Hydrogen-bonded complexes upon spatial confinement: Structural and energetic aspects

Paweł Lipkowski*, J. Kozłowska, A. Roztoczyńska and W. Bartkowiak

Theoretical Chemistry Group, Institute of Physical and Theoretical Chemistry, Wroclaw University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland
Corresponding author, e-mail: pawel.lipkowski@pwr.wroc.pl

1 Electronic Supplementary Information

Table 1 QTAIM parameters (electron density (ρ_{HBCP}), Laplacian ($\nabla^2\rho_{\text{HBCP}}$), kinetic electron energy density (G_{HBCP}), potential electron energy density (V_{HBCP}) and the total electron energy density (H_{HBCP}) at the hydrogen bond critical point), hydrogen bond donor charge ($Q_{\text{X-H}}$) and the interaction energy calculated with the counterpoise procedure (ΔE_{CP}) changes for the HF$\cdots$HF complex in the presence of the confining potential of cylindrical symmetry. All calculations have been performed using 6-311++G(2df,2pd) basis set. The results are based on the geometry optimized in vacuum (ω=0.0). All parameters except ΔE_{CP}, which is in kcal/mol, are given in atomic units.

M06-2X

ω	ρ_{HBCP}	$\nabla^2\rho_{\text{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$	ΔE_{CP}
0.00	0.0189	0.0879	0.0202	-0.0184	0.0018	-0.0046	-3.95
0.04	0.0190	0.0879	0.0202	-0.0184	0.0018	-0.0046	-3.97
0.08	0.0191	0.0879	0.0203	-0.0185	0.0017	-0.0047	-4.03
0.12	0.0192	0.0879	0.0203	-0.0187	0.0016	-0.0049	-4.11
0.16	0.0194	0.0879	0.0204	-0.0189	0.0015	-0.0054	-4.22
0.20	0.0197	0.0879	0.0206	-0.0192	0.0014	-0.0064	-4.33
0.24	0.0199	0.0877	0.0207	-0.0194	0.0013	-0.0070	-4.44
0.28	0.0202	0.0876	0.0208	-0.0197	0.0011	-0.0066	-4.55
0.32	0.0205	0.0874	0.0209	-0.0200	0.0009	-0.0062	-4.65
0.36	0.0208	0.0871	0.0210	-0.0202	0.0008	-0.0063	-4.74
0.40	0.0211	0.0869	0.0211	-0.0205	0.0006	-0.0064	-4.81
0.44	0.0214	0.0866	0.0212	-0.0207	0.0005	-0.0069	-4.88
0.48	0.0217	0.0863	0.0212	-0.0209	0.0003	-0.0080	-4.94
0.52	0.0220	0.0861	0.0213	-0.0211	0.0002	-0.0078	-4.98
0.56	0.0222	0.0858	0.0214	-0.0213	0.0001	-0.0078	-5.02
0.60	0.0225	0.0856	0.0214	-0.0214	0.0000	-0.0080	-5.05
0.70	0.0230	0.0852	0.0215	-0.0218	-0.0002	-0.0088	-5.09
0.80	0.0235	0.0850	0.0216	-0.0220	-0.0004	-0.0095	-5.09

