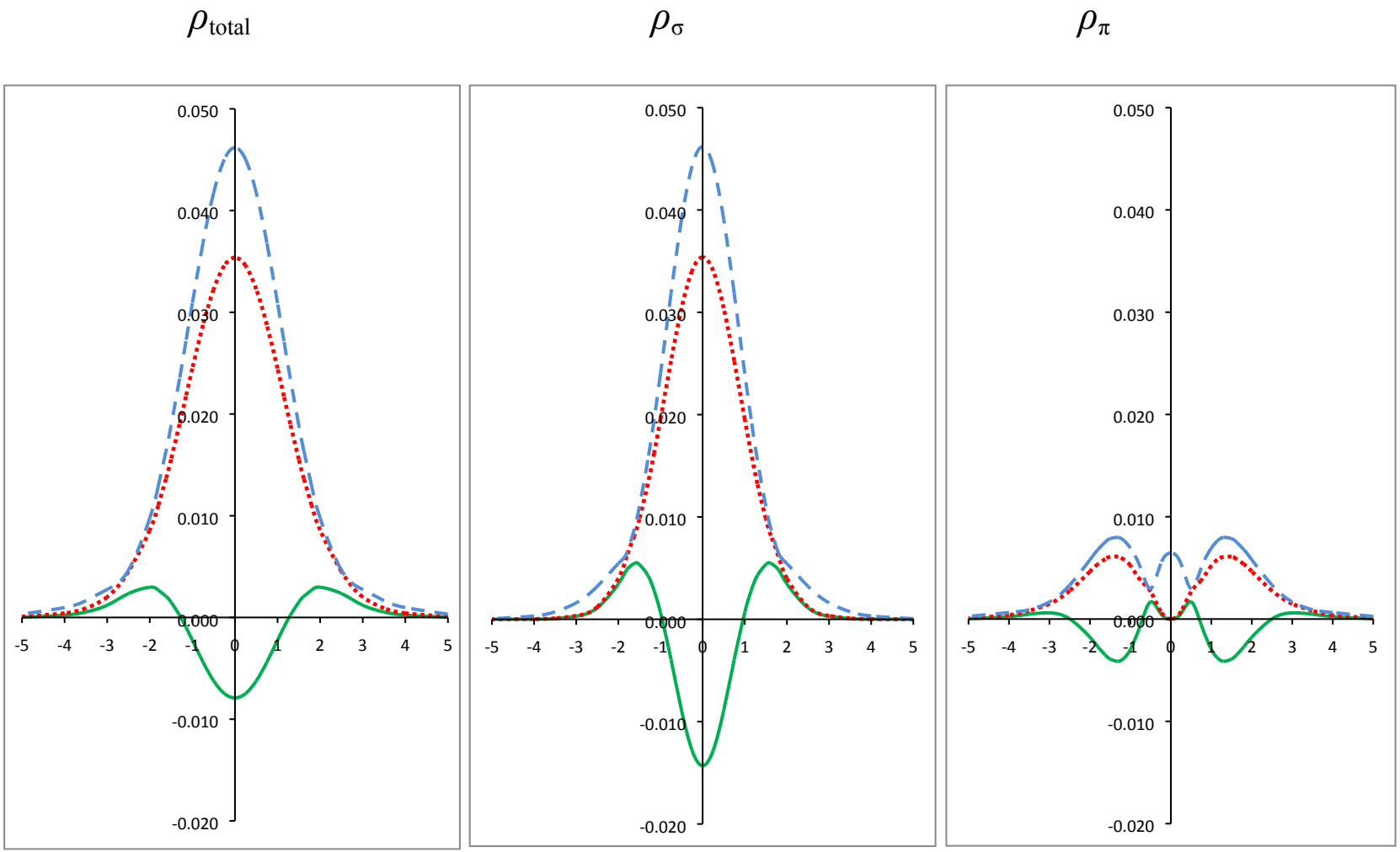
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_4H_4**S**.



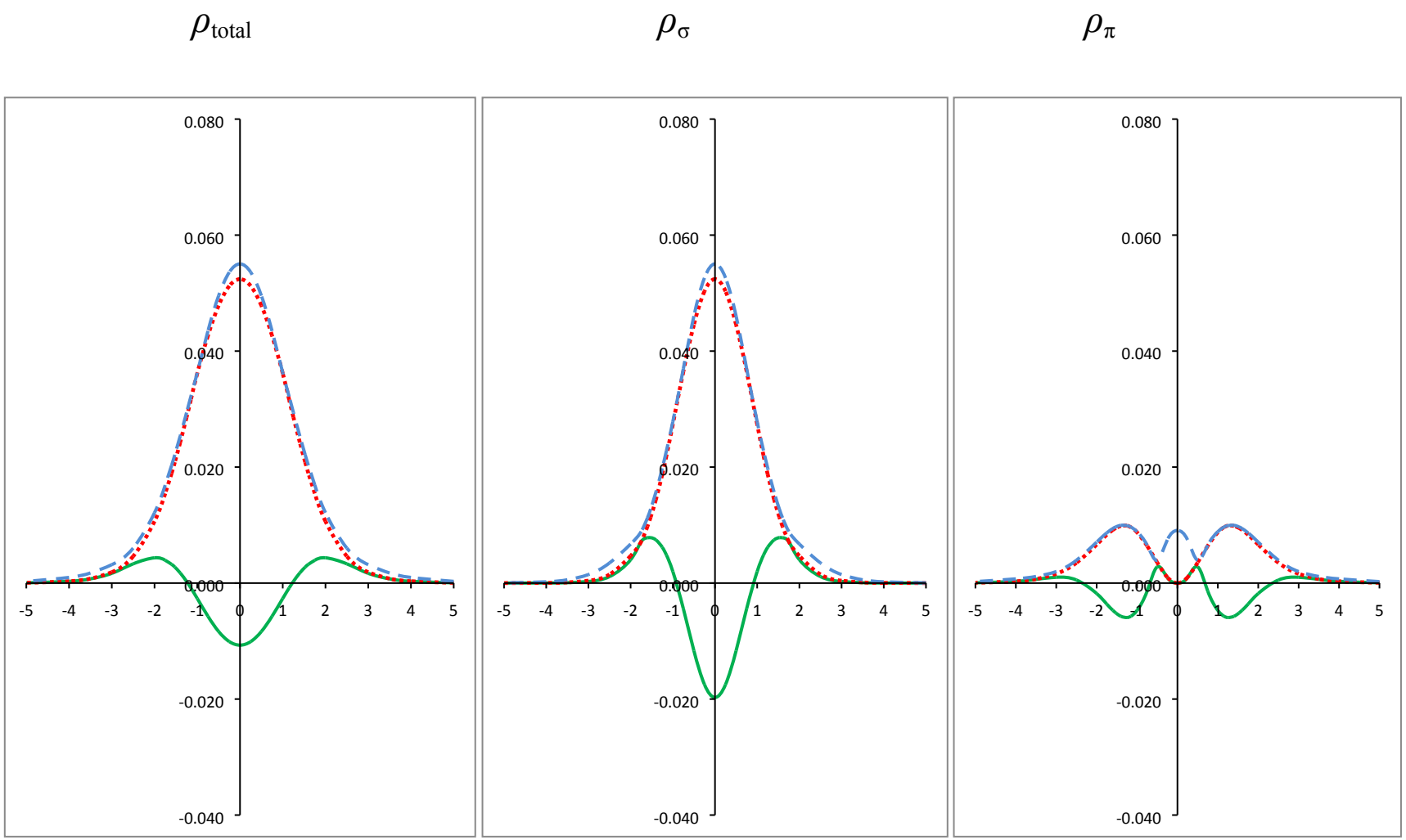
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_5\mathbf{BH}^-$.



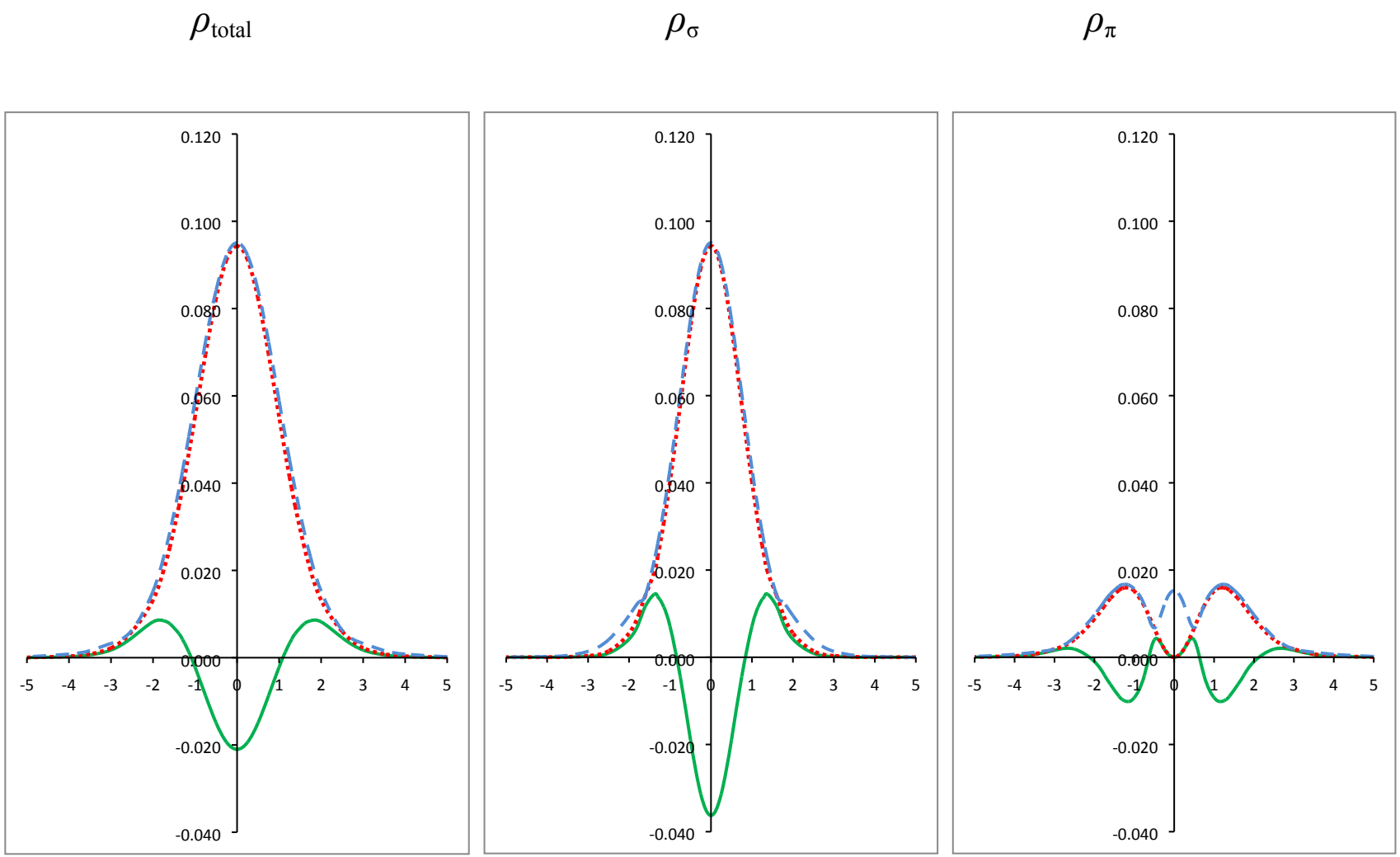
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_5H_5**AlH**$^-$.



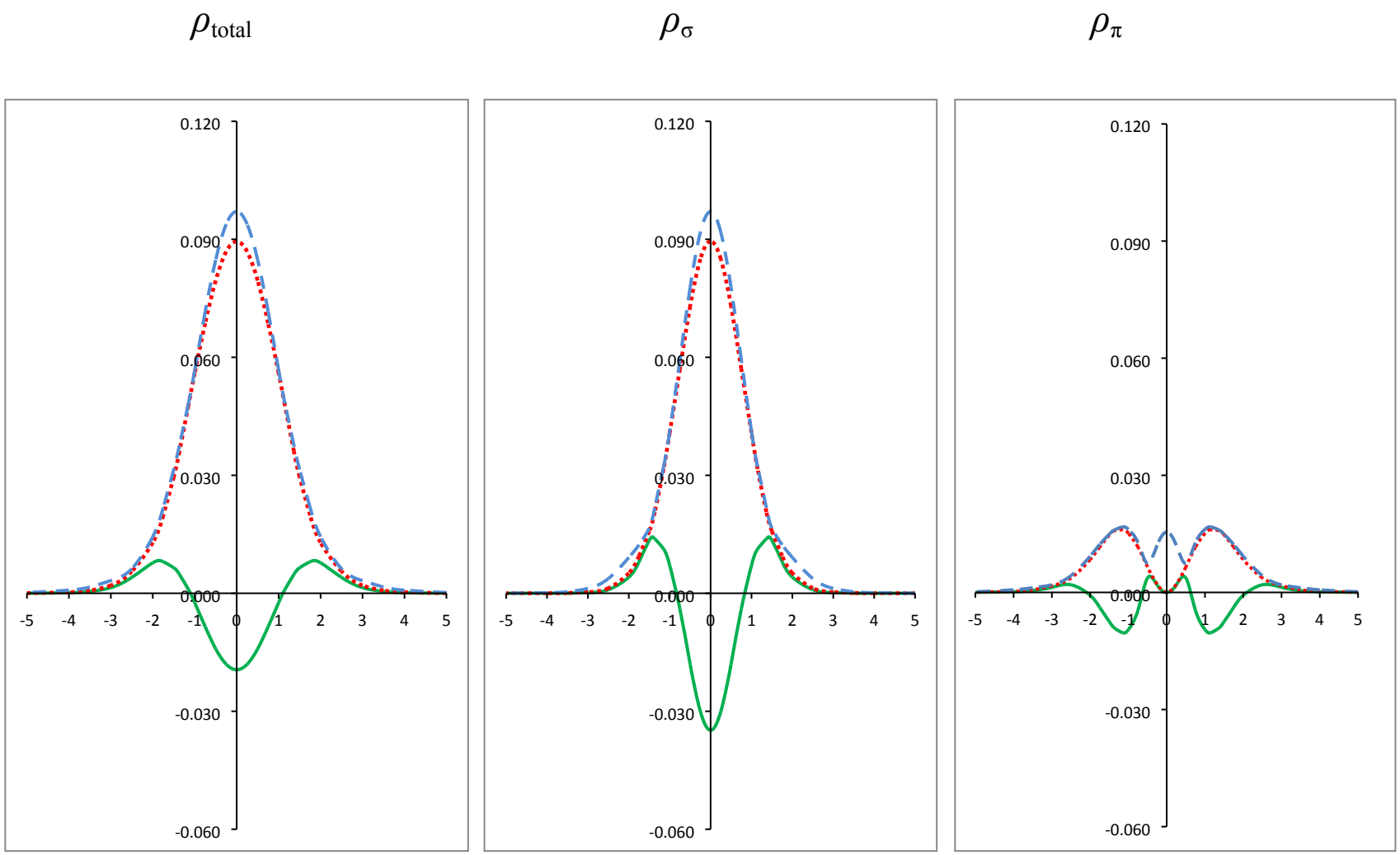
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_5H_5**SiH**.



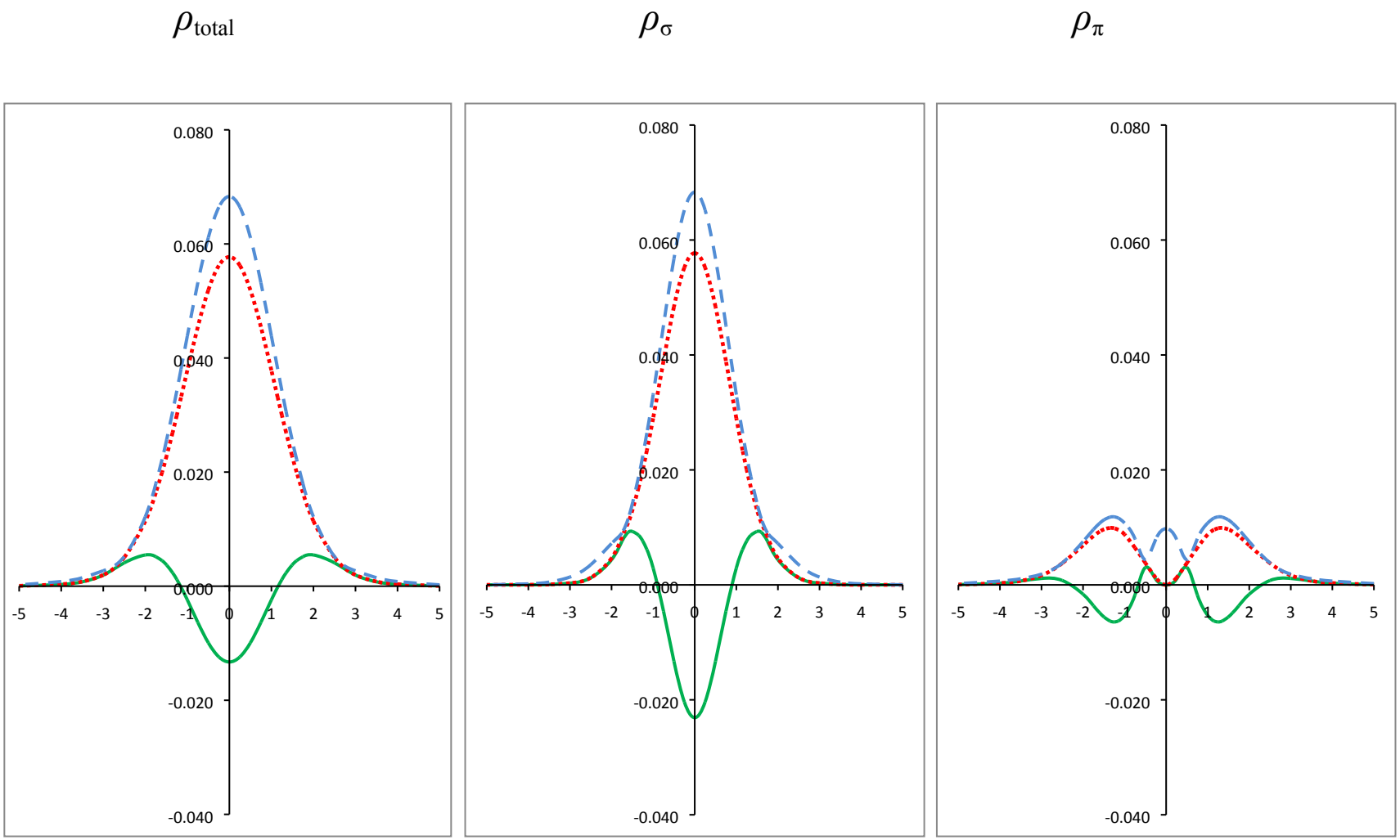
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_5\mathbf{N}$.



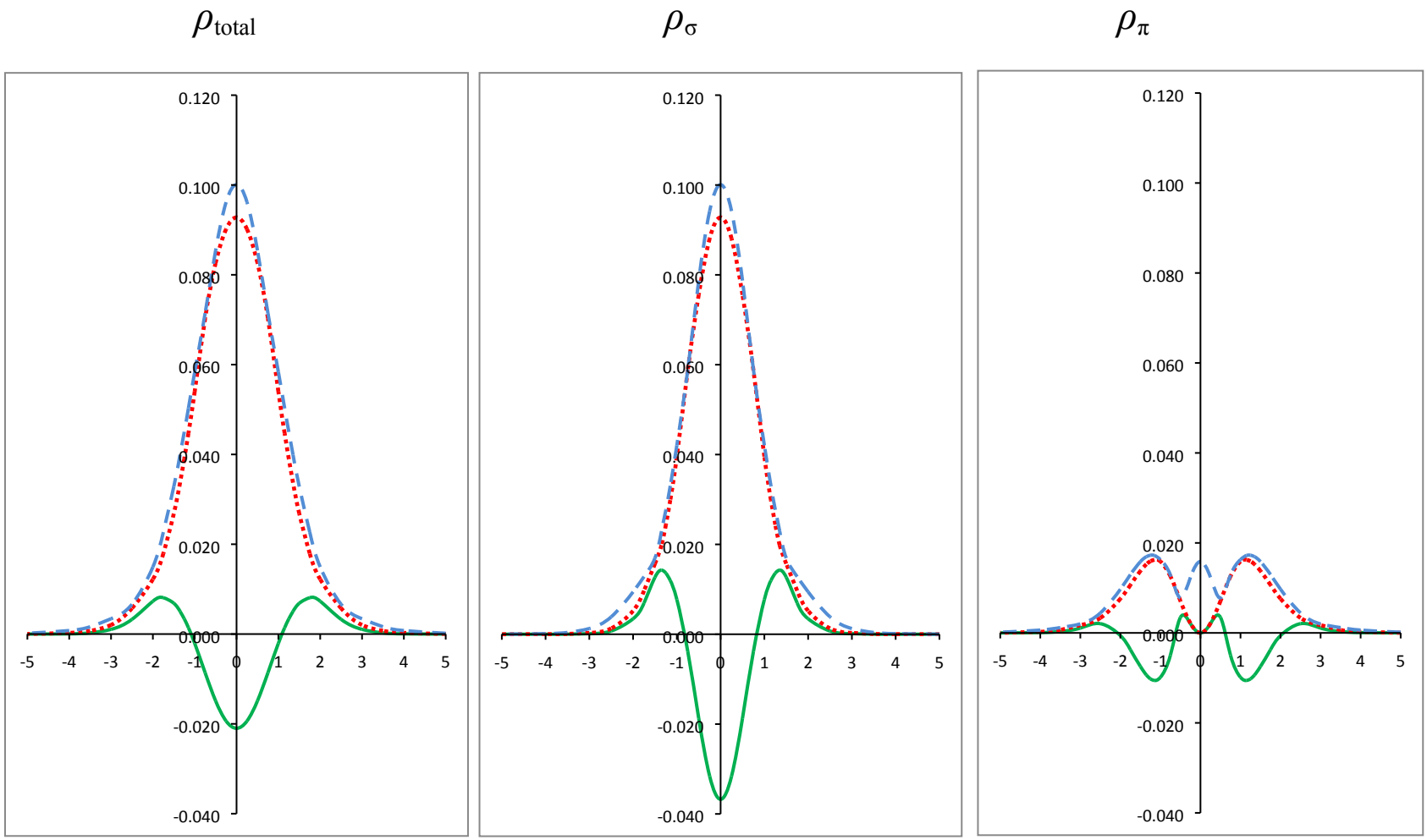
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_5\mathbf{NH}^+$.



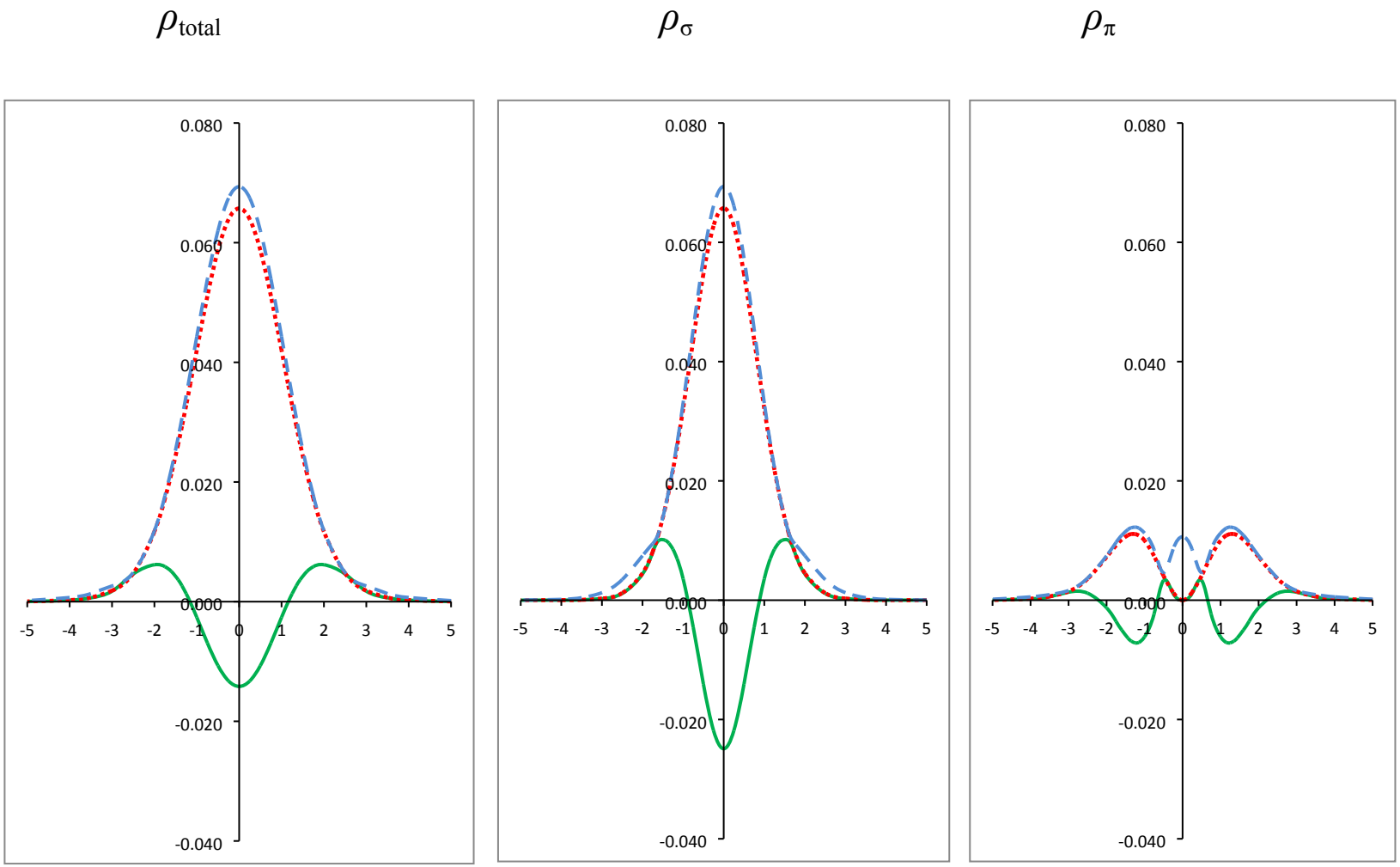
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_5\mathbf{P}$.



F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_5\mathbf{O}^+$.

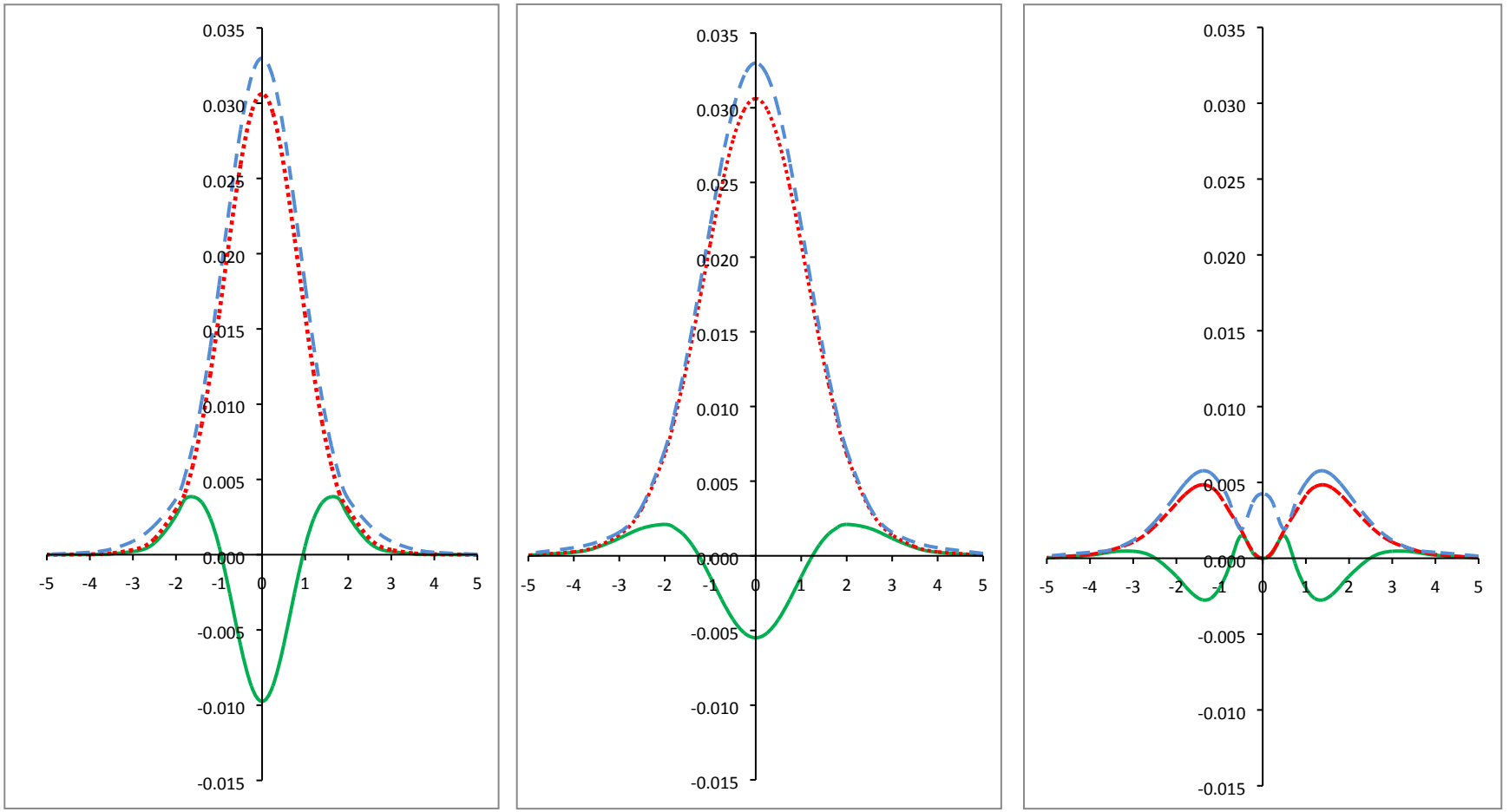


F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_5S^+$.

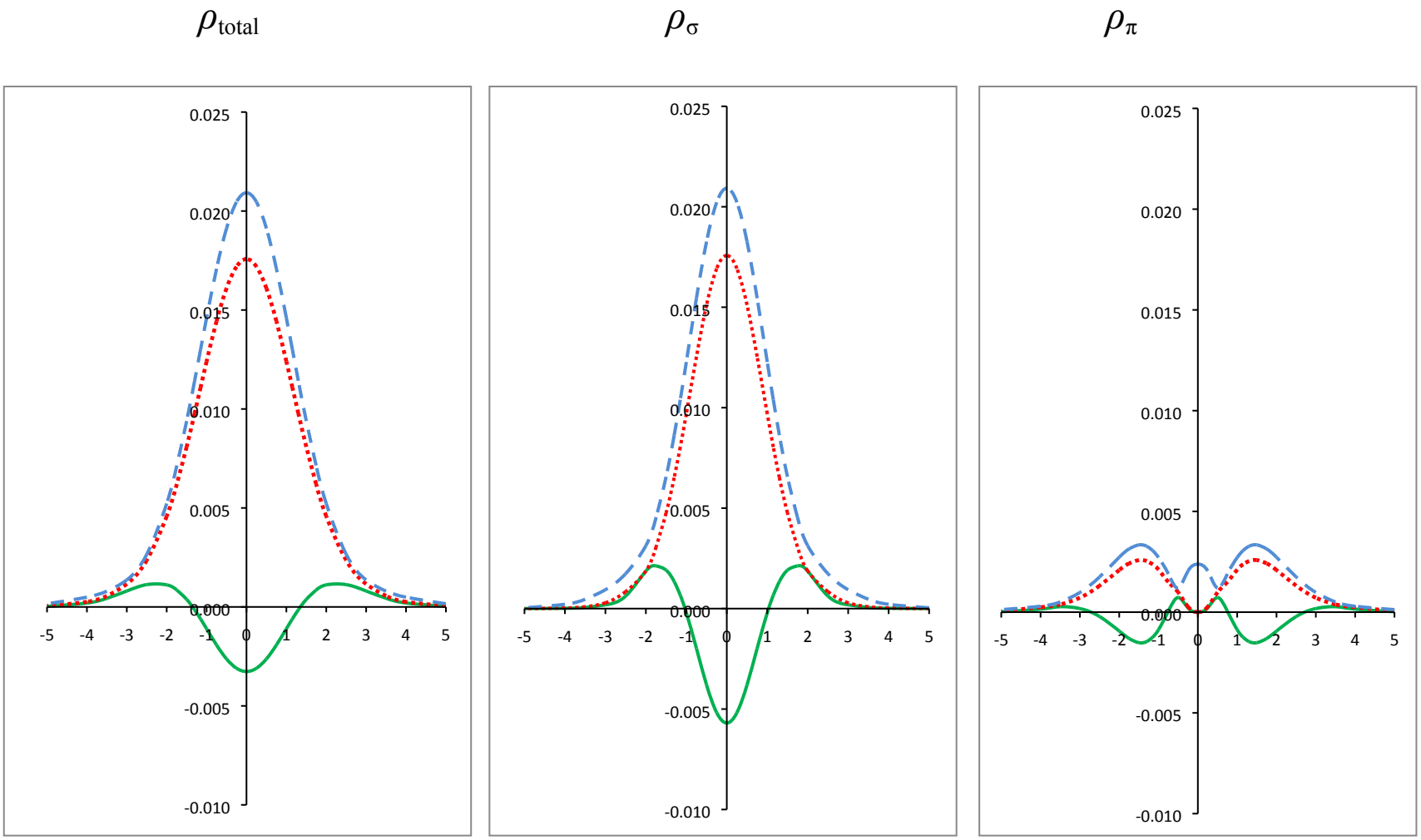


F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_6H_6**BH**.

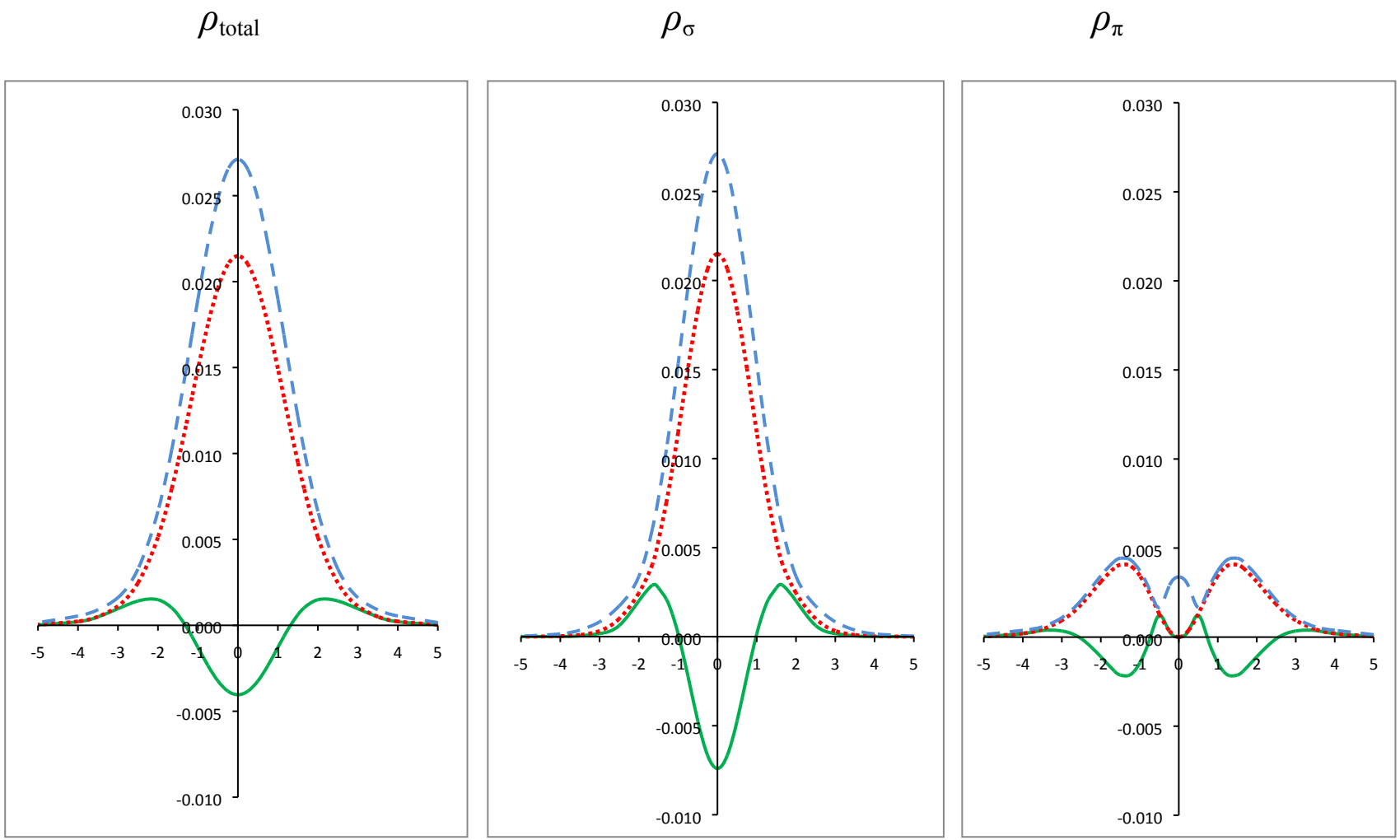
ρ_{total} ρ_{σ} ρ_{π}



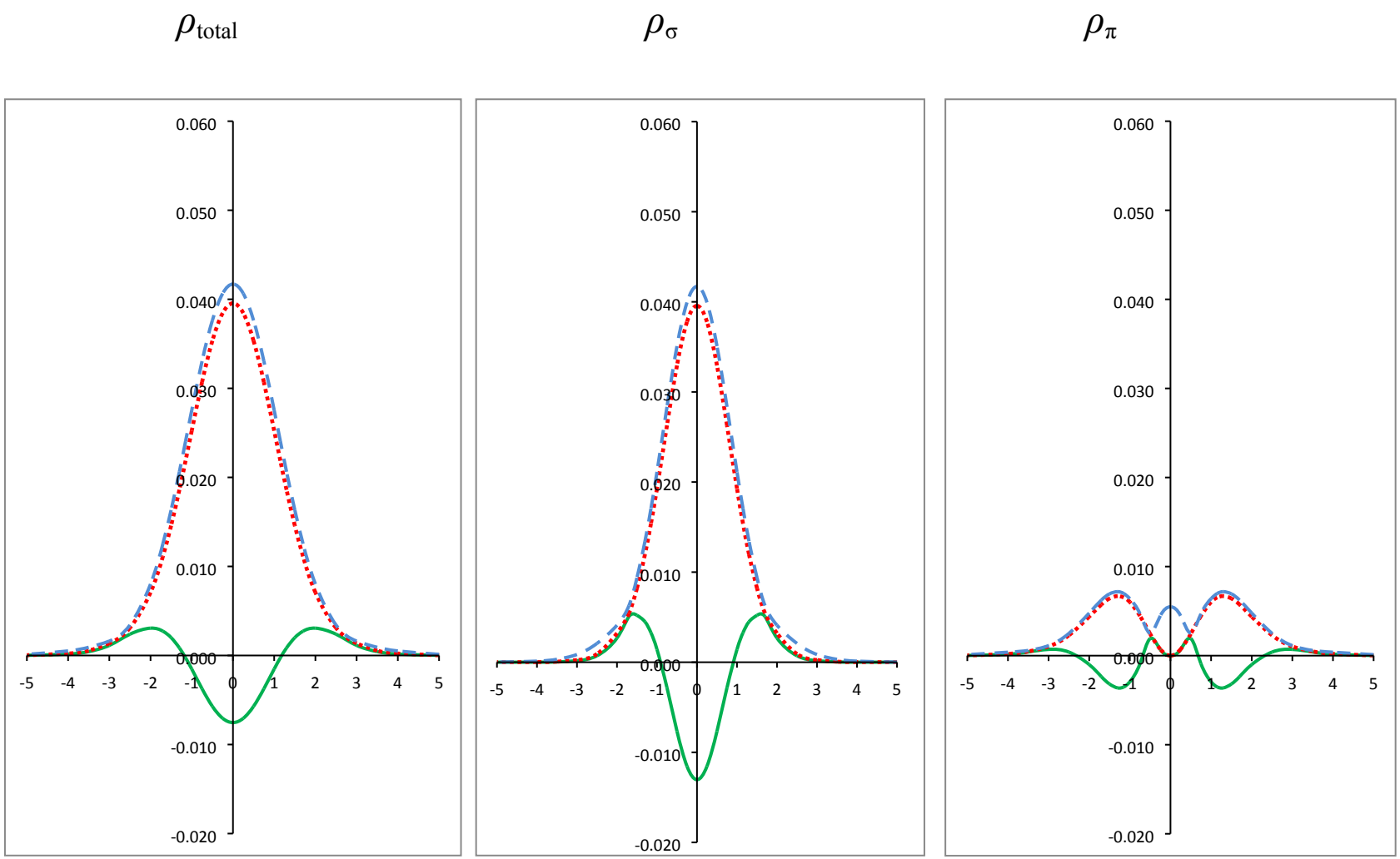
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_6H_6**AlH**.