B3LYP

ω	ρ_{HBCP}	$\nabla^2\rho_{\text{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$	ΔE_{CP}
0.00	0.0174	0.0769	0.0177	-0.0162	0.0015	-0.0047	-3.41
0.04	0.0174	0.0769	0.0177	-0.0162	0.0015	-0.0048	-3.43
0.08	0.0176	0.0768	0.0178	-0.0163	0.0014	-0.0051	-3.50
0.12	0.0177	0.0767	0.0178	-0.0165	0.0013	-0.0058	-3.60
0.16	0.0180	0.0765	0.0179	-0.0167	0.0012	-0.0068	-3.73
0.20	0.0182	0.0763	0.0180	-0.0170	0.0010	-0.0066	-3.86
0.24	0.0185	0.0759	0.0181	-0.0173	0.0009	-0.0064	-4.00
0.28	0.0188	0.0755	0.0182	-0.0176	0.0007	-0.0062	-4.13
0.32	0.0192	0.0751	0.0183	-0.0178	0.0005	-0.0061	-4.25
0.36	0.0195	0.0747	0.0184	-0.0181	0.0003	-0.0065	-4.36
0.40	0.0198	0.0742	0.0185	-0.0183	0.0001	-0.0069	-4.46
0.44	0.0201	0.0738	0.0185	-0.0186	-0.0001	-0.0080	-4.55
0.48	0.0204	0.0733	0.0186	-0.0188	-0.0002	-0.0078	-4.63
0.52	0.0207	0.0730	0.0186	-0.0190	-0.0004	-0.0078	-4.70
0.56	0.0209	0.0726	0.0186	-0.0191	-0.0005	-0.0081	-4.75
0.60	0.0212	0.0723	0.0187	-0.0193	-0.0006	-0.0084	-4.80
0.70	0.0217	0.0719	0.0187	-0.0195	-0.0008	-0.0092	-4.89
0.80	0.0221	0.0720	0.0188	-0.0196	-0.0008	-0.0099	-4.94

Table 2 QTAIM parameters (electron density (ρ_{HBCP}), Laplacian ($\nabla^2\rho_{\mathrm{HBCP}}$), kinetic electron energy density (G_{HBCP}), potential electron energy density (V_{HBCP}) and the total electron energy density (H_{HBCP}) at the hydrogen bond critical point) and hydrogen bond donor charge ($Q_{\text{X-H}}$) changes for the HF$\cdots$HF complex in the presence of the confining potential of cylindrical symmetry. All calculations have been performed using 6-311++G(2df,2pd) basis set. The results are based on the geometry optimized for each ω value. All parameters are given in atomic units.

M06-2X

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$
0.00	0.0189	0.0879	0.0202	-0.0184	0.0018	-0.0046
0.04	0.0190	0.0883	0.0203	-0.0185	0.0018	-0.0052
0.08	0.0194	0.0894	0.0206	-0.0189	0.0017	-0.0054
0.12	0.0199	0.0913	0.0212	-0.0195	0.0017	-0.0057
0.16	0.0206	0.0937	0.0219	-0.0203	0.0016	-0.0061
0.20	0.0214	0.0966	0.0227	-0.0213	0.0014	-0.0066
0.24	0.0224	0.1001	0.0238	-0.0225	0.0013	-0.0071
0.28	0.0235	0.1039	0.0249	-0.0238	0.0011	-0.0076
0.32	0.0247	0.1083	0.0262	-0.0252	0.0009	-0.0080
0.36	0.0261	0.1131	0.0276	-0.0269	0.0007	-0.0086
0.40	0.0275	0.1185	0.0292	-0.0287	0.0005	-0.0092
0.44	0.0293	0.1248	0.0311	-0.0309	0.0001	-0.0099
0.48	0.0312	0.1321	0.0333	-0.0335	-0.0002	-0.0107
0.52	0.0336	0.1408	0.0360	-0.0368	-0.0008	-0.0117
0.56	0.0367	0.1518	0.0396	-0.0413	-0.0017	-0.0128
0.60	0.0406	0.1654	0.0444	-0.0474	-0.0030	-0.0140
0.70	0.0552	0.2112	0.0627	-0.0727	-0.0099	-0.0184
0.80	0.0752	0.2658	0.0897	-0.1130	-0.0233	-0.0233

B3LYP

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$
0.00	0.0174	0.0769	0.0177	-0.0162	0.0015	-0.0047
0.04	0.0176	0.0774	0.0178	-0.0163	0.0015	-0.0052
0.08	0.0180	0.0788	0.0183	-0.0168	0.0014	-0.0055
0.12	0.0188	0.0810	0.0189	-0.0176	0.0013	-0.0060
0.16	0.0198	0.0840	0.0199	-0.0187	0.0011	-0.0065
0.20	0.0210	0.0876	0.0210	-0.0201	0.0009	-0.0072
0.24	0.0225	0.0918	0.0223	-0.0217	0.0006	-0.0079
0.28	0.0241	0.0964	0.0238	-0.0236	0.0003	-0.0087
0.32	0.0259	0.1015	0.0255	-0.0256	-0.0001	-0.0092
0.36	0.0278	0.1070	0.0273	-0.0279	-0.0006	-0.0103
0.40	0.0300	0.1132	0.0295	-0.0306	-0.0012	-0.0113
0.44	0.0325	0.1201	0.0319	-0.0338	-0.0019	-0.0124
0.48	0.0353	0.1281	0.0348	-0.0375	-0.0027	-0.0134
0.52	0.0386	0.1373	0.0382	-0.0421	-0.0039	-0.0145
0.56	0.0425	0.1481	0.0425	-0.0479	-0.0054	-0.0161
0.60	0.0471	0.1608	0.0477	-0.0551	-0.0075	-0.0177
0.70	0.0618	0.2005	0.0654	-0.0806	-0.0152	-0.0218
0.80	0.0798	0.2494	0.0896	-0.1169	-0.0273	-0.0261

Table 3 QTAIM parameters (electron density (ρ_{HBCP}), Laplacian ($\nabla^2\rho_{\mathrm{HBCP}}$), kinetic electron energy density (G_{HBCP}), potential electron energy density (V_{HBCP}) and the total electron energy density (H_{HBCP}) at the hydrogen bond critical point), hydrogen bond donor charge ($Q_{\text{X-H}}$) and interaction energy calculated with the counterpoise procedure ($\Delta E_C P$) changes for the HCN$\cdots$HCN complex in the presence of the confining potential of cylindrical symmetry. All calculations have been performed using 6-311++G(2df,2pd) basis set. The results are based on the geometry optimized in vacuum (ω=0.0). All parameters except ΔE_{CP}, which is in kcal/mol, are given in atomic units.

M06-2X

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$	ΔE_{CP}
0.00	0.0144	0.0538	0.0113	-0.0092	0.0021	-0.0125	-4.46
0.04	0.0145	0.0538	0.0114	-0.0093	0.0021	-0.0125	-4.48
0.08	0.0146	0.0540	0.0115	-0.0094	0.0020	-0.0126	-4.55
0.12	0.0149	0.0544	0.0116	-0.0097	0.0019	-0.0128	-4.65
0.16	0.0152	0.0547	0.0119	-0.0100	0.0018	-0.0131	-4.74
0.20	0.0156	0.0551	0.0121	-0.0105	0.0016	-0.0135	-4.83
0.24	0.0160	0.0554	0.0124	-0.0110	0.0014	-0.0139	-4.88
0.28	0.0165	0.0556	0.0127	-0.0115	0.0012	-0.0145	-4.90
0.32	0.0170	0.0558	0.0130	-0.0120	0.0010	-0.0150	-4.87
0.36	0.0175	0.0560	0.0133	-0.0126	0.0007	-0.0155	-4.80
0.40	0.0180	0.0560	0.0136	-0.0132	0.0004	-0.0160	-4.69
0.44	0.0185	0.0560	0.0139	-0.0137	0.0001	-0.0165	-4.54
0.48	0.0189	0.0560	0.0141	-0.0143	-0.0001	-0.0169	-4.37
0.52	0.0194	0.0559	0.0144	-0.0148	-0.0004	-0.0174	-4.17
0.56	0.0198	0.0559	0.0146	-0.0152	-0.0006	-0.0178	-3.96
0.60	0.0202	0.0558	0.0148	-0.0157	-0.0009	-0.0180	-3.75
0.70	0.0211	0.0557	0.0152	-0.0165	-0.0013	-0.0188	-3.20
0.80	0.0218	0.0560	0.0155	-0.0171	-0.0015	-0.0192	-2.66