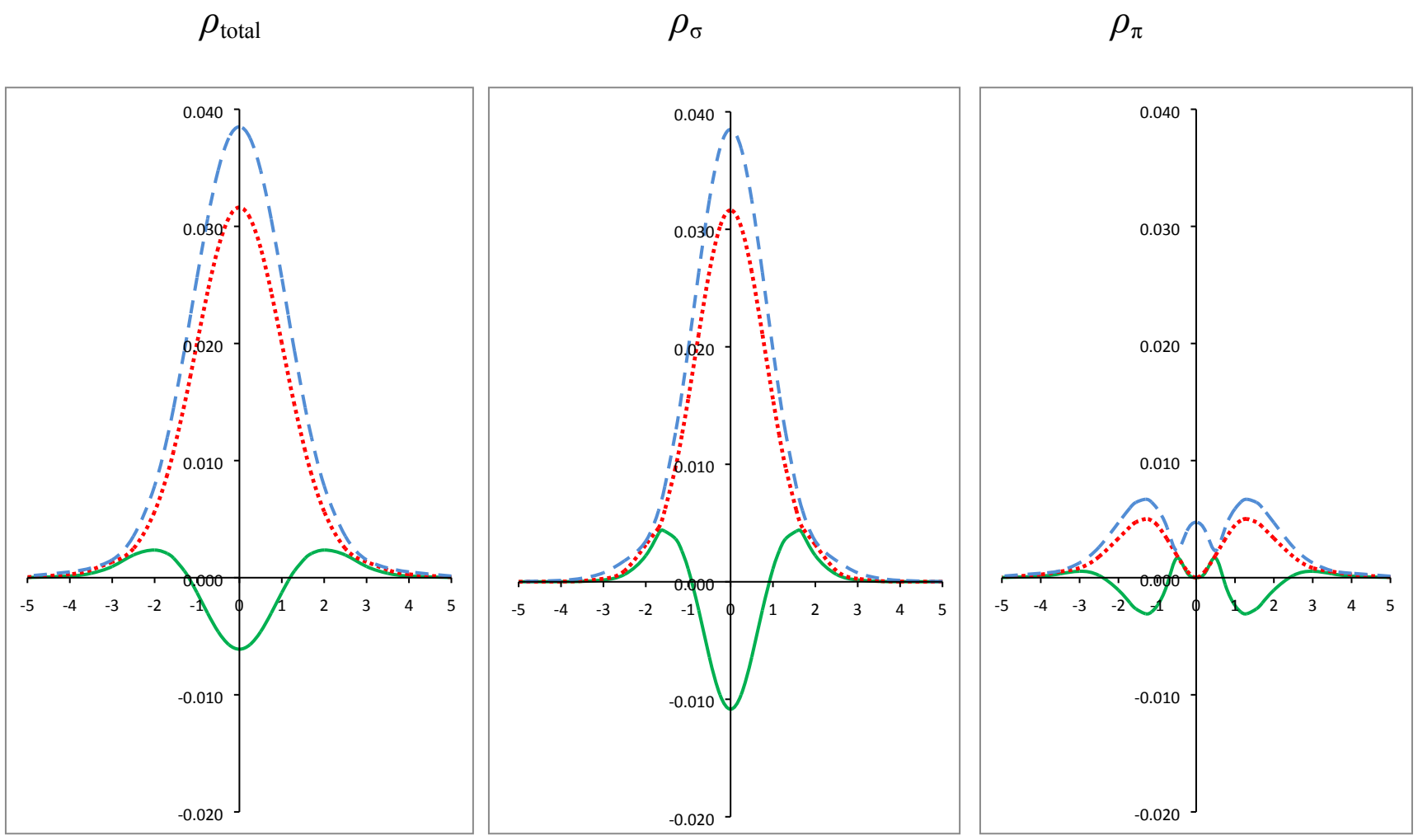
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_6H_6**SiH**$^+$.



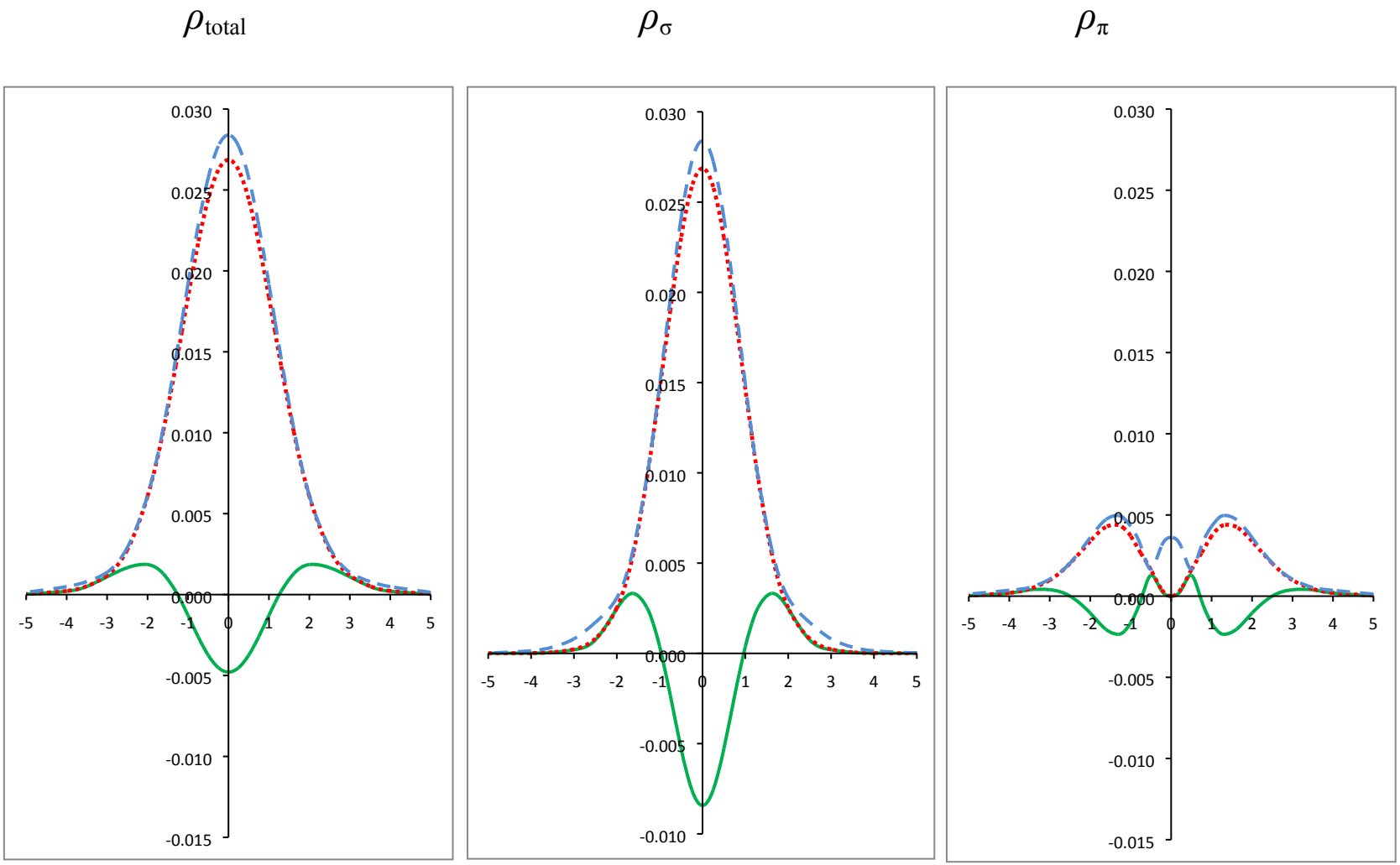
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_6H_6\mathbf{N}^+$.



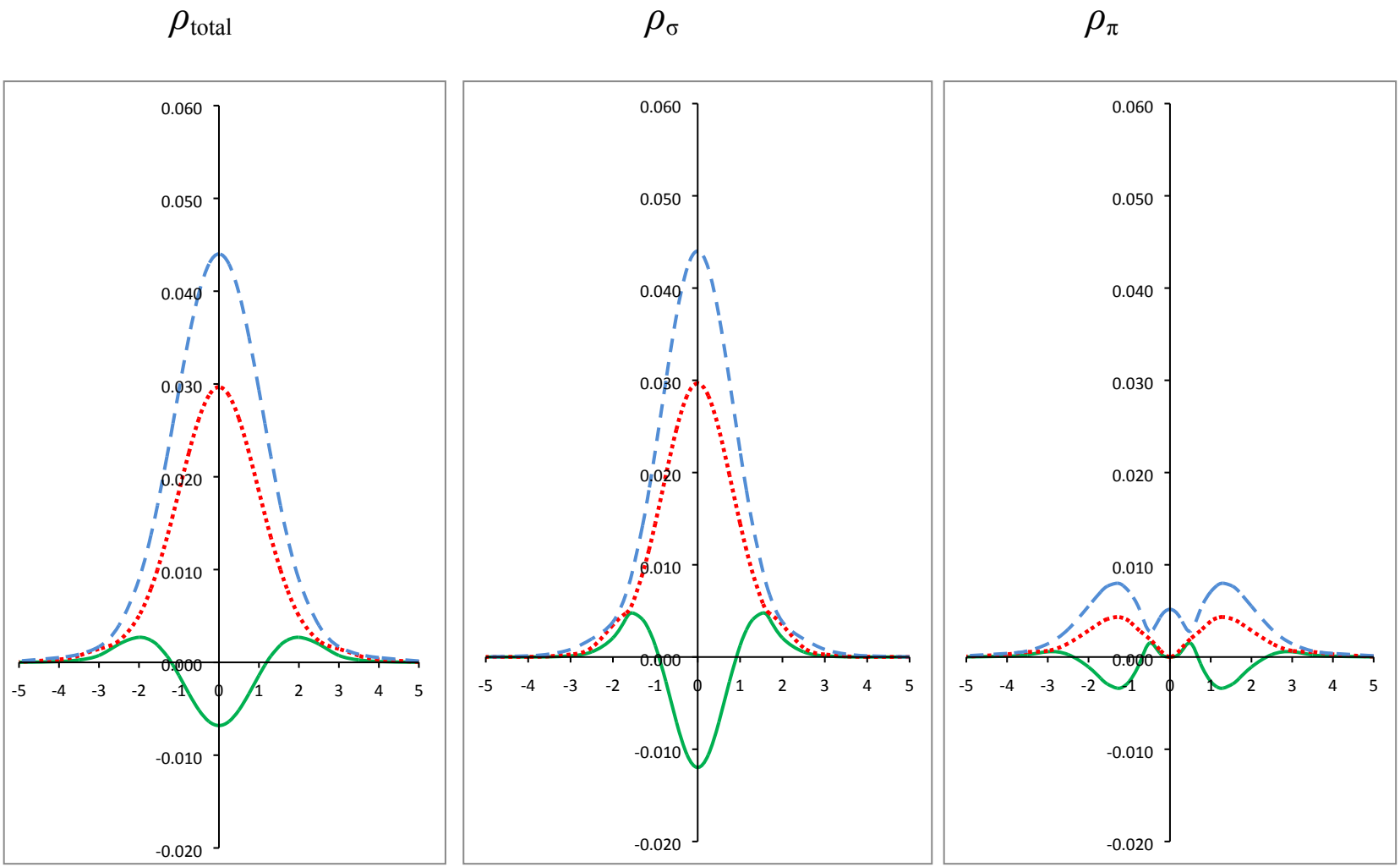
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_6H_6**NH**.



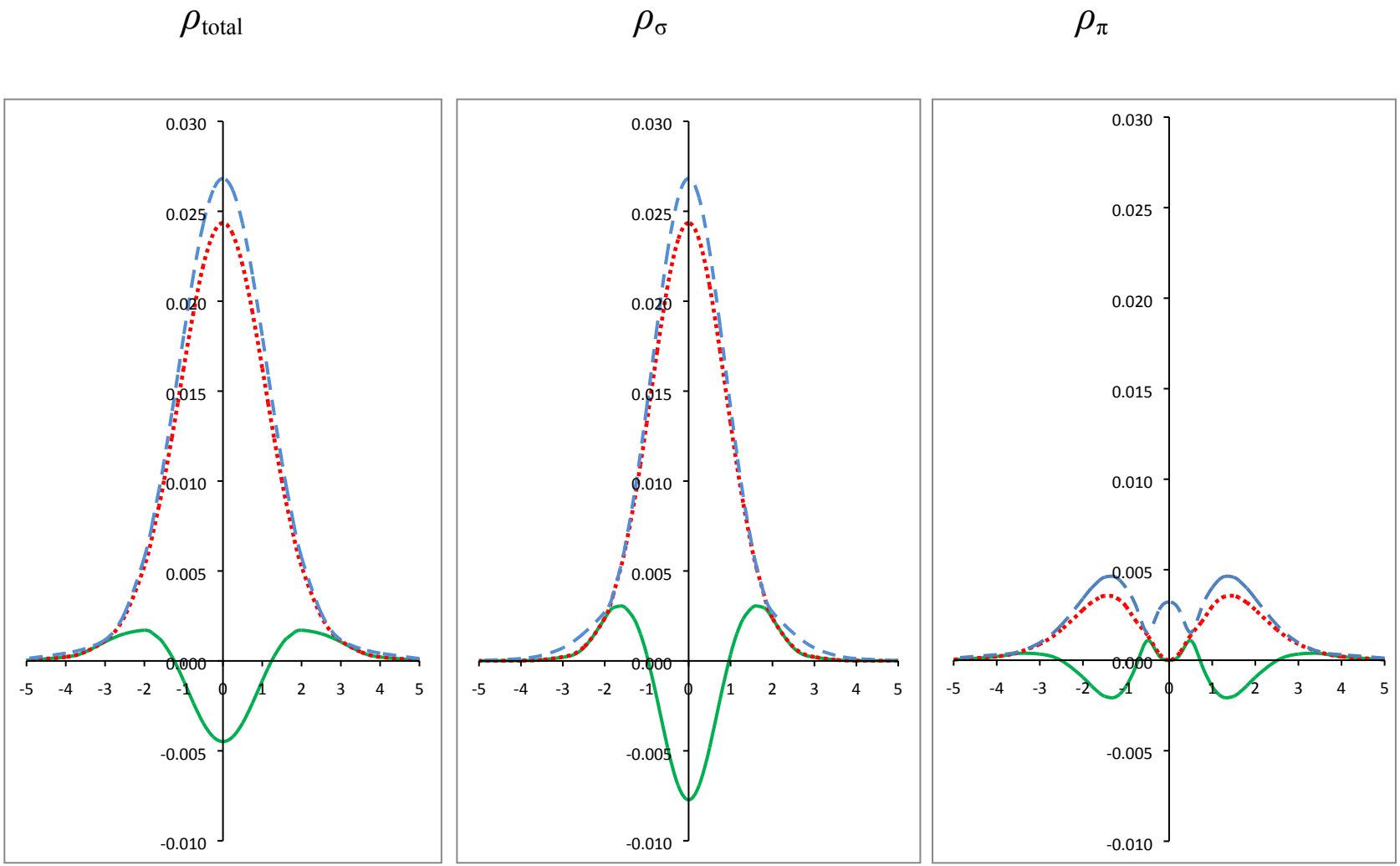
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_6H_6\mathbf{P}^+$.



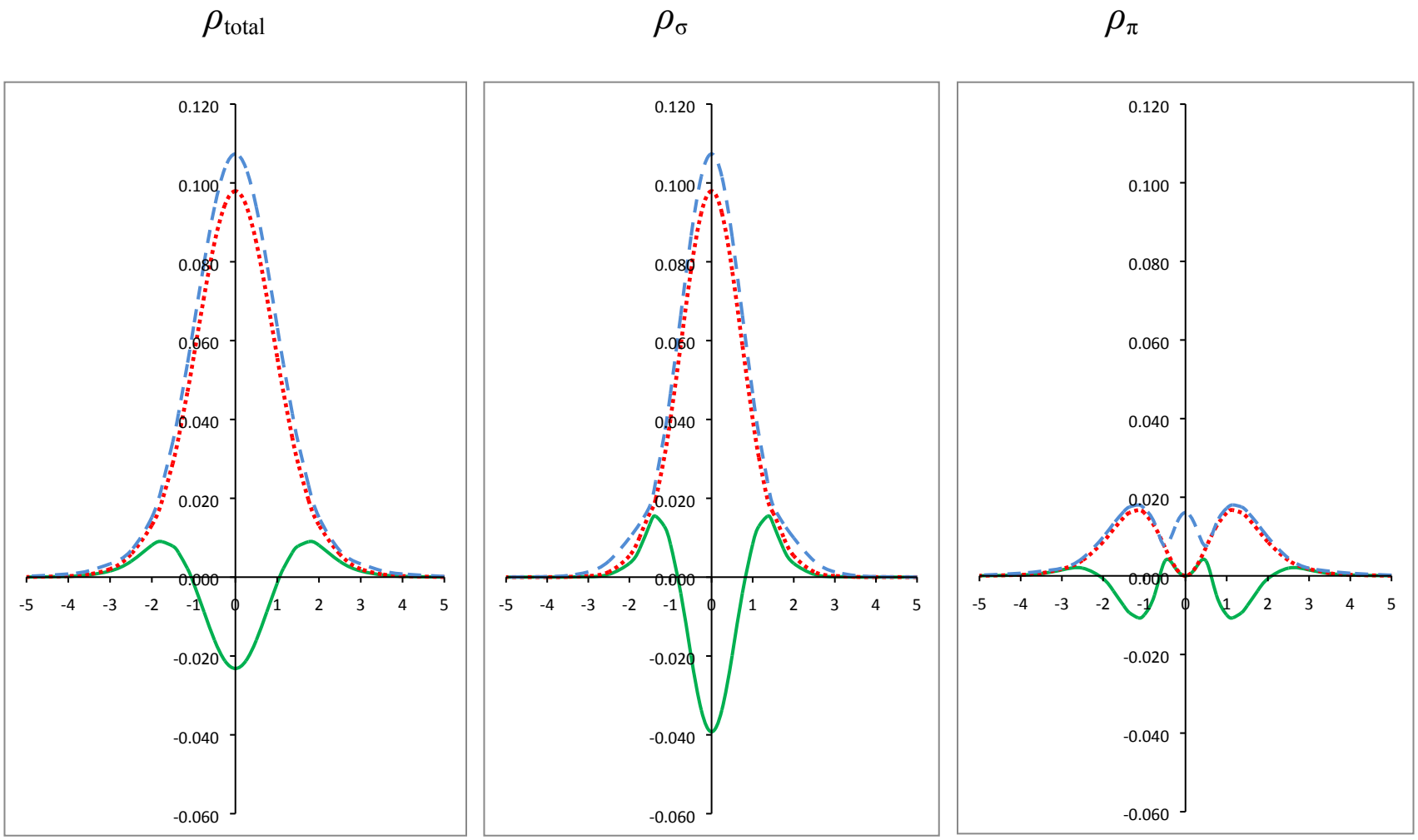
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_6H_6\mathbf{O}$.



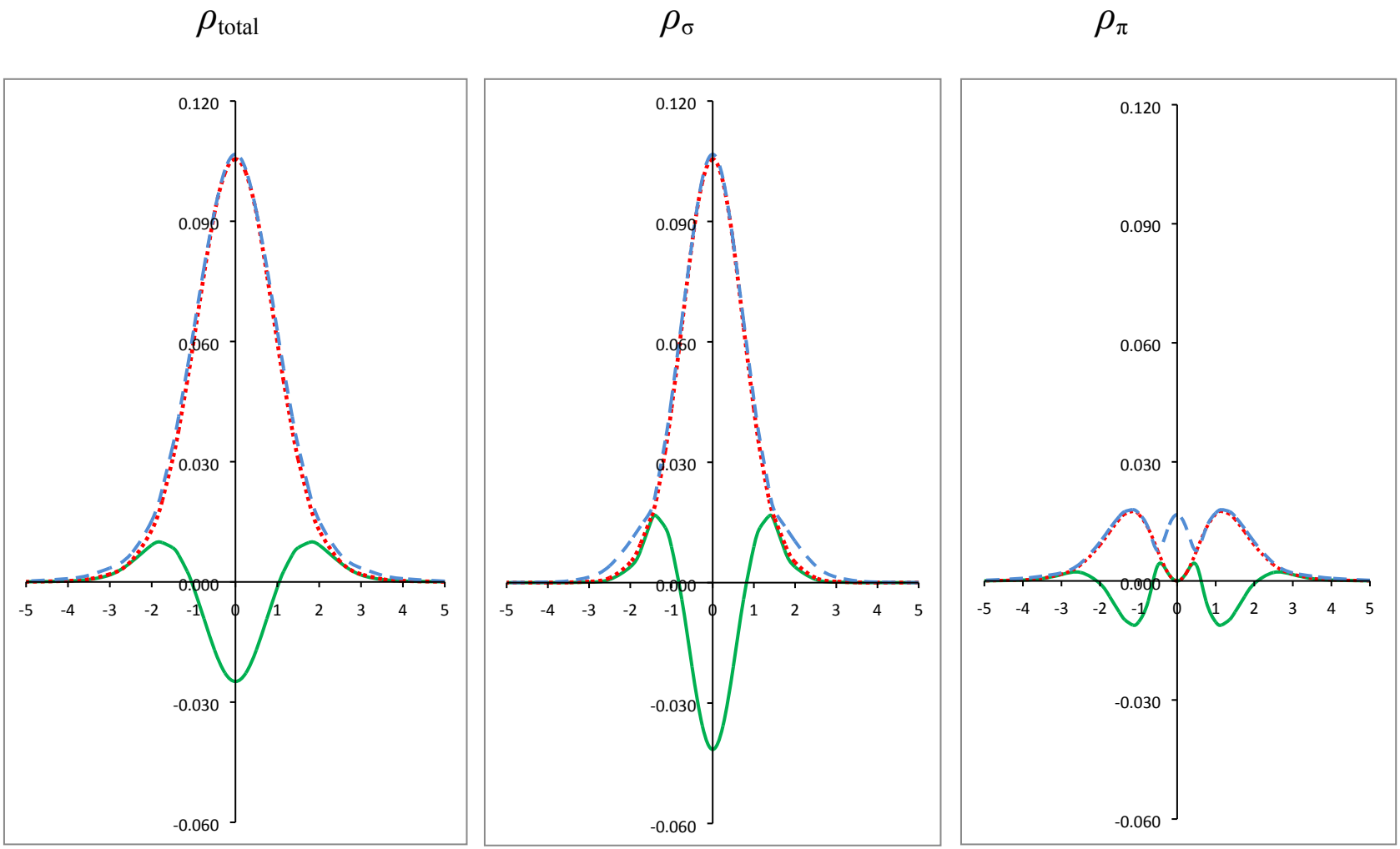
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of C_6H_6**S**.



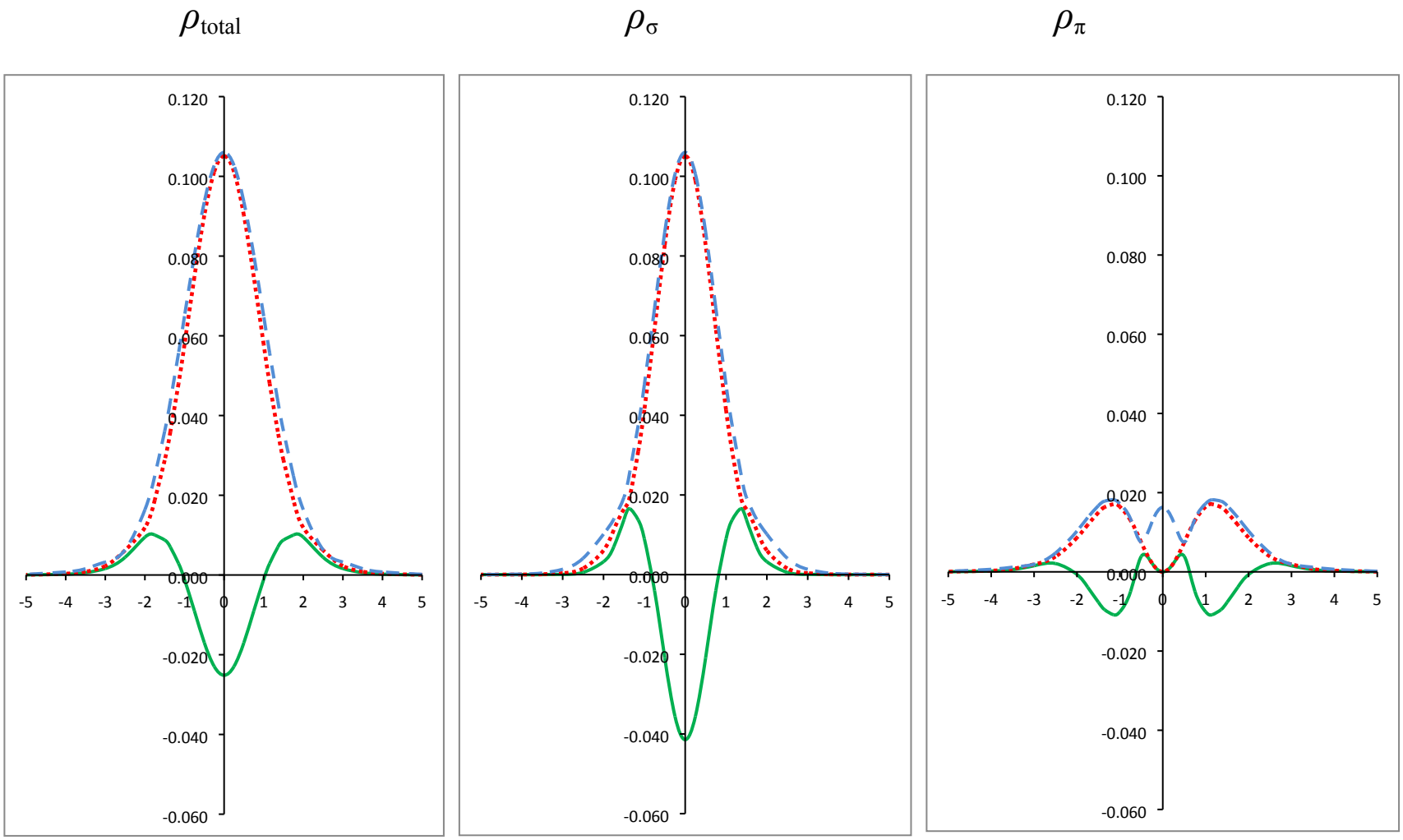
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of Pyridazine.



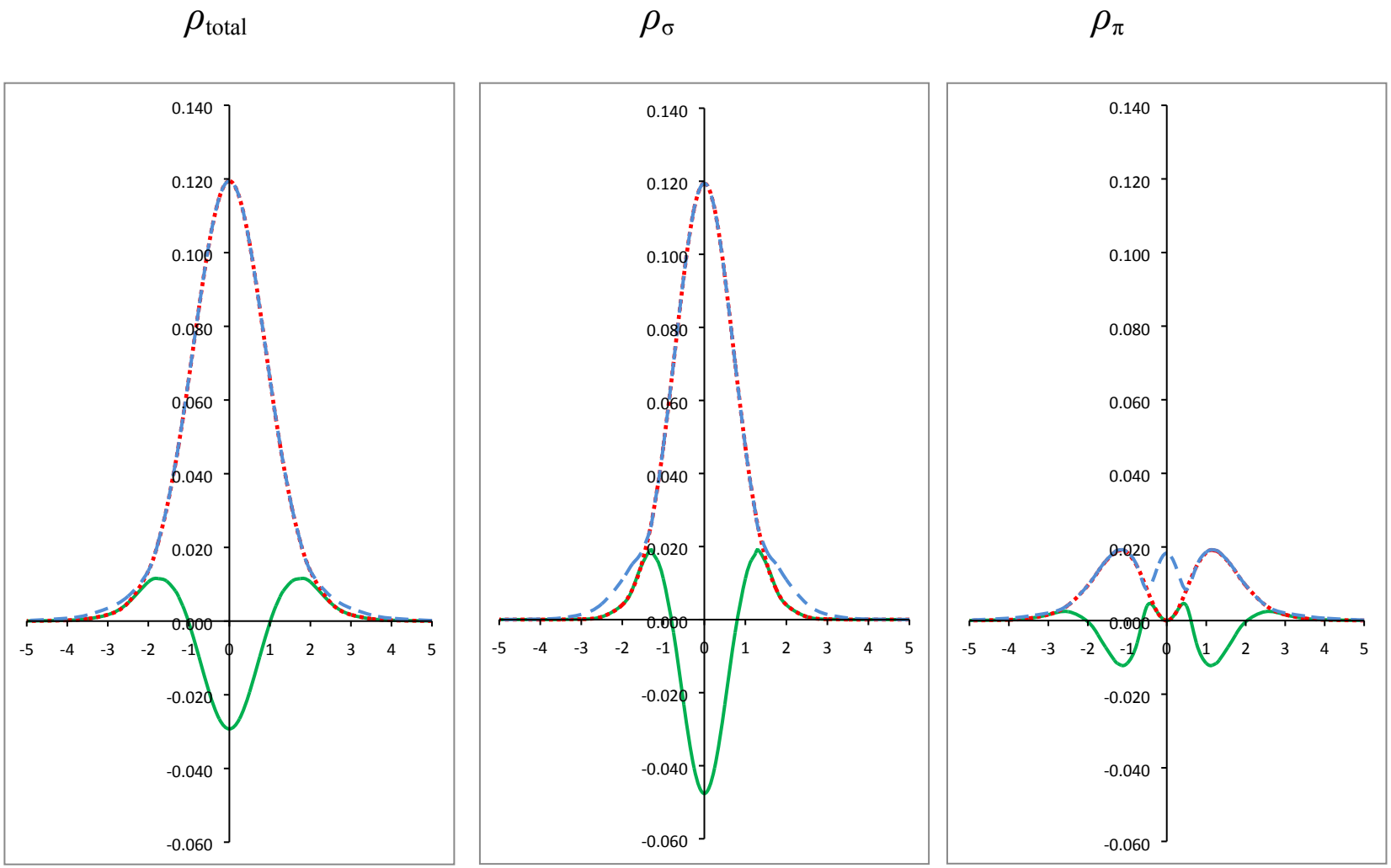
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of Pyrimidine.



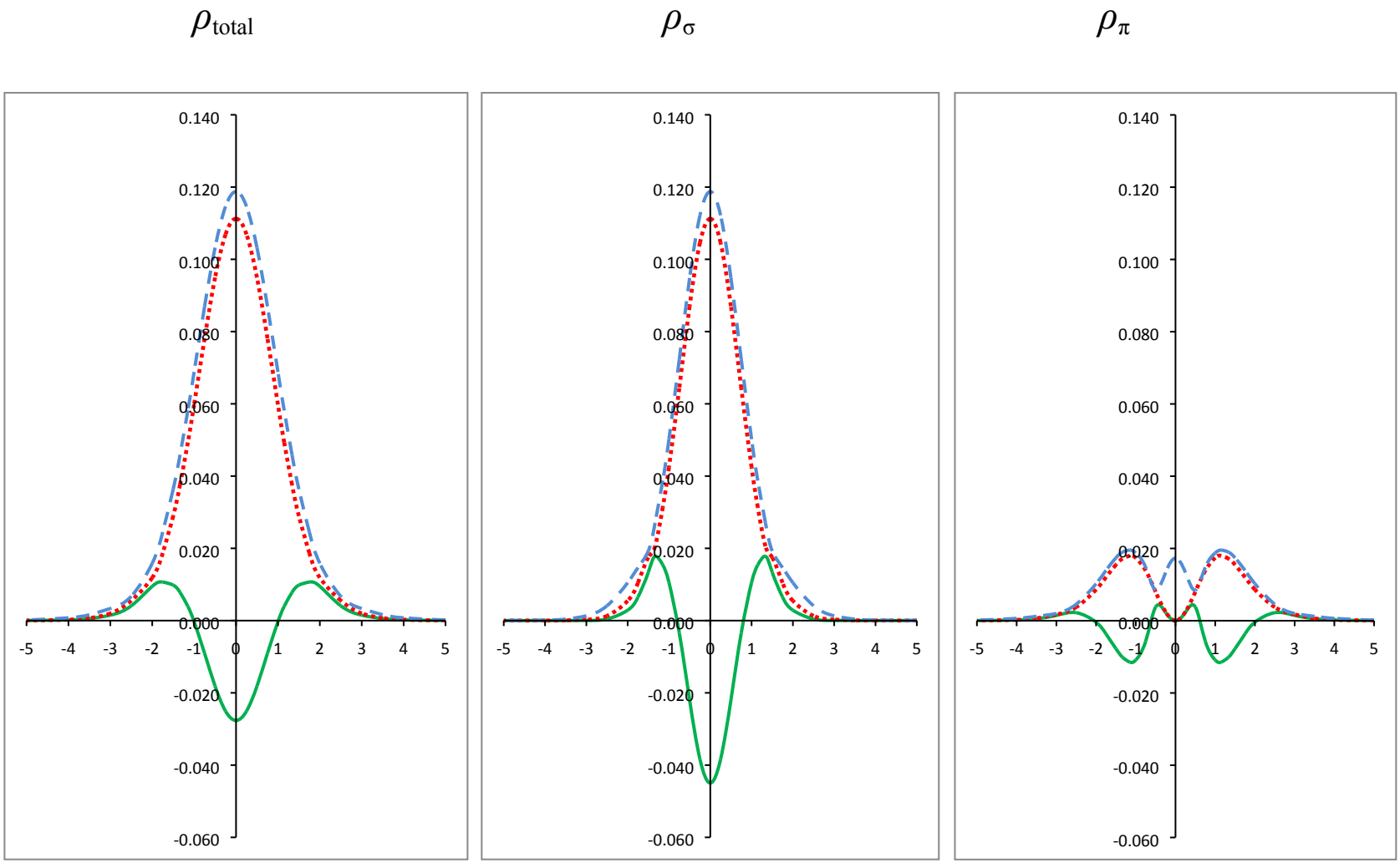
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of Pyrazine.



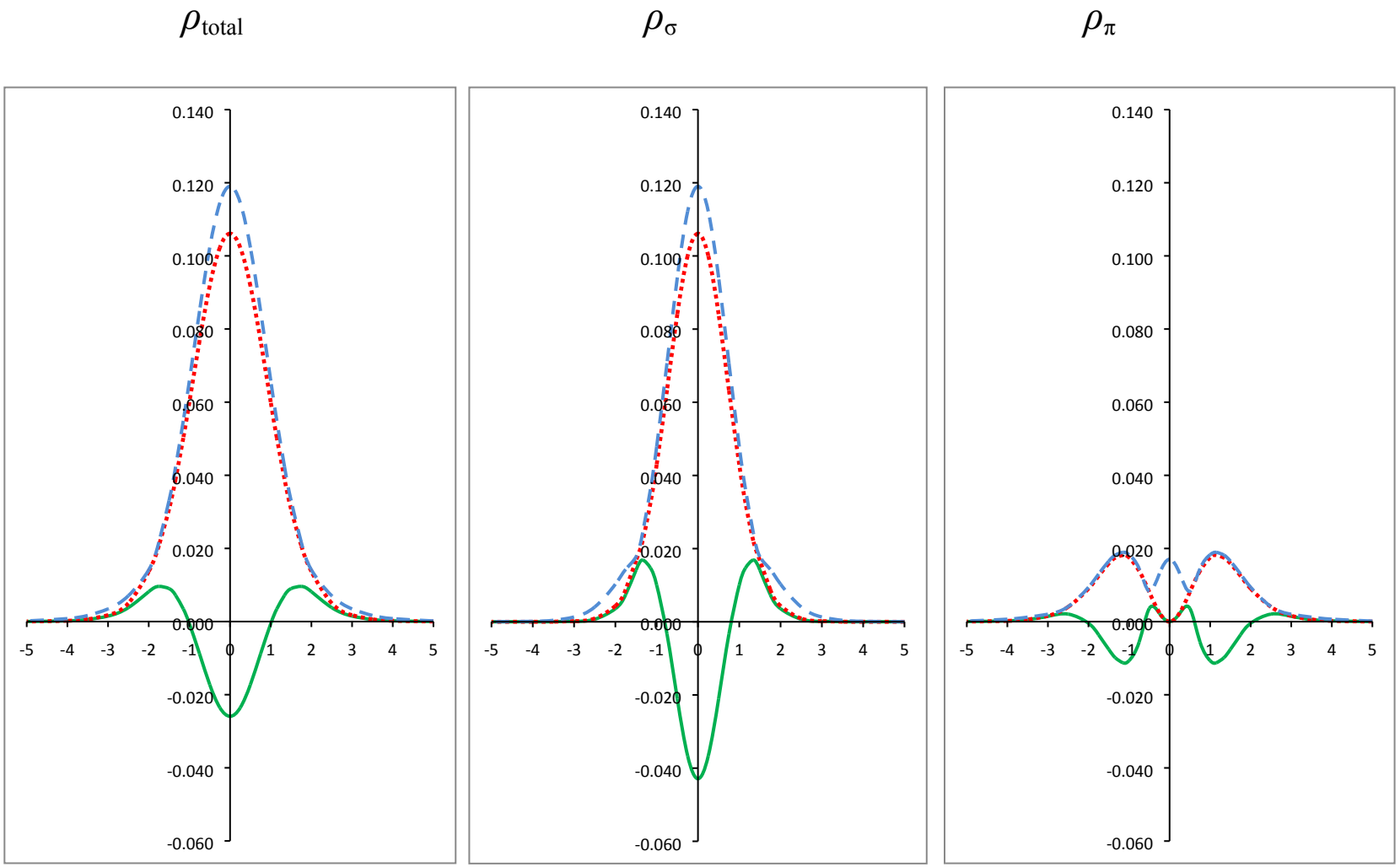
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of 1,3,5-Triazine.