B3LYP

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$	ΔE_{CP}
0.00	0.0144	0.0507	0.0106	-0.0086	0.0021	-0.0144	-4.20
0.04	0.0144	0.0507	0.0107	-0.0086	0.0020	-0.0145	-4.23
0.08	0.0146	0.0509	0.0107	-0.0088	0.0020	-0.0146	-4.32
0.12	0.0148	0.0511	0.0109	-0.0090	0.0019	-0.0149	-4.43
0.16	0.0152	0.0513	0.0111	-0.0093	0.0018	-0.0152	-4.55
0.20	0.0156	0.0515	0.0113	-0.0097	0.0016	-0.0156	-4.66
0.24	0.0160	0.0517	0.0115	-0.0101	0.0014	-0.0161	-4.74
0.28	0.0165	0.0518	0.0118	-0.0106	0.0012	-0.0168	-4.79
0.32	0.0170	0.0519	0.0121	-0.0112	0.0009	-0.0173	-4.79
0.36	0.0175	0.0519	0.0123	-0.0117	0.0006	-0.0179	-4.76
0.40	0.0180	0.0518	0.0126	-0.0123	0.0003	-0.0185	-4.68
0.44	0.0185	0.0517	0.0129	-0.0128	0.0000	-0.0191	-4.58
0.48	0.0190	0.0516	0.0131	-0.0134	-0.0002	-0.0197	-4.44
0.52	0.0195	0.0514	0.0134	-0.0138	-0.0005	-0.0202	-4.28
0.56	0.0200	0.0513	0.0136	-0.0143	-0.0007	-0.0207	-4.11
0.60	0.0204	0.0511	0.0138	-0.0147	-0.0010	-0.0212	-3.93
0.70	0.0213	0.0509	0.0142	-0.0156	-0.0014	-0.0220	-3.46
0.80	0.0220	0.0512	0.0145	-0.0161	-0.0017	-0.0227	-2.98

Table 4 QTAIM parameters (electron density (ρ_{HBCP}), Laplacian ($\nabla^2\rho_{\mathrm{HBCP}}$), kinetic electron energy density (G_{HBCP}), potential electron energy density (V_{HBCP}) and the total electron energy density (H_{HBCP}) at the hydrogen bond critical point) and hydrogen bond donor charge ($Q_{\text{X-H}}$) changes for the HCN$\cdots$HCN complex in the presence of the confining potential of cylindrical symmetry. All calculations have been performed using 6-311++G(2df,2pd) basis set. The results are based on the geometry optimized for each ω value. All parameters are given in atomic units.

M06-2X

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$
0.00	0.0144	0.0538	0.0113	-0.0092	0.0021	-0.0125
0.04	0.0146	0.0542	0.0115	-0.0094	0.0021	-0.0126
0.08	0.0149	0.0552	0.0118	-0.0097	0.0020	-0.0128
0.12	0.0155	0.0568	0.0122	-0.0103	0.0020	-0.0133
0.16	0.0162	0.0587	0.0129	-0.0110	0.0018	-0.0138
0.20	0.0171	0.0609	0.0136	-0.0120	0.0016	-0.0145
0.24	0.0181	0.0632	0.0144	-0.0131	0.0014	-0.0152
0.28	0.0192	0.0655	0.0154	-0.0143	0.0010	-0.0161
0.32	0.0204	0.0679	0.0163	-0.0157	0.0006	-0.0169
0.36	0.0217	0.0703	0.0174	-0.0172	0.0002	-0.1770
0.40	0.0231	0.0728	0.0185	-0.0189	-0.0003	-0.0185
0.44	0.0246	0.0753	0.0197	-0.0206	-0.0009	-0.0193
0.48	0.0261	0.0779	0.0210	-0.0225	-0.0015	-0.0200
0.52	0.0278	0.0805	0.0223	-0.0245	-0.0022	-0.0208
0.56	0.0294	0.0830	0.0237	-0.0266	-0.0029	-0.0213
0.60	0.0311	0.0853	0.0250	-0.0286	-0.0037	-0.0220
0.70	0.0350	0.0905	0.0282	-0.0338	-0.0056	-0.0234
0.80	0.0387	0.0948	0.0313	-0.0389	-0.0076	-0.0244