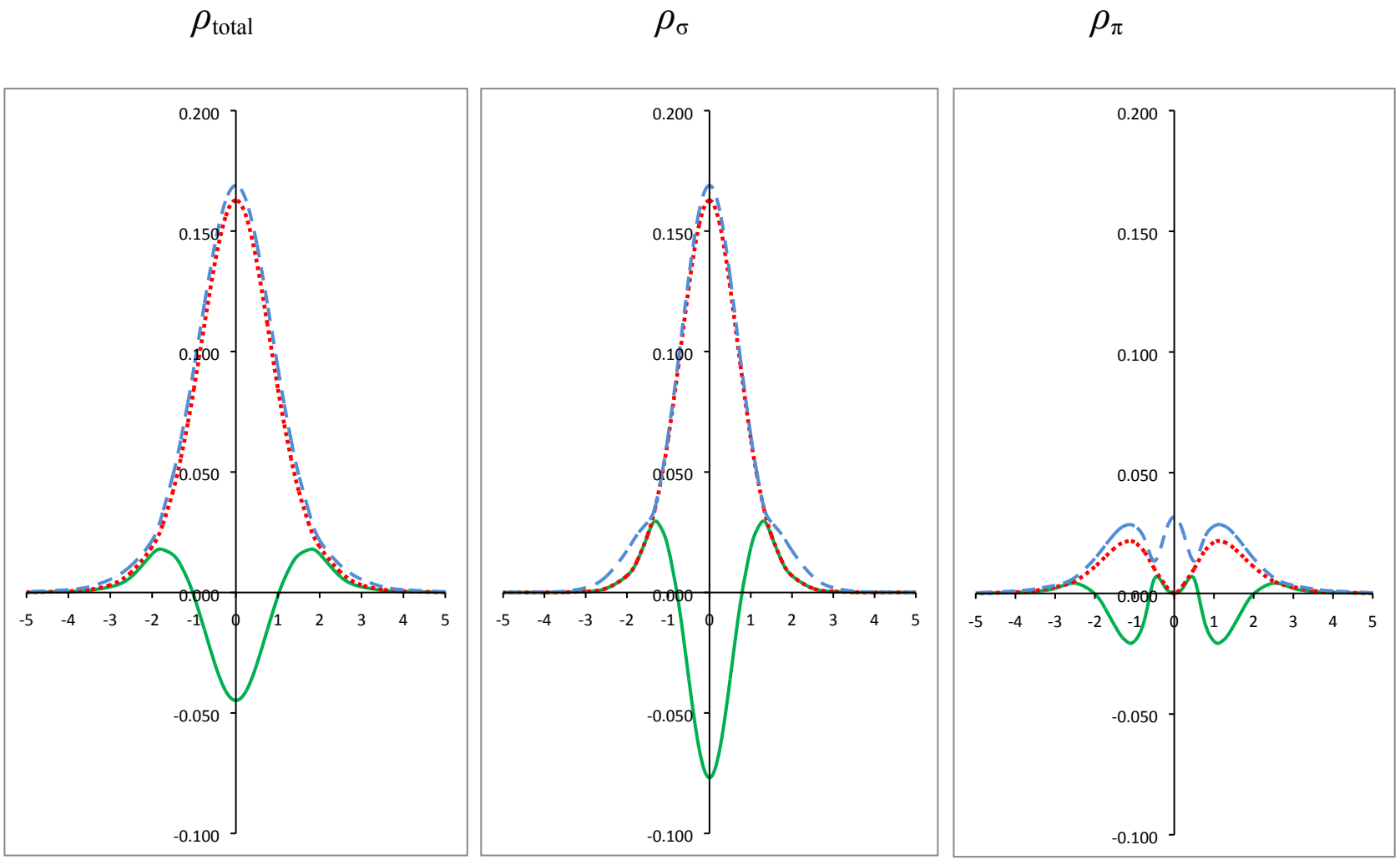
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of 1,2,4-Triazine.



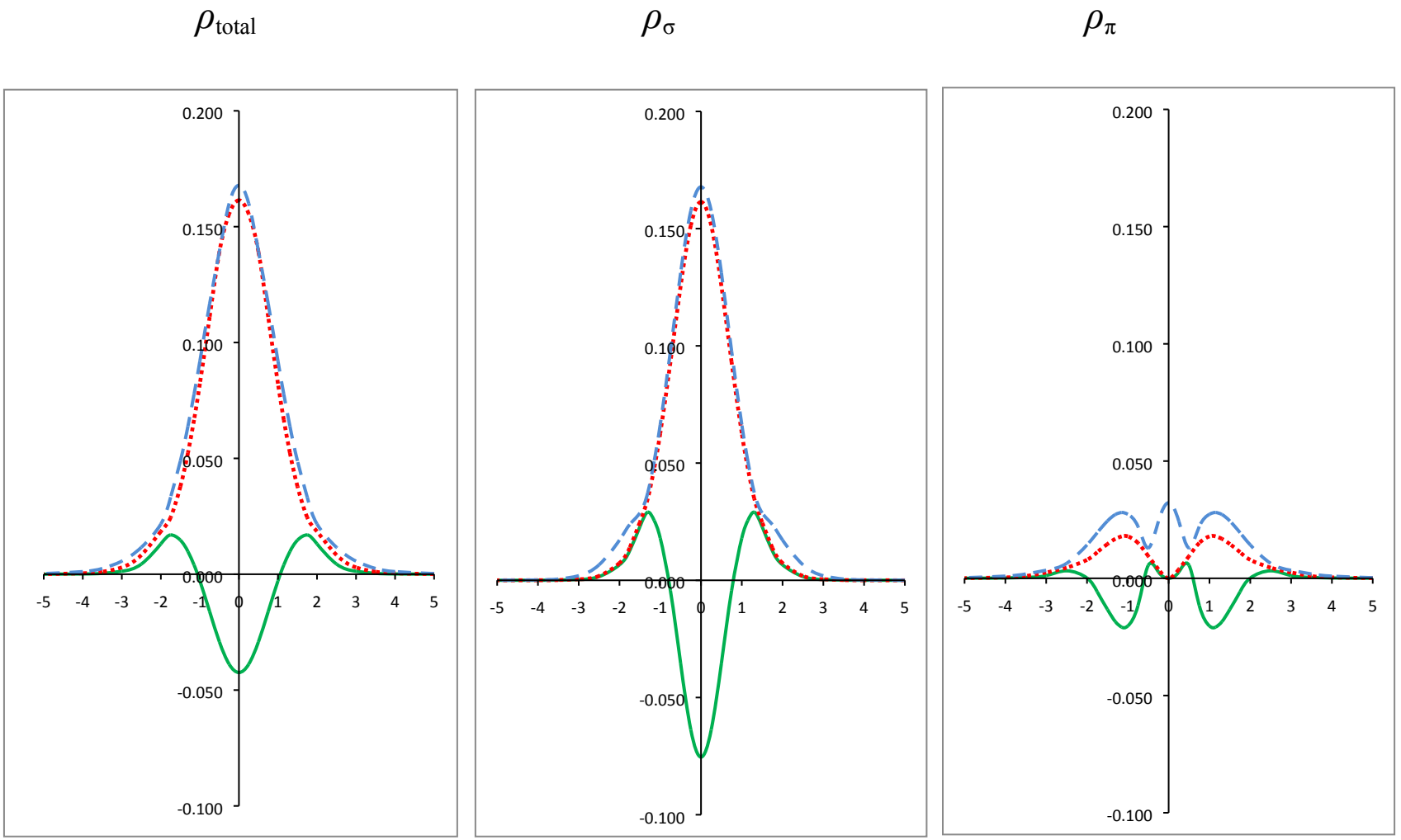
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of 1,2,3-Triazine.



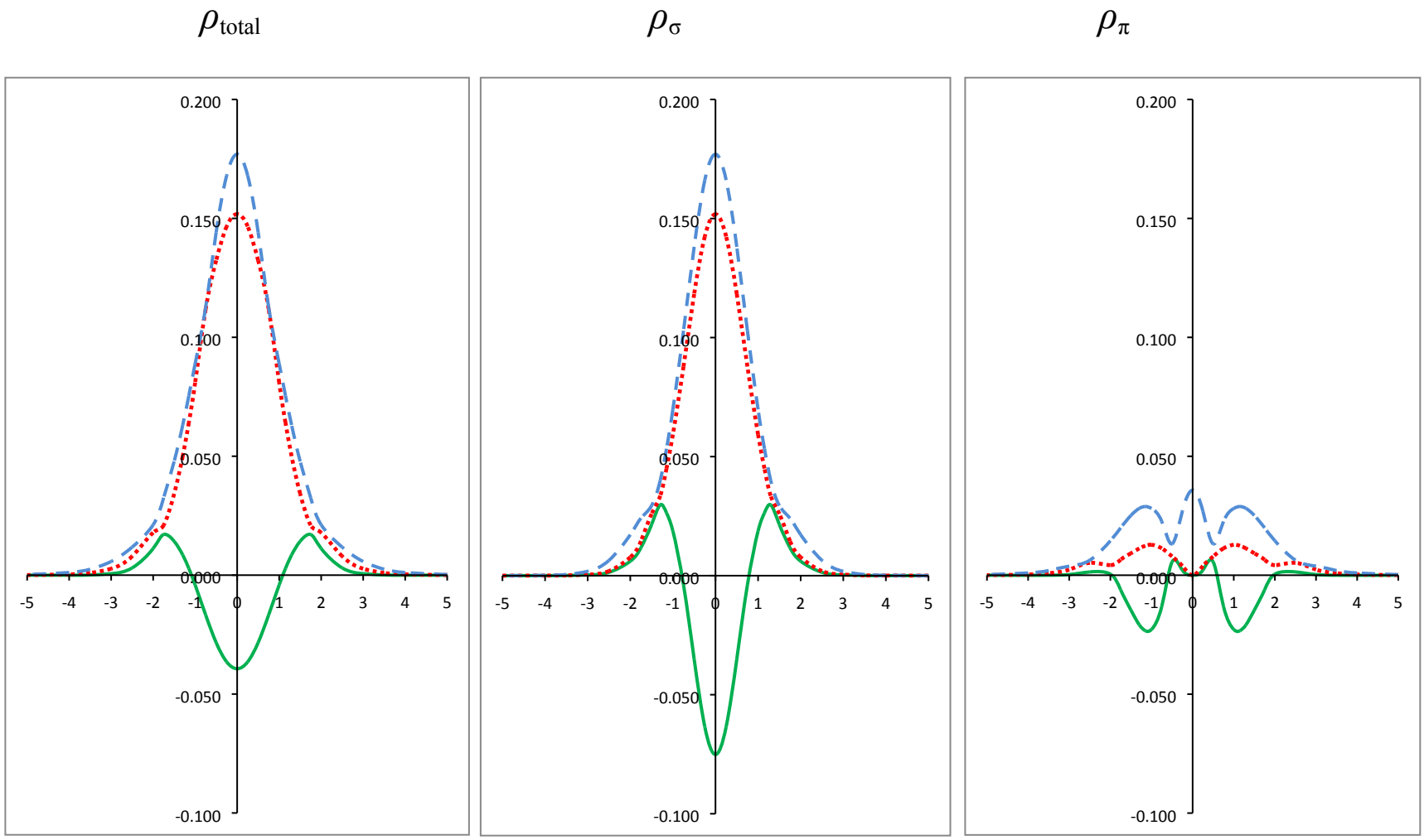
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_4\mathbf{BH_2}^-$.



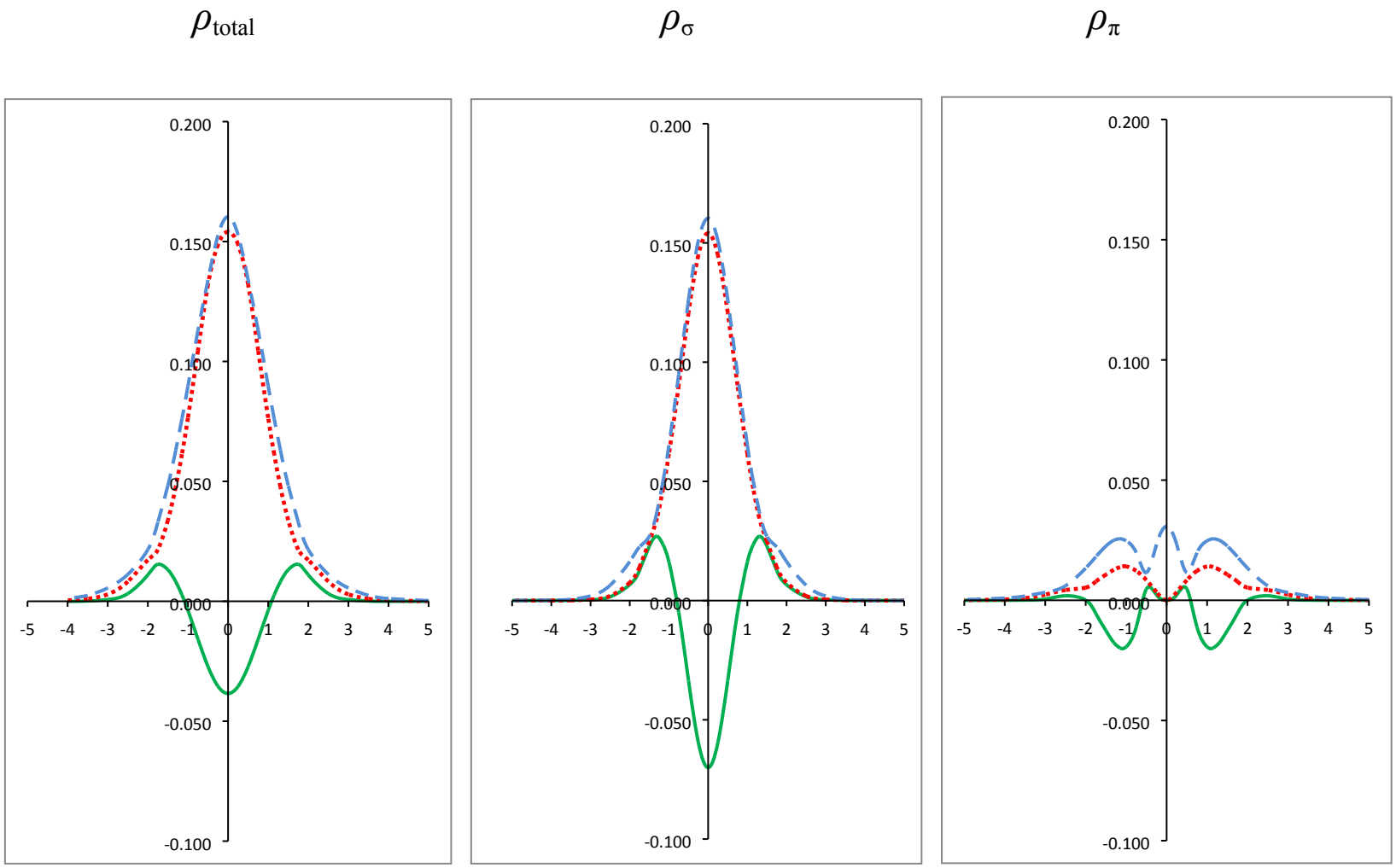
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_4\mathbf{CH_2}$.



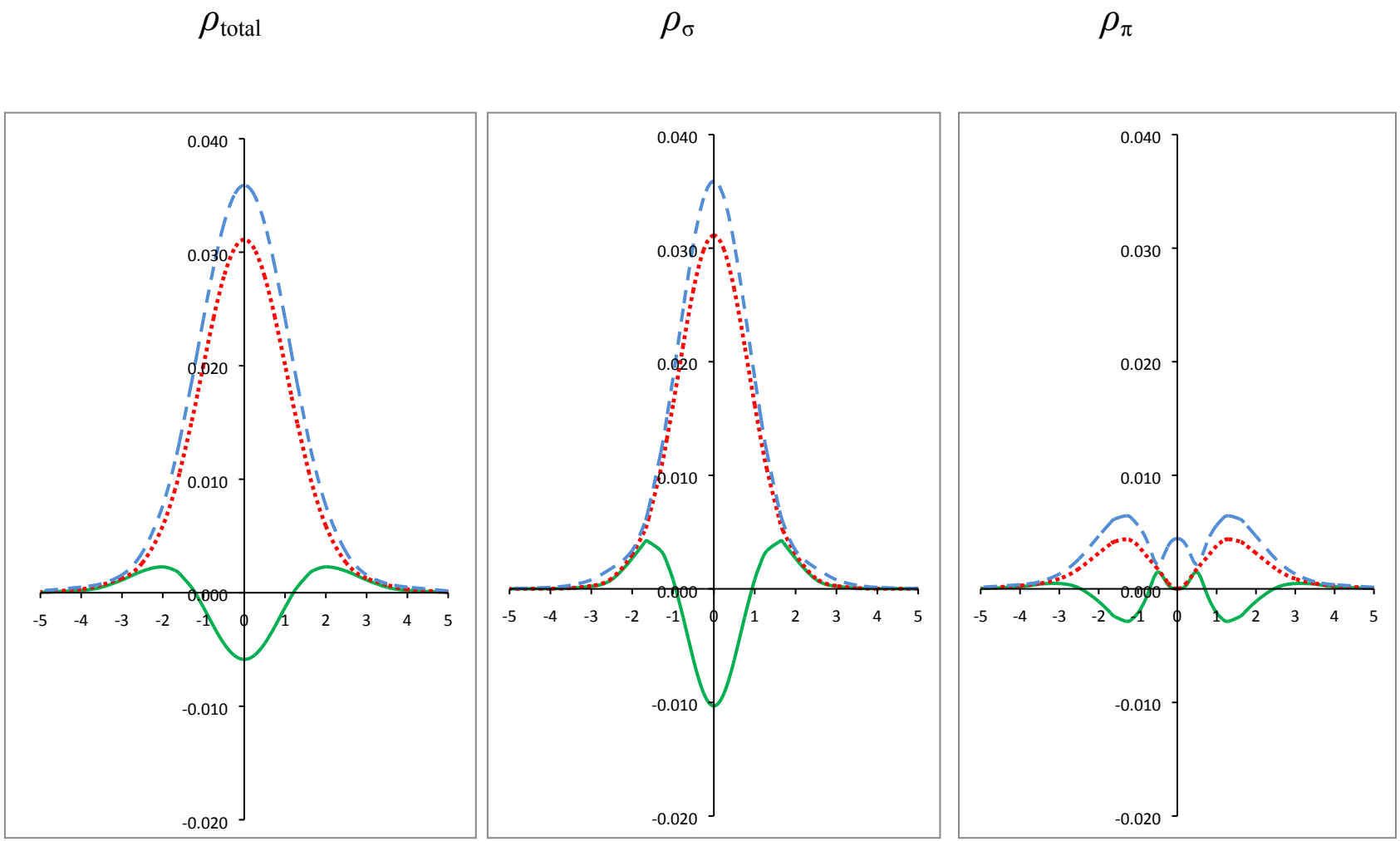
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_4\mathbf{NH_2}^+$.



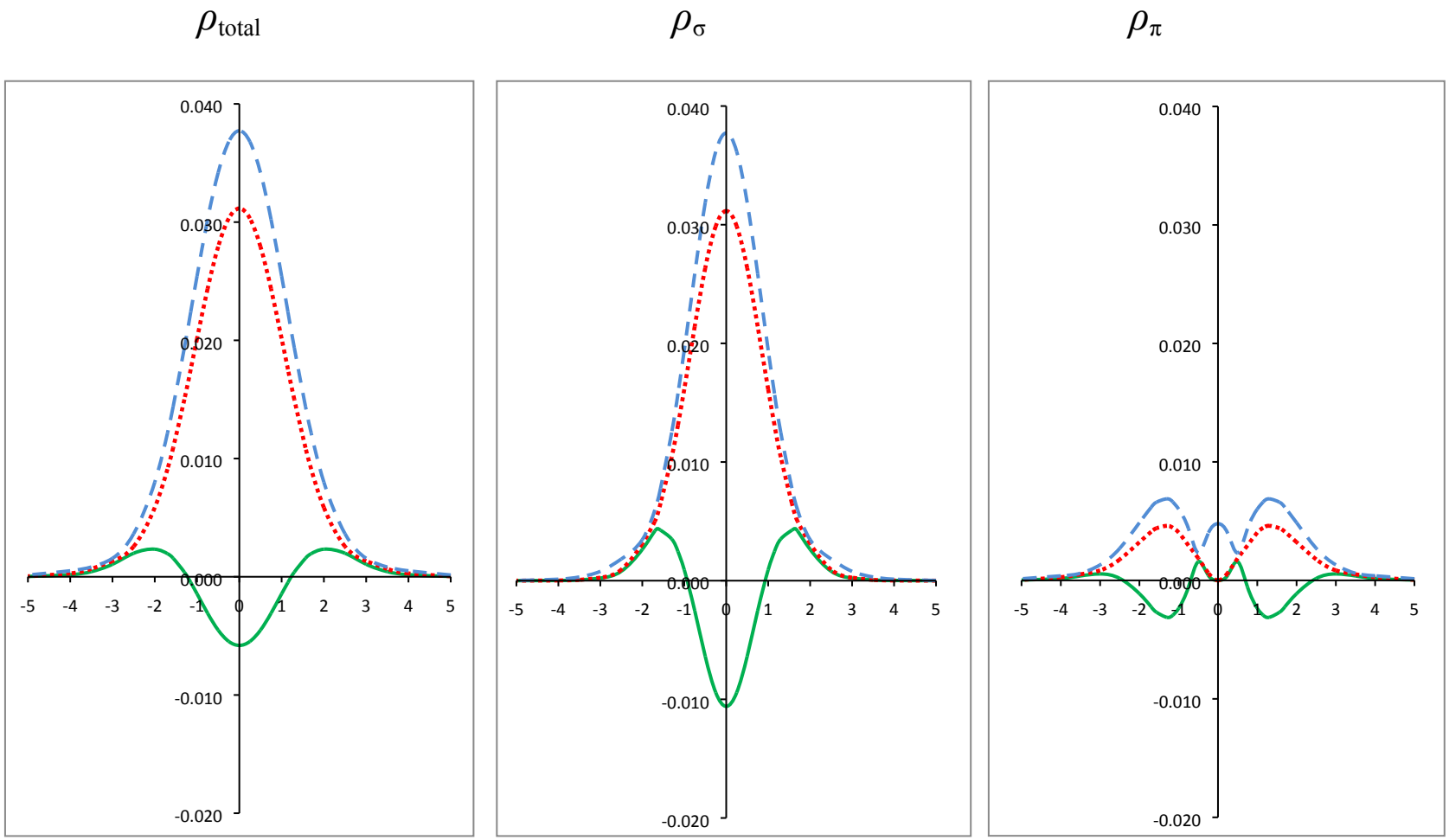
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_5H_4\mathbf{O}$.



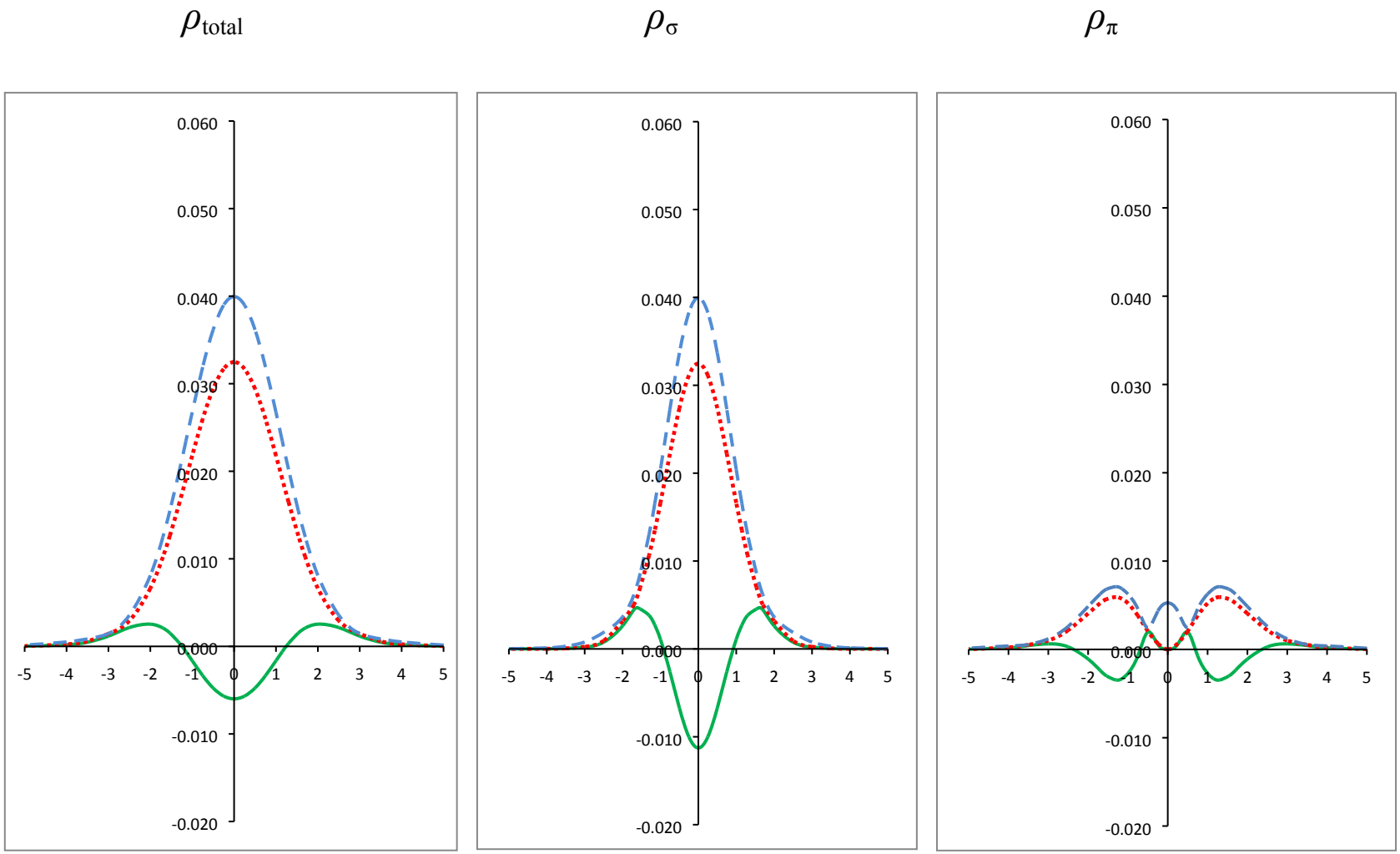
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_7H_6\mathbf{BH_2}^-$.



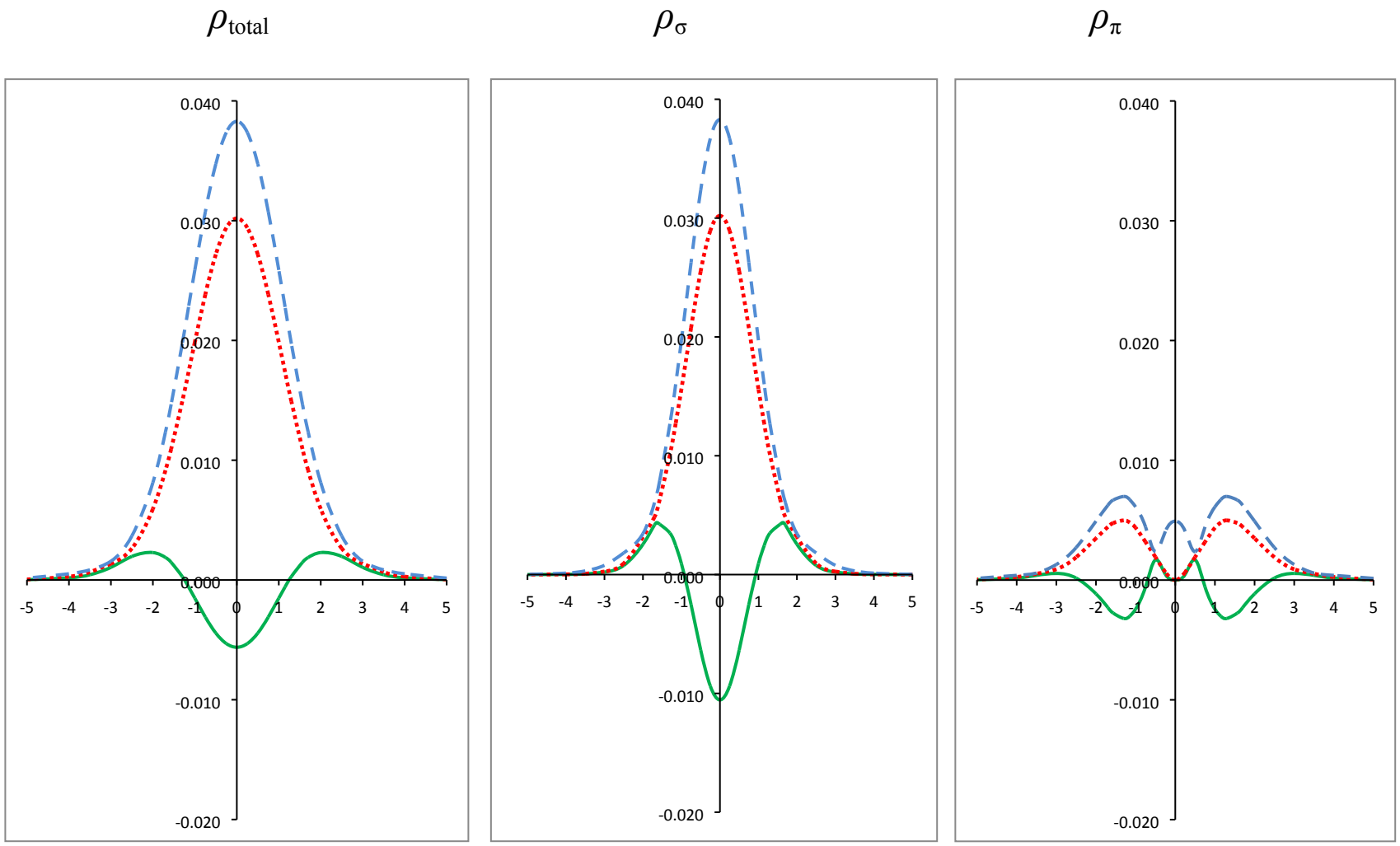
F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_7H_6\mathbf{CH_2}$.



F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_7H_6\mathbf{NH_2}^+$.



F2 (continued). The plot of Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} versus distance (horizontal axis) from the ring center of $C_7H_6\mathbf{O}$.



S1.

An ellipse in canonical position (center at origin, here center at scanned points along the axis perpendicular to the ring plane), can be expressed *parametrically* as the path of a point $(X(u),Y(u))$, where

$$X(u) = \lambda_2 \, \mathrm{Sin}u$$

$$Y(u) = \lambda_3 \, \mathrm{Cos}u$$

Note that the parameter u (called the eccentric anomaly in astronomy) is an angularparameter that defines the position of the point $(X(u),Y(u))$ that is moving along an ellipticorbit.

In Figure 3, the anisotropy of electron density at scanned points has been shown by the ratio of the two positive eigenvalues, λ_2 andλ_3, as a parametric form of the equation of an ellipse.

T1. The electron density values of total electron density (ρ_{total}) and its σ- and π-components (ρ_σ and ρ_π) at the RCP for all studied compounds, in atomic units. These values are maximum values of electron density along the scan axis.

NAME	$\rho_{RCP,Total}$	$\rho_{RCP,\sigma}$	$\rho_{RCP,\pi}$
$C_6H_6SiH^+$	0.007624	0.007624	0.001551
$C_6H_6P^+$	0.008283	0.008283	0.001587
C_6H_6S	0.007600	0.007600	0.001428
$C_4H_4BH_2^-$	0.050473	0.050473	0.009259
C_4H_4BH	0.044024	0.044024	0.006868
$C_4H_4CH_2$	0.049669	0.049669	0.009235
C_4H_4AlH	0.028570	0.028570	0.003260
$C_4H_4NH_2^+$	0.049473	0.049473	0.010149
C_4H_4NH	0.053534	0.053534	0.010374
C_4H_4O	0.047024	0.047024	0.008779
$C_4H_4BH_2^-$	0.055592	0.055592	0.010412
$C_4H_4SiH_2$	0.009514	0.009514	0.001870
$C_4H_4CH_2$	0.037078	0.037078	0.007236
$C_4H_4SiH_2$	0.009634	0.009634	0.001972
$C_4H_4NH_2^+$	0.035587	0.035587	0.007142
$C_4H_4PH_2$	0.010048	0.010048	0.003096
C_4H_4O	0.041174	0.041174	0.008317
C_4H_4S	0.009591	0.009591	0.003025
Pyridazine	0.042739	0.042739	0.008044
$C_5H_5BH^+$	0.027707	0.027707	0.005061
Pyrimidine	0.021214	0.021214	0.004100
$C_5H_5NH^+$	0.029249	0.029249	0.005234
Pyrazine	0.025094	0.025094	0.004908
C_5H_5N	0.029068	0.029068	0.005107
1,3,5-Triazine	0.026565	0.026565	0.004979
$C_5H_5O^+$	0.032238	0.032238	0.005517
1,2,4-Triazine	0.026007	0.026007	0.004914
$C_5H_5AlH^+$	0.030411	0.030411	0.005253
1,2,3-Triazine	0.014091	0.014091	0.002803
$C_5H_5SiH^+$	0.029068	0.029068	0.005174
C_5H_5P	0.017387	0.017387	0.003554
$C_5H_5S^+$	0.019360	0.019360	0.003675
C_6H_6BH	0.020126	0.020126	0.003778
C_6H_6NH	0.009378	0.009378	0.001847
$C_6H_6N^+$	0.009619	0.009619	0.001915
C_6H_6O	0.011343	0.011343	0.002100
C_6H_6AlH	0.010564	0.010564	0.002058
	0.006550	0.006550	0.001206

T2. The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_4H_4**BH**. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.0000686	-0.0000155	0.0000506	0.0002214	0.0000049	0.0000009	0.0000018	0.0000293	0.0000918	-0.0000125	0.0000629	0.0002962
4.00	0.0003748	-0.0000705	0.0002971	0.0008833	0.0000477	0.0000191	0.0000288	0.0002477	0.0005189	-0.0000233	0.0003990	0.0012631
3.00	0.0015990	-0.0002277	0.0017772	0.0024033	0.0004401	0.0003599	0.0004575	0.0023834	0.0024396	0.0005843	0.0028298	0.0053644
2.50	0.0029512	-0.0001890	0.0027086	0.0043231	0.0013605	0.0016478	0.0018984	0.0067906	0.0051110	0.0025781	0.0078980	0.0100194
2.00	0.0048666	-0.0000888	0.0007456	0.0090564	0.0040299	0.0067397	0.0069815	0.0155696	0.0102527	0.0088516	0.0145998	0.0203787
1.75	0.0058629	-0.0038303	0.0017808	0.0119060	0.0066574	0.0125925	0.0126677	0.0206278	0.0140786	0.0131832	0.0171321	0.0309856
1.50	0.0066279	-0.0091154	0.0031195	0.0143657	0.0105562	0.0216516	0.0224730	0.0239287	0.0187701	0.0112875	0.0268668	0.0450601
1.30	0.0068683	-0.0134233	0.0041544	0.0154960	0.0148249	0.0229883	0.0327274	0.0342807	0.0231320	0.0067231	0.0387637	0.0590663
1.15	0.0067228	-0.0154301	0.0046914	0.0155293	0.0184562	0.0194178	0.0427521	0.0450924	0.0264264	0.0020860	0.0492722	0.0702135
1.00	0.0062436	-0.0155916	0.0049562	0.0147327	0.0226175	0.0125099	0.0550121	0.0582837	0.0298604	-0.0036585	0.0616560	0.0823605
0.75	0.0047127	-0.0097356	0.0046058	0.0114802	0.0300543	-0.0063730	0.0788226	0.0838684	0.0353297	-0.0144294	0.0845399	0.1028521
0.50	0.0026153	0.0014293	0.0052984	0.0065930	0.0370640	-0.0309869	0.1033389	0.1102276	0.0399037	-0.0247030	0.1068381	0.1211081
0.25	0.0007511	0.0008271	0.0020069	0.0187378	0.0421539	-0.0526324	0.1223191	0.1306771	0.0429528	-0.0320678	0.1233931	0.1338624
0.00	0.0000000	0.0000000	0.0000113	0.0252117	0.0440241	-0.0613405	0.1295308	0.1384601	0.0440241	-0.0347353	0.1295314	0.1384610
-0.25	0.0007511	0.0008271	0.0020069	0.0187378	0.0421539	-0.0526324	0.1223191	0.1306771	0.0429528	-0.0320678	0.1233931	0.1338624
-0.50	0.0026153	0.0014293	0.0052984	0.0065930	0.0370640	-0.0309869	0.1033389	0.1102276	0.0399037	-0.0247030	0.1068381	0.1211081
-0.75	0.0047127	-0.0097356	0.0046058	0.0114802	0.0300543	-0.0063730	0.0788226	0.0838684	0.0353297	-0.0144294	0.0845399	0.1028521
-1.00	0.0062436	-0.0155916	0.0049562	0.0147327	0.0226175	0.0125099	0.0550121	0.0582837	0.0298604	-0.0036585	0.0616560	0.0823605
-1.15	0.0067228	-0.0154301	0.0046914	0.0155293	0.0184562	0.0194178	0.0427521	0.0450924	0.0264264	0.0020860	0.0492722	0.0702135
-1.30	0.0068683	-0.0134233	0.0041544	0.0154960	0.0148249	0.0229883	0.0327274	0.0342807	0.0231320	0.0067231	0.0387637	0.0590663
-1.50	0.0066279	-0.0091154	0.0031195	0.0143657	0.0105562	0.0216516	0.0224730	0.0239287	0.0187701	0.0112875	0.0268668	0.0450601
-1.75	0.0058629	-0.0038303	0.0017808	0.0119060	0.0066574	0.0125925	0.0126677	0.0206278	0.0140786	0.0131832	0.0171321	0.0309856
-2.00	0.0048666	-0.0000888	0.0007456	0.0090564	0.0040299	0.0067397	0.0069815	0.0155696	0.0102527	0.0088516	0.0145998	0.0203787
-2.50	0.0029512	-0.0001890	0.0027086	0.0043231	0.0013605	0.0016478	0.0018984	0.0067906	0.0051110	0.0025781	0.0078980	0.0100194
-3.00	0.0015990	-0.0002277	0.0017772	0.0024033	0.0004401	0.0003599	0.0004575	0.0023834	0.0024396	0.0005843	0.0028298	0.0053644
-4.00	0.0003748	-0.0000705	0.0002971	0.0008833	0.0000477	0.0000191	0.0000288	0.0002477	0.0005189	-0.0000233	0.0003990	0.0012631
-5.00	0.0000686	-0.0000155	0.0000506	0.0002214	0.0000049	0.0000009	0.0000018	0.0000293	0.0000918	-0.0000125	0.0000629	0.0002962

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_4H_4**AlH**. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00006095	-0.00001209	0.00004317	0.00016837	0.00001990	-0.00000788	0.00000604	0.00007789	0.00010651	-0.00000229	0.00006581	0.00029764
4.00	0.00028460	-0.00004893	0.00024059	0.00059318	0.00012289	-0.00002718	0.00004852	0.00051317	0.00054085	0.00006085	0.00039599	0.00117787
3.00	0.00105844	-0.00016031	0.00114205	0.00126594	0.00076631	0.00010740	0.00056546	0.00285866	0.00231539	0.00083041	0.00243764	0.00407555
2.50	0.00180030	-0.00028298	0.00102318	0.00235800	0.00185996	0.00087079	0.00210419	0.00603759	0.00452293	0.00253768	0.00631442	0.00655087
2.00	0.00266616	-0.00114777	0.00067567	0.00420911	0.00432911	0.00364467	0.00714299	0.01055479	0.00834599	0.00675128	0.00789328	0.01539452
1.75	0.00302247	-0.00258977	0.00190355	0.00505743	0.00641328	0.00651439	0.01226056	0.01234613	0.01097820	0.00699483	0.010415772	0.02287917
1.50	0.00323238	-0.00442427	0.00487106	0.00543304	0.00922187	0.01069874	0.01238234	0.02022063	0.01404078	0.00460216	0.01526612	0.03255747
1.38	0.00326026	-0.00532877	0.00532534	0.00715903	0.01085298	0.01113592	0.01361740	0.02514180	0.01563938	0.00286823	0.01805878	0.03797078
1.15	0.00314955	-0.00667655	0.00445946	0.01310436	0.01435591	0.00706156	0.01955005	0.03640621	0.01874697	-0.00125500	0.02399123	0.04913947
1.00	0.00294400	-0.00697893	0.00343565	0.01774728	0.01686954	0.00259454	0.02408218	0.04499621	0.02076216	-0.00435650	0.02819795	0.05681580
0.75	0.00233410	-0.00572617	0.00135476	0.02401743	0.02113465	-0.00745005	0.03216305	0.06042005	0.02386729	-0.00961980	0.03525205	0.06929150
0.50	0.00140846	-0.00223373	-0.00012078	0.02359211	0.02494611	-0.01874922	0.03977152	0.07502836	0.02637500	-0.01416690	0.04147730	0.07993179
0.25	0.00043801	-0.00025317	0.00057511	0.01751100	0.02761077	-0.02782823	0.04530154	0.08567456	0.02800531	-0.01720652	0.04578988	0.08710432
0.00	0.00000000	0.00000000	0.00000082	0.01518111	0.02857063	-0.03132338	0.04733583	0.08959398	0.02857063	-0.01826886	0.04733583	0.08959543
-0.25	0.00043801	-0.00025317	0.00057511	0.01751100	0.02761077	-0.02782823	0.04530154	0.08567456	0.02800531	-0.01720652	0.04578988	0.08710432
-0.50	0.00140846	-0.00223373	-0.00012078	0.02359211	0.02494611	-0.01874922	0.03977152	0.07502836	0.02637500	-0.01416690	0.04147730	0.07993179
-0.75	0.00233410	-0.00572617	0.00135476	0.02401743	0.02113465	-0.00745005	0.03216305	0.06042005	0.02386729	-0.00961980	0.03525205	0.06929150
-1.00	0.00294400	-0.00697893	0.00343565	0.01774728	0.01686954	0.00259454	0.02408218	0.04499621	0.02076216	-0.00435650	0.02819795	0.05681580
-1.15	0.00314955	-0.00667655	0.00445946	0.01310436	0.01435591	0.00706156	0.01955005	0.03640621	0.01874697	-0.00125500	0.02399123	0.04913947
-1.38	0.00326026	-0.00532877	0.00532534	0.00715903	0.01085298	0.01113592	0.01361740	0.02514180	0.01563938	0.00286823	0.01805878	0.03797078
-1.50	0.00323238	-0.00442427	0.00487106	0.00543304	0.00922187	0.01069874	0.01238234	0.02022063	0.01404078	0.00460216	0.01526612	0.03255747
-1.75	0.00302247	-0.00258977	0.00190355	0.00505743	0.00641328	0.00651439	0.01226056	0.01234613	0.01097820	0.00699483	0.010415772	0.02287917
-2.00	0.00266616	-0.00114777	0.00067567	0.00420911	0.00432911	0.00364467	0.00714299	0.01055479	0.00834599	0.00675128	0.00789328	0.01539452
-2.50	0.00180030	-0.00028298	0.00102318	0.00235800	0.00185996	0.00087079	0.00210419	0.00603759	0.00452293	0.00253768	0.00631442	0.00655087
-3.00	0.00105844	-0.00016031	0.00114205	0.00126594	0.00076631	0.00010740	0.00056546	0.00285866	0.00231539	0.00083041	0.00243764	0.00407555
-4.00	0.00028460	-0.00004893	0.00024059	0.00059318	0.00012289	-0.00002718	0.00004852	0.00051317	0.00054085	0.00006085	0.00039599	0.00117787
-5.00	0.00006095	-0.00001209	0.00004317	0.00016837	0.00001990	-0.00000788	0.00000604	0.00007789	0.00010651	-0.00000229	0.00006581	0.00029764

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_4H_4**SiH**$^+$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00007545	-0.00001576	0.00003939	0.00025733	0.00000726	-0.00000088	0.00000114	0.00003735	0.00008595	-0.00001008	0.00004414	0.00030077
4.00	0.00043837	-0.00006396	0.00026890	0.00098881	0.00005958	0.00001890	0.00001961	0.00031653	0.00051841	0.00000288	0.00031632	0.00128809
3.00	0.00187997	0.00004946	0.00173202	0.00269529	0.00051137	0.00033167	0.00044246	0.00269048	0.00246802	0.00088991	0.00233665	0.00524558
2.50	0.00347400	0.00057263	0.00256634	0.00425949	0.00148975	0.00150104	0.00189645	0.00689170	0.00511547	0.00337083	0.00653593	0.00914946
2.00	0.00561814	-0.00186260	0.00187806	0.00897371	0.00410693	0.00599699	0.00678875	0.01416023	0.01000338	0.00996248	0.01184462	0.01678346
1.75	0.00659694	-0.00629207	0.00283917	0.01178987	0.00654505	0.01108137	0.01175445	0.01779180	0.01348684	0.010210039	0.016697339	0.02536755
1.50	0.00718073	-0.01113407	0.00384551	0.01414949	0.01002841	0.01776041	0.01923784	0.02092135	0.01759933	0.00669501	0.02537961	0.03653318
1.40	0.00723658	-0.01266616	0.00418631	0.01474805	0.01166639	0.01801070	0.02335141	0.02396155	0.01930038	0.00469462	0.02941444	0.04144341
1.25	0.00707884	-0.01419419	0.00460628	0.01516766	0.01464597	0.01591862	0.03068718	0.03121480	0.02211841	0.00085564	0.03667902	0.04993562
1.00	0.00611429	-0.01280695	0.00473660	0.01406619	0.02022629	0.00712763	0.04426084	0.04709057	0.02668389	-0.00635073	0.05009354	0.06463457
0.75	0.00438137	-0.00551987	0.00395594	0.01069627	0.02622614	-0.00782253	0.05974500	0.06563040	0.03085364	-0.01348486	0.06433818	0.07910688
0.50	0.00232691	0.00232627	0.00596897	0.00612332	0.03173231	-0.02576987	0.07468674	0.08386699	0.03418937	-0.01919888	0.07730902	0.09144509
0.25	0.00064878	0.00070946	0.00175192	0.01703129	0.03565287	-0.04075533	0.08573689	0.09752698	0.03633776	-0.02272775	0.08650241	0.09975232
0.00	0.00000000	0.00000000	0.00000176	0.02153824	0.03707842	-0.04663108	0.08983793	0.10262904	0.03707842	-0.02389645	0.08983793	0.10263053
-0.25	0.00064878	0.00070946	0.00175192	0.01703129	0.03565287	-0.04075533	0.08573689	0.09752698	0.03633776	-0.02272775	0.08650241	0.09975232
-0.50	0.00232691	0.00232627	0.00596897	0.00612332	0.03173231	-0.02576987	0.07468674	0.08386699	0.03418937	-0.01919888	0.07730902	0.09144509
-0.75	0.00438137	-0.00551987	0.00395594	0.01069627	0.02622614	-0.00782253	0.05974500	0.06563040	0.03085364	-0.01348486	0.06433818	0.07910688
-1.00	0.00611429	-0.01280695	0.00473660	0.01406619	0.02022629	0.00712763	0.04426084	0.04709057	0.02668389	-0.00635073	0.05009354	0.06463457
-1.25	0.00707884	-0.01419419	0.00460628	0.01516766	0.01464597	0.01591862	0.03068718	0.03121480	0.02211841	0.00085564	0.03667902	0.04993562
-1.40	0.00723658	-0.01266616	0.00418631	0.01474805	0.01166639	0.01801070	0.02335141	0.02396155	0.01930038	0.00469462	0.02941444	0.04144341
-1.50	0.00718073	-0.01113407	0.00384551	0.01414949	0.01002841	0.01776041	0.01923784	0.02092135	0.01759933	0.00669501	0.02537961	0.03653318
-1.75	0.00659694	-0.00629207	0.00283917	0.01178987	0.00654505	0.01108137	0.01175445	0.01779180	0.01348684	0.010210039	0.016697339	0.02536755
-2.00	0.00561814	-0.00186260	0.00187806	0.00897371	0.00410693	0.00599699	0.00678875	0.01416023	0.01000338	0.00996248	0.01184462	0.01678346
-2.50	0.00347400	0.00057263	0.00256634	0.00425949	0.00148975	0.00150104	0.00189645	0.00689170	0.00511547	0.00337083	0.00653593	0.00914946
-3.00	0.00187997	0.00004946	0.00173202	0.00269529	0.00051137	0.00033167	0.00044246	0.00269048	0.00246802	0.00088991	0.00233665	0.00524558
-4.00	0.00043837	-0.00006396	0.00026890	0.00098881	0.00005958	0.00001890	0.00001961	0.00031653	0.00051841	0.00000288	0.00031632	0.00128809
-5.00	0.00007545	-0.00001576	0.00003939	0.00025733	0.00000726	-0.00000088	0.00000114	0.00003735	0.00008595	-0.00001008	0.00004414	0.00030077

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_4H_4**SiH**$^-$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00023114	0.00001584	0.00005149	0.00052818	0.00001203	-0.00000244	0.00000083	0.00004501	0.00025911	-0.00000421	0.00004817	0.00059940
4.00	0.00081692	0.00042497	0.00046174	0.00135236	0.00007344	0.00000676	0.00001804	0.00032160	0.00093408	0.00035923	0.00046782	0.00175331
3.00	0.00247212	0.00201250	0.00262216	0.00350655	0.00051969	0.00037004	0.00037778	0.00251475	0.00308304	0.00257098	0.00296199	0.00579450
2.50	0.00402676	0.00172558	0.00584139	0.00661174	0.00144907	0.00164206	0.00170545	0.00640821	0.00558772	0.00595124	0.00747344	0.01024544
2.00	0.00593386	-0.00255824	0.01139410	0.01181264	0.00392786	0.00585166	0.00663726	0.01327539	0.00996707	0.00973860	0.01789203	0.01817471
1.70	0.00685236	-0.00733814	0.01509193	0.01518733	0.00682323	0.01125997	0.01355133	0.01725208	0.01375544	0.00939766	0.02624468	0.02854373
1.46	0.00714263	-0.01116907	0.01693272	0.01754150	0.01024816	0.01723782	0.01902831	0.02265893	0.01743988	0.00671864	0.03462323	0.03995739
1.30	0.00699909	-0.01271476	0.01734614	0.01825765	0.01301488	0.01640281	0.02413443	0.03057178	0.02004139	0.00377263	0.04070981	0.04855978
1.15	0.00657451	-0.01287607	0.01696713	0.01808965	0.01603269	0.01291956	0.03063506	0.03968669	0.02261529	0.00016381	0.04683109	0.05749045
1.00	0.00586485	-0.01131811	0.01573339	0.01694620	0.01933779	0.00710852	0.03807784	0.05019728	0.02519504	-0.00403423	0.05304886	0.06685637
0.75	0.00416181	-0.00453598	0.01188523	0.01289923	0.02511108	-0.00729574	0.05177274	0.06978407	0.02925194	-0.01158957	0.06296967	0.08244050
0.50	0.00219712	0.00500753	0.00717060	0.00768114	0.03042164	-0.02472247	0.06510871	0.08910220	0.03260122	-0.01851123	0.07127057	0.09612873
0.25	0.00061067	0.00180857	0.00203827	0.01620112	0.03420934	-0.03935063	0.07503839	0.10361205	0.03481397	-0.02333738	0.07679760	0.10561140
0.00	0.00000000	0.00000000	0.00000061	0.02025326	0.03558782	-0.04510192	0.07873675	0.10904056	0.03558782	-0.02506235	0.07873675	0.10904096
-0.25	0.00061067	0.00180857	0.00203827	0.01620112	0.03420934	-0.03935063	0.07503839	0.10361205	0.03481397	-0.02333738	0.07679760	0.10561140
-0.50	0.00219712	0.00500753	0.00717060	0.00768114	0.03042164	-0.02472247	0.06510871	0.08910220	0.03260122	-0.01851123	0.07127057	0.09612873
-0.75	0.00416181	-0.00453598	0.01188523	0.01289923	0.02511108	-0.00729574	0.05177274	0.06978407	0.02925194	-0.01158957	0.06296967	0.08244050
-1.00	0.00586485	-0.01131811	0.01573339	0.01694620	0.01933779	0.00710852	0.03807784	0.05019728	0.02519504	-0.00403423	0.05304886	0.06685637
-1.15	0.00657451	-0.01287607	0.01696713	0.01808965	0.01603269	0.01291956	0.03063506	0.03968669	0.02261529	0.00016381	0.04683109	0.05749045
-1.30	0.00699909	-0.01271476	0.01734614	0.01825765	0.01301488	0.01640281	0.02413443	0.03057178	0.02004139	0.00377263	0.04070981	0.04855978
-1.46	0.00714263	-0.01116907	0.01693272	0.01754150	0.01024816	0.01723782	0.01902831	0.02265893	0.01743988	0.00671864	0.03462323	0.03995739
-1.70	0.00685236	-0.00733814	0.01509193	0.01518733	0.00682323	0.01125997	0.01355133	0.01725208	0.01375544	0.00939766	0.02624468	0.02854373
-2.00	0.00593386	-0.00255824	0.01139410	0.01181264	0.00392786	0.00585166	0.00663726	0.01327539	0.00996707	0.00973860	0.01789203	0.01817471
-2.50	0.00402676	0.00172558	0.00584139	0.00661174	0.00144907	0.00164206	0.00170545	0.00640821	0.00558772	0.00595124	0.00747344	0.01024544
-3.00	0.00247212	0.00201250	0.00262216	0.00350655	0.00051969	0.00037004	0.00037778	0.00251475	0.00308304	0.00257098	0.00296199	0.00579450
-4.00	0.00081692	0.00042497	0.00046174	0.00135236	0.00007344	0.00000676	0.00001804	0.00032160	0.00093408	0.00035923	0.00046782	0.00175331
-5.00	0.00023114	0.00001584	0.00005149	0.00052818	0.00001203	-0.00000244	0.00000083	0.00004501	0.00025911	-0.00000421	0.00004817	0.00059940

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_4H_4**NH**. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00006338	0.00001621	0.00006645	0.00023408	0.00000157	-0.00000040	0.00000206	0.00001410	0.00006620	0.00001374	0.00006827	0.00025217
4.00	0.00037549	0.00020436	0.00039257	0.00098490	0.00002286	0.00000539	0.00002663	0.00013411	0.00040383	0.00019515	0.00041864	0.00113451
3.00	0.00178840	0.00179550	0.00257963	0.00385910	0.00025652	0.00021566	0.00037657	0.00173646	0.00206392	0.00192828	0.00295976	0.00567746
2.50	0.00365931	0.00454854	0.00617549	0.00674193	0.00092309	0.00115099	0.00164422	0.00625924	0.00461636	0.00596063	0.00840289	0.01210078
2.00	0.00672187	0.00127805	0.01387546	0.01537323	0.00326506	0.00574446	0.00674763	0.01778542	0.01003534	0.01632879	0.02198094	0.02217902
1.75	0.00844872	-0.00509859	0.02033426	0.02123972	0.00587514	0.01202214	0.01287710	0.02596996	0.01437192	0.01991849	0.03269861	0.03420998
1.60	0.00935913	-0.01030363	0.02459536	0.02488371	0.00817431	0.01818167	0.01855240	0.03065955	0.01757699	0.01972856	0.04267608	0.04353231
1.40	0.01019233	-0.01776062	0.02908075	0.03006658	0.01230827	0.02936097	0.03013338	0.03510943	0.02253311	0.01663697	0.05860408	0.06000915
1.27	0.01037495	-0.02202078	0.03109515	0.03286162	0.01581292	0.03444220	0.03911896	0.04230981	0.02621066	0.01262484	0.07040192	0.07401164
1.00	0.00953291	-0.02470355	0.03151903	0.03443409	0.02460800	0.02452759	0.06595325	0.07380061	0.03414360	-0.00007269	0.09769356	0.10720447
0.75	0.00721519	-0.01534281	0.02598500	0.02901724	0.03436858	-0.00103349	0.09950959	0.11364129	0.04157449	-0.01622188	0.12572382	0.14173754
0.50	0.00400175	0.00538888	0.01542659	0.01775390	0.04400290	-0.03870688	0.13630256	0.15721827	0.04799460	-0.03303812	0.15193089	0.17414955
0.25	0.00114749	0.00451574	0.00538384	0.02850068	0.05123215	-0.07423796	0.16616493	0.19246802	0.05237586	-0.04587633	0.17086548	0.19761437
0.00	0.00000000	0.00000000	0.00004271	0.03846645	0.05393422	-0.08901782	0.17780081	0.20617805	0.05393422	-0.05068838	0.17780081	0.20622090
-0.25	0.00114749	0.00451574	0.00538384	0.02850068	0.05123215	-0.07423796	0.16616493	0.19246802	0.05237586	-0.04587633	0.17086548	0.19761437
-0.50	0.00400175	0.00538888	0.01542659	0.01775390	0.04400290	-0.03870688	0.13630256	0.15721827	0.04799460	-0.03303812	0.15193089	0.17414955
-0.75	0.00721519	-0.01534281	0.02598500	0.02901724	0.03436858	-0.00103349	0.09950959	0.11364129	0.04157449	-0.01622188	0.12572382	0.14173754
-1.00	0.00953291	-0.02470355	0.03151903	0.03443409	0.02460800	0.02452759	0.06595325	0.07380061	0.03414360	-0.00007269	0.09769356	0.10720447
-1.27	0.01037495	-0.02202078	0.03109515	0.03286162	0.01581292	0.03444220	0.03911896	0.04230981	0.02621066	0.01262484	0.07040192	0.07401164
-1.40	0.01019233	-0.01776062	0.02908075	0.03006658	0.01230827	0.02936097	0.03013338	0.03510943	0.02253311	0.01663697	0.05860408	0.06000915
-1.60	0.00935913	-0.01030363	0.02459536	0.02488371	0.00817431	0.01818167	0.01855240	0.03065955	0.01757699	0.01972856	0.04267608	0.04353231
-1.75	0.00844872	-0.00509859	0.02033426	0.02123972	0.00587514	0.01202214	0.01287710	0.02596996	0.01437192	0.01991849	0.03269861	0.03420998
-2.00	0.00672187	0.00127805	0.01387546	0.01537323	0.00326506	0.00574446	0.00674763	0.01778542	0.01003534	0.01632879	0.02198094	0.02217902
-2.50	0.00365931	0.00454854	0.00617549	0.00674193	0.00092309	0.00115099	0.00164422	0.00625924	0.00461636	0.00596063	0.00840289	0.01210078
-3.00	0.00178840	0.00179550	0.00257963	0.00385910	0.00025652	0.00021566	0.00037657	0.00173646	0.00206392	0.00192828	0.00295976	0.00567746
-4.00	0.00037549	0.00020436	0.00039257	0.00098490	0.00002286	0.00000539	0.00002663	0.00013411	0.00040383	0.00019515	0.00041864	0.00113451
-5.00	0.00006338	0.00001621	0.00006645	0.00023408	0.00000157	-0.00000040	0.00000206	0.00001410	0.00006620	0.00001374	0.00006827	0.00025217

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_4H_4**PH**. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00009559	0.00005271	0.00007690	0.00029824	0.00000311	0.00000131	0.00000272	0.00002196	0.00010064	0.00005331	0.00007618	0.00032685
4.00	0.00048748	0.00032940	0.00044440	0.00109414	0.00003625	0.00001855	0.00003523	0.00020368	0.00053062	0.00034481	0.00046496	0.00132686
3.00	0.00200858	0.00210940	0.00249609	0.00357056	0.00036610	0.00032185	0.00050798	0.00212545	0.00239666	0.00241325	0.00303698	0.00571416
2.50	0.00375793	0.00326724	0.00532411	0.00688262	0.00117654	0.00147734	0.00205038	0.00631030	0.00496784	0.00675848	0.00762589	0.01094580
2.00	0.00622986	-0.00141631	0.01163557	0.01366592	0.00360995	0.00607930	0.00736009	0.01486033	0.00987834	0.01285072	0.01762391	0.02168627
1.75	0.00742134	-0.00659364	0.01563242	0.01772894	0.00604933	0.01144528	0.01302919	0.01981980	0.01350607	0.01286053	0.02695443	0.03120272
1.50	0.00819838	-0.01257451	0.01925038	0.02123103	0.00970075	0.02029415	0.02148122	0.02342918	0.01792707	0.01010845	0.03938874	0.04355272
1.37	0.00831713	-0.01518330	0.02056714	0.02242225	0.01212317	0.02259189	0.02658190	0.02845069	0.02046310	0.00747756	0.04698004	0.05090300
1.25	0.00820130	-0.01680563	0.02123996	0.02294617	0.01474509	0.02105569	0.03371085	0.03528917	0.02296390	0.00426624	0.05477448	0.05831786
1.00	0.00718329	-0.01590012	0.02028753	0.02164405	0.02106467	0.01167327	0.05213544	0.05283415	0.02825495	-0.00419419	0.07225406	0.07452466
0.75	0.00521193	-0.00762735	0.01580597	0.01684584	0.02806946	-0.00631399	0.07372636	0.07443220	0.03328113	-0.01388308	0.08996535	0.09069740
0.50	0.00279579	0.00634236	0.00893031	0.00976381	0.03465525	-0.02935994	0.09466484	0.09706894	0.03744859	-0.02281776	0.10405641	0.10609817
0.25	0.00078459	0.00248565	0.00290432	0.02033841	0.03942461	-0.04936257	0.11057665	0.11442863	0.04020808	-0.02905910	0.11332115	0.11705612
0.00	0.00000000	0.00000000	0.00002712	0.02610574	0.04117402	-0.05735291	0.11656577	0.12099412	0.04117402	-0.03128930	0.11659139	0.12099412
-0.25	0.00078459	0.00248565	0.00290432	0.02033841	0.03942461	-0.04936257	0.11057665	0.11442863	0.04020808	-0.02905910	0.11332115	0.11705612
-0.50	0.00279579	0.00634236	0.00893031	0.00976381	0.03465525	-0.02935994	0.09466484	0.09706894	0.03744859	-0.02281776	0.10405641	0.10609817
-0.75	0.00521193	-0.00762735	0.01580597	0.01684584	0.02806946	-0.00631399	0.07372636	0.07443220	0.03328113	-0.01388308	0.08996535	0.09069740
-1.00	0.00718329	-0.01590012	0.02028753	0.02164405	0.02106467	0.01167327	0.05213544	0.05283415	0.02825495	-0.00419419	0.07225406	0.07452466
-1.25	0.00820130	-0.01680563	0.02123996	0.02294617	0.01474509	0.02105569	0.03371085	0.03528917	0.02296390	0.00426624	0.05477448	0.05831786
-1.37	0.00831713	-0.01518330	0.02056714	0.02242225	0.01212317	0.02259189	0.02658190	0.02845069	0.02046310	0.00747756	0.04698004	0.05090300
-1.50	0.00819838	-0.01257451	0.01925038	0.02123103	0.00970075	0.02029415	0.02148122	0.02342918	0.01792707	0.01010845	0.03938874	0.04355272
-1.75	0.00742134	-0.00659364	0.01563242	0.01772894	0.00604933	0.01144528	0.01302919	0.01981980	0.01350607	0.01286053	0.02695443	0.03120272
-2.00	0.00622986	-0.00141631	0.01163557	0.01366592	0.00360995	0.00607930	0.00736009	0.01486033	0.00987834	0.01285072	0.01762391	0.02168627
-2.50	0.00375793	0.00326724	0.00532411	0.00688262	0.00117654	0.00147734	0.00205038	0.00631030	0.00496784	0.00675848	0.00762589	0.01094580
-3.00	0.00200858	0.00210940	0.00249609	0.00357056	0.00036610	0.00032185	0.00050798	0.00212545	0.00239666	0.00241325	0.00303698	0.00571416
-4.00	0.00048748	0.00032940	0.00044440	0.00109414	0.00003625	0.00001855	0.00003523	0.00020368	0.00053062	0.00034481	0.00046496	0.00132686
-5.00	0.00009559	0.00005271	0.00007690	0.00029824	0.00000311	0.00000131	0.00000272	0.00002196	0.00010064	0.00005331	0.00007618	0.00032685

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_4H_4O. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00005925	-0.00000700	0.00006266	0.00022601	0.00000209	-0.00000080	0.00000178	0.00001439	0.00006499	-0.00001107	0.00006399	0.00025152
4.00	0.00035035	0.00007245	0.00038695	0.00097458	0.00002408	-0.00000501	0.00002499	0.00013682	0.00039281	0.00003381	0.00041110	0.00115516
3.00	0.00170988	0.00137554	0.00265238	0.00394092	0.00025899	0.00008263	0.00037091	0.00178174	0.00203478	0.00122454	0.00304403	0.00596686
2.50	0.00356460	0.00384579	0.00598680	0.00707569	0.00092978	0.00063302	0.00164490	0.00638219	0.00461267	0.00403581	0.00879715	0.01271025
2.00	0.00662991	0.00148411	0.01177629	0.01641541	0.00327804	0.00386680	0.00683465	0.01817443	0.01009070	0.01188761	0.02251027	0.02347591
1.80	0.00803524	-0.00320068	0.01645996	0.02151030	0.00525856	0.00757050	0.01155690	0.02499396	0.01348971	0.01660246	0.02767104	0.03338942
1.60	0.00930748	-0.00988072	0.02212068	0.02685721	0.00820268	0.01423442	0.01897019	0.03185581	0.01770043	0.01920163	0.03681646	0.04625865
1.40	0.01018715	-0.01750124	0.02800333	0.03167075	0.01237193	0.02536667	0.03019076	0.03692612	0.02272010	0.01763787	0.05213940	0.06239207
1.25	0.01041205	-0.02244840	0.03168098	0.03422111	0.01634918	0.03480610	0.04053470	0.04164965	0.02688676	0.01374570	0.06745670	0.07644908
1.15	0.01029126	-0.02478832	0.03345995	0.03516190	0.01956874	0.03426485	0.05021569	0.05145105	0.02995642	0.00968235	0.07998629	0.08720338
1.00	0.00964859	-0.02548781	0.03432366	0.03488332	0.02492153	0.02703811	0.06875845	0.07017882	0.03462245	0.00179423	0.10084281	0.10421074
0.75	0.00736489	-0.01656361	0.02909834	0.02984054	0.03502423	0.00064875	0.10471653	0.11326081	0.04238360	-0.01542605	0.13425283	0.13987773
0.50	0.00411511	0.00442628	0.01749964	0.01892735	0.04510416	-0.03960298	0.14461782	0.16168477	0.04919553	-0.03433194	0.16235319	0.17809502
0.25	0.00118594	0.00528319	0.00542591	0.02934999	0.05272965	-0.07822345	0.17729201	0.20137160	0.05390488	-0.04927951	0.18264554	0.20643365
0.00	0.00000000	0.00000000	0.00000153	0.03982653	0.05559221	-0.09441138	0.19008342	0.21688582	0.05559221	-0.05499001	0.19008371	0.21688870
-0.25	0.00118594	0.00528319	0.00542591	0.02934999	0.05272965	-0.07822345	0.17729201	0.20137160	0.05390488	-0.04927951	0.18264554	0.20643365
-0.50	0.00411511	0.00442628	0.01749964	0.01892735	0.04510416	-0.03960298	0.14461782	0.16168477	0.04919553	-0.03433194	0.16235319	0.17809502
-0.75	0.00736489	-0.01656361	0.02909834	0.02984054	0.03502423	0.00064875	0.10471653	0.11326081	0.04238360	-0.01542605	0.13425283	0.13987773
-1.00	0.00964859	-0.02548781	0.03432366	0.03488332	0.02492153	0.02703811	0.06875845	0.07017882	0.03462245	0.00179423	0.10084281	0.10421074
-1.15	0.01029126	-0.02478832	0.03345995	0.03516190	0.01956874	0.03426485	0.05021569	0.05145105	0.02995642	0.00968235	0.07998629	0.08720338
-1.25	0.01041205	-0.02244840	0.03168098	0.03422111	0.01634918	0.03480610	0.04053470	0.04164965	0.02688676	0.01374570	0.06745670	0.07644908
-1.40	0.01018715	-0.01750124	0.02800333	0.03167075	0.01237193	0.02536667	0.03019076	0.03692612	0.02272010	0.01763787	0.05213940	0.06239207
-1.60	0.00930748	-0.00988072	0.02212068	0.02685721	0.00820268	0.01423442	0.01897019	0.03185581	0.01770043	0.01920163	0.03681646	0.04625865
-1.80	0.00803524	-0.00320068	0.01645996	0.02151030	0.00525856	0.00757050	0.01155690	0.02499396	0.01348971	0.01660246	0.02767104	0.03338942
-2.00	0.00662991	0.00148411	0.01177629	0.01641541	0.00327804	0.00386680	0.00683465	0.01817443	0.01009070	0.01188761	0.02251027	0.02347591
-2.50	0.00356460	0.00384579	0.00598680	0.00707569	0.00092978	0.00063302	0.00164490	0.00638219	0.00461267	0.00403581	0.00879715	0.01271025
-3.00	0.00170988	0.00137554	0.00265238	0.00394092	0.00025899	0.00008263	0.00037091	0.00178174	0.00203478	0.00122454	0.00304403	0.00596686
-4.00	0.00035035	0.00007245	0.00038695	0.00097458	0.00002408	-0.00000501	0.00002499	0.00013682	0.00039281	0.00003381	0.00041110	0.00115516
-5.00	0.00005925	-0.00000700	0.00006266	0.00022601	0.00000209	-0.00000080	0.00000178	0.00001439	0.00006499	-0.00001107	0.00006399	0.00025152

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_4H_4S. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00007404	0.00005387	0.00006464	0.00023858	0.00000181	0.00000173	0.00000188	0.00001376	0.00000181	0.00000173	0.00000188	0.00001376
4.00	0.00041080	0.00033654	0.00038403	0.00091726	0.00002521	0.00002207	0.00002238	0.00015233	0.00002521	0.00002207	0.00002238	0.00015233
3.00	0.00178379	0.00224043	0.00235987	0.00312937	0.00030161	0.00034095	0.00036385	0.00193425	0.00030161	0.00034095	0.00036385	0.00193425
2.50	0.00343702	0.00348576	0.00578378	0.00591469	0.00105562	0.00154127	0.00163022	0.00620111	0.00105562	0.00154127	0.00163022	0.00620111
2.00	0.00586304	-0.00095718	0.01218159	0.01289437	0.00345758	0.00637952	0.00650504	0.01526767	0.00345758	0.00637952	0.00650504	0.01526767
1.75	0.00706994	-0.00610375	0.01598665	0.01749113	0.00592927	0.01208781	0.01208957	0.02062264	0.00592927	0.01208781	0.01208957	0.02062264
1.50	0.00789085	-0.01217230	0.01931170	0.02176666	0.00967570	0.02116398	0.02163420	0.02423517	0.00967570	0.02116398	0.02163420	0.02423517
1.35	0.00804406	-0.01518989	0.02057944	0.02357576	0.01255875	0.02397975	0.02893148	0.02957991	0.01255875	0.02397975	0.02893148	0.02957991
1.15	0.00771111	-0.01714849	0.02092477	0.02449385	0.01739463	0.01990385	0.04231389	0.04395629	0.01739463	0.01990385	0.04231389	0.04395629
1.00	0.00701886	-0.01597526	0.01984390	0.02358792	0.02149503	0.01302460	0.05444955	0.05711493	0.02149503	0.01302460	0.05444955	0.05711493
0.75	0.00511900	-0.00792983	0.01539394	0.01875152	0.02885455	-0.00589689	0.07781206	0.08285123	0.02885455	-0.00589689	0.07781206	0.08285123
0.50	0.00275621	0.00604017	0.00878183	0.01086268	0.03581469	-0.03060435	0.10163830	0.10959440	0.03581469	-0.03060435	0.10163830	0.10959440
0.25	0.00077526	0.00251848	0.00325947	0.01998905	0.04087808	-0.05233804	0.11996096	0.13046522	0.04087808	-0.05233804	0.11996096	0.13046522
0.00	0.00000000	0.00000000	0.00000269	0.02581503	0.04274000	-0.06108180	0.12689926	0.13843254	0.04274000	-0.06108180	0.12689926	0.13843254
-0.25	0.00077526	0.00251848	0.00325947	0.01998905	0.04087808	-0.05233804	0.11996096	0.13046522	0.04087808	-0.05233804	0.11996096	0.13046522
-0.50	0.00275621	0.00604017	0.00878183	0.01086268	0.03581469	-0.03060435	0.10163830	0.10959440	0.03581469	-0.03060435	0.10163830	0.10959440
-0.75	0.00511900	-0.00792983	0.01539394	0.01875152	0.02885455	-0.00589689	0.07781206	0.08285123	0.02885455	-0.00589689	0.07781206	0.08285123
-1.00	0.00701886	-0.01597526	0.01984390	0.02358792	0.02149503	0.01302460	0.05444955	0.05711493	0.02149503	0.01302460	0.05444955	0.05711493
-1.15	0.00771111	-0.01714849	0.02092477	0.02449385	0.01739463	0.01990385	0.04231389	0.04395629	0.01739463	0.01990385	0.04231389	0.04395629
-1.35	0.00804406	-0.01518989	0.02057944	0.02357576	0.01255875	0.02397975	0.02893148	0.02957991	0.01255875	0.02397975	0.02893148	0.02957991
-1.50	0.00789085	-0.01217230	0.01931170	0.02176666	0.00967570	0.02116398	0.02163420	0.02423517	0.00967570	0.02116398	0.02163420	0.02423517
-1.75	0.00706994	-0.00610375	0.01598665	0.01749113	0.00592927	0.01208781	0.01208957	0.02062264	0.00592927	0.01208781	0.01208957	0.02062264
-2.00	0.00586304	-0.00095718	0.01218159	0.01289437	0.00345758	0.00637952	0.00650504	0.01526767	0.00345758	0.00637952	0.00650504	0.01526767
-2.50	0.00343702	0.00348576	0.00578378	0.00591469	0.00105562	0.00154127	0.00163022	0.00620111	0.00105562	0.00154127	0.00163022	0.00620111
-3.00	0.00178379	0.00224043	0.00235987	0.00312937	0.00030161	0.00034095	0.00036385	0.00193425	0.00030161	0.00034095	0.00036385	0.00193425
-4.00	0.00041080	0.00033654	0.00038403	0.00091726	0.00002521	0.00002207	0.00002238	0.00015233	0.00002521	0.00002207	0.00002238	0.00015233
-5.00	0.00007404	0.00005387	0.00006464	0.00023858	0.00000181	0.00000173	0.00000188	0.00001376	0.00000181	0.00000173	0.00000188	0.00001376