B3LYP

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$
0.00	0.0144	0.0507	0.0106	-0.0086	0.0021	-0.0144
0.04	0.0147	0.0518	0.0109	-0.0089	0.0020	-0.0148
0.08	0.0152	0.0529	0.0112	-0.0092	0.0020	-0.0151
0.12	0.0159	0.0546	0.0118	-0.0099	0.0019	-0.0157
0.16	0.0168	0.0567	0.0124	-0.0107	0.0017	-0.0164
0.20	0.0178	0.0590	0.0132	-0.0117	0.0015	-0.0173
0.24	0.0191	0.0615	0.0142	-0.0129	0.0012	-0.0182
0.28	0.0204	0.0639	0.0152	-0.0143	0.0008	-0.0193
0.32	0.0218	0.0664	0.0162	-0.0159	0.0004	-0.0203
0.36	0.0233	0.0689	0.0174	-0.0175	-0.0001	-0.0213
0.40	0.0248	0.0713	0.0186	-0.0193	-0.0007	-0.0222
0.44	0.0265	0.0737	0.0198	-0.0212	-0.0014	-0.0231
0.48	0.0281	0.0761	0.0211	-0.0231	-0.0021	-0.0239
0.52	0.0298	0.0785	0.0224	-0.0252	-0.0028	-0.0246
0.56	0.0314	0.0807	0.0237	-0.0272	-0.0035	-0.0252
0.60	0.0331	0.0829	0.0250	-0.0293	-0.0043	-0.0259
0.70	0.0371	0.0878	0.0282	-0.0345	-0.0063	-0.0272
0.80	0.0407	0.0920	0.0313	-0.0396	-0.0083	-0.0282

Table 5 QTAIM parameters (electron density (ρ_{HBCP}), Laplacian ($\nabla^2\rho_{\mathrm{HBCP}}$), kinetic electron energy density (G_{HBCP}), potential electron energy density (V_{HBCP}) and the total electron energy density (H_{HBCP}) at the hydrogen bond critical point), hydrogen bond donor charge ($Q_{\text{X-H}}$) and interaction energy calculated with the counterpoise procedure ($\Delta E_C P$) changes for the HCN$\cdots$HCCH complex in the presence of the confining potential of cylindrical symmetry. All calculations have been performed using 6-311++G(2df,2pd) basis set. The results are based on the geometry optimized in vacuum (ω=0.0). All parameters except ΔE_{CP}, which is in kcal/mol, are given in atomic units.

M06-2X

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$	ΔE_{CP}
0.00	0.0102	0.0382	0.0077	-0.0059	0.0018	-0.0068	-2.17
0.04	0.0102	0.0383	0.0078	-0.0060	0.0018	-0.0068	-2.16
0.08	0.0103	0.0385	0.0079	-0.0061	0.0018	-0.0070	-2.14
0.12	0.0105	0.0389	0.0080	-0.0062	0.0017	-0.0072	-2.10
0.16	0.0108	0.0393	0.0081	-0.0065	0.0017	-0.0075	-2.06
0.20	0.0110	0.0397	0.0083	-0.0067	0.0016	-0.0077	-1.98
0.24	0.0113	0.0401	0.0085	-0.0071	0.0015	-0.0080	-1.88
0.28	0.0116	0.0405	0.0088	-0.0074	0.0014	-0.0085	-1.74
0.32	0.0120	0.0409	0.0090	-0.0077	0.0012	-0.0089	-1.57
0.36	0.0123	0.0413	0.0092	-0.0081	0.0011	-0.0092	-1.38
0.40	0.0126	0.0416	0.0094	-0.0084	0.0010	-0.0096	-1.17
0.44	0.0129	0.0418	0.0096	-0.0088	0.0008	-0.0100	-0.96
0.48	0.0132	0.0420	0.0098	-0.0091	0.0007	-0.0104	-0.74
0.52	0.0135	0.0423	0.0100	-0.0094	0.0006	-0.0108	-0.52
0.56	0.0137	0.0425	0.0101	-0.0096	0.0005	-0.0111	-0.30
0.60	0.0139	0.0427	0.0102	-0.0098	0.0004	-0.0114	-0.07
0.70	0.0143	0.0433	0.0105	-0.0102	0.0003	-0.0120	0.50
0.80	0.0146	0.0441	0.0108	-0.0105	0.0003	-0.0122	1.09

B3LYP

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$	ΔE_{CP}
0.00	0.0097	0.0351	0.0070	-0.0053	0.0017	-0.0076	-1.89
0.04	0.0097	0.0352	0.0070	-0.0053	0.0017	-0.0077	-1.89
0.08	0.0098	0.0353	0.0071	-0.0054	0.0017	-0.0078	-1.88
0.12	0.0100	0.0356	0.0072	-0.0055	0.0017	-0.0080	-1.86
0.16	0.0102	0.0359	0.0074	-0.0057	0.0016	-0.0082	-1.82
0.20	0.0105	0.0362	0.0075	-0.0060	0.0015	-0.0085	-1.77
0.24	0.0108	0.0365	0.0077	-0.0063	0.0014	-0.0088	-1.69
0.28	0.0111	0.0368	0.0079	-0.0066	0.0013	-0.0092	-1.58
0.32	0.0114	0.0371	0.0081	-0.0069	0.0012	-0.0097	-1.44
0.36	0.0117	0.0373	0.0083	-0.0072	0.0011	-0.0102	-1.28
0.40	0.0120	0.0375	0.0084	-0.0075	0.0009	-0.0106	-1.11
0.44	0.0123	0.0377	0.0086	-0.0078	0.0008	-0.0111	-0.92
0.48	0.0126	0.0379	0.0088	-0.0081	0.0007	-0.0115	-0.73
0.52	0.0129	0.0381	0.0089	-0.0083	0.0006	-0.0119	-0.54
0.56	0.0131	0.0383	0.0091	-0.0085	0.0005	-0.0123	-0.35
0.60	0.0133	0.0385	0.0092	-0.0087	0.0004	-0.0127	-0.15
0.70	0.0137	0.0391	0.0094	-0.0091	0.0003	-0.0133	0.35
0.80	0.0139	0.0399	0.0096	-0.0093	0.0004	-0.0136	0.89

Table 6 QTAIM parameters (electron density (ρ_{HBCP}), Laplacian ($\nabla^2\rho_{\mathrm{HBCP}}$), kinetic electron energy density (G_{HBCP}), potential electron energy density (V_{HBCP}) and the total electron energy density (H_{HBCP}) at the hydrogen bond critical point) and hydrogen bond donor charge ($Q_{\text{X-H}}$) changes for the HCN$\cdots$HCCH complex in the presence of the confining potential of cylindrical symmetry. All calculations have been performed using 6-311++G(2df,2pd) basis set. The results are based on the geometry optimized for each ω value. All parameters are given in atomic units.