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_5H_5\mathbf{BH}^-$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00011159	0.00005961	0.00007356	0.00024212	0.00000456	0.00000073	0.00000235	0.00002755	0.00011637	0.00006149	0.00007428	0.00027011
4.00	0.00044132	0.00032013	0.00038618	0.00070970	0.00004405	0.00001891	0.00003078	0.00020234	0.00048595	0.00035090	0.00040509	0.00091178
3.00	0.00144871	0.00120571	0.00188571	0.00196365	0.00034700	0.00031820	0.00039695	0.00149147	0.00179706	0.00194987	0.00228205	0.00302616
2.50	0.00238176	0.00084112	0.00376727	0.00433715	0.00095139	0.00131062	0.00147852	0.00379477	0.00333480	0.00419991	0.00564828	0.00567064
2.00	0.00347949	-0.00175056	0.00692746	0.00840103	0.00250918	0.00488276	0.00499040	0.00783598	0.00598996	0.00587441	0.01210663	0.01328458
1.80	0.00384078	-0.00348718	0.00831834	0.01024435	0.00360630	0.00769180	0.00785750	0.00953525	0.00744796	0.00577184	0.01626028	0.01810260
1.49	0.00410060	-0.00620076	0.01000497	0.01253972	0.00607042	0.01028565	0.01479031	0.01533935	0.01017110	0.00413141	0.02471977	0.02787946
1.30	0.00398520	-0.00711065	0.01036754	0.01308269	0.00802686	0.00924875	0.02051940	0.02184176	0.01201167	0.00214702	0.03084970	0.03492445
1.15	0.00371607	-0.00702354	0.01013376	0.01283344	0.00982490	0.00707562	0.02605648	0.02815916	0.01354029	0.00005672	0.03615916	0.04099226
1.00	0.00329090	-0.00599033	0.00937104	0.01189176	0.01177988	0.00360315	0.03231650	0.03534762	0.01506993	-0.00238015	0.04165689	0.04723875
0.75	0.00230887	-0.00207296	0.00700543	0.00888520	0.01516336	-0.00474180	0.04367551	0.04848255	0.01747138	-0.00679431	0.05064285	0.05736688
0.50	0.00120751	0.00333379	0.00418641	0.00486255	0.01824399	-0.01457099	0.05454875	0.06113214	0.01945096	-0.01087943	0.05836576	0.06599402
0.25	0.00033353	0.00107955	0.00137337	0.00892659	0.02042422	-0.02266979	0.06253120	0.07045343	0.02075758	-0.01375638	0.06361669	0.07182657
0.00	0.00000000	0.00000000	0.00000014	0.01103750	0.02121434	-0.02582312	0.06548085	0.07390404	0.02121434	-0.01479127	0.06548085	0.07390418
-0.25	0.00033353	0.00107955	0.00137337	0.00892659	0.02042422	-0.02266979	0.06253120	0.07045343	0.02075758	-0.01375638	0.06361669	0.07182657
-0.50	0.00120751	0.00333379	0.00418641	0.00486255	0.01824399	-0.01457099	0.05454875	0.06113214	0.01945096	-0.01087943	0.05836576	0.06599402
-0.75	0.00230887	-0.00207296	0.00700543	0.00888520	0.01516336	-0.00474180	0.04367551	0.04848255	0.01747138	-0.00679431	0.05064285	0.05736688
-1.00	0.00329090	-0.00599033	0.00937104	0.01189176	0.01177988	0.00360315	0.03231650	0.03534762	0.01506993	-0.00238015	0.04165689	0.04723875
-1.15	0.00371607	-0.00702354	0.01013376	0.01283344	0.00982490	0.00707562	0.02605648	0.02815916	0.01354029	0.00005672	0.03615916	0.04099226
-1.30	0.00398520	-0.00711065	0.01036754	0.01308269	0.00802686	0.00924875	0.02051940	0.02184176	0.01201167	0.00214702	0.03084970	0.03492445
-1.49	0.00410060	-0.00620076	0.01000497	0.01253972	0.00607042	0.01028565	0.01479031	0.01533935	0.01017110	0.00413141	0.02471977	0.02787946
-1.80	0.00384078	-0.00348718	0.00831834	0.01024435	0.00360630	0.00769180	0.00785750	0.00953525	0.00744796	0.00577184	0.01626028	0.01810260
-2.00	0.00347949	-0.00175056	0.00692746	0.00840103	0.00250918	0.00488276	0.00499040	0.00783598	0.00598996	0.00587441	0.01210663	0.01328458
-2.50	0.00238176	0.00084112	0.00376727	0.00433715	0.00095139	0.00131062	0.00147852	0.00379477	0.00333480	0.00419991	0.00564828	0.00567064
-3.00	0.00144871	0.00120571	0.00188571	0.00196365	0.00034700	0.00031820	0.00039695	0.00149147	0.00179706	0.00194987	0.00228205	0.00302616
-4.00	0.00044132	0.00032013	0.00038618	0.00070970	0.00004405	0.00001891	0.00003078	0.00020234	0.00048595	0.00035090	0.00040509	0.00091178
-5.00	0.00011159	0.00005961	0.00007356	0.00024212	0.00000456	0.00000073	0.00000235	0.00002755	0.00011637	0.00006149	0.00007428	0.00027011

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_5H_5**AlH**$^{-}$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00016060	0.00003488	0.00007801	0.00026163	0.00001634	-0.00000289	0.00000224	0.00005605	0.00018177	0.00002605	0.00008010	0.00032367
4.00	0.00049056	0.00023882	0.00038748	0.00063452	0.00008684	0.00001379	0.00002775	0.00032316	0.00058839	0.00022967	0.00041549	0.00097547
3.00	0.00132447	0.00060283	0.00148740	0.00167655	0.00048074	0.00030663	0.00033642	0.00160864	0.00182588	0.00120259	0.00201347	0.00275403
2.50	0.00196801	0.00001834	0.00276143	0.00331938	0.00110279	0.00112667	0.00121011	0.00322212	0.00309345	0.00234888	0.00452657	0.00465737
2.00	0.00259299	-0.00177084	0.00464826	0.00579299	0.00242892	0.00346139	0.00399210	0.00544771	0.00503828	0.00297120	0.00858745	0.00977033
1.80	0.00275087	-0.00272853	0.00537736	0.00680057	0.00326410	0.00483981	0.00615223	0.00647823	0.00602602	0.00268988	0.01101296	0.01293035
1.62	0.00280335	-0.00352286	0.00588107	0.00753644	0.00420403	0.00546490	0.00817765	0.00884594	0.00701271	0.00208605	0.01362951	0.01635222
1.50	0.00277790	-0.00391048	0.00607934	0.00785610	0.00491999	0.00534992	0.00981452	0.01104837	0.00769934	0.00150277	0.01553962	0.01886936
1.30	0.00261106	-0.00412601	0.00609138	0.00797438	0.00629054	0.00429934	0.01324382	0.01556029	0.00889709	0.00021417	0.01901054	0.02349278
1.00	0.00206412	-0.00296236	0.00522295	0.00693347	0.00863840	0.00066320	0.01954956	0.02400862	0.01069264	-0.00223264	0.02446913	0.03089778
0.75	0.00140647	-0.00055821	0.00379475	0.00501793	0.01065338	-0.00392812	0.02523733	0.03183633	0.01205014	-0.00438260	0.02875055	0.03681785
0.50	0.00071974	0.00168435	0.00267754	0.00297268	0.01242649	-0.00891251	0.03040505	0.03909178	0.01314011	-0.00623424	0.03226415	0.04174795
0.25	0.00019614	0.00052661	0.00074360	0.00541548	0.01365241	-0.01282005	0.03405579	0.04428751	0.01384669	-0.00747339	0.03457278	0.04502475
0.00	0.00000000	0.00000000	0.00000010	0.00646154	0.01409144	-0.01430510	0.03537761	0.04618160	0.01409144	-0.00790727	0.03537761	0.04618170
-0.25	0.00019614	0.00052661	0.00074360	0.00541548	0.01365241	-0.01282005	0.03405579	0.04428751	0.01384669	-0.00747339	0.03457278	0.04502475
-0.50	0.00071974	0.00168435	0.00267754	0.00297268	0.01242649	-0.00891251	0.03040505	0.03909178	0.01314011	-0.00623424	0.03226415	0.04174795
-0.75	0.00140647	-0.00055821	0.00379475	0.00501793	0.01065338	-0.00392812	0.02523733	0.03183633	0.01205014	-0.00438260	0.02875055	0.03681785
-1.00	0.00206412	-0.00296236	0.00522295	0.00693347	0.00863840	0.00066320	0.01954956	0.02400862	0.01069264	-0.00223264	0.02446913	0.03089778
-1.30	0.00261106	-0.00412601	0.00609138	0.00797438	0.00629054	0.00429934	0.01324382	0.01556029	0.00889709	0.00021417	0.01901054	0.02349278
-1.50	0.00277790	-0.00391048	0.00607934	0.00785610	0.00491999	0.00534992	0.00981452	0.01104837	0.00769934	0.00150277	0.01553962	0.01886936
-1.62	0.00280335	-0.00352286	0.00588107	0.00753644	0.00420403	0.00546490	0.00817765	0.00884594	0.00701271	0.00208605	0.01362951	0.01635222
-1.80	0.00275087	-0.00272853	0.00537736	0.00680057	0.00326410	0.00483981	0.00615223	0.00647823	0.00602602	0.00268988	0.01101296	0.01293035
-2.00	0.00259299	-0.00177084	0.00464826	0.00579299	0.00242892	0.00346139	0.00399210	0.00544771	0.00503828	0.00297120	0.00858745	0.00977033
-2.50	0.00196801	0.00001834	0.00276143	0.00331938	0.00110279	0.00112667	0.00121011	0.00322212	0.00309345	0.00234888	0.00452657	0.00465737
-3.00	0.00132447	0.00060283	0.00148740	0.00167655	0.00048074	0.00030663	0.00033642	0.00160864	0.00182588	0.00120259	0.00201347	0.00275403
-4.00	0.00049056	0.00023882	0.00038748	0.00063452	0.00008684	0.00001379	0.00002775	0.00032316	0.00058839	0.00022967	0.00041549	0.00097547
-5.00	0.00016060	0.00003488	0.00007801	0.00026163	0.00001634	-0.00000289	0.00000224	0.00005605	0.00018177	0.00002605	0.00008010	0.00032367

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_5H_5**SiH**. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00009392	0.00004807	0.00004984	0.00025282	0.00000625	-0.00000005	0.00000108	0.00003135	0.00010400	0.00004424	0.00004765	0.00029402
4.00	0.00040616	0.00030026	0.00030502	0.00072540	0.00004928	0.00001617	0.00003009	0.00021594	0.00046728	0.00030722	0.00031621	0.00097411
3.00	0.00134517	0.00099933	0.00160153	0.00198781	0.00035598	0.00027960	0.00041475	0.00146700	0.00172933	0.00167883	0.00188220	0.00317530
2.50	0.00217526	0.00053016	0.00349966	0.00393875	0.00093491	0.00111671	0.00148561	0.00347173	0.00314569	0.00331631	0.00461716	0.00603279
2.00	0.00309981	-0.00179728	0.00663156	0.00705896	0.00234444	0.00402444	0.00468813	0.00672963	0.00547704	0.00435617	0.01065083	0.01213612
1.75	0.00343751	-0.00361848	0.00832230	0.00865412	0.00358419	0.00713811	0.00714461	0.00888591	0.00704728	0.00392988	0.01544832	0.01689780
1.60	0.00354052	-0.00468830	0.00916342	0.00940815	0.00454927	0.00780986	0.00979593	0.01125725	0.00810946	0.00323216	0.01894182	0.02029549
1.53	0.00355439	-0.00514922	0.00949024	0.00968580	0.00509678	0.00783583	0.01137633	0.01276851	0.00866761	0.00275189	0.02084611	0.02212327
1.40	0.00351272	-0.00572342	0.00984836	0.00995799	0.00611040	0.00744117	0.01442044	0.01569444	0.00963401	0.00175726	0.02424337	0.02534310
1.25	0.00334566	-0.00593827	0.00989234	0.00990288	0.00747659	0.00617973	0.01873299	0.01979430	0.01082675	0.00028178	0.02859445	0.02939371
1.00	0.00277890	-0.00471791	0.00875609	0.00886361	0.01003555	0.00200640	0.02734495	0.02779311	0.01281075	-0.00265273	0.03617225	0.03626376
0.75	0.00192893	-0.00138136	0.00641295	0.00653134	0.01270976	-0.00441524	0.03649454	0.03696094	0.01463178	-0.00572035	0.04266016	0.04345924
0.50	0.00100045	0.00280786	0.00353728	0.00393387	0.01510626	-0.01166652	0.04454466	0.04603459	0.01610141	-0.00835040	0.04785521	0.04955075
0.25	0.00027487	0.00094255	0.00099718	0.00745155	0.01678330	-0.01748283	0.05030786	0.05261564	0.01705642	-0.01009316	0.05123693	0.05360596
0.00	0.00000000	0.00000000	0.00000000	0.00907984	0.01738751	-0.01971728	0.05240929	0.05503076	0.01738751	-0.01069870	0.05240929	0.05503076
-0.25	0.00027487	0.00094255	0.00099718	0.00745155	0.01678330	-0.01748283	0.05030786	0.05261564	0.01705642	-0.01009316	0.05123693	0.05360596
-0.50	0.00100045	0.00280786	0.00353728	0.00393387	0.01510626	-0.01166652	0.04454466	0.04603459	0.01610141	-0.00835040	0.04785521	0.04955075
-0.75	0.00192893	-0.00138136	0.00641295	0.00653134	0.01270976	-0.00441524	0.03649454	0.03696094	0.01463178	-0.00572035	0.04266016	0.04345924
-1.00	0.00277890	-0.00471791	0.00875609	0.00886361	0.01003555	0.00200640	0.02734495	0.02779311	0.01281075	-0.00265273	0.03617225	0.03626376
-1.25	0.00334566	-0.00593827	0.00989234	0.00990288	0.00747659	0.00617973	0.01873299	0.01979430	0.01082675	0.00028178	0.02859445	0.02939371
-1.40	0.00351272	-0.00572342	0.00984836	0.00995799	0.00611040	0.00744117	0.01442044	0.01569444	0.00963401	0.00175726	0.02424337	0.02534310
-1.53	0.00355439	-0.00514922	0.00949024	0.00968580	0.00509678	0.00783583	0.01137633	0.01276851	0.00866761	0.00275189	0.02084611	0.02212327
-1.60	0.00354052	-0.00468830	0.00916342	0.00940815	0.00454927	0.00780986	0.00979593	0.01125725	0.00810946	0.00323216	0.01894182	0.02029549
-1.75	0.00343751	-0.00361848	0.00832230	0.00865412	0.00358419	0.00713811	0.00714461	0.00888591	0.00704728	0.00392988	0.01544832	0.01689780
-2.00	0.00309981	-0.00179728	0.00663156	0.00705896	0.00234444	0.00402444	0.00468813	0.00672963	0.00547704	0.00435617	0.01065083	0.01213612
-2.50	0.00217526	0.00053016	0.00349966	0.00393875	0.00093491	0.00111671	0.00148561	0.00347173	0.00314569	0.00331631	0.00461716	0.00603279
-3.00	0.00134517	0.00099933	0.00160153	0.00198781	0.00035598	0.00027960	0.00041475	0.00146700	0.00172933	0.00167883	0.00188220	0.00317530
-4.00	0.00040616	0.00030026	0.00030502	0.00072540	0.00004928	0.00001617	0.00003009	0.00021594	0.00046728	0.00030722	0.00031621	0.00097411
-5.00	0.00009392	0.00004807	0.00004984	0.00025282	0.00000625	-0.00000005	0.00000108	0.00003135	0.00010400	0.00004424	0.00004765	0.00029402

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_5H_5\mathbf{N}$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00004814	0.00002783	0.00004828	0.00017389	0.00000184	0.00000013	0.00000178	0.00001334	0.00005090	0.00002621	0.00005002	0.00019079
4.00	0.00028620	0.00023489	0.00030233	0.00066541	0.00002381	0.00000501	0.00002378	0.00013577	0.00031390	0.00022868	0.00032630	0.00081300
3.00	0.00124084	0.00160122	0.00187415	0.00188047	0.00024965	0.00018066	0.00033903	0.00135246	0.00150120	0.00174473	0.00221869	0.00327347
2.50	0.00230824	0.00186657	0.00407612	0.00459814	0.00079247	0.00092577	0.00142440	0.00402278	0.00311778	0.00457773	0.00602387	0.00631903
2.00	0.00378251	-0.00098630	0.00875781	0.00971360	0.00239699	0.00414839	0.00552088	0.00955787	0.00620329	0.00821113	0.01320408	0.01523707
1.75	0.00447996	-0.00406175	0.01175561	0.01281403	0.00399448	0.00811467	0.01015194	0.01275913	0.00849926	0.00845231	0.01998758	0.02296662
1.60	0.00478947	-0.00619750	0.01348041	0.01452126	0.00531924	0.01171777	0.01423111	0.01426012	0.01013266	0.00778390	0.02530788	0.02875036
1.38	0.00497926	-0.00895065	0.01539032	0.01629553	0.00779090	0.01445872	0.01951097	0.02225860	0.01279075	0.00551835	0.03467579	0.03854513
1.25	0.00489609	-0.00996902	0.01595500	0.01672676	0.00965136	0.01331167	0.02562408	0.02859430	0.01456491	0.00332973	0.04136413	0.04530561
1.15	0.00471882	-0.01015918	0.01595742	0.01661610	0.01120147	0.01149297	0.03100954	0.03404197	0.01593508	0.00132405	0.04674972	0.05063695
1.00	0.00426464	-0.00925796	0.01517802	0.01566463	0.01373263	0.00709028	0.04027351	0.04324169	0.01800791	-0.00216724	0.05524283	0.05887622
0.75	0.00307784	-0.00424592	0.01177847	0.01202161	0.01822882	-0.00446919	0.05797158	0.06044837	0.02131131	-0.00869793	0.06959248	0.07242864
0.50	0.00164350	0.00397172	0.00668531	0.00675107	0.02243047	-0.01896782	0.07576675	0.07746925	0.02407516	-0.01491611	0.08232744	0.08416638
0.25	0.00045978	0.00190616	0.00194388	0.01199423	0.02545827	-0.03136725	0.08926766	0.09027536	0.02591815	-0.01937923	0.09117094	0.09220121
0.00	0.00000000	0.00000000	0.00000005	0.01528128	0.02656579	-0.03628251	0.09433951	0.09507020	0.02656579	-0.02100058	0.09433955	0.09507022
-0.25	0.00045978	0.00190616	0.00194388	0.01199423	0.02545827	-0.03136725	0.08926766	0.09027536	0.02591815	-0.01937923	0.09117094	0.09220121
-0.50	0.00164350	0.00397172	0.00668531	0.00675107	0.02243047	-0.01896782	0.07576675	0.07746925	0.02407516	-0.01491611	0.08232744	0.08416638
-0.75	0.00307784	-0.00424592	0.01177847	0.01202161	0.01822882	-0.00446919	0.05797158	0.06044837	0.02131131	-0.00869793	0.06959248	0.07242864
-1.00	0.00426464	-0.00925796	0.01517802	0.01566463	0.01373263	0.00709028	0.04027351	0.04324169	0.01800791	-0.00216724	0.05524283	0.05887622
-1.15	0.00471882	-0.01015918	0.01595742	0.01661610	0.01120147	0.01149297	0.03100954	0.03404197	0.01593508	0.00132405	0.04674972	0.05063695
-1.25	0.00489609	-0.00996902	0.01595500	0.01672676	0.00965136	0.01331167	0.02562408	0.02859430	0.01456491	0.00332973	0.04136413	0.04530561
-1.38	0.00497926	-0.00895065	0.01539032	0.01629553	0.00779090	0.01445872	0.01951097	0.02225860	0.01279075	0.00551835	0.03467579	0.03854513
-1.60	0.00478947	-0.00619750	0.01348041	0.01452126	0.00531924	0.01171777	0.01423111	0.01426012	0.01013266	0.00778390	0.02530788	0.02875036
-1.75	0.00447996	-0.00406175	0.01175561	0.01281403	0.00399448	0.00811467	0.01015194	0.01275913	0.00849926	0.00845231	0.01998758	0.02296662
-2.00	0.00378251	-0.00098630	0.00875781	0.00971360	0.00239699	0.00414839	0.00552088	0.00955787	0.00620329	0.00821113	0.01320408	0.01523707
-2.50	0.00230824	0.00186657	0.00407612	0.00459814	0.00079247	0.00092577	0.00142440	0.00402278	0.00311778	0.00457773	0.00602387	0.00631903
-3.00	0.00124084	0.00160122	0.00187415	0.00188047	0.00024965	0.00018066	0.00033903	0.00135246	0.00150120	0.00174473	0.00221869	0.00327347
-4.00	0.00028620	0.00023489	0.00030233	0.00066541	0.00002381	0.00000501	0.00002378	0.00013577	0.00031390	0.00022868	0.00032630	0.00081300
-5.00	0.00004814	0.00002783	0.00004828	0.00017389	0.00000184	0.00000013	0.00000178	0.00001334	0.00005090	0.00002621	0.00005002	0.00019079

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_5H_5\mathbf{NH}^+$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00003497	0.00001187	0.00003570	0.00015454	0.00000128	-0.00000019	0.00000130	0.00001208	0.00003710	0.00001034	0.00003684	0.00016976
4.00	0.00024017	0.00015284	0.00024995	0.00064306	0.00002082	0.00000421	0.00001879	0.00012295	0.00026506	0.00014662	0.00026831	0.00077736
3.50	0.00054214	0.00046504	0.00064435	0.00116848	0.00006941	0.00003193	0.00007104	0.00038163	0.00061902	0.00047136	0.00071516	0.00157548
3.00	0.00113051	0.00129562	0.00169667	0.00193872	0.00022300	0.00017977	0.00029606	0.00123083	0.00136640	0.00142673	0.00199334	0.00321526
2.50	0.00216705	0.00194848	0.00371486	0.00429082	0.00071199	0.00091262	0.00128983	0.00373763	0.00289995	0.00403439	0.00558337	0.00624027
2.00	0.00363897	-0.00074924	0.00842165	0.00925650	0.00217931	0.00409425	0.00512251	0.00909603	0.00584564	0.00775216	0.01291922	0.01438727
1.75	0.00435550	-0.00383863	0.01164301	0.01229329	0.00365819	0.00802521	0.00949550	0.01231963	0.00804000	0.00801348	0.01981662	0.02180132
1.50	0.00483042	-0.00746728	0.01473727	0.01491223	0.00588204	0.01346108	0.01579089	0.01655557	0.01073308	0.00648584	0.02958959	0.03148395
1.36	0.00490864	-0.00912918	0.01582071	0.01598839	0.00743999	0.01385508	0.02064861	0.02174279	0.01236443	0.00480742	0.03605805	0.03758043
1.15	0.00468516	-0.01033080	0.01606037	0.01677177	0.01043019	0.01125895	0.03158555	0.03213193	0.01512232	0.00096365	0.04779283	0.04820771
1.00	0.00425216	-0.00952882	0.01514502	0.01613814	0.01283091	0.00708809	0.04082957	0.04110927	0.01708429	-0.00239035	0.05598690	0.05668951
0.75	0.00308714	-0.00456489	0.01161792	0.01273662	0.01711294	-0.00401783	0.05704516	0.05937645	0.02019525	-0.00850619	0.06866839	0.07163671
0.50	0.00165575	0.00371641	0.00650468	0.00741803	0.02112988	-0.01803803	0.07301658	0.07779688	0.02278057	-0.01413295	0.07952135	0.08477941
0.25	0.00046447	0.00188076	0.00208119	0.01207967	0.02403177	-0.03005759	0.08498931	0.09179503	0.02449437	-0.01804737	0.08686904	0.09382812
0.00	0.00000000	0.00000000	0.00000004	0.01545133	0.02509452	-0.03482620	0.08946286	0.09705773	0.02509452	-0.01944249	0.08946290	0.09705773
-0.25	0.00046447	0.00188076	0.00208119	0.01207967	0.02403177	-0.03005759	0.08498931	0.09179503	0.02449437	-0.01804737	0.08686904	0.09382812
-0.50	0.00165575	0.00371641	0.00650468	0.00741803	0.02112988	-0.01803803	0.07301658	0.07779688	0.02278057	-0.01413295	0.07952135	0.08477941
-0.75	0.00308714	-0.00456489	0.01161792	0.01273662	0.01711294	-0.00401783	0.05704516	0.05937645	0.02019525	-0.00850619	0.06866839	0.07163671
-1.00	0.00425216	-0.00952882	0.01514502	0.01613814	0.01283091	0.00708809	0.04082957	0.04110927	0.01708429	-0.00239035	0.05598690	0.05668951
-1.15	0.00468516	-0.01033080	0.01606037	0.01677177	0.01043019	0.01125895	0.03158555	0.03213193	0.01512232	0.00096365	0.04779283	0.04820771
-1.36	0.00490864	-0.00912918	0.01582071	0.01598839	0.00743999	0.01385508	0.02064861	0.02174279	0.01236443	0.00480742	0.03605805	0.03758043
-1.50	0.00483042	-0.00746728	0.01473727	0.01491223	0.00588204	0.01346108	0.01579089	0.01655557	0.01073308	0.00648584	0.02958959	0.03148395
-1.75	0.00435550	-0.00383863	0.01164301	0.01229329	0.00365819	0.00802521	0.00949550	0.01231963	0.00804000	0.00801348	0.01981662	0.02180132
-2.00	0.00363897	-0.00074924	0.00842165	0.00925650	0.00217931	0.00409425	0.00512251	0.00909603	0.00584564	0.00775216	0.01291922	0.01438727
-2.50	0.00216705	0.00194848	0.00371486	0.00429082	0.00071199	0.00091262	0.00128983	0.00373763	0.00289995	0.00403439	0.00558337	0.00624027
-3.00	0.00113051	0.00129562	0.00169667	0.00193872	0.00022300	0.00017977	0.00029606	0.00123083	0.00136640	0.00142673	0.00199334	0.00321526
-3.50	0.00054214	0.00046504	0.00064435	0.00116848	0.00006941	0.00003193	0.00007104	0.00038163	0.00061902	0.00047136	0.00071516	0.00157548
-4.00	0.00024017	0.00015284	0.00024995	0.00064306	0.00002082	0.00000421	0.00001879	0.00012295	0.00026506	0.00014662	0.00026831	0.00077736
-5.00	0.00003497	0.00001187	0.00003570	0.00015454	0.00000128	-0.00000019	0.00000130	0.00001208	0.00003710	0.00001034	0.00003684	0.00016976

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_5H_5**P**. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00007267	0.00004545	0.00005296	0.00021571	0.00000287	0.00000121	0.00000176	0.00002035	0.00007483	0.00004678	0.00005668	0.00023309
4.00	0.00035519	0.00028883	0.00030834	0.00066295	0.00003479	0.00001772	0.00001942	0.00017379	0.00038756	0.00030858	0.00034121	0.00081942
3.00	0.00126508	0.00112192	0.00165858	0.00186789	0.00030635	0.00029682	0.00030498	0.00136503	0.00156552	0.00194784	0.00196582	0.00270413
2.50	0.00211586	0.00076581	0.00377062	0.00381401	0.00086586	0.00122120	0.00124869	0.00350736	0.00297482	0.00409362	0.00504949	0.00520414
2.00	0.00311611	-0.00162379	0.00687745	0.00753215	0.00231775	0.00437195	0.00463608	0.00720326	0.00542937	0.00547187	0.01140805	0.01216670
1.75	0.00350812	-0.00362711	0.00849056	0.00963443	0.00364440	0.00757497	0.00833653	0.00903793	0.00715095	0.00516651	0.01637417	0.01796945
1.60	0.00364358	-0.00484954	0.00926860	0.01072107	0.00469603	0.00915193	0.01081602	0.01152921	0.00834015	0.00447287	0.01998318	0.02224916
1.49	0.00367561	-0.00561757	0.00967077	0.01133221	0.00559459	0.00926567	0.01319728	0.01439878	0.00927232	0.00369230	0.02289437	0.02573032
1.35	0.00361783	-0.00628809	0.00990858	0.01178991	0.00691022	0.00863880	0.01694654	0.01879732	0.01053206	0.00234748	0.02692823	0.03058727
1.15	0.00332262	-0.00627733	0.00957882	0.01161666	0.00906749	0.00614000	0.02341122	0.02643578	0.01239616	-0.00016535	0.03308292	0.03805356
1.00	0.00293781	-0.00529924	0.00876408	0.01075665	0.01085074	0.00293652	0.02897928	0.03309243	0.01379533	-0.00239448	0.03783418	0.04385082
0.75	0.00205524	-0.00174821	0.00644644	0.00802492	0.01391974	-0.00458840	0.03895902	0.04517784	0.01598115	-0.00634770	0.04546558	0.05320460
0.50	0.00107203	0.00303160	0.00381232	0.00439104	0.01669673	-0.01328395	0.04837353	0.05673011	0.01777255	-0.00992429	0.05190003	0.06112178
0.25	0.00029556	0.00098227	0.00124871	0.00793959	0.01865293	-0.02035937	0.05520662	0.06519304	0.01894963	-0.01240085	0.05620940	0.06644117
0.00	0.00000000	0.00000000	0.00000030	0.00977468	0.01936009	-0.02309681	0.05771589	0.06831582	0.01936009	-0.01328351	0.05771639	0.06831585
-0.25	0.00029556	0.00098227	0.00124871	0.00793959	0.01865293	-0.02035937	0.05520662	0.06519304	0.01894963	-0.01240085	0.05620940	0.06644117
-0.50	0.00107203	0.00303160	0.00381232	0.00439104	0.01669673	-0.01328395	0.04837353	0.05673011	0.01777255	-0.00992429	0.05190003	0.06112178
-0.75	0.00205524	-0.00174821	0.00644644	0.00802492	0.01391974	-0.00458840	0.03895902	0.04517784	0.01598115	-0.00634770	0.04546558	0.05320460
-1.00	0.00293781	-0.00529924	0.00876408	0.01075665	0.01085074	0.00293652	0.02897928	0.03309243	0.01379533	-0.00239448	0.03783418	0.04385082
-1.15	0.00332262	-0.00627733	0.00957882	0.01161666	0.00906749	0.00614000	0.02341122	0.02643578	0.01239616	-0.00016535	0.03308292	0.03805356
-1.35	0.00361783	-0.00628809	0.00990858	0.01178991	0.00691022	0.00863880	0.01694654	0.01879732	0.01053206	0.00234748	0.02692823	0.03058727
-1.49	0.00367561	-0.00561757	0.00967077	0.01133221	0.00559459	0.00926567	0.01319728	0.01439878	0.00927232	0.00369230	0.02289437	0.02573032
-1.60	0.00364358	-0.00484954	0.00926860	0.01072107	0.00469603	0.00915193	0.01081602	0.01152921	0.00834015	0.00447287	0.01998318	0.02224916
-1.75	0.00350812	-0.00362711	0.00849056	0.00963443	0.00364440	0.00757497	0.00833653	0.00903793	0.00715095	0.00516651	0.01637417	0.01796945
-2.00	0.00311611	-0.00162379	0.00687745	0.00753215	0.00231775	0.00437195	0.00463608	0.00720326	0.00542937	0.00547187	0.01140805	0.01216670
-2.50	0.00211586	0.00076581	0.00377062	0.00381401	0.00086586	0.00122120	0.00124869	0.00350736	0.00297482	0.00409362	0.00504949	0.00520414
-3.00	0.00126508	0.00112192	0.00165858	0.00186789	0.00030635	0.00029682	0.00030498	0.00136503	0.00156552	0.00194784	0.00196582	0.00270413
-4.00	0.00035519	0.00028883	0.00030834	0.00066295	0.00003479	0.00001772	0.00001942	0.00017379	0.00038756	0.00030858	0.00034121	0.00081942
-5.00	0.00007267	0.00004545	0.00005296	0.00021571	0.00000287	0.00000121	0.00000176	0.00002035	0.00007483	0.00004678	0.00005668	0.00023309

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_5H_5\mathbf{O}^+$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00003302	-0.00000141	0.00003442	0.00014733	0.00000135	-0.00000033	0.00000122	0.00001191	0.00003651	-0.00000359	0.00003534	0.00016706
4.00	0.00022201	0.00006732	0.00024770	0.00062588	0.00002057	-0.00000055	0.00001820	0.00012264	0.00025448	0.00004581	0.00026488	0.00077833
3.00	0.00106286	0.00107341	0.00172686	0.00199916	0.00022238	0.00012254	0.00029519	0.00126742	0.00132575	0.00104597	0.00202646	0.00340811
2.50	0.00208424	0.00205218	0.00332702	0.00443145	0.00071999	0.00071927	0.00129951	0.00386649	0.00286947	0.00327159	0.00574525	0.00663083
2.00	0.00357268	-0.00059691	0.00759431	0.00970062	0.00222460	0.00344247	0.00520798	0.00943249	0.00588692	0.00731632	0.01219510	0.01493904
1.75	0.00431170	-0.00372058	0.01064805	0.01296971	0.00374435	0.00694732	0.00969021	0.01282413	0.00814853	0.008092263	0.017933878	0.02269933
1.50	0.00481705	-0.00744654	0.01376175	0.01583345	0.00603371	0.01268797	0.01570287	0.01695038	0.01093319	0.00686079	0.02680382	0.03282793
1.35	0.00491438	-0.00935341	0.01525667	0.01693341	0.00783055	0.01426017	0.01982921	0.02294029	0.01281460	0.00505247	0.03370600	0.03991582
1.25	0.00486611	-0.01021263	0.01593235	0.01726639	0.00921614	0.01358613	0.02439603	0.02769878	0.01414109	0.00339465	0.03897858	0.04500323
1.15	0.00471689	-0.01056374	0.01624610	0.01720464	0.01073356	0.01196002	0.02985936	0.03303317	0.01549740	0.00141396	0.04470449	0.05026961
1.00	0.00429773	-0.00986547	0.01588848	0.01628771	0.01322494	0.00772995	0.03955744	0.04204468	0.01755143	-0.00206744	0.05400167	0.05835142
0.75	0.00313931	-0.00494486	0.01257920	0.01286599	0.01768733	-0.00384301	0.05876792	0.05889784	0.02083124	-0.00862870	0.07035162	0.07147302
0.50	0.00169231	0.00345173	0.00709523	0.00775820	0.02189503	-0.01871343	0.07555905	0.07872742	0.02358239	-0.01488556	0.08263889	0.08543013
0.25	0.00047635	0.00207532	0.00213227	0.01234932	0.02494740	-0.03160005	0.08808652	0.09419671	0.02542095	-0.01936260	0.09015179	0.09616883
0.00	0.00000000	0.00000000	0.00000046	0.01586544	0.02606786	-0.03673990	0.09277527	0.10006919	0.02606786	-0.02098375	0.09277561	0.10006919
-0.25	0.00047635	0.00207532	0.00213227	0.01234932	0.02494740	-0.03160005	0.08808652	0.09419671	0.02542095	-0.01936260	0.09015179	0.09616883
-0.50	0.00169231	0.00345173	0.00709523	0.00775820	0.02189503	-0.01871343	0.07555905	0.07872742	0.02358239	-0.01488556	0.08263889	0.08543013
-0.75	0.00313931	-0.00494486	0.01257920	0.01286599	0.01768733	-0.00384301	0.05876792	0.05889784	0.02083124	-0.00862870	0.07035162	0.07147302
-1.00	0.00429773	-0.00986547	0.01588848	0.01628771	0.01322494	0.00772995	0.03955744	0.04204468	0.01755143	-0.00206744	0.05400167	0.05835142
-1.15	0.00471689	-0.01056374	0.01624610	0.01720464	0.01073356	0.01196002	0.02985936	0.03303317	0.01549740	0.00141396	0.04470449	0.05026961
-1.25	0.00486611	-0.01021263	0.01593235	0.01726639	0.00921614	0.01358613	0.02439603	0.02769878	0.01414109	0.00339465	0.03897858	0.04500323
-1.35	0.00491438	-0.00935341	0.01525667	0.01693341	0.00783055	0.01426017	0.01982921	0.02294029	0.01281460	0.00505247	0.03370600	0.03991582
-1.50	0.00481705	-0.00744654	0.01376175	0.01583345	0.00603371	0.01268797	0.01570287	0.01695038	0.01093319	0.00686079	0.02680382	0.03282793
-1.75	0.00431170	-0.00372058	0.01064805	0.01296971	0.00374435	0.00694732	0.00969021	0.01282413	0.00814853	0.008092263	0.017933878	0.02269933
-2.00	0.00357268	-0.00059691	0.00759431	0.00970062	0.00222460	0.00344247	0.00520798	0.00943249	0.00588692	0.00731632	0.01219510	0.01493904
-2.50	0.00208424	0.00205218	0.00332702	0.00443145	0.00071999	0.00071927	0.00129951	0.00386649	0.00286947	0.00327159	0.00574525	0.00663083
-3.00	0.00106286	0.00107341	0.00172686	0.00199916	0.00022238	0.00012254	0.00029519	0.00126742	0.00132575	0.00104597	0.00202646	0.00340811
-4.00	0.00022201	0.00006732	0.00024770	0.00062588	0.00002057	-0.00000055	0.00001820	0.00012264	0.00025448	0.00004581	0.00026488	0.00077833
-5.00	0.00003302	-0.00000141	0.00003442	0.00014733	0.00000135	-0.00000033	0.00000122	0.00001191	0.00003651	-0.00000359	0.00003534	0.00016706

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_5H_5S^+$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00004442	0.00003150	0.00003770	0.00015885	0.00000174	0.00000071	0.00000090	0.00001385	0.00004598	0.00003257	0.00003779	0.00017226
4.00	0.00026428	0.00022665	0.00025434	0.00055455	0.00002474	0.00001373	0.00001556	0.00013765	0.00028855	0.00024309	0.00026279	0.00069047
3.00	0.00108008	0.00134231	0.00147553	0.00162367	0.00025151	0.00026299	0.00027702	0.00125949	0.00133067	0.00174356	0.00183932	0.00262816
2.50	0.00193551	0.00117601	0.00358444	0.00370046	0.00076412	0.00113246	0.00120265	0.00345899	0.00269997	0.00461461	0.00472831	0.00486519
2.00	0.00303719	-0.00127505	0.00723968	0.00744168	0.00217825	0.00439169	0.00453285	0.00746686	0.00522193	0.00617080	0.01170206	0.01185501
1.75	0.00351320	-0.00355008	0.00918487	0.00969524	0.00351420	0.00803449	0.00810944	0.00947408	0.00703929	0.00584158	0.01726226	0.01775572
1.60	0.00370177	-0.00500602	0.01016664	0.01089284	0.00458926	0.01001166	0.01121095	0.01136780	0.00830647	0.00505704	0.02135306	0.02213239
1.44	0.00377852	-0.00634110	0.01088822	0.01184051	0.00599340	0.01003295	0.01556350	0.01560693	0.00979087	0.00366491	0.02633402	0.02747804
1.25	0.00365882	-0.00715215	0.01108916	0.01225026	0.00797038	0.00854391	0.02183859	0.02217672	0.01165111	0.00133179	0.03283436	0.03445816
1.15	0.00349383	-0.00707328	0.01084864	0.01207496	0.00914327	0.00698598	0.02570368	0.02625256	0.01265974	-0.00015805	0.03647139	0.03835797
1.00	0.00311585	-0.00613202	0.01000160	0.01124576	0.01102630	0.00358945	0.03209891	0.03303936	0.01416451	-0.00261964	0.04203929	0.04431296
0.75	0.00220467	-0.00231236	0.00741866	0.00845526	0.01428971	-0.00453958	0.04367309	0.04543396	0.01651242	-0.00690573	0.05106086	0.05390893
0.50	0.00115905	0.00333105	0.00407724	0.00465222	0.01726205	-0.01405909	0.05469986	0.05735117	0.01843149	-0.01069081	0.05873608	0.06201245
0.25	0.00032103	0.00115172	0.00132757	0.00853672	0.01936488	-0.02186396	0.06275804	0.06611678	0.01968894	-0.01325637	0.06390999	0.06744510
0.00	0.00000000	0.00000000	0.00000023	0.01063281	0.02012667	-0.02489436	0.06572755	0.06935795	0.02012667	-0.01415930	0.06572768	0.06935796
-0.25	0.00032103	0.00115172	0.00132757	0.00853672	0.01936488	-0.02186396	0.06275804	0.06611678	0.01968894	-0.01325637	0.06390999	0.06744510
-0.50	0.00115905	0.00333105	0.00407724	0.00465222	0.01726205	-0.01405909	0.05469986	0.05735117	0.01843149	-0.01069081	0.05873608	0.06201245
-0.75	0.00220467	-0.00231236	0.00741866	0.00845526	0.01428971	-0.00453958	0.04367309	0.04543396	0.01651242	-0.00690573	0.05106086	0.05390893
-1.00	0.00311585	-0.00613202	0.01000160	0.01124576	0.01102630	0.00358945	0.03209891	0.03303936	0.01416451	-0.00261964	0.04203929	0.04431296
-1.15	0.00349383	-0.00707328	0.01084864	0.01207496	0.00914327	0.00698598	0.02570368	0.02625256	0.01265974	-0.00015805	0.03647139	0.03835797
-1.25	0.00365882	-0.00715215	0.01108916	0.01225026	0.00797038	0.00854391	0.02183859	0.02217672	0.01165111	0.00133179	0.03283436	0.03445816
-1.44	0.00377852	-0.00634110	0.01088822	0.01184051	0.00599340	0.01003295	0.01556350	0.01560693	0.00979087	0.00366491	0.02633402	0.02747804
-1.60	0.00370177	-0.00500602	0.01016664	0.01089284	0.00458926	0.01001166	0.01121095	0.01136780	0.00830647	0.00505704	0.02135306	0.02213239
-1.75	0.00351320	-0.00355008	0.00918487	0.00969524	0.00351420	0.00803449	0.00810944	0.00947408	0.00703929	0.00584158	0.01726226	0.01775572
-2.00	0.00303719	-0.00127505	0.00723968	0.00744168	0.00217825	0.00439169	0.00453285	0.00746686	0.00522193	0.00617080	0.01170206	0.01185501
-2.50	0.00193551	0.00117601	0.00358444	0.00370046	0.00076412	0.00113246	0.00120265	0.00345899	0.00269997	0.00461461	0.00472831	0.00486519
-3.00	0.00108008	0.00134231	0.00147553	0.00162367	0.00025151	0.00026299	0.00027702	0.00125949	0.00133067	0.00174356	0.00183932	0.00262816
-4.00	0.00026428	0.00022665	0.00025434	0.00055455	0.00002474	0.00001373	0.00001556	0.00013765	0.00028855	0.00024309	0.00026279	0.00069047
-5.00	0.00004442	0.00003150	0.00003770	0.00015885	0.00000174	0.00000071	0.00000090	0.00001385	0.00004598	0.00003257	0.00003779	0.00017226

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_σ and ρ_π in atomic units for C_6H_6**BH**. The highlighted cells display the position of RCPs of ρ_π.