M06-2X

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$
0.00	0.0102	0.0382	0.0077	-0.0059	0.0018	-0.0068
0.04	0.0102	0.0383	0.0078	-0.0060	0.0018	-0.0069
0.08	0.0103	0.0386	0.0079	-0.0061	0.0018	-0.0070
0.12	0.0106	0.0392	0.0080	-0.0063	0.0017	-0.0072
0.16	0.0109	0.0400	0.0083	-0.0066	0.0017	-0.0074
0.20	0.0112	0.0409	0.0086	-0.0070	0.0016	-0.0077
0.24	0.0116	0.0418	0.0089	-0.0074	0.0015	-0.0080
0.28	0.0121	0.0429	0.0093	-0.0079	0.0014	-0.0084
0.32	0.0126	0.0441	0.0098	-0.0085	0.0013	-0.0090
0.36	0.0133	0.0457	0.0103	-0.0092	0.0011	-0.0096
0.40	0.0141	0.0478	0.0110	-0.0101	0.0009	-0.0102
0.44	0.0151	0.0500	0.0118	-0.0110	0.0007	-0.0108
0.48	0.0162	0.0526	0.0127	-0.0122	0.0005	-0.0115
0.52	0.0173	0.0553	0.0136	-0.0135	0.0002	-0.0121
0.56	0.0185	0.0582	0.0147	-0.0148	-0.0001	-0.0128
0.60	0.0197	0.0609	0.0157	-0.0162	-0.0005	-0.0134
0.70	0.0229	0.0676	0.0183	-0.0198	-0.0015	-0.0147
0.80	0.0260	0.0736	0.0209	-0.0235	-0.0025	-0.0158

B3LYP

ω	ρ_{HBCP}	$\nabla^2\rho_{\mathrm{HBCP}}$	G_{HBCP}	V_{HBCP}	H_{HBCP}	$Q_{\text{X-H}}$
0.00	0.0097	0.0351	0.0070	-0.0053	0.0017	-0.0076
0.04	0.0097	0.0350	0.0070	-0.0053	0.0017	-0.0076
0.08	0.0099	0.0356	0.0072	-0.0054	0.0017	-0.0078
0.12	0.0102	0.0363	0.0074	-0.0057	0.0017	-0.0080
0.16	0.0105	0.0372	0.0076	-0.0060	0.0017	-0.0084
0.20	0.0110	0.0383	0.0080	-0.0064	0.0016	-0.0087
0.24	0.0115	0.0395	0.0084	-0.0069	0.0015	-0.0092
0.28	0.0121	0.0409	0.0088	-0.0074	0.0014	-0.0097
0.32	0.0129	0.0425	0.0094	-0.0081	0.0013	-0.0105
0.36	0.0137	0.0444	0.0100	-0.0089	0.0011	-0.0111
0.40	0.0147	0.0466	0.0108	-0.0099	0.0009	-0.0119
0.44	0.0158	0.0491	0.0116	-0.0110	0.0006	-0.0127
0.48	0.0171	0.0518	0.0126	-0.0122	0.0003	-0.0135
0.52	0.0184	0.0547	0.0136	-0.0136	0.0000	-0.0143
0.56	0.0198	0.0574	0.0147	-0.0151	-0.0004	-0.0151
0.60	0.0212	0.0602	0.0158	-0.0166	-0.0008	-0.0158
0.70	0.0247	0.0665	0.0185	-0.0204	-0.0019	-0.0174
0.80	0.0280	0.0722	0.0212	-0.0243	-0.0031	-0.0187

Table 7 The values of bond lengths [Å] for the HF···HF complex in the presence of the confining potential of cylindrical symmetry. All calculations have been performed using 6-311++G(2df,2pd) basis set. The results are based on the geometry optimized for each ω value.