	$\rho(r)_\pi$				$\rho(r)_\sigma$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00005258	0.00003352	0.00004335	0.00013941	0.00000361	0.00000022	0.00000192	0.00002165	0.00005595	0.00003624	0.00004352	0.00016036
4.00	0.00024366	0.00020382	0.00025402	0.00039279	0.00003539	0.00001299	0.00002715	0.00015429	0.00027834	0.00023538	0.00026665	0.00054377
3.00	0.00080493	0.00046164	0.00106671	0.00119441	0.00025753	0.00020824	0.00031679	0.00089187	0.00106081	0.00117015	0.00140065	0.00157585
2.50	0.00125470	0.00002738	0.00210212	0.00239928	0.00064005	0.00077439	0.00105862	0.00194629	0.00189290	0.00184476	0.00316918	0.00331311
2.00	0.00169458	-0.00118624	0.00360768	0.00420091	0.00149541	0.00260003	0.00300136	0.00370430	0.00318891	0.00210152	0.00679298	0.00707156
1.80	0.00180709	-0.00182765	0.00419824	0.00492776	0.00204648	0.00366032	0.00402802	0.00515217	0.00385313	0.00190728	0.00894672	0.00933014
1.61	0.00184713	-0.00238157	0.00463273	0.00547568	0.00271011	0.00384721	0.00592650	0.00724007	0.00455751	0.00148579	0.01139253	0.01191264
1.40	0.00179197	-0.00273736	0.00484662	0.00576561	0.00359696	0.00347176	0.00869685	0.01026241	0.00538995	0.00073394	0.01445285	0.01517162
1.20	0.00162913	-0.00263537	0.00469475	0.00561149	0.00458502	0.00239638	0.01202800	0.01382979	0.00621570	-0.00024600	0.01763068	0.01859101
1.00	0.00136291	-0.00196259	0.00414890	0.00497415	0.00566648	0.00056364	0.01590956	0.01791639	0.00703118	-0.00140531	0.02087630	0.02212399
0.75	0.00092783	-0.00033929	0.00299143	0.00358668	0.00703642	-0.00258640	0.02111406	0.02331180	0.00796582	-0.00292242	0.02469558	0.02633909
0.50	0.00047430	0.00149231	0.00185613	0.00191436	0.00824383	-0.00602357	0.02592493	0.02823765	0.00871906	-0.00425807	0.02783152	0.02985030
0.25	0.00012915	0.00044270	0.00053166	0.00355298	0.00907917	-0.00872329	0.02936069	0.03172811	0.00920860	-0.00516646	0.02989130	0.03218072
0.00	0.00000000	0.00000000	0.00000021	0.00425330	0.00937839	-0.00974983	0.03061107	0.03299364	0.00937839	-0.00548727	0.03061134	0.03299370
-0.25	0.00012915	0.00044270	0.00053166	0.00355298	0.00907917	-0.00872329	0.02936069	0.03172811	0.00920860	-0.00516646	0.02989130	0.03218072
-0.50	0.00047430	0.00149231	0.00185613	0.00191436	0.00824383	-0.00602357	0.02592493	0.02823765	0.00871906	-0.00425807	0.02783152	0.02985030
-0.75	0.00092783	-0.00033929	0.00299143	0.00358668	0.00703642	-0.00258640	0.02111406	0.02331180	0.00796582	-0.00292242	0.02469558	0.02633909
-1.00	0.00136291	-0.00196259	0.00414890	0.00497415	0.00566648	0.00056364	0.01590956	0.01791639	0.00703118	-0.00140531	0.02087630	0.02212399
-1.20	0.00162913	-0.00263537	0.00469475	0.00561149	0.00458502	0.00239638	0.01202800	0.01382979	0.00621570	-0.00024600	0.01763068	0.01859101
-1.40	0.00179197	-0.00273736	0.00484662	0.00576561	0.00359696	0.00347176	0.00869685	0.01026241	0.00538995	0.00073394	0.01445285	0.01517162
-1.61	0.00184713	-0.00238157	0.00463273	0.00547568	0.00271011	0.00384721	0.00592650	0.00724007	0.00455751	0.00148579	0.01139253	0.01191264
-1.80	0.00180709	-0.00182765	0.00419824	0.00492776	0.00204648	0.00366032	0.00402802	0.00515217	0.00385313	0.00190728	0.00894672	0.00933014
-2.00	0.00169458	-0.00118624	0.00360768	0.00420091	0.00149541	0.00260003	0.00300136	0.00370430	0.00318891	0.00210152	0.00679298	0.00707156
-2.50	0.00125470	0.00002738	0.00210212	0.00239928	0.00064005	0.00077439	0.00105862	0.00194629	0.00189290	0.00184476	0.00316918	0.00331311
-3.00	0.00080493	0.00046164	0.00106671	0.00119441	0.00025753	0.00020824	0.00031679	0.00089187	0.00106081	0.00117015	0.00140065	0.00157585
-4.00	0.00024366	0.00020382	0.00025402	0.00039279	0.00003539	0.00001299	0.00002715	0.00015429	0.00027834	0.00023538	0.00026665	0.00054377
-5.00	0.00005258	0.00003352	0.00004335	0.00013941	0.00000361	0.00000022	0.00000192	0.00002165	0.00005595	0.00003624	0.00004352	0.00016036

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_6H_6**AlH**. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00005775	0.00002453	0.00004512	0.00012382	0.00001050	0.00000046	0.00000069	0.00003772	0.00006672	0.00002967	0.00004540	0.00015792
4.00	0.00022708	0.00014978	0.00024462	0.00029211	0.00005992	0.00001601	0.00002658	0.00021318	0.00028340	0.00019812	0.00025814	0.00049310
3.00	0.00065321	0.00017707	0.00071423	0.00097691	0.00032427	0.00019015	0.00028679	0.00093939	0.00097211	0.00080417	0.00115837	0.00136467
2.50	0.00094114	-0.00021765	0.00131288	0.00174719	0.00070334	0.00062352	0.00084533	0.00173662	0.00164077	0.00112672	0.00235798	0.00265773
2.00	0.00116792	-0.00093845	0.00208894	0.00272605	0.00142920	0.00186850	0.00187260	0.00313113	0.00259892	0.00111401	0.00458026	0.00522354
1.75	0.00120618	-0.00131152	0.00242059	0.00314109	0.00198286	0.00212277	0.00307986	0.00454922	0.00319476	0.00084982	0.00620796	0.00714692
1.50	0.00116419	-0.00151512	0.00258118	0.00333763	0.00264923	0.00191396	0.00475946	0.00656012	0.00382269	0.00038128	0.00808683	0.00939040
1.30	0.00106397	-0.00145931	0.00253329	0.00326835	0.00327634	0.00134532	0.00651653	0.00863026	0.00435153	-0.00014639	0.00977757	0.01142443
1.00	0.00080972	-0.00087008	0.00210950	0.00270949	0.00430506	-0.00020904	0.00969348	0.01227341	0.00512623	-0.00110273	0.01240010	0.01460212
0.75	0.00053751	0.00004828	0.00149304	0.00189601	0.00515408	-0.00197989	0.01254025	0.01545032	0.00570056	-0.00192435	0.01443597	0.01708551
0.50	0.00026972	0.00072664	0.00098306	0.00119886	0.00588128	-0.00379921	0.01511346	0.01826674	0.00615602	-0.00262750	0.01609725	0.01912045
0.25	0.00007261	0.00020890	0.00026476	0.00204414	0.00637492	-0.00517809	0.01692288	0.02022125	0.00644898	-0.00309811	0.01718820	0.02045659
0.00	0.00000000	0.00000000	0.00000033	0.00238221	0.00655007	-0.00569363	0.01757616	0.02092226	0.00655007	-0.00326315	0.01757646	0.02092226
-0.25	0.00007261	0.00020890	0.00026476	0.00204414	0.00637492	-0.00517809	0.01692288	0.02022125	0.00644898	-0.00309811	0.01718820	0.02045659
-0.50	0.00026972	0.00072664	0.00098306	0.00119886	0.00588128	-0.00379921	0.01511346	0.01826674	0.00615602	-0.00262750	0.01609725	0.01912045
-0.75	0.00053751	0.00004828	0.00149304	0.00189601	0.00515408	-0.00197989	0.01254025	0.01545032	0.00570056	-0.00192435	0.01443597	0.01708551
-1.00	0.00080972	-0.00087008	0.00210950	0.00270949	0.00430506	-0.00020904	0.00969348	0.01227341	0.00512623	-0.00110273	0.01240010	0.01460212
-1.30	0.00106397	-0.00145931	0.00253329	0.00326835	0.00327634	0.00134532	0.00651653	0.00863026	0.00435153	-0.00014639	0.00977757	0.01142443
-1.50	0.00116419	-0.00151512	0.00258118	0.00333763	0.00264923	0.00191396	0.00475946	0.00656012	0.00382269	0.00038128	0.00808683	0.00939040
-1.75	0.00120618	-0.00131152	0.00242059	0.00314109	0.00198286	0.00212277	0.00307986	0.00454922	0.00319476	0.00084982	0.00620796	0.00714692
-2.00	0.00116792	-0.00093845	0.00208894	0.00272605	0.00142920	0.00186850	0.00187260	0.00313113	0.00259892	0.00111401	0.00458026	0.00522354
-2.50	0.00094114	-0.00021765	0.00131288	0.00174719	0.00070334	0.00062352	0.00084533	0.00173662	0.00164077	0.00112672	0.00235798	0.00265773
-3.00	0.00065321	0.00017707	0.00071423	0.00097691	0.00032427	0.00019015	0.00028679	0.00093939	0.00097211	0.00080417	0.00115837	0.00136467
-4.00	0.00022708	0.00014978	0.00024462	0.00029211	0.00005992	0.00001601	0.00002658	0.00021318	0.00028340	0.00019812	0.00025814	0.00049310
-5.00	0.00005775	0.00002453	0.00004512	0.00012382	0.00001050	0.00000046	0.00000069	0.00003772	0.00006672	0.00002967	0.00004540	0.00015792

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_6H_6**SiH**$^+$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00004321	0.00003079	0.00003509	0.00013581	0.00000444	-0.00000028	0.00000181	0.00002423	0.00004830	0.00003059	0.00003525	0.00016230
4.00	0.00021727	0.00019851	0.00020589	0.00038245	0.00003835	0.00001053	0.00002860	0.00015555	0.00025779	0.00020981	0.00022825	0.00054412
3.00	0.00072212	0.00034375	0.00093842	0.00108975	0.00025614	0.00017523	0.00032158	0.00083368	0.00098315	0.00096393	0.00111718	0.00161549
2.50	0.00110576	-0.00009169	0.00183672	0.00207426	0.00061122	0.00062522	0.00101087	0.00172549	0.00172255	0.00141647	0.00246801	0.00327582
2.00	0.00145432	-0.00110398	0.00310741	0.00344505	0.00136502	0.00200926	0.00245142	0.00338730	0.00282347	0.00148911	0.00512498	0.00663726
1.66	0.00155153	-0.00190114	0.00387222	0.00424398	0.00224314	0.00289108	0.00406951	0.00606338	0.00379640	0.00101593	0.00795018	0.01021267
1.50	0.00152764	-0.00213085	0.00405709	0.00442606	0.00275104	0.00273457	0.00541242	0.00780027	0.00427918	0.00061842	0.00947747	0.01213961
1.30	0.00142177	-0.00216395	0.00405553	0.00440174	0.00349927	0.00210178	0.00754538	0.01050050	0.00492011	-0.00005110	0.01160771	0.01481952
1.15	0.00128613	-0.00192930	0.00384477	0.00416065	0.00411665	0.00127274	0.00942071	0.01282501	0.00540103	-0.00064455	0.01327111	0.01690583
1.00	0.00110761	-0.00144454	0.00344943	0.00372604	0.00476224	0.00014790	0.01147616	0.01533050	0.00586761	-0.00128233	0.01492994	0.01898097
0.75	0.00074663	-0.00014288	0.00245525	0.00265858	0.00583022	-0.00221924	0.01505717	0.01961313	0.00657464	-0.00234015	0.01751469	0.02220337
0.50	0.00037887	0.00122792	0.00129112	0.00165870	0.00675960	-0.00472987	0.01833054	0.02345649	0.00713707	-0.00323708	0.01962241	0.02481974
0.25	0.00010270	0.00035331	0.00037877	0.00285554	0.00739703	-0.00666811	0.02064970	0.02614648	0.00749930	-0.00383026	0.02100302	0.02652417
0.00	0.00000000	0.00000000	0.00000015	0.00337683	0.00762435	-0.00739900	0.02149020	0.02711550	0.00762435	-0.00403659	0.02149037	0.02711550
-0.25	0.00010270	0.00035331	0.00037877	0.00285554	0.00739703	-0.00666811	0.02064970	0.02614648	0.00749930	-0.00383026	0.02100302	0.02652417
-0.50	0.00037887	0.00122792	0.00129112	0.00165870	0.00675960	-0.00472987	0.01833054	0.02345649	0.00713707	-0.00323708	0.01962241	0.02481974
-0.75	0.00074663	-0.00014288	0.00245525	0.00265858	0.00583022	-0.00221924	0.01505717	0.01961313	0.00657464	-0.00234015	0.01751469	0.02220337
-1.00	0.00110761	-0.00144454	0.00344943	0.00372604	0.00476224	0.00014790	0.01147616	0.01533050	0.00586761	-0.00128233	0.01492994	0.01898097
-1.15	0.00128613	-0.00192930	0.00384477	0.00416065	0.00411665	0.00127274	0.00942071	0.01282501	0.00540103	-0.00064455	0.01327111	0.01690583
-1.30	0.00142177	-0.00216395	0.00405553	0.00440174	0.00349927	0.00210178	0.00754538	0.01050050	0.00492011	-0.00005110	0.01160771	0.01481952
-1.50	0.00152764	-0.00213085	0.00405709	0.00442606	0.00275104	0.00273457	0.00541242	0.00780027	0.00427918	0.00061842	0.00947747	0.01213961
-1.66	0.00155153	-0.00190114	0.00387222	0.00424398	0.00224314	0.00289108	0.00406951	0.00606338	0.00379640	0.00101593	0.00795018	0.01021267
-2.00	0.00145432	-0.00110398	0.00310741	0.00344505	0.00136502	0.00200926	0.00245142	0.00338730	0.00282347	0.00148911	0.00512498	0.00663726
-2.50	0.00110576	-0.00009169	0.00183672	0.00207426	0.00061122	0.00062522	0.00101087	0.00172549	0.00172255	0.00141647	0.00246801	0.00327582
-3.00	0.00072212	0.00034375	0.00093842	0.00108975	0.00025614	0.00017523	0.00032158	0.00083368	0.00098315	0.00096393	0.00111718	0.00161549
-4.00	0.00021727	0.00019851	0.00020589	0.00038245	0.00003835	0.00001053	0.00002860	0.00015555	0.00025779	0.00020981	0.00022825	0.00054412
-5.00	0.00004321	0.00003079	0.00003509	0.00013581	0.00000444	-0.00000028	0.00000181	0.00002423	0.00004830	0.00003059	0.00003525	0.00016230

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_6H_6\mathbf{N}^+$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00002697	0.00001814	0.00002937	0.00010815	0.00000142	0.00000007	0.00000116	0.00001214	0.00002894	0.00001716	0.00003062	0.00012269
4.00	0.00017248	0.00015906	0.00019909	0.00038378	0.00002142	0.00000575	0.00001737	0.00011748	0.00019645	0.00015749	0.00021729	0.00050850
3.00	0.00070480	0.00070135	0.00102749	0.00112172	0.00020324	0.00016579	0.00023891	0.00085729	0.00091449	0.00113211	0.00136548	0.00161678
2.50	0.00120925	0.00040052	0.00228585	0.00249662	0.00056649	0.00071694	0.00091631	0.00208744	0.00178492	0.00238870	0.00309722	0.00342272
2.00	0.00179013	-0.00100495	0.00437940	0.00478356	0.00005116	0.00268351	0.00322002	0.00411053	0.00327151	0.00306659	0.00707883	0.00801926
1.70	0.00204205	-0.00236102	0.00574212	0.00624006	0.00246820	0.00507201	0.00545000	0.00628900	0.00452273	0.00272653	0.01112973	0.01254756
1.50	0.00210007	-0.00318305	0.00641576	0.00693368	0.00337833	0.00520680	0.00821256	0.00936758	0.00549040	0.00200801	0.01458033	0.01632033
1.30	0.00203201	-0.00362399	0.00669026	0.00718223	0.00450318	0.00449090	0.01197646	0.01343045	0.00654589	0.00085126	0.01860648	0.02063062
1.15	0.00188738	-0.00351704	0.00653058	0.00697397	0.00546210	0.00326946	0.01540539	0.01706775	0.00735876	-0.00026109	0.02187089	0.02405757
1.00	0.00166453	-0.00293532	0.00601934	0.00639496	0.00649340	0.00142184	0.01928254	0.02112460	0.00816552	-0.00152345	0.02523762	0.02753240
0.75	0.00115989	-0.00090623	0.00445732	0.00469948	0.00825477	-0.00282861	0.02629069	0.02834123	0.00941928	-0.00373566	0.03069702	0.03304752
0.50	0.00060307	0.00191890	0.00244166	0.00254113	0.00983623	-0.00765691	0.03294063	0.03508179	0.01044141	-0.00570816	0.03533402	0.03762405
0.25	0.00016591	0.00068027	0.00071777	0.00447082	0.01094412	-0.01154010	0.03777724	0.03993226	0.01111056	-0.00705660	0.03845313	0.04064965
0.00	0.00000000	0.00000000	0.00000006	0.00548299	0.01134346	-0.01303330	0.03955402	0.04170464	0.01134346	-0.00753345	0.03955406	0.04170467
-0.25	0.00016591	0.00068027	0.00071777	0.00447082	0.01094412	-0.01154010	0.03777724	0.03993226	0.01111056	-0.00705660	0.03845313	0.04064965
-0.50	0.00060307	0.00191890	0.00244166	0.00254113	0.00983623	-0.00765691	0.03294063	0.03508179	0.01044141	-0.00570816	0.03533402	0.03762405
-0.75	0.00115989	-0.00090623	0.00445732	0.00469948	0.00825477	-0.00282861	0.02629069	0.02834123	0.00941928	-0.00373566	0.03069702	0.03304752
-1.00	0.00166453	-0.00293532	0.00601934	0.00639496	0.00649340	0.00142184	0.01928254	0.02112460	0.00816552	-0.00152345	0.02523762	0.02753240
-1.15	0.00188738	-0.00351704	0.00653058	0.00697397	0.00546210	0.00326946	0.01540539	0.01706775	0.00735876	-0.00026109	0.02187089	0.02405757
-1.30	0.00203201	-0.00362399	0.00669026	0.00718223	0.00450318	0.00449090	0.01197646	0.01343045	0.00654589	0.00085126	0.01860648	0.02063062
-1.50	0.00210007	-0.00318305	0.00641576	0.00693368	0.00337833	0.00520680	0.00821256	0.00936758	0.00549040	0.00200801	0.01458033	0.01632033
-1.70	0.00204205	-0.00236102	0.00574212	0.00624006	0.00246820	0.00507201	0.00545000	0.00628900	0.00452273	0.00272653	0.01112973	0.01254756
-2.00	0.00179013	-0.00100495	0.00437940	0.00478356	0.00005116	0.00268351	0.00322002	0.00411053	0.00327151	0.00306659	0.00707883	0.00801926
-2.50	0.00120925	0.00040052	0.00228585	0.00249662	0.00056649	0.00071694	0.00091631	0.00208744	0.00178492	0.00238870	0.00309722	0.00342272
-3.00	0.00070480	0.00070135	0.00102749	0.00112172	0.00020324	0.00016579	0.00023891	0.00085729	0.00091449	0.00113211	0.00136548	0.00161678
-4.00	0.00017248	0.00015906	0.00019909	0.00038378	0.00002142	0.00000575	0.00001737	0.00011748	0.00019645	0.00015749	0.00021729	0.00050850
-5.00	0.00002697	0.00001814	0.00002937	0.00010815	0.00000142	0.00000007	0.00000116	0.00001214	0.00002894	0.00001716	0.00003062	0.00012269

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_6H_6**NH**. The highlighted cells display the position of RCPs ofρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00004079	0.00001651	0.00004698	0.00012418	0.00000178	0.00000018	0.00000149	0.00001397	0.00004265	0.00001676	0.00004837	0.00013843
4.00	0.00021054	0.00013207	0.00026829	0.00037632	0.00002382	0.00000708	0.00002092	0.00011857	0.00023468	0.00013935	0.00028868	0.00049554
3.00	0.00074830	0.00054768	0.00082949	0.00127146	0.00020136	0.00015576	0.00025774	0.00076596	0.00095039	0.00095648	0.00134420	0.00152694
2.50	0.00120981	0.00019086	0.00179718	0.00261019	0.00053228	0.00062650	0.00093528	0.00179669	0.00174292	0.00193313	0.00248125	0.00354058
2.00	0.00169982	-0.00106027	0.00336306	0.00470175	0.00132316	0.00223262	0.00315096	0.00346258	0.00302364	0.00236046	0.00564188	0.00784306
1.70	0.00188817	-0.00216595	0.00435603	0.00596996	0.00217982	0.00410890	0.00458523	0.00604187	0.00406835	0.00206031	0.00882807	0.01199887
1.55	0.00191575	-0.00265771	0.00473587	0.00642802	0.00274058	0.00430459	0.00609184	0.00810417	0.00465651	0.00166600	0.01081230	0.01451788
1.30	0.00182562	-0.00308011	0.00501259	0.00669580	0.00390287	0.00366207	0.00972011	0.01267554	0.00572833	0.00058546	0.01473176	0.01935583
1.15	0.00168097	-0.00292362	0.00487633	0.00645520	0.00470924	0.00263676	0.01245122	0.01602774	0.00638989	-0.00028452	0.01732689	0.02246766
1.00	0.00147132	-0.00237568	0.00448250	0.00588413	0.00557397	0.00109693	0.01553602	0.01975291	0.00704485	-0.00127607	0.02001661	0.02562282
0.75	0.00101492	-0.00060918	0.00331032	0.00429245	0.00704647	-0.00242584	0.02110413	0.02635215	0.00806093	-0.00303009	0.02440881	0.03063391
0.50	0.00052395	0.00167174	0.00191707	0.00231164	0.00836509	-0.00641177	0.02637998	0.03249095	0.00888873	-0.00461585	0.02817088	0.03479666
0.25	0.00014354	0.00050411	0.00065490	0.00390056	0.00928734	-0.00961033	0.03021317	0.03689588	0.00943079	-0.00571387	0.03071848	0.03754904
0.00	0.00000000	0.00000000	0.00000012	0.00473695	0.00961952	-0.01083898	0.03162055	0.03850309	0.00961952	-0.00610527	0.03162055	0.03850321
-0.25	0.00014354	0.00050411	0.00065490	0.00390056	0.00928734	-0.00961033	0.03021317	0.03689588	0.00943079	-0.00571387	0.03071848	0.03754904
-0.50	0.00052395	0.00167174	0.00191707	0.00231164	0.00836509	-0.00641177	0.02637998	0.03249095	0.00888873	-0.00461585	0.02817088	0.03479666
-0.75	0.00101492	-0.00060918	0.00331032	0.00429245	0.00704647	-0.00242584	0.02110413	0.02635215	0.00806093	-0.00303009	0.02440881	0.03063391
-1.00	0.00147132	-0.00237568	0.00448250	0.00588413	0.00557397	0.00109693	0.01553602	0.01975291	0.00704485	-0.00127607	0.02001661	0.02562282
-1.15	0.00168097	-0.00292362	0.00487633	0.00645520	0.00470924	0.00263676	0.01245122	0.01602774	0.00638989	-0.00028452	0.01732689	0.02246766
-1.30	0.00182562	-0.00308011	0.00501259	0.00669580	0.00390287	0.00366207	0.00972011	0.01267554	0.00572833	0.00058546	0.01473176	0.01935583
-1.55	0.00191575	-0.00265771	0.00473587	0.00642802	0.00274058	0.00430459	0.00609184	0.00810417	0.00465651	0.00166600	0.01081230	0.01451788
-1.70	0.00188817	-0.00216595	0.00435603	0.00596996	0.00217982	0.00410890	0.00458523	0.00604187	0.00406835	0.00206031	0.00882807	0.01199887
-2.00	0.00169982	-0.00106027	0.00336306	0.00470175	0.00132316	0.00223262	0.00315096	0.00346258	0.00302364	0.00236046	0.00564188	0.00784306
-2.50	0.00120981	0.00019086	0.00179718	0.00261019	0.00053228	0.00062650	0.00093528	0.00179669	0.00174292	0.00193313	0.00248125	0.00354058
-3.00	0.00074830	0.00054768	0.00082949	0.00127146	0.00020136	0.00015576	0.00025774	0.00076596	0.00095039	0.00095648	0.00134420	0.00152694
-4.00	0.00021054	0.00013207	0.00026829	0.00037632	0.00002382	0.00000708	0.00002092	0.00011857	0.00023468	0.00013935	0.00028868	0.00049554
-5.00	0.00004079	0.00001651	0.00004698	0.00012418	0.00000178	0.00000018	0.00000149	0.00001397	0.00004265	0.00001676	0.00004837	0.00013843

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_6H_6\mathbf{P}^+$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00003747	0.00002890	0.00003395	0.00012489	0.00000246	0.00000075	0.00000104	0.00001796	0.00003965	0.00002964	0.00003582	0.00014154
4.00	0.00020142	0.00019401	0.00020384	0.00035779	0.00003015	0.00001393	0.00001546	0.00014082	0.00023055	0.00020775	0.00022719	0.00049027
3.50	0.00039456	0.00038788	0.00044813	0.00053702	0.00008792	0.00005313	0.00005941	0.00034494	0.00048087	0.00050072	0.00052388	0.00080574
3.00	0.00069262	0.00039406	0.00098788	0.00104311	0.00023496	0.00020103	0.00022705	0.00080407	0.00092542	0.00109398	0.00118759	0.00137821
2.50	0.00108289	0.00000553	0.00201679	0.00203150	0.00058687	0.00074168	0.00081921	0.00171567	0.00166763	0.00166317	0.00277043	0.00290758
2.00	0.00146044	-0.00104102	0.00338447	0.00360477	0.00136321	0.00247429	0.00252254	0.00307191	0.00282291	0.00185575	0.00607470	0.00611145
1.61	0.00158787	-0.00204106	0.00425756	0.00471118	0.00243062	0.00332018	0.00554242	0.00578386	0.00401967	0.00129472	0.01006512	0.01024884
1.30	0.00147858	-0.00234898	0.00437151	0.00496630	0.00366014	0.00254877	0.00967344	0.00973836	0.00514130	0.00019138	0.01415925	0.01463563
1.15	0.00134607	-0.00214303	0.00413905	0.00475232	0.00434042	0.00164313	0.01207288	0.01215564	0.00568944	-0.00051129	0.01626253	0.01690445
1.00	0.00116591	-0.00165484	0.00371148	0.00430041	0.00505706	0.00038127	0.01461700	0.01489207	0.00622601	-0.00128406	0.01837502	0.01918967
0.75	0.00079226	-0.00026462	0.00264851	0.00310087	0.00625251	-0.00233522	0.01901999	0.01969159	0.00704730	-0.00259924	0.02169682	0.02279084
0.50	0.00040438	0.00128603	0.00162913	0.00165126	0.00730129	-0.00526824	0.02301943	0.02410845	0.00770715	-0.00374431	0.02443230	0.02575901
0.25	0.00011000	0.00038261	0.00046076	0.00303330	0.00802455	-0.00755678	0.02584156	0.02725252	0.00813499	-0.00451660	0.02623370	0.02771312
0.00	0.00000000	0.00000000	0.00000000	0.00362148	0.00828319	-0.00842414	0.02686236	0.02839477	0.00828319	-0.00478813	0.02686236	0.02839477
-0.25	0.00011000	0.00038261	0.00046076	0.00303330	0.00802455	-0.00755678	0.02584156	0.02725252	0.00813499	-0.00451660	0.02623370	0.02771312
-0.50	0.00040438	0.00128603	0.00162913	0.00165126	0.00730129	-0.00526824	0.02301943	0.02410845	0.00770715	-0.00374431	0.02443230	0.02575901
-0.75	0.00079226	-0.00026462	0.00264851	0.00310087	0.00625251	-0.00233522	0.01901999	0.01969159	0.00704730	-0.00259924	0.02169682	0.02279084
-1.00	0.00116591	-0.00165484	0.00371148	0.00430041	0.00505706	0.00038127	0.01461700	0.01489207	0.00622601	-0.00128406	0.01837502	0.01918967
-1.15	0.00134607	-0.00214303	0.00413905	0.00475232	0.00434042	0.00164313	0.01207288	0.01215564	0.00568944	-0.00051129	0.01626253	0.01690445
-1.30	0.00147858	-0.00234898	0.00437151	0.00496630	0.00366014	0.00254877	0.00967344	0.00973836	0.00514130	0.00019138	0.01415925	0.01463563
-1.61	0.00158787	-0.00204106	0.00425756	0.00471118	0.00243062	0.00332018	0.00554242	0.00578386	0.00401967	0.00129472	0.01006512	0.01024884
-2.00	0.00146044	-0.00104102	0.00338447	0.00360477	0.00136321	0.00247429	0.00252254	0.00307191	0.00282291	0.00185575	0.00607470	0.00611145
-2.50	0.00108289	0.00000553	0.00201679	0.00203150	0.00058687	0.00074168	0.00081921	0.00171567	0.00166763	0.00166317	0.00277043	0.00290758
-3.00	0.00069262	0.00039406	0.00098788	0.00104311	0.00023496	0.00020103	0.00022705	0.00080407	0.00092542	0.00109398	0.00118759	0.00137821
-3.50	0.00039456	0.00038788	0.00044813	0.00053702	0.00008792	0.00005313	0.00005941	0.00034494	0.00048087	0.00050072	0.00052388	0.00080574
-4.00	0.00020142	0.00019401	0.00020384	0.00035779	0.00003015	0.00001393	0.00001546	0.00014082	0.00023055	0.00020775	0.00022719	0.00049027
-5.00	0.00003747	0.00002890	0.00003395	0.00012489	0.00000246	0.00000075	0.00000104	0.00001796	0.00003965	0.00002964	0.00003582	0.00014154

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_6H_6\mathbf{O}$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00004370	0.00001123	0.00004938	0.00012937	0.00000191	-0.00000008	0.00000158	0.00001426	0.00004580	0.00001193	0.00005050	0.00014450
4.00	0.00022206	0.00008731	0.00029018	0.00038779	0.00002457	0.00000283	0.00002162	0.00012241	0.00024773	0.00009341	0.00030917	0.00051348
3.50	0.00043692	0.00023468	0.00054525	0.00065230	0.00007448	0.00002230	0.00007547	0.00032059	0.00051349	0.00026263	0.00072209	0.00087081
3.00	0.00078372	0.00056853	0.00066989	0.00143445	0.00020995	0.00012390	0.00027448	0.00082384	0.00099695	0.00074637	0.00145609	0.00169680
2.50	0.00127396	0.00026377	0.00147497	0.00300646	0.00056354	0.00055736	0.00101577	0.00196555	0.00184165	0.00196246	0.00232666	0.00399634
2.00	0.00180848	-0.00108504	0.00286981	0.00551101	0.00142286	0.00207337	0.00348155	0.00380821	0.00323521	0.00269840	0.00501564	0.00894192
1.70	0.00202235	-0.00231842	0.00375303	0.00705943	0.00236144	0.00410847	0.00472250	0.00673407	0.00438674	0.00236550	0.00796043	0.01372534
1.54	0.00205858	-0.00292341	0.00411626	0.00767453	0.00304275	0.00477159	0.00582509	0.00932115	0.00510357	0.00186289	0.00999169	0.01691952
1.30	0.00197069	-0.00337743	0.00433692	0.00799659	0.00425707	0.00406448	0.00905339	0.01426486	0.00622888	0.00069117	0.01345284	0.02217885
1.15	0.00181895	-0.00322695	0.00422047	0.00773388	0.00514571	0.00293076	0.01160824	0.01809322	0.00696511	-0.00029134	0.01588752	0.02574517
1.00	0.00159545	-0.00264281	0.00387955	0.00707009	0.00609923	0.00122954	0.01449773	0.02236117	0.00769459	-0.00140714	0.01842856	0.02935446
0.75	0.00110366	-0.00071882	0.00286293	0.00517870	0.00772381	-0.00266274	0.01972823	0.02995197	0.00882691	-0.00337332	0.02262380	0.03507188
0.50	0.00057090	0.00150964	0.00195945	0.00279726	0.00917931	-0.00707007	0.02470490	0.03704324	0.00974972	-0.00514530	0.02626981	0.03980690
0.25	0.00015659	0.00042919	0.00079354	0.00424536	0.01019764	-0.01060998	0.02833407	0.04214775	0.01035406	-0.00637047	0.02877177	0.04293076
0.00	0.00000000	0.00000000	0.00000166	0.00516966	0.01056447	-0.01197056	0.02966939	0.04401338	0.01056447	-0.00680712	0.02967034	0.04401398
-0.25	0.00015659	0.00042919	0.00079354	0.00424536	0.01019764	-0.01060998	0.02833407	0.04214775	0.01035406	-0.00637047	0.02877177	0.04293076
-0.50	0.00057090	0.00150964	0.00195945	0.00279726	0.00917931	-0.00707007	0.02470490	0.03704324	0.00974972	-0.00514530	0.02626981	0.03980690
-0.75	0.00110366	-0.00071882	0.00286293	0.00517870	0.00772381	-0.00266274	0.01972823	0.02995197	0.00882691	-0.00337332	0.02262380	0.03507188
-1.00	0.00159545	-0.00264281	0.00387955	0.00707009	0.00609923	0.00122954	0.01449773	0.02236117	0.00769459	-0.00140714	0.01842856	0.02935446
-1.15	0.00181895	-0.00322695	0.00422047	0.00773388	0.00514571	0.00293076	0.01160824	0.01809322	0.00696511	-0.00029134	0.01588752	0.02574517
-1.30	0.00197069	-0.00337743	0.00433692	0.00799659	0.00425707	0.00406448	0.00905339	0.01426486	0.00622888	0.00069117	0.01345284	0.02217885
-1.54	0.00205858	-0.00292341	0.00411626	0.00767453	0.00304275	0.00477159	0.00582509	0.00932115	0.00510357	0.00186289	0.00999169	0.01691952
-1.70	0.00202235	-0.00231842	0.00375303	0.00705943	0.00236144	0.00410847	0.00472250	0.00673407	0.00438674	0.00236550	0.00796043	0.01372534
-2.00	0.00180848	-0.00108504	0.00286981	0.00551101	0.00142286	0.00207337	0.00348155	0.00380821	0.00323521	0.00269840	0.00501564	0.00894192
-2.50	0.00127396	0.00026377	0.00147497	0.00300646	0.00056354	0.00055736	0.00101577	0.00196555	0.00184165	0.00196246	0.00232666	0.00399634
-3.00	0.00078372	0.00056853	0.00066989	0.00143445	0.00020995	0.00012390	0.00027448	0.00082384	0.00099695	0.00074637	0.00145609	0.00169680
-3.50	0.00043692	0.00023468	0.00054525	0.00065230	0.00007448	0.00002230	0.00007547	0.00032059	0.00051349	0.00026263	0.00072209	0.00087081
-4.00	0.00022206	0.00008731	0.00029018	0.00038779	0.00002457	0.00000283	0.00002162	0.00012241	0.00024773	0.00009341	0.00030917	0.00051348
-5.00	0.00004370	0.00001123	0.00004938	0.00012937	0.00000191	-0.00000008	0.00000158	0.00001426	0.00004580	0.00001193	0.00005050	0.00014450

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for C_6H_6**S**. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00003944	0.00003185	0.00003804	0.00011293	0.00000222	0.00000104	0.00000119	0.00001610	0.00004154	0.00003297	0.00003904	0.00012872
4.00	0.00019518	0.00020182	0.00020517	0.00030294	0.00002755	0.00001642	0.00001693	0.00012776	0.00022249	0.00021789	0.00022199	0.00043008
3.00	0.00064363	0.00033839	0.00089112	0.00097220	0.00021605	0.00020721	0.00022004	0.00072436	0.00085973	0.00105941	0.00111923	0.00117381
2.50	0.00099205	-0.00002098	0.00169038	0.00195075	0.00053975	0.00073169	0.00076842	0.00154266	0.00153259	0.00151125	0.00248778	0.00266950
2.00	0.00132285	-0.00094391	0.00278267	0.00340313	0.00125313	0.00236926	0.00238476	0.00271624	0.00257841	0.00170496	0.00526532	0.00576225
1.80	0.00140366	-0.00142010	0.00318775	0.00398592	0.00170769	0.00295176	0.00366258	0.00369408	0.00311465	0.00155367	0.00691864	0.00761711
1.63	0.00142856	-0.00179049	0.00344689	0.00438876	0.00219435	0.00305175	0.00509689	0.00516599	0.00362694	0.00126175	0.00861203	0.00951896
1.50	0.00141341	-0.00198861	0.00355339	0.00458205	0.00261226	0.00293358	0.00637875	0.00654699	0.00403016	0.00093883	0.01001278	0.01109076
1.30	0.00132420	-0.00207048	0.00352665	0.00463235	0.00336149	0.00233293	0.00880214	0.00919186	0.00469062	0.00025067	0.01242003	0.01378413
1.15	0.00120342	-0.00188166	0.00332757	0.00442654	0.00398555	0.00150338	0.01091830	0.01153253	0.00519393	-0.00039152	0.01433821	0.01591979
1.00	0.00104077	-0.00144419	0.00297282	0.00400087	0.00464284	0.00034808	0.01322545	0.01411130	0.00568830	-0.00110845	0.01628558	0.01807579
0.75	0.00070578	-0.00020653	0.00210342	0.00287986	0.00573904	-0.00213984	0.01722169	0.01863147	0.00644839	-0.00235165	0.01939129	0.02148393
0.50	0.00035973	0.00108823	0.00137627	0.00153053	0.00670052	-0.00482759	0.02085529	0.02278907	0.00706222	-0.00345709	0.02199170	0.02430390
0.25	0.00009777	0.00029628	0.00042508	0.00269677	0.00736349	-0.00692564	0.02342112	0.02574766	0.00746182	-0.00421522	0.02372994	0.02616758
0.00	0.00000000	0.00000000	0.00000051	0.00321814	0.00760054	-0.00772097	0.02434956	0.02682237	0.00760054	-0.00448430	0.02435018	0.02682249
-0.25	0.00009777	0.00029628	0.00042508	0.00269677	0.00736349	-0.00692564	0.02342112	0.02574766	0.00746182	-0.00421522	0.02372994	0.02616758
-0.50	0.00035973	0.00108823	0.00137627	0.00153053	0.00670052	-0.00482759	0.02085529	0.02278907	0.00706222	-0.00345709	0.02199170	0.02430390
-0.75	0.00070578	-0.00020653	0.00210342	0.00287986	0.00573904	-0.00213984	0.01722169	0.01863147	0.00644839	-0.00235165	0.01939129	0.02148393
-1.00	0.00104077	-0.00144419	0.00297282	0.00400087	0.00464284	0.00034808	0.01322545	0.01411130	0.00568830	-0.00110845	0.01628558	0.01807579
-1.15	0.00120342	-0.00188166	0.00332757	0.00442654	0.00398555	0.00150338	0.01091830	0.01153253	0.00519393	-0.00039152	0.01433821	0.01591979
-1.30	0.00132420	-0.00207048	0.00352665	0.00463235	0.00336149	0.00233293	0.00880214	0.00919186	0.00469062	0.00025067	0.01242003	0.01378413
-1.50	0.00141341	-0.00198861	0.00355339	0.00458205	0.00261226	0.00293358	0.00637875	0.00654699	0.00403016	0.00093883	0.01001278	0.01109076
-1.63	0.00142856	-0.00179049	0.00344689	0.00438876	0.00219435	0.00305175	0.00509689	0.00516599	0.00362694	0.00126175	0.00861203	0.00951896
-1.80	0.00140366	-0.00142010	0.00318775	0.00398592	0.00170769	0.00295176	0.00366258	0.00369408	0.00311465	0.00155367	0.00691864	0.00761711
-2.00	0.00132285	-0.00094391	0.00278267	0.00340313	0.00125313	0.00236926	0.00238476	0.00271624	0.00257841	0.00170496	0.00526532	0.00576225
-2.50	0.00099205	-0.00002098	0.00169038	0.00195075	0.00053975	0.00073169	0.00076842	0.00154266	0.00153259	0.00151125	0.00248778	0.00266950
-3.00	0.00064363	0.00033839	0.00089112	0.00097220	0.00021605	0.00020721	0.00022004	0.00072436	0.00085973	0.00105941	0.00111923	0.00117381
-4.00	0.00019518	0.00020182	0.00020517	0.00030294	0.00002755	0.00001642	0.00001693	0.00012776	0.00022249	0.00021789	0.00022199	0.00043008
-5.00	0.00003944	0.00003185	0.00003804	0.00011293	0.00000222	0.00000104	0.00000119	0.00001610	0.00004154	0.00003297	0.00003904	0.00012872

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for Pyridazine. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00004118	0.00001884	0.00003538	0.00016340	0.00000188	-0.00000009	0.00000109	0.00001151	0.00004466	0.00001613	0.00003621	0.00018082
4.00	0.00025851	0.00021395	0.00025430	0.00066217	0.00002065	0.00000168	0.00001868	0.00012333	0.00028586	0.00019912	0.00027106	0.00080443
3.00	0.00118477	0.00150226	0.00176634	0.00193892	0.00022704	0.00012195	0.00030361	0.00133052	0.00143008	0.00155593	0.00206321	0.00337123
2.50	0.00224888	0.00196576	0.00394222	0.00448814	0.00074690	0.00069501	0.00133148	0.00406091	0.00302639	0.00398315	0.00580192	0.00672745
2.00	0.00375125	-0.00072162	0.00863955	0.00983965	0.00232673	0.00348961	0.00540517	0.00995450	0.00612252	0.00809570	0.01320115	0.01518035
1.75	0.00448496	-0.00383768	0.01181047	0.01324596	0.00392927	0.00718495	0.01018747	0.01354515	0.00846065	0.00897816	0.01954563	0.02331917
1.50	0.00497634	-0.00757265	0.01482769	0.01633356	0.00635222	0.01348775	0.01629010	0.01811350	0.01136993	0.00787298	0.02887134	0.03426948
1.36	0.00506105	-0.00936586	0.01605446	0.01752140	0.00811063	0.01544748	0.01977744	0.02425185	0.01320717	0.00621425	0.03537217	0.04156129
1.15	0.00483945	-0.01066801	0.01672249	0.01804080	0.01134653	0.01289550	0.03044259	0.03623112	0.01620982	0.00222877	0.04682765	0.05402254
1.00	0.00439889	-0.00992182	0.01603298	0.01719442	0.01400049	0.00835798	0.04010529	0.04663428	0.01841456	-0.00154036	0.05580942	0.06357231
0.75	0.00320200	-0.00486728	0.01257861	0.01340315	0.01876013	-0.00402968	0.05884244	0.06645363	0.02196595	-0.00884024	0.07115483	0.07963609
0.50	0.00172123	0.00377171	0.00726966	0.00759968	0.02325180	-0.01994260	0.07789312	0.08641683	0.02497201	-0.01600369	0.08488886	0.09387856
0.25	0.00048357	0.00203894	0.00221129	0.01252576	0.02651101	-0.03373116	0.09243497	0.10162155	0.02699374	-0.02124667	0.09446839	0.10378820
0.00	0.00000000	0.00000000	0.00000060	0.01609508	0.02770743	-0.03923033	0.09791258	0.10734953	0.02770743	-0.02316946	0.09791267	0.10734953
-0.25	0.00048357	0.00203894	0.00221129	0.01252576	0.02651101	-0.03373116	0.09243497	0.10162155	0.02699374	-0.02124667	0.09446839	0.10378820
-0.50	0.00172123	0.00377171	0.00726966	0.00759968	0.02325180	-0.01994260	0.07789312	0.08641683	0.02497201	-0.01600369	0.08488886	0.09387856
-0.75	0.00320200	-0.00486728	0.01257861	0.01340315	0.01876013	-0.00402968	0.05884244	0.06645363	0.02196595	-0.00884024	0.07115483	0.07963609
-1.00	0.00439889	-0.00992182	0.01603298	0.01719442	0.01400049	0.00835798	0.04010529	0.04663428	0.01841456	-0.00154036	0.05580942	0.06357231
-1.15	0.00483945	-0.01066801	0.01672249	0.01804080	0.01134653	0.01289550	0.03044259	0.03623112	0.01620982	0.00222877	0.04682765	0.05402254
-1.36	0.00506105	-0.00936586	0.01605446	0.01752140	0.00811063	0.01544748	0.01977744	0.02425185	0.01320717	0.00621425	0.03537217	0.04156129
-1.50	0.00497634	-0.00757265	0.01482769	0.01633356	0.00635222	0.01348775	0.01629010	0.01811350	0.01136993	0.00787298	0.02887134	0.03426948
-1.75	0.00448496	-0.00383768	0.01181047	0.01324596	0.00392927	0.00718495	0.01018747	0.01354515	0.00846065	0.00897816	0.01954563	0.02331917
-2.00	0.00375125	-0.00072162	0.00863955	0.00983965	0.00232673	0.00348961	0.00540517	0.00995450	0.00612252	0.00809570	0.01320115	0.01518035
-2.50	0.00224888	0.00196576	0.00394222	0.00448814	0.00074690	0.00069501	0.00133148	0.00406091	0.00302639	0.00398315	0.00580192	0.00672745
-3.00	0.00118477	0.00150226	0.00176634	0.00193892	0.00022704	0.00012195	0.00030361	0.00133052	0.00143008	0.00155593	0.00206321	0.00337123
-4.00	0.00025851	0.00021395	0.00025430	0.00066217	0.00002065	0.00000168	0.00001868	0.00012333	0.00028586	0.00019912	0.00027106	0.00080443
-5.00	0.00004118	0.00001884	0.00003538	0.00016340	0.00000188	-0.00000009	0.00000109	0.00001151	0.00004466	0.00001613	0.00003621	0.00018082

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for Pyrimidine. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00003874	0.00002451	0.00003405	0.00015536	0.00000117	0.00000038	0.00000068	0.00001073	0.00004084	0.00002498	0.00003211	0.00017032
4.00	0.00025046	0.00021501	0.00025790	0.00066558	0.00001937	0.00000363	0.00001415	0.00013282	0.00027379	0.00021650	0.00026132	0.00081193
3.50	0.00056551	0.00059652	0.00067062	0.00121719	0.00007041	0.00002126	0.00005753	0.00043059	0.00064275	0.00061346	0.00070563	0.00167640
3.00	0.00118438	0.00159784	0.00170707	0.00202775	0.00024100	0.00013515	0.00025562	0.00138907	0.00143673	0.00172752	0.00193164	0.00346197
2.50	0.00228002	0.00212796	0.00405457	0.00450417	0.00079343	0.00079015	0.00119279	0.00419555	0.00309197	0.00483695	0.00510762	0.00692458
2.00	0.00384712	-0.00068493	0.00904241	0.00981297	0.00245719	0.00391304	0.00505589	0.01030820	0.00633053	0.00919951	0.01291464	0.01526039
1.75	0.00461881	-0.00394854	0.01236948	0.01319827	0.00414174	0.00798602	0.00965123	0.01408885	0.00878804	0.00981163	0.02027133	0.02311380
1.50	0.00514056	-0.00785793	0.01552610	0.01626548	0.00669012	0.01520530	0.01609055	0.01795846	0.01185595	0.00853940	0.03058986	0.03383120
1.36	0.00523479	-0.00978625	0.01684562	0.01747158	0.00860466	0.01649916	0.02124949	0.02386356	0.01386178	0.00671755	0.03792207	0.04124192
1.15	0.00501269	-0.01111041	0.01753261	0.01795531	0.01195177	0.01371624	0.03281621	0.03539497	0.01698103	0.00259516	0.05014580	0.05328215
1.00	0.00455972	-0.01034659	0.01683085	0.01711097	0.01475214	0.00895640	0.04331236	0.04564258	0.01932381	-0.00139025	0.05993735	0.06268928
0.75	0.00332190	-0.00509689	0.01322856	0.01334180	0.01978046	-0.00411594	0.06372857	0.06518688	0.02310762	-0.00919519	0.07678755	0.07847473
0.50	0.00178663	0.00397105	0.00752619	0.00761553	0.02453173	-0.02100593	0.08462276	0.08487439	0.02631972	-0.01696533	0.09205097	0.09240608
0.25	0.00050209	0.00218519	0.00218640	0.01297847	0.02798244	-0.03569282	0.09986531	0.10066467	0.02848465	-0.02272047	0.10205414	0.10282195
0.00	0.00000000	0.00000000	0.00000002	0.01671317	0.02924975	-0.04156004	0.10551174	0.10672713	0.02924975	-0.02484592	0.10551174	0.10672716
-0.25	0.00050209	0.00218519	0.00218640	0.01297847	0.02798244	-0.03569282	0.09986531	0.10066467	0.02848465	-0.02272047	0.10205414	0.10282195
-0.50	0.00178663	0.00397105	0.00752619	0.00761553	0.02453173	-0.02100593	0.08462276	0.08487439	0.02631972	-0.01696533	0.09205097	0.09240608
-0.75	0.00332190	-0.00509689	0.01322856	0.01334180	0.01978046	-0.00411594	0.06372857	0.06518688	0.02310762	-0.00919519	0.07678755	0.07847473
-1.00	0.00455972	-0.01034659	0.01683085	0.01711097	0.01475214	0.00895640	0.04331236	0.04564258	0.01932381	-0.00139025	0.05993735	0.06268928
-1.15	0.00501269	-0.01111041	0.01753261	0.01795531	0.01195177	0.01371624	0.03281621	0.03539497	0.01698103	0.00259516	0.05014580	0.05328215
-1.36	0.00523479	-0.00978625	0.01684562	0.01747158	0.00860466	0.01649916	0.02124949	0.02386356	0.01386178	0.00671755	0.03792207	0.04124192
-1.50	0.00514056	-0.00785793	0.01552610	0.01626548	0.00669012	0.01520530	0.01609055	0.01795846	0.01185595	0.00853940	0.03058986	0.03383120
-1.75	0.00461881	-0.00394854	0.01236948	0.01319827	0.00414174	0.00798602	0.00965123	0.01408885	0.00878804	0.00981163	0.02027133	0.02311380
-2.00	0.00384712	-0.00068493	0.00904241	0.00981297	0.00245719	0.00391304	0.00505589	0.01030820	0.00633053	0.00919951	0.01291464	0.01526039
-2.50	0.00228002	0.00212796	0.00405457	0.00450417	0.00079343	0.00079015	0.00119279	0.00419555	0.00309197	0.00483695	0.00510762	0.00692458
-3.00	0.00118438	0.00159784	0.00170707	0.00202775	0.00024100	0.00013515	0.00025562	0.00138907	0.00143673	0.00172752	0.00193164	0.00346197
-3.50	0.00056551	0.00059652	0.00067062	0.00121719	0.00007041	0.00002126	0.00005753	0.00043059	0.00064275	0.00061346	0.00070563	0.00167640
-4.00	0.00025046	0.00021501	0.00025790	0.00066558	0.00001937	0.00000363	0.00001415	0.00013282	0.00027379	0.00021650	0.00026132	0.00081193
-5.00	0.00003874	0.00002451	0.00003405	0.00015536	0.00000117	0.00000038	0.00000068	0.00001073	0.00004084	0.00002498	0.00003211	0.00017032

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for Pyrazine. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00003623	0.00002181	0.00004956	0.00014046	0.00000202	-0.00000011	0.00000224	0.00001128	0.00003825	0.00002170	0.00005180	0.00015174
4.00	0.00023852	0.00020838	0.00030120	0.00063361	0.00002183	-0.00000423	0.00002645	0.00012453	0.00026035	0.00020415	0.00032765	0.00075814
3.00	0.00114655	0.00154274	0.00189602	0.00191163	0.00023623	0.00007009	0.00036897	0.00133661	0.00138278	0.00161300	0.00226493	0.00324814
2.50	0.00221804	0.00209419	0.00386820	0.00475909	0.00077203	0.00056850	0.00156449	0.00410700	0.00299007	0.00443730	0.00620115	0.00632303
2.00	0.00375175	-0.00067784	0.00863698	0.01028937	0.00240691	0.00324760	0.00608379	0.01016399	0.00615866	0.00948613	0.01188636	0.01637147
1.75	0.00450641	-0.00386532	0.01187529	0.01371171	0.00407322	0.00696049	0.01118199	0.01388807	0.00857962	0.01002275	0.01883852	0.02489108
1.50	0.00501598	-0.00767293	0.01500132	0.01671729	0.00660169	0.01377916	0.01644476	0.01937689	0.01161765	0.00877185	0.02878446	0.03609036
1.36	0.00510764	-0.00954414	0.01633439	0.01784387	0.00849965	0.01652917	0.01959640	0.02578751	0.01360728	0.00698506	0.03593552	0.04362682
1.15	0.00489010	-0.01083041	0.01708698	0.01818775	0.01183403	0.01372112	0.03094418	0.03749652	0.01672411	0.00289074	0.04803693	0.05567869
1.00	0.00444748	-0.01008066	0.01645353	0.01724103	0.01462186	0.00898101	0.04134596	0.04768867	0.01906932	-0.00109961	0.05780584	0.06492352
0.75	0.00323921	-0.00495508	0.01298428	0.01334524	0.01963045	-0.00404567	0.06175530	0.06687624	0.02286966	-0.00900068	0.07474616	0.08021501
0.50	0.00174172	0.00393186	0.00740910	0.00752913	0.02436526	-0.02090021	0.08277396	0.08602515	0.02610698	-0.01696773	0.09018798	0.09354884
0.25	0.00048939	0.00215886	0.00218248	0.01264108	0.02780496	-0.03557075	0.09895883	0.10054220	0.02829435	-0.02293000	0.10112004	0.10272269
0.00	0.00000000	0.00000000	0.00000000	0.01628957	0.02906840	-0.04143429	0.10508185	0.10600132	0.02906840	-0.02514490	0.10508194	0.10600135
-0.25	0.00048939	0.00215886	0.00218248	0.01264108	0.02780496	-0.03557075	0.09895883	0.10054220	0.02829435	-0.02293000	0.10112004	0.10272269
-0.50	0.00174172	0.00393186	0.00740910	0.00752913	0.02436526	-0.02090021	0.08277396	0.08602515	0.02610698	-0.01696773	0.09018798	0.09354884
-0.75	0.00323921	-0.00495508	0.01298428	0.01334524	0.01963045	-0.00404567	0.06175530	0.06687624	0.02286966	-0.00900068	0.07474616	0.08021501
-1.00	0.00444748	-0.01008066	0.01645353	0.01724103	0.01462186	0.00898101	0.04134596	0.04768867	0.01906932	-0.00109961	0.05780584	0.06492352
-1.15	0.00489010	-0.01083041	0.01708698	0.01818775	0.01183403	0.01372112	0.03094418	0.03749652	0.01672411	0.00289074	0.04803693	0.05567869
-1.36	0.00510764	-0.00954414	0.01633439	0.01784387	0.00849965	0.01652917	0.01959640	0.02578751	0.01360728	0.00698506	0.03593552	0.04362682
-1.50	0.00501598	-0.00767293	0.01500132	0.01671729	0.00660169	0.01377916	0.01644476	0.01937689	0.01161765	0.00877185	0.02878446	0.03609036
-1.75	0.00450641	-0.00386532	0.01187529	0.01371171	0.00407322	0.00696049	0.01118199	0.01388807	0.00857962	0.01002275	0.01883852	0.02489108
-2.00	0.00375175	-0.00067784	0.00863698	0.01028937	0.00240691	0.00324760	0.00608379	0.01016399	0.00615866	0.00948613	0.01188636	0.01637147
-2.50	0.00221804	0.00209419	0.00386820	0.00475909	0.00077203	0.00056850	0.00156449	0.00410700	0.00299007	0.00443730	0.00620115	0.00632303
-3.00	0.00114655	0.00154274	0.00189602	0.00191163	0.00023623	0.00007009	0.00036897	0.00133661	0.00138278	0.00161300	0.00226493	0.00324814
-4.00	0.00023852	0.00020838	0.00030120	0.00063361	0.00002183	-0.00000423	0.00002645	0.00012453	0.00026035	0.00020415	0.00032765	0.00075814
-5.00	0.00003623	0.00002181	0.00004956	0.00014046	0.00000202	-0.00000011	0.00000224	0.00001128	0.00003825	0.00002170	0.00005180	0.00015174

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for 1,3,5-Triazine. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00002890	0.00002485	0.00002488	0.00012601	0.00000038	0.00000084	0.00000084	0.00000660	0.00002928	0.00002570	0.00002572	0.00013262
4.00	0.00021308	0.00021190	0.00021271	0.00064272	0.00001502	0.00000446	0.00000447	0.00013092	0.00022810	0.00021637	0.00021717	0.00077365
3.00	0.00112159	0.00160363	0.00161539	0.00206738	0.00023644	0.00012136	0.00012144	0.00141767	0.00135802	0.00172506	0.00173675	0.00348505
2.50	0.00224186	0.00242729	0.00417257	0.00420694	0.00080193	0.00076964	0.00076990	0.00431318	0.00304379	0.004942451	0.004976596	0.00674046
2.00	0.00390549	-0.00031021	0.00952878	0.00960857	0.00252694	0.00403522	0.00403603	0.01094068	0.00643243	0.01063047	0.01356474	0.01364386
1.75	0.00475928	-0.00376466	0.01317350	0.01328137	0.00430103	0.00839449	0.00839587	0.01528091	0.00906031	0.01151625	0.02156924	0.02167599
1.55	0.00528186	-0.00724273	0.01605974	0.01618667	0.00639285	0.01431163	0.01431369	0.01811478	0.01167471	0.01087206	0.03037323	0.03049850
1.33	0.00551777	-0.01074818	0.01845560	0.01859226	0.00953864	0.01889025	0.02432210	0.02432523	0.01505641	0.00814208	0.04278054	0.04291465
1.25	0.00548309	-0.01160407	0.01893365	0.01906926	0.01089088	0.01817518	0.02895270	0.02895631	0.01637397	0.00657111	0.04788963	0.04802229
1.15	0.00533516	-0.01216543	0.01914359	0.01927365	0.01275988	0.01629838	0.03562965	0.03563392	0.01809504	0.00413295	0.05477713	0.05490369
1.00	0.00488657	-0.01158377	0.01849503	0.01860738	0.01585787	0.01117592	0.04732713	0.04733255	0.02074444	-0.00040785	0.06582710	0.06593498
0.75	0.00359533	-0.00609415	0.01468765	0.01474872	0.02148185	-0.00357862	0.07029657	0.07030423	0.02507718	-0.00967277	0.08499120	0.08504597
0.50	0.00194814	0.00397652	0.00843361	0.00843575	0.02685538	-0.02323265	0.09405158	0.09406154	0.02880352	-0.01925613	0.10248712	0.10249535
0.25	0.00055003	0.00244132	0.00246942	0.01406909	0.03078840	-0.04061052	0.11243683	0.11244858	0.03133843	-0.02654143	0.11487877	0.11491738
0.00	0.00000000	0.00000000	0.00000058	0.01833778	0.03223861	-0.04760595	0.11941527	0.11942771	0.03223861	-0.02926816	0.11941580	0.11942775
-0.25	0.00055003	0.00244132	0.00246942	0.01406909	0.03078840	-0.04061052	0.11243683	0.11244858	0.03133843	-0.02654143	0.11487877	0.11491738
-0.50	0.00194814	0.00397652	0.00843361	0.00843575	0.02685538	-0.02323265	0.09405158	0.09406154	0.02880352	-0.01925613	0.10248712	0.10249535
-0.75	0.00359533	-0.00609415	0.01468765	0.01474872	0.02148185	-0.00357862	0.07029657	0.07030423	0.02507718	-0.00967277	0.08499120	0.08504597
-1.00	0.00488657	-0.01158377	0.01849503	0.01860738	0.01585787	0.01117592	0.04732713	0.04733255	0.02074444	-0.00040785	0.06582710	0.06593498
-1.15	0.00533516	-0.01216543	0.01914359	0.01927365	0.01275988	0.01629838	0.03562965	0.03563392	0.01809504	0.00413295	0.05477713	0.05490369
-1.25	0.00548309	-0.01160407	0.01893365	0.01906926	0.01089088	0.01817518	0.02895270	0.02895631	0.01637397	0.00657111	0.04788963	0.04802229
-1.33	0.00551777	-0.01074818	0.01845560	0.01859226	0.00953864	0.01889025	0.02432210	0.02432523	0.01505641	0.00814208	0.04278054	0.04291465
-1.55	0.00528186	-0.00724273	0.01605974	0.01618667	0.00639285	0.01431163	0.01431369	0.01811478	0.01167471	0.01087206	0.03037323	0.03049850
-1.75	0.00475928	-0.00376466	0.01317350	0.01328137	0.00430103	0.00839449	0.00839587	0.01528091	0.00906031	0.01151625	0.02156924	0.02167599
-2.00	0.00390549	-0.00031021	0.00952878	0.00960857	0.00252694	0.00403522	0.00403603	0.01094068	0.00643243	0.01063047	0.01356474	0.01364386
-2.50	0.00224186	0.00242729	0.00417257	0.00420694	0.00080193	0.00076964	0.00076990	0.00431318	0.00304379	0.004942451	0.004976596	0.00674046
-3.00	0.00112159	0.00160363	0.00161539	0.00206738	0.00023644	0.00012136	0.00012144	0.00141767	0.00135802	0.00172506	0.00173675	0.00348505
-4.00	0.00021308	0.00021190	0.00021271	0.00064272	0.00001502	0.00000446	0.00000447	0.00013092	0.00022810	0.00021637	0.00021717	0.00077365
-5.00	0.00002890	0.00002485	0.00002488	0.00012601	0.00000038	0.00000084	0.00000084	0.00000660	0.00002928	0.00002570	0.00002572	0.00013262

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for 1,2,4-Triazine. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00002895	0.00001732	0.00003202	0.00012848	0.00000127	0.00000031	0.00000075	0.00000867	0.00003057	0.00001741	0.00003204	0.00013871
4.00	0.00021101	0.00019226	0.00024241	0.00063819	0.00001680	-0.00000260	0.00001717	0.00011748	0.00022927	0.00018883	0.00025560	0.00076031
3.00	0.00110127	0.00146716	0.00172112	0.00200434	0.00021758	0.00003969	0.00028300	0.00131917	0.00132296	0.00150343	0.00198857	0.00334907
2.50	0.00218218	0.00221842	0.00376180	0.00455567	0.00073751	0.00043114	0.00129556	0.00410590	0.00292691	0.00409368	0.00554248	0.00673842
2.00	0.00376140	-0.00041497	0.00861250	0.01023131	0.00235077	0.00287434	0.00547074	0.01048876	0.00612296	0.00949020	0.01187322	0.01586061
1.75	0.00456124	-0.00366664	0.01204605	0.01394228	0.00402122	0.00649100	0.01047112	0.01466238	0.00859371	0.01066439	0.01868798	0.02451004
1.50	0.00512764	-0.00773462	0.01547522	0.01740091	0.00659207	0.01335571	0.01747749	0.01926762	0.01172957	0.00981408	0.02892993	0.03636743
1.34	0.00525369	-0.01009522	0.01717512	0.01897775	0.00886422	0.01781540	0.02057619	0.02706239	0.01412588	0.00780080	0.03764807	0.04590957
1.15	0.00506902	-0.01146274	0.01797805	0.01954236	0.01201026	0.01540588	0.03136765	0.03874314	0.01708452	0.00394760	0.04930447	0.05815968
1.00	0.00463612	-0.01087774	0.01742498	0.01875472	0.01493774	0.01054549	0.04241404	0.05020613	0.01957688	-0.00032309	0.05979640	0.06883852
0.75	0.00340475	-0.00566646	0.01386507	0.01477686	0.02025166	-0.00342391	0.06431129	0.07229692	0.02365665	-0.00907210	0.07813508	0.08697680
0.50	0.00184255	0.00379404	0.00797237	0.00845808	0.02532786	-0.02198323	0.08703204	0.09483274	0.02716969	-0.01814579	0.09495427	0.10322723
0.25	0.00051983	0.00231124	0.00246609	0.01332634	0.02904245	-0.03836553	0.10458863	0.11217219	0.02956193	-0.02505411	0.10689762	0.11462601
0.00	0.00000000	0.00000000	0.00000013	0.01732691	0.03041195	-0.04495475	0.11123809	0.11874243	0.03041195	-0.02764136	0.11123823	0.11874243
-0.25	0.00051983	0.00231124	0.00246609	0.01332634	0.02904245	-0.03836553	0.10458863	0.11217219	0.02956193	-0.02505411	0.10689762	0.11462601
-0.50	0.00184255	0.00379404	0.00797237	0.00845808	0.02532786	-0.02198323	0.08703204	0.09483274	0.02716969	-0.01814579	0.09495427	0.10322723
-0.75	0.00340475	-0.00566646	0.01386507	0.01477686	0.02025166	-0.00342391	0.06431129	0.07229692	0.02365665	-0.00907210	0.07813508	0.08697680
-1.00	0.00463612	-0.01087774	0.01742498	0.01875472	0.01493774	0.01054549	0.04241404	0.05020613	0.01957688	-0.00032309	0.05979640	0.06883852
-1.15	0.00506902	-0.01146274	0.01797805	0.01954236	0.01201026	0.01540588	0.03136765	0.03874314	0.01708452	0.00394760	0.04930447	0.05815968
-1.34	0.00525369	-0.01009522	0.01717512	0.01897775	0.00886422	0.01781540	0.02057619	0.02706239	0.01412588	0.00780080	0.03764807	0.04590957
-1.50	0.00512764	-0.00773462	0.01547522	0.01740091	0.00659207	0.01335571	0.01747749	0.01926762	0.01172957	0.00981408	0.02892993	0.03636743
-1.75	0.00456124	-0.00366664	0.01204605	0.01394228	0.00402122	0.00649100	0.01047112	0.01466238	0.00859371	0.01066439	0.01868798	0.02451004
-2.00	0.00376140	-0.00041497	0.00861250	0.01023131	0.00235077	0.00287434	0.00547074	0.01048876	0.00612296	0.00949020	0.01187322	0.01586061
-2.50	0.00218218	0.00221842	0.00376180	0.00455567	0.00073751	0.00043114	0.00129556	0.00410590	0.00292691	0.00409368	0.00554248	0.00673842
-3.00	0.00110127	0.00146716	0.00172112	0.00200434	0.00021758	0.00003969	0.00028300	0.00131917	0.00132296	0.00150343	0.00198857	0.00334907
-4.00	0.00021101	0.00019226	0.00024241	0.00063819	0.00001680	-0.00000260	0.00001717	0.00011748	0.00022927	0.00018883	0.00025560	0.00076031
-5.00	0.00002895	0.00001732	0.00003202	0.00012848	0.00000127	0.00000031	0.00000075	0.00000867	0.00003057	0.00001741	0.00003204	0.00013871

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for 1,2,3-Triazine. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00003266	0.00001703	0.00002282	0.00014601	0.00000151	-0.00000014	0.00000067	0.00000978	0.00003580	0.00001395	0.00002320	0.00016229
4.00	0.00022594	0.00020697	0.00020799	0.00066177	0.00001754	0.00000406	0.00000733	0.00011857	0.00025059	0.00019330	0.00021308	0.00080131
3.50	0.00052703	0.00057492	0.00058282	0.00121696	0.00006181	0.00002468	0.00003302	0.00039519	0.00060103	0.00056021	0.00061255	0.00166364
3.00	0.00112882	0.00145326	0.00158360	0.00201946	0.00021342	0.00012761	0.00016942	0.00130480	0.00136321	0.00149171	0.00175245	0.00345492
2.50	0.00219676	0.00205514	0.00403526	0.00410667	0.00071595	0.00069804	0.00090290	0.00404272	0.00295016	0.00380969	0.00501087	0.00706447
2.00	0.00373533	-0.00044797	0.00902036	0.00939146	0.00226535	0.00357199	0.00433726	0.01028154	0.00605733	0.00817073	0.01368530	0.01412680
1.75	0.00450993	-0.00360402	0.01249508	0.01300956	0.00386473	0.00744727	0.00880909	0.01434352	0.00843403	0.00960916	0.02078692	0.02171185
1.50	0.00505607	-0.00758362	0.01588444	0.01652681	0.00632297	0.01412229	0.01675262	0.01775409	0.01143165	0.00900753	0.03074334	0.03308416
1.34	0.00517485	-0.00987138	0.01748587	0.01819678	0.00845523	0.01686426	0.02216454	0.02439295	0.01367324	0.00716983	0.03899748	0.04233896
1.15	0.00498943	-0.01125053	0.01818663	0.01894778	0.01149976	0.01469635	0.03251746	0.03622823	0.01651819	0.00345925	0.05021609	0.05488159
1.00	0.00456203	-0.01067812	0.01753363	0.01829316	0.01429592	0.01003447	0.04295313	0.04789190	0.01887543	-0.00060182	0.06001523	0.06588378
0.75	0.00334977	-0.00556552	0.01386791	0.01449454	0.01937045	-0.00335484	0.06330819	0.07067806	0.02272303	-0.00883466	0.07678730	0.08492494
0.50	0.00181277	0.00361237	0.00807761	0.00829531	0.02421664	-0.02106377	0.08411494	0.09411378	0.02602670	-0.01724275	0.09181033	0.10227187
0.25	0.00051143	0.00225448	0.00241674	0.01314998	0.02776194	-0.03664155	0.10006212	0.11217664	0.02827186	-0.02356009	0.10229692	0.11455944
0.00	0.00000000	0.00000000	0.00000038	0.01704714	0.02906878	-0.04289593	0.10608285	0.11901733	0.02906878	-0.02590793	0.10608302	0.11901738
-0.25	0.00051143	0.00225448	0.00241674	0.01314998	0.02776194	-0.03664155	0.10006212	0.11217664	0.02827186	-0.02356009	0.10229692	0.11455944
-0.50	0.00181277	0.00361237	0.00807761	0.00829531	0.02421664	-0.02106377	0.08411494	0.09411378	0.02602670	-0.01724275	0.09181033	0.10227187
-0.75	0.00334977	-0.00556552	0.01386791	0.01449454	0.01937045	-0.00335484	0.06330819	0.07067806	0.02272303	-0.00883466	0.07678730	0.08492494
-1.00	0.00456203	-0.01067812	0.01753363	0.01829316	0.01429592	0.01003447	0.04295313	0.04789190	0.01887543	-0.00060182	0.06001523	0.06588378
-1.15	0.00498943	-0.01125053	0.01818663	0.01894778	0.01149976	0.01469635	0.03251746	0.03622823	0.01651819	0.00345925	0.05021609	0.05488159
-1.34	0.00517485	-0.00987138	0.01748587	0.01819678	0.00845523	0.01686426	0.02216454	0.02439295	0.01367324	0.00716983	0.03899748	0.04233896
-1.50	0.00505607	-0.00758362	0.01588444	0.01652681	0.00632297	0.01412229	0.01675262	0.01775409	0.01143165	0.00900753	0.03074334	0.03308416
-1.75	0.00450993	-0.00360402	0.01249508	0.01300956	0.00386473	0.00744727	0.00880909	0.01434352	0.00843403	0.00960916	0.02078692	0.02171185
-2.00	0.00373533	-0.00044797	0.00902036	0.00939146	0.00226535	0.00357199	0.00433726	0.01028154	0.00605733	0.00817073	0.01368530	0.01412680
-2.50	0.00219676	0.00205514	0.00403526	0.00410667	0.00071595	0.00069804	0.00090290	0.00404272	0.00295016	0.00380969	0.00501087	0.00706447
-3.00	0.00112882	0.00145326	0.00158360	0.00201946	0.00021342	0.00012761	0.00016942	0.00130480	0.00136321	0.00149171	0.00175245	0.00345492
-3.50	0.00052703	0.00057492	0.00058282	0.00121696	0.00006181	0.00002468	0.00003302	0.00039519	0.00060103	0.00056021	0.00061255	0.00166364
-4.00	0.00022594	0.00020697	0.00020799	0.00066177	0.00001754	0.00000406	0.00000733	0.00011857	0.00025059	0.00019330	0.00021308	0.00080131
-5.00	0.00003266	0.00001703	0.00002282	0.00014601	0.00000151	-0.00000014	0.00000067	0.00000978	0.00003580	0.00001395	0.00002320	0.00016229

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_5H_4\mathbf{BH_2}^-$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00009837	0.00007921	0.00009179	0.00026390	0.00000224	0.00000229	0.00000289	0.00001477	0.00010085	0.00007882	0.00009522	0.00028186
4.00	0.00047981	0.00037046	0.00046235	0.00095649	0.00002640	0.00002907	0.00003160	0.00014534	0.00050934	0.00038181	0.00049697	0.00112218
3.00	0.00195994	0.00206545	0.00267348	0.00333109	0.00029839	0.00040130	0.00040354	0.00198080	0.00227726	0.00235097	0.00311018	0.00543278
2.50	0.00375908	0.00420719	0.00508123	0.00661358	0.00107229	0.00172184	0.00172251	0.00671122	0.00487319	0.00648454	0.00843092	0.01121520
2.00	0.00650228	-0.00022619	0.01103091	0.01447838	0.00365421	0.00693718	0.00695889	0.01737454	0.01023608	0.01597290	0.01898852	0.02166153
1.75	0.00793670	-0.00599421	0.01496012	0.01966803	0.00639091	0.01310766	0.01318031	0.02409475	0.01442721	0.01781425	0.02807638	0.03316260
1.50	0.00898814	-0.01329581	0.01877841	0.02470555	0.01062512	0.02355140	0.02377253	0.02915160	0.01972697	0.01562555	0.04215494	0.04888110
1.32	0.00925918	-0.01802081	0.02083665	0.02741809	0.01480205	0.02966263	0.03479853	0.03523888	0.02417785	0.01139760	0.05541327	0.06310700
1.15	0.00898710	-0.02043367	0.02166988	0.02851801	0.01957310	0.02604714	0.04867631	0.04949633	0.02867211	0.00534755	0.07013903	0.07848142
1.00	0.00826373	-0.01978386	0.02115446	0.02784690	0.02442550	0.01844964	0.06388819	0.06521494	0.03279060	-0.00158720	0.08487007	0.09351369
0.75	0.00612531	-0.01102649	0.01719532	0.02266201	0.03328487	-0.00429494	0.09436725	0.09694439	0.03948298	-0.01546203	0.11147175	0.11995999
0.50	0.00334348	0.00607743	0.01015297	0.01337466	0.04182705	-0.03595384	0.12688817	0.13106485	0.04520897	-0.02976484	0.13698485	0.14462095
0.25	0.00094916	0.00297699	0.00404036	0.02400433	0.04813493	-0.06496849	0.15276881	0.15836893	0.04909473	-0.04070598	0.15580463	0.16241600
0.00	0.00000000	0.00000000	0.00002968	0.03170918	0.05047353	-0.07688490	0.16275083	0.16892983	0.05047353	-0.04482354	0.16278343	0.16892983
-0.25	0.00094916	0.00297699	0.00404036	0.02400433	0.04813493	-0.06496849	0.15276881	0.15836893	0.04909473	-0.04070598	0.15580463	0.16241600
-0.50	0.00334348	0.00607743	0.01015297	0.01337466	0.04182705	-0.03595384	0.12688817	0.13106485	0.04520897	-0.02976484	0.13698485	0.14462095
-0.75	0.00612531	-0.01102649	0.01719532	0.02266201	0.03328487	-0.00429494	0.09436725	0.09694439	0.03948298	-0.01546203	0.11147175	0.11995999
-1.00	0.00826373	-0.01978386	0.02115446	0.02784690	0.02442550	0.01844964	0.06388819	0.06521494	0.03279060	-0.00158720	0.08487007	0.09351369
-1.15	0.00898710	-0.02043367	0.02166988	0.02851801	0.01957310	0.02604714	0.04867631	0.04949633	0.02867211	0.00534755	0.07013903	0.07848142
-1.32	0.00925918	-0.01802081	0.02083665	0.02741809	0.01480205	0.02966263	0.03479853	0.03523888	0.02417785	0.01139760	0.05541327	0.06310700
-1.50	0.00898814	-0.01329581	0.01877841	0.02470555	0.01062512	0.02355140	0.02377253	0.02915160	0.01972697	0.01562555	0.04215494	0.04888110
-1.75	0.00793670	-0.00599421	0.01496012	0.01966803	0.00639091	0.01310766	0.01318031	0.02409475	0.01442721	0.01781425	0.02807638	0.03316260
-2.00	0.00650228	-0.00022619	0.01103091	0.01447838	0.00365421	0.00693718	0.00695889	0.01737454	0.01023608	0.01597290	0.01898852	0.02166153
-2.50	0.00375908	0.00420719	0.00508123	0.00661358	0.00107229	0.00172184	0.00172251	0.00671122	0.00487319	0.00648454	0.00843092	0.01121520
-3.00	0.00195994	0.00206545	0.00267348	0.00333109	0.00029839	0.00040130	0.00040354	0.00198080	0.00227726	0.00235097	0.00311018	0.00543278
-4.00	0.00047981	0.00037046	0.00046235	0.00095649	0.00002640	0.00002907	0.00003160	0.00014534	0.00050934	0.00038181	0.00049697	0.00112218
-5.00	0.00009837	0.00007921	0.00009179	0.00026390	0.00000224	0.00000229	0.00000289	0.00001477	0.00010085	0.00007882	0.00009522	0.00028186

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_5H_4\mathbf{CH_2}$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00007061	0.00002304	0.00006132	0.00023683	0.00000209	0.00000157	0.00000236	0.00001399	0.00007599	0.00001761	0.00006458	0.00026308
4.00	0.00040316	0.00014310	0.00037520	0.00092938	0.00002520	0.00002370	0.00003053	0.00014205	0.00044689	0.00012506	0.00041061	0.00112866
3.00	0.00179992	0.00114954	0.00247849	0.00342240	0.00029109	0.00035590	0.00043222	0.00194766	0.00217680	0.00129038	0.00294298	0.00564592
2.50	0.00356919	0.00320137	0.00453108	0.00637663	0.00105140	0.00158655	0.00184865	0.00661563	0.00479143	0.00437942	0.00829241	0.01160439
2.00	0.00633435	0.00010506	0.00787436	0.01425337	0.00359458	0.00659000	0.00736964	0.01715344	0.01022277	0.01310531	0.01845620	0.02168298
1.75	0.00780902	-0.00573508	0.01114116	0.01944360	0.00629334	0.01259235	0.01384133	0.02378055	0.01445139	0.01694647	0.02451407	0.03324849
1.50	0.00891731	-0.01324746	0.01459830	0.02443128	0.01047003	0.02283363	0.02472986	0.02872574	0.01976366	0.01470089	0.03786779	0.04886952
1.31	0.00923536	-0.01849472	0.01683972	0.02720118	0.01493537	0.02905260	0.03487967	0.03740488	0.02453730	0.00978172	0.05239772	0.06393256
1.15	0.00900068	-0.02081999	0.01788050	0.02805865	0.01929230	0.02553809	0.04764262	0.05073899	0.02862924	0.00400828	0.06659631	0.07765970
1.00	0.00830426	-0.02031859	0.01787846	0.02730191	0.02407221	0.01799309	0.06273662	0.06642405	0.03266640	-0.00287239	0.08224073	0.09198317
0.75	0.00618506	-0.01160252	0.01507049	0.02207315	0.03279001	-0.00442577	0.09306851	0.09776138	0.03916496	-0.01611048	0.11104095	0.11675162
0.50	0.00338858	0.00551695	0.00948406	0.01294124	0.04118408	-0.03545377	0.12551993	0.13111214	0.04466381	-0.02917806	0.13912219	0.13941239
0.25	0.00096423	0.00271403	0.00386780	0.02432308	0.04737540	-0.06378625	0.15138987	0.15761032	0.04836300	-0.03884255	0.15553497	0.16003585
0.00	0.00000000	0.00000000	0.00000026	0.03223881	0.04966928	-0.07540127	0.16137609	0.16782262	0.04966928	-0.04241203	0.16137621	0.16782262
-0.25	0.00096423	0.00271403	0.00386780	0.02432308	0.04737540	-0.06378625	0.15138987	0.15761032	0.04836300	-0.03884255	0.15553497	0.16003585
-0.50	0.00338858	0.00551695	0.00948406	0.01294124	0.04118408	-0.03545377	0.12551993	0.13111214	0.04466381	-0.02917806	0.13912219	0.13941239
-0.75	0.00618506	-0.01160252	0.01507049	0.02207315	0.03279001	-0.00442577	0.09306851	0.09776138	0.03916496	-0.01611048	0.11104095	0.11675162
-1.00	0.00830426	-0.02031859	0.01787846	0.02730191	0.02407221	0.01799309	0.06273662	0.06642405	0.03266640	-0.00287239	0.08224073	0.09198317
-1.15	0.00900068	-0.02081999	0.01788050	0.02805865	0.01929230	0.02553809	0.04764262	0.05073899	0.02862924	0.00400828	0.06659631	0.07765970
-1.31	0.00923536	-0.01849472	0.01683972	0.02720118	0.01493537	0.02905260	0.03487967	0.03740488	0.02453730	0.00978172	0.05239772	0.06393256
-1.50	0.00891731	-0.01324746	0.01459830	0.02443128	0.01047003	0.02283363	0.02472986	0.02872574	0.01976366	0.01470089	0.03786779	0.04886952
-1.75	0.00780902	-0.00573508	0.01114116	0.01944360	0.00629334	0.01259235	0.01384133	0.02378055	0.01445139	0.01694647	0.02451407	0.03324849
-2.00	0.00633435	0.00010506	0.00787436	0.01425337	0.00359458	0.00659000	0.00736964	0.01715344	0.01022277	0.01310531	0.01845620	0.02168298
-2.50	0.00356919	0.00320137	0.00453108	0.00637663	0.00105140	0.00158655	0.00184865	0.00661563	0.00479143	0.00437942	0.00829241	0.01160439
-3.00	0.00179992	0.00114954	0.00247849	0.00342240	0.00029109	0.00035590	0.00043222	0.00194766	0.00217680	0.00129038	0.00294298	0.00564592
-4.00	0.00040316	0.00014310	0.00037520	0.00092938	0.00002520	0.00002370	0.00003053	0.00014205	0.00044689	0.00012506	0.00041061	0.00112866
-5.00	0.00007061	0.00002304	0.00006132	0.00023683	0.00000209	0.00000157	0.00000236	0.00001399	0.00007599	0.00001761	0.00006458	0.00026308

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_5H_4\mathbf{NH_2}^+$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00006208	-0.00000996	0.00004494	0.00022750	0.00000176	0.00000105	0.00000194	0.00001181	0.00006573	-0.00000928	0.00004642	0.00024568
4.00	0.00038171	-0.00003656	0.00031694	0.00094787	0.00002273	0.00001771	0.00002821	0.00012498	0.00041610	-0.00002050	0.00033917	0.00109910
3.00	0.00181611	0.00028458	0.00235659	0.00381228	0.00027847	0.00029715	0.00044217	0.00181959	0.00214717	0.00062785	0.00272165	0.00574372
2.50	0.00372714	0.00137830	0.00519643	0.00631580	0.00102556	0.00140265	0.00193073	0.00642550	0.00485326	0.00304511	0.00794812	0.01178690
2.00	0.00680418	0.00045945	0.00424535	0.01448699	0.00354724	0.00606208	0.00773421	0.01720630	0.01051502	0.01121487	0.01787749	0.02116942
1.75	0.00847608	-0.00613666	0.00653198	0.01991563	0.00623251	0.01173023	0.01452810	0.02412884	0.01489526	0.01709253	0.02099402	0.03256219
1.50	0.00975516	-0.01467197	0.00921757	0.02513305	0.01039404	0.02144512	0.02594504	0.02939791	0.02033897	0.01424734	0.03421478	0.04782107
1.30	0.01014921	-0.02088453	0.01129467	0.02810916	0.01509464	0.02974485	0.03355106	0.04006175	0.02541522	0.00848856	0.05001895	0.06313111
1.15	0.00991683	-0.02331499	0.01236867	0.02888160	0.01919081	0.02636203	0.04497893	0.05330362	0.02925439	0.00278703	0.06413885	0.07543833
1.00	0.00916723	-0.02279443	0.01278863	0.02806296	0.02395750	0.01875539	0.05925473	0.06981576	0.03323922	-0.00412165	0.08095487	0.08891496
0.75	0.00684220	-0.01308486	0.01129250	0.02260043	0.03265005	-0.00388130	0.08784029	0.10286586	0.03955056	-0.01672579	0.11180671	0.11261179
0.50	0.00375275	0.00557696	0.00788911	0.01318148	0.04101763	-0.03510587	0.11829137	0.13811246	0.04478891	-0.02836124	0.13230661	0.14416525
0.25	0.00106838	0.00214135	0.00390640	0.02691086	0.04718786	-0.06351104	0.14248567	0.16616093	0.04825883	-0.03646530	0.14664615	0.16802554
0.00	0.00000000	0.00000000	0.00000000	0.03572600	0.04947358	-0.07513030	0.15180841	0.17697973	0.04947358	-0.03935022	0.15180841	0.17697973
-0.25	0.00106838	0.00214135	0.00390640	0.02691086	0.04718786	-0.06351104	0.14248567	0.16616093	0.04825883	-0.03646530	0.14664615	0.16802554
-0.50	0.00375275	0.00557696	0.00788911	0.01318148	0.04101763	-0.03510587	0.11829137	0.13811246	0.04478891	-0.02836124	0.13230661	0.14416525
-0.75	0.00684220	-0.01308486	0.01129250	0.02260043	0.03265005	-0.00388130	0.08784029	0.10286586	0.03955056	-0.01672579	0.11180671	0.11261179
-1.00	0.00916723	-0.02279443	0.01278863	0.02806296	0.02395750	0.01875539	0.05925473	0.06981576	0.03323922	-0.00412165	0.08095487	0.08891496
-1.15	0.00991683	-0.02331499	0.01236867	0.02888160	0.01919081	0.02636203	0.04497893	0.05330362	0.02925439	0.00278703	0.06413885	0.07543833
-1.30	0.01014921	-0.02088453	0.01129467	0.02810916	0.01509464	0.02974485	0.03355106	0.04006175	0.02541522	0.00848856	0.05001895	0.06313111
-1.50	0.00975516	-0.01467197	0.00921757	0.02513305	0.01039404	0.02144512	0.02594504	0.02939791	0.02033897	0.01424734	0.03421478	0.04782107
-1.75	0.00847608	-0.00613666	0.00653198	0.01991563	0.00623251	0.01173023	0.01452810	0.02412884	0.01489526	0.01709253	0.02099402	0.03256219
-2.00	0.00680418	0.00045945	0.00424535	0.01448699	0.00354724	0.00606208	0.00773421	0.01720630	0.01051502	0.01121487	0.01787749	0.02116942
-2.50	0.00372714	0.00137830	0.00519643	0.00631580	0.00102556	0.00140265	0.00193073	0.00642550	0.00485326	0.00304511	0.00794812	0.01178690
-3.00	0.00181611	0.00028458	0.00235659	0.00381228	0.00027847	0.00029715	0.00044217	0.00181959	0.00214717	0.00062785	0.00272165	0.00574372
-4.00	0.00038171	-0.00003656	0.00031694	0.00094787	0.00002273	0.00001771	0.00002821	0.00012498	0.00041610	-0.00002050	0.00033917	0.00109910
-5.00	0.00006208	-0.00000996	0.00004494	0.00022750	0.00000176	0.00000105	0.00000194	0.00001181	0.00006573	-0.00000928	0.00004642	0.00024568

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_5H_4\mathbf{O}$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00006909	-0.00000527	0.00005467	0.00023086	0.00000210	0.00000162	0.00000254	0.00001432	0.00007751	-0.00000726	0.00005881	0.00026491
4.00	0.00038805	-0.00000429	0.00034982	0.00090230	0.00002590	0.00002266	0.00003149	0.00014751	0.00044986	-0.00000598	0.00039138	0.00112671
3.00	0.00171884	0.00050273	0.00235008	0.00328300	0.00029753	0.00035405	0.00045807	0.00193487	0.00217056	0.00071634	0.00289848	0.00554328
2.50	0.00340152	0.00187359	0.00428504	0.00602718	0.00105536	0.00160124	0.00193993	0.00643174	0.00474848	0.00319117	0.00822935	0.01121292
2.00	0.00602700	0.00007911	0.00526321	0.01335844	0.00354124	0.00665310	0.00757614	0.01639067	0.01004544	0.01100225	0.01722532	0.02154967
1.75	0.00742559	-0.00547323	0.00780867	0.01810848	0.00614988	0.01266189	0.01406922	0.02252759	0.01412844	0.01543962	0.02154295	0.03298707
1.50	0.00847664	-0.01260736	0.01068299	0.02257335	0.01015784	0.02280937	0.02484599	0.02693772	0.01921455	0.01314236	0.03382180	0.04830535
1.31	0.00877913	-0.01760303	0.01271575	0.02495280	0.01442657	0.02696261	0.03463849	0.03726308	0.02375618	0.00821424	0.04768567	0.06295334
1.15	0.00855788	-0.01981502	0.01381124	0.02557290	0.01855265	0.02342863	0.04698706	0.05013285	0.02760303	0.00265632	0.06131547	0.07610562
1.00	0.00789870	-0.01935749	0.01409094	0.02472728	0.02307164	0.01616322	0.06149041	0.06517315	0.03138265	-0.00380393	0.07647061	0.08973064
0.75	0.00588839	-0.01111519	0.01223672	0.01979507	0.03127183	-0.00490132	0.09029877	0.09490030	0.03741386	-0.01582396	0.10455070	0.11299603
0.50	0.00322942	0.00470447	0.00840012	0.01151929	0.03912409	-0.03356706	0.12074953	0.12619193	0.04246620	-0.02725651	0.13208236	0.13398662
0.25	0.00091970	0.00222766	0.00343650	0.02322159	0.04489199	-0.05947888	0.14481756	0.15086418	0.04583853	-0.03547025	0.14876213	0.15266003
0.00	0.00000000	0.00000000	0.00000059	0.03075979	0.04702428	-0.07004959	0.15406743	0.16033561	0.04702428	-0.03845538	0.15406781	0.16033561
-0.25	0.00091970	0.00222766	0.00343650	0.02322159	0.04489199	-0.05947888	0.14481756	0.15086418	0.04583853	-0.03547025	0.14876213	0.15266003
-0.50	0.00322942	0.00470447	0.00840012	0.01151929	0.03912409	-0.03356706	0.12074953	0.12619193	0.04246620	-0.02725651	0.13208236	0.13398662
-0.75	0.00588839	-0.01111519	0.01223672	0.01979507	0.03127183	-0.00490132	0.09029877	0.09490030	0.03741386	-0.01582396	0.10455070	0.11299603
-1.00	0.00789870	-0.01935749	0.01409094	0.02472728	0.02307164	0.01616322	0.06149041	0.06517315	0.03138265	-0.00380393	0.07647061	0.08973064
-1.15	0.00855788	-0.01981502	0.01381124	0.02557290	0.01855265	0.02342863	0.04698706	0.05013285	0.02760303	0.00265632	0.06131547	0.07610562
-1.31	0.00877913	-0.01760303	0.01271575	0.02495280	0.01442657	0.02696261	0.03463849	0.03726308	0.02375618	0.00821424	0.04768567	0.06295334
-1.50	0.00847664	-0.01260736	0.01068299	0.02257335	0.01015784	0.02280937	0.02484599	0.02693772	0.01921455	0.01314236	0.03382180	0.04830535
-1.75	0.00742559	-0.00547323	0.00780867	0.01810848	0.00614988	0.01266189	0.01406922	0.02252759	0.01412844	0.01543962	0.02154295	0.03298707
-2.00	0.00602700	0.00007911	0.00526321	0.01335844	0.00354124	0.00665310	0.00757614	0.01639067	0.01004544	0.01100225	0.01722532	0.02154967
-2.50	0.00340152	0.00187359	0.00428504	0.00602718	0.00105536	0.00160124	0.00193993	0.00643174	0.00474848	0.00319117	0.00822935	0.01121292
-3.00	0.00171884	0.00050273	0.00235008	0.00328300	0.00029753	0.00035405	0.00045807	0.00193487	0.00217056	0.00071634	0.00289848	0.00554328
-4.00	0.00038805	-0.00000429	0.00034982	0.00090230	0.00002590	0.00002266	0.00003149	0.00014751	0.00044986	-0.00000598	0.00039138	0.00112671
-5.00	0.00006909	-0.00000527	0.00005467	0.00023086	0.00000210	0.00000162	0.00000254	0.00001432	0.00007751	-0.00000726	0.00005881	0.00026491

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_7H_6\mathbf{BH_2}^-$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00005541	0.00003560	0.00005224	0.00013852	0.00000261	0.00000101	0.00000106	0.00001681	0.00005796	0.00003684	0.00005323	0.00015523
4.00	0.00025036	0.00019154	0.00028702	0.00036884	0.00002883	0.00001711	0.00001963	0.00012849	0.00027909	0.00021035	0.00030604	0.00049732
3.00	0.00080692	0.00046922	0.00088385	0.00131541	0.00022357	0.00022727	0.00025900	0.00079798	0.00103054	0.00111977	0.00126901	0.00157028
2.50	0.00125303	0.00007750	0.00178165	0.00263976	0.00057522	0.00081491	0.00092393	0.00182426	0.00182863	0.00190036	0.00262169	0.00355386
2.00	0.00170108	-0.00111415	0.00314455	0.00464593	0.00139544	0.00268178	0.00304564	0.00339219	0.00309748	0.00227477	0.00587531	0.00767174
1.70	0.00185664	-0.00211225	0.00394664	0.00582473	0.00226652	0.00407416	0.00507829	0.00577679	0.00412449	0.00196178	0.00908455	0.01157504
1.59	0.00187082	-0.00243829	0.00416590	0.00614623	0.00267606	0.00412606	0.00629644	0.00717307	0.00454833	0.00168602	0.01052759	0.01329080
1.30	0.00175983	-0.00285273	0.00436614	0.00643591	0.00398581	0.00336187	0.01048527	0.01198654	0.00574726	0.00050543	0.01492347	0.01839127
1.15	0.00161014	-0.00265915	0.00418998	0.00617292	0.00477956	0.00232337	0.01319345	0.01510813	0.00639128	-0.00033982	0.01745400	0.02125058
1.00	0.00140129	-0.00210966	0.00380284	0.00559882	0.00562470	0.00081774	0.01618930	0.01856845	0.00702746	-0.00129573	0.02005733	0.02413920
0.75	0.00095891	-0.00043716	0.00275535	0.00404969	0.00705160	-0.00253244	0.02146816	0.02468122	0.00801161	-0.00297157	0.02427190	0.02871022
0.50	0.00049212	0.00147295	0.00176956	0.00215753	0.00831825	-0.00624355	0.02635186	0.03035152	0.00881096	-0.00447310	0.02785147	0.03249794
0.25	0.00013433	0.00041220	0.00059681	0.00367334	0.00919872	-0.00918399	0.02984249	0.03441222	0.00933322	-0.00550636	0.03026216	0.03500603
0.00	0.00000000	0.00000000	0.00000016	0.00442752	0.00951484	-0.01030664	0.03111348	0.03589231	0.00951484	-0.00587351	0.03111348	0.03589246
-0.25	0.00013433	0.00041220	0.00059681	0.00367334	0.00919872	-0.00918399	0.02984249	0.03441222	0.00933322	-0.00550636	0.03026216	0.03500603
-0.50	0.00049212	0.00147295	0.00176956	0.00215753	0.00831825	-0.00624355	0.02635186	0.03035152	0.00881096	-0.00447310	0.02785147	0.03249794
-0.75	0.00095891	-0.00043716	0.00275535	0.00404969	0.00705160	-0.00253244	0.02146816	0.02468122	0.00801161	-0.00297157	0.02427190	0.02871022
-1.00	0.00140129	-0.00210966	0.00380284	0.00559882	0.00562470	0.00081774	0.01618930	0.01856845	0.00702746	-0.00129573	0.02005733	0.02413920
-1.15	0.00161014	-0.00265915	0.00418998	0.00617292	0.00477956	0.00232337	0.01319345	0.01510813	0.00639128	-0.00033982	0.01745400	0.02125058
-1.30	0.00175983	-0.00285273	0.00436614	0.00643591	0.00398581	0.00336187	0.01048527	0.01198654	0.00574726	0.00050543	0.01492347	0.01839127
-1.59	0.00187082	-0.00243829	0.00416590	0.00614623	0.00267606	0.00412606	0.00629644	0.00717307	0.00454833	0.00168602	0.01052759	0.01329080
-1.70	0.00185664	-0.00211225	0.00394664	0.00582473	0.00226652	0.00407416	0.00507829	0.00577679	0.00412449	0.00196178	0.00908455	0.01157504
-2.00	0.00170108	-0.00111415	0.00314455	0.00464593	0.00139544	0.00268178	0.00304564	0.00339219	0.00309748	0.00227477	0.00587531	0.00767174
-2.50	0.00125303	0.00007750	0.00178165	0.00263976	0.00057522	0.00081491	0.00092393	0.00182426	0.00182863	0.00190036	0.00262169	0.00355386
-3.00	0.00080692	0.00046922	0.00088385	0.00131541	0.00022357	0.00022727	0.00025900	0.00079798	0.00103054	0.00111977	0.00126901	0.00157028
-4.00	0.00025036	0.00019154	0.00028702	0.00036884	0.00002883	0.00001711	0.00001963	0.00012849	0.00027909	0.00021035	0.00030604	0.00049732
-5.00	0.00005541	0.00003560	0.00005224	0.00013852	0.00000261	0.00000101	0.00000106	0.00001681	0.00005796	0.00003684	0.00005323	0.00015523

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_7H_6\mathbf{CH_2}$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00004477	0.00002525	0.00004443	0.00013433	0.00000231	0.00000071	0.00000083	0.00001560	0.00004709	0.00002587	0.00004528	0.00014995
4.00	0.00023037	0.00016276	0.00026621	0.00038350	0.00002674	0.00001547	0.00001777	0.00012203	0.00025712	0.00017774	0.00028416	0.00050558
3.00	0.00079611	0.00054341	0.00084121	0.00130908	0.00021270	0.00021912	0.00025346	0.00078279	0.00100884	0.00105725	0.00132705	0.00156347
2.50	0.00127001	0.00016227	0.00177028	0.00270644	0.00055523	0.00079402	0.00092940	0.00182562	0.00182528	0.00198713	0.00256034	0.00363788
2.00	0.00176485	-0.00112206	0.00322614	0.00487245	0.00136793	0.00263594	0.00312319	0.00345418	0.00313282	0.00233186	0.00585361	0.00799953
1.70	0.00194909	-0.00223858	0.00410649	0.00616979	0.00224119	0.00419277	0.00500955	0.00597208	0.00419032	0.00195424	0.00910474	0.01214696
1.56	0.00197240	-0.00268742	0.00440008	0.00659768	0.00275498	0.00425278	0.00652735	0.00780056	0.00472741	0.00156536	0.01091533	0.01440376
1.30	0.00187098	-0.00311991	0.00460565	0.00688169	0.00398019	0.00351227	0.01040599	0.01248670	0.00585118	0.00039239	0.01499887	0.01937426
1.15	0.00171836	-0.00293674	0.00443690	0.00661703	0.00478736	0.00245863	0.01311804	0.01577169	0.00650573	-0.00047806	0.01754259	0.02239443
1.00	0.00150040	-0.00235953	0.00404005	0.00601346	0.00564894	0.00091763	0.01612356	0.01941816	0.00714934	-0.00144184	0.02015231	0.02543686
0.75	0.00103123	-0.00055228	0.00293959	0.00435840	0.00710755	-0.00253370	0.02143042	0.02586932	0.00813878	-0.00308590	0.02436172	0.03023158
0.50	0.00053085	0.00157578	0.00186216	0.00232183	0.00840566	-0.00637435	0.02635002	0.03186183	0.00893651	-0.00451266	0.02792183	0.03418573
0.25	0.00014516	0.00044175	0.00063878	0.00395607	0.00930951	-0.00942507	0.02987115	0.03615724	0.00945467	-0.00546905	0.03031167	0.03679660
0.00	0.00000000	0.00000000	0.00000043	0.00478744	0.00963428	-0.01059116	0.03115415	0.03772360	0.00963428	-0.00580377	0.03115415	0.03772403
-0.25	0.00014516	0.00044175	0.00063878	0.00395607	0.00930951	-0.00942507	0.02987115	0.03615724	0.00945467	-0.00546905	0.03031167	0.03679660
-0.50	0.00053085	0.00157578	0.00186216	0.00232183	0.00840566	-0.00637435	0.02635002	0.03186183	0.00893651	-0.00451266	0.02792183	0.03418573
-0.75	0.00103123	-0.00055228	0.00293959	0.00435840	0.00710755	-0.00253370	0.02143042	0.02586932	0.00813878	-0.00308590	0.02436172	0.03023158
-1.00	0.00150040	-0.00235953	0.00404005	0.00601346	0.00564894	0.00091763	0.01612356	0.01941816	0.00714934	-0.00144184	0.02015231	0.02543686
-1.15	0.00171836	-0.00293674	0.00443690	0.00661703	0.00478736	0.00245863	0.01311804	0.01577169	0.00650573	-0.00047806	0.01754259	0.02239443
-1.30	0.00187098	-0.00311991	0.00460565	0.00688169	0.00398019	0.00351227	0.01040599	0.01248670	0.00585118	0.00039239	0.01499887	0.01937426
-1.56	0.00197240	-0.00268742	0.00440008	0.00659768	0.00275498	0.00425278	0.00652735	0.00780056	0.00472741	0.00156536	0.01091533	0.01440376
-1.70	0.00194909	-0.00223858	0.00410649	0.00616979	0.00224119	0.00419277	0.00500955	0.00597208	0.00419032	0.00195424	0.00910474	0.01214696
-2.00	0.00176485	-0.00112206	0.00322614	0.00487245	0.00136793	0.00263594	0.00312319	0.00345418	0.00313282	0.00233186	0.00585361	0.00799953
-2.50	0.00127001	0.00016227	0.00177028	0.00270644	0.00055523	0.00079402	0.00092940	0.00182562	0.00182528	0.00198713	0.00256034	0.00363788
-3.00	0.00079611	0.00054341	0.00084121	0.00130908	0.00021270	0.00021912	0.00025346	0.00078279	0.00100884	0.00105725	0.00132705	0.00156347
-4.00	0.00023037	0.00016276	0.00026621	0.00038350	0.00002674	0.00001547	0.00001777	0.00012203	0.00025712	0.00017774	0.00028416	0.00050558
-5.00	0.00004477	0.00002525	0.00004443	0.00013433	0.00000231	0.00000071	0.00000083	0.00001560	0.00004709	0.00002587	0.00004528	0.00014995

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_7H_6\mathbf{NH_2}^+$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00003867	0.00002646	0.00003224	0.00013012	0.00000185	0.00000060	0.00000075	0.00001360	0.00004066	0.00002618	0.00003320	0.00014423
4.00	0.00021650	0.00018215	0.00021914	0.00038911	0.00002350	0.00001299	0.00001638	0.00011418	0.00024059	0.00019013	0.00023701	0.00050531
3.00	0.00078570	0.00062676	0.00100763	0.00120349	0.00019941	0.00020173	0.00024698	0.00078311	0.00098702	0.00116992	0.00143475	0.00145918
2.50	0.00128634	0.00028533	0.00218211	0.00260744	0.00053673	0.00076337	0.00093145	0.00187949	0.00182624	0.00214779	0.00293127	0.00355850
2.00	0.00183587	-0.00109392	0.00406722	0.00486501	0.00135936	0.00261868	0.00320090	0.00363869	0.00319992	0.00253772	0.00663246	0.00810399
1.70	0.00205787	-0.00236781	0.00523023	0.00626086	0.00225839	0.00446799	0.00505172	0.00618298	0.00432163	0.00209419	0.01020790	0.01249397
1.53	0.00209676	-0.00300606	0.00569743	0.00682293	0.00292600	0.00453937	0.00702469	0.00860703	0.00502829	0.00152530	0.01264175	0.01548522
1.30	0.00200909	-0.00346464	0.00592535	0.00709970	0.00407057	0.00381601	0.01064523	0.01305782	0.00608502	0.00034162	0.01648733	0.02021590
1.15	0.00185496	-0.00330945	0.00572455	0.00686110	0.00491777	0.00271341	0.01347627	0.01654046	0.00677771	-0.00060602	0.01912094	0.02345850
1.00	0.00162720	-0.00270742	0.00522511	0.00626383	0.00582503	0.00108233	0.01662404	0.02041459	0.00745662	-0.00163411	0.02177689	0.02673085
0.75	0.00112544	-0.00073038	0.00381383	0.00457198	0.00736645	-0.00260152	0.02220292	0.02728480	0.00849494	-0.00333606	0.02596487	0.03189555
0.50	0.00058194	0.00195772	0.00205738	0.00245451	0.00874285	-0.00672524	0.02739375	0.03368115	0.00932637	-0.00475593	0.02941582	0.03615676
0.25	0.00015956	0.00057499	0.00068560	0.00432639	0.00970331	-0.01001166	0.03111845	0.03827313	0.00986330	-0.00567418	0.03168597	0.03896477
0.00	0.00000000	0.00000000	0.00000003	0.00526691	0.01004880	-0.01126977	0.03247738	0.03994894	0.01004880	-0.00598850	0.03247738	0.03994898
-0.25	0.00015956	0.00057499	0.00068560	0.00432639	0.00970331	-0.01001166	0.03111845	0.03827313	0.00986330	-0.00567418	0.03168597	0.03896477
-0.50	0.00058194	0.00195772	0.00205738	0.00245451	0.00874285	-0.00672524	0.02739375	0.03368115	0.00932637	-0.00475593	0.02941582	0.03615676
-0.75	0.00112544	-0.00073038	0.00381383	0.00457198	0.00736645	-0.00260152	0.02220292	0.02728480	0.00849494	-0.00333606	0.02596487	0.03189555
-1.00	0.00162720	-0.00270742	0.00522511	0.00626383	0.00582503	0.00108233	0.01662404	0.02041459	0.00745662	-0.00163411	0.02177689	0.02673085
-1.15	0.00185496	-0.00330945	0.00572455	0.00686110	0.00491777	0.00271341	0.01347627	0.01654046	0.00677771	-0.00060602	0.01912094	0.02345850
-1.30	0.00200909	-0.00346464	0.00592535	0.00709970	0.00407057	0.00381601	0.01064523	0.01305782	0.00608502	0.00034162	0.01648733	0.02021590
-1.53	0.00209676	-0.00300606	0.00569743	0.00682293	0.00292600	0.00453937	0.00702469	0.00860703	0.00502829	0.00152530	0.01264175	0.01548522
-1.70	0.00205787	-0.00236781	0.00523023	0.00626086	0.00225839	0.00446799	0.00505172	0.00618298	0.00432163	0.00209419	0.01020790	0.01249397
-2.00	0.00183587	-0.00109392	0.00406722	0.00486501	0.00135936	0.00261868	0.00320090	0.00363869	0.00319992	0.00253772	0.00663246	0.00810399
-2.50	0.00128634	0.00028533	0.00218211	0.00260744	0.00053673	0.00076337	0.00093145	0.00187949	0.00182624	0.00214779	0.00293127	0.00355850
-3.00	0.00078570	0.00062676	0.00100763	0.00120349	0.00019941	0.00020173	0.00024698	0.00078311	0.00098702	0.00116992	0.00143475	0.00145918
-4.00	0.00021650	0.00018215	0.00021914	0.00038911	0.00002350	0.00001299	0.00001638	0.00011418	0.00024059	0.00019013	0.00023701	0.00050531
-5.00	0.00003867	0.00002646	0.00003224	0.00013012	0.00000185	0.00000060	0.00000075	0.00001360	0.00004066	0.00002618	0.00003320	0.00014423

T2 (continued). The values of electron density and its Hessian's eigenvalues of ρ_{total}, ρ_{σ} and ρ_{π} in atomic units for $C_7H_6\mathbf{O}$. The highlighted cells display the position of RCPs of ρ_{π}.

	$\rho(r)_{\pi}$				$\rho(r)_{\sigma}$				$\rho(r)_{total}$			
R(Å)	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3	ρ	λ1	λ2	λ3
5.00	0.00004740	0.00002619	0.00004202	0.00013984	0.00000211	0.00000091	0.00000108	0.00001485	0.00004979	0.00002557	0.00004337	0.00015549
4.00	0.00023999	0.00017051	0.00025835	0.00039337	0.00002557	0.00001540	0.00001836	0.00012029	0.00026656	0.00017763	0.00027850	0.00051634
3.00	0.00082076	0.00055299	0.00090220	0.00130226	0.00020891	0.00021130	0.00025554	0.00078102	0.00103233	0.00105507	0.00136424	0.00156794
2.50	0.00130589	0.00016730	0.00190627	0.00271710	0.00054941	0.00076661	0.00094038	0.00182176	0.00185905	0.00196602	0.00263652	0.00367980
2.00	0.00181270	-0.00114787	0.00348576	0.00491977	0.00135897	0.00255000	0.00316876	0.00344340	0.00317616	0.00228869	0.00593284	0.00813074
1.70	0.00200162	-0.00229522	0.00444160	0.00624353	0.00222918	0.00417644	0.00485018	0.00606377	0.00423524	0.00187632	0.00915591	0.01236197
1.56	0.00202556	-0.00275768	0.00476066	0.00668231	0.00274165	0.00423463	0.00632274	0.00792354	0.00477147	0.00147219	0.01093699	0.01466482
1.30	0.00192159	-0.00320430	0.00498397	0.00697960	0.00396179	0.00349416	0.01008070	0.01268178	0.00588699	0.00028561	0.01491055	0.01972380
1.15	0.00176497	-0.00301762	0.00480138	0.00671665	0.00476583	0.00244363	0.01270937	0.01601758	0.00653390	-0.00057757	0.01736209	0.02279468
1.00	0.00154123	-0.00242579	0.00437174	0.00610954	0.00562393	0.00090853	0.01562232	0.01971950	0.00716769	-0.00151973	0.01985855	0.02588431
0.75	0.00105943	-0.00057006	0.00318084	0.00443718	0.00707640	-0.00252716	0.02076522	0.02626655	0.00813741	-0.00309668	0.02384695	0.03074417
0.50	0.00054542	0.00169148	0.00192495	0.00237307	0.00836880	-0.00634833	0.02553221	0.03234593	0.00891497	-0.00443398	0.02718438	0.03474071
0.25	0.00014916	0.00047739	0.00066055	0.00406487	0.00926855	-0.00938260	0.02894376	0.03670246	0.00941790	-0.00531285	0.02940674	0.03736904
0.00	0.00000000	0.00000000	0.00000006	0.00491924	0.00959183	-0.01054222	0.03018676	0.03829088	0.00959183	-0.00561681	0.03018676	0.03829094
-0.25	0.00014916	0.00047739	0.00066055	0.00406487	0.00926855	-0.00938260	0.02894376	0.03670246	0.00941790	-0.00531285	0.02940674	0.03736904
-0.50	0.00054542	0.00169148	0.00192495	0.00237307	0.00836880	-0.00634833	0.02553221	0.03234593	0.00891497	-0.00443398	0.02718438	0.03474071
-0.75	0.00105943	-0.00057006	0.00318084	0.00443718	0.00707640	-0.00252716	0.02076522	0.02626655	0.00813741	-0.00309668	0.02384695	0.03074417
-1.00	0.00154123	-0.00242579	0.00437174	0.00610954	0.00562393	0.00090853	0.01562232	0.01971950	0.00716769	-0.00151973	0.01985855	0.02588431
-1.15	0.00176497	-0.00301762	0.00480138	0.00671665	0.00476583	0.00244363	0.01270937	0.01601758	0.00653390	-0.00057757	0.01736209	0.02279468
-1.30	0.00192159	-0.00320430	0.00498397	0.00697960	0.00396179	0.00349416	0.01008070	0.01268178	0.00588699	0.00028561	0.01491055	0.01972380
-1.56	0.00202556	-0.00275768	0.00476066	0.00668231	0.00274165	0.00423463	0.00632274	0.00792354	0.00477147	0.00147219	0.01093699	0.01466482
-1.70	0.00200162	-0.00229522	0.00444160	0.00624353	0.00222918	0.00417644	0.00485018	0.00606377	0.00423524	0.00187632	0.00915591	0.01236197
-2.00	0.00181270	-0.00114787	0.00348576	0.00491977	0.00135897	0.00255000	0.00316876	0.00344340	0.00317616	0.00228869	0.00593284	0.00813074
-2.50	0.00130589	0.00016730	0.00190627	0.00271710	0.00054941	0.00076661	0.00094038	0.00182176	0.00185905	0.00196602	0.00263652	0.00367980
-3.00	0.00082076	0.00055299	0.00090220	0.00130226	0.00020891	0.00021130	0.00025554	0.00078102	0.00103233	0.00105507	0.00136424	0.00156794
-4.00	0.00023999	0.00017051	0.00025835	0.00039337	0.00002557	0.00001540	0.00001836	0.00012029	0.00026656	0.00017763	0.00027850	0.00051634
-5.00	0.00004740	0.00002619	0.00004202	0.00013984	0.00000211	0.00000091	0.00000108	0.00001485	0.00004979	0.00002557	0.00004337	0.00015549