MP2

ω	H-F	F···H	H-F	ΔE_{CP}	μ
0.00	0.9190	1.9222	0.9206	-3.22	4.32
0.04	0.9184	1.9187	0.9201	-3.24	4.09
0.08	0.9167	1.9123	0.9183	-3.29	4.07
0.12	0.9138	1.9010	0.9155	-3.36	4.05
0.16	0.9101	1.8864	0.9119	-3.45	4.01
0.20	0.9057	1.8692	0.9075	-3.54	3.98
0.24	0.9006	1.8504	0.9026	-3.64	3.94
0.28	0.8952	1.8304	0.8973	-3.74	3.89
0.32	0.8894	1.8093	0.8916	-3.82	3.85
0.36	0.8833	1.7881	0.8856	-3.91	3.81
0.40	0.8770	1.7653	0.8794	-3.98	3.77
0.44	0.8705	1.7409	0.8730	-4.03	3.74
0.48	0.8639	1.7145	0.8664	-4.07	3.70
0.52	0.8571	1.6854	0.8598	-4.09	3.67
0.56	0.8470	1.6368	0.8497	-4.06	3.64
0.60	0.8436	1.6195	0.8463	-4.03	3.63
0.70	0.8267	1.5313	0.8296	-3.69	3.60
0.80	0.8105	1.4521	0.8135	-3.03	3.59

M06-2X

ω	H-F	F···H	H-F	ΔE_{CP}	μ
0.00	0.9199	1.8664	0.9217	-3.95	4.20
0.04	0.9194	1.8650	0.9212	-4.02	4.19
0.08	0.9178	1.8604	0.9197	-4.01	4.18
0.12	0.9153	1.8533	0.9172	-4.08	4.15
0.16	0.9119	1.8441	0.9139	-4.16	4.11
0.20	0.9078	1.8331	0.9099	-4.24	4.07
0.24	0.9031	1.8206	0.9053	-4.32	4.03
0.28	0.8980	1.8075	0.9003	-4.40	3.98
0.32	0.8925	1.7933	0.8949	-4.47	3.93
0.36	0.8867	1.7781	0.8892	-4.53	3.89
0.40	0.8806	1.7622	0.8831	-4.58	3.84
0.44	0.8744	1.7444	0.8769	-4.61	3.79
0.48	0.8679	1.7252	0.8705	-4.63	3.75
0.52	0.8614	1.7029	0.8640	-4.63	3.71
0.56	0.8548	1.6761	0.8574	-4.60	3.68
0.60	0.8482	1.6448	0.8508	-4.54	3.66
0.70	0.8318	1.5523	0.8347	-4.15	3.63
0.80	0.8159	1.4635	0.8193	-3.37	3.62

B3LYP

ω	H-F	F···H	H-F	ΔE_{CP}	μ
0.00	0.9238	1.9114	0.9260	-3.41	4.16
0.04	0.9233	1.9089	0.9255	-3.43	4.15
0.08	0.9217	1.9012	0.9240	-3.48	4.13
0.12	0.9190	1.8894	0.9214	-3.57	4.11
0.16	0.9155	1.8740	0.9179	-3.67	4.07
0.20	0.9112	1.8560	0.9138	-3.79	4.03
0.24	0.9064	1.8363	0.9092	-3.91	3.99
0.28	0.9012	1.8153	0.9041	-4.04	3.95
0.32	0.8955	1.7938	0.8987	-4.15	3.90
0.36	0.8859	1.7720	0.8929	-4.26	3.86
0.40	0.8835	1.7490	0.8869	-4.36	3.82
0.44	0.8772	1.7249	0.8807	-4.44	3.78
0.48	0.8707	1.6993	0.8743	-4.51	3.75
0.52	0.8641	1.6717	0.8678	-4.57	3.72
0.56	0.8574	1.6420	0.8612	-4.60	3.69
0.60	0.8508	1.6102	0.8547	-4.61	3.67
0.70	0.8342	1.5283	0.8384	-4.44	3.63
0.80	0.8182	1.4534	0.8226	-4.01	3.61

Table 8 The values of bond lengths [Å] for the HCN···HCN complex in the presence of the confining potential of cylindrical symmetry. All calculations have been performed using 6-311++G(2df,2pd) basis set. The results are based on the geometry optimized for each ω value.

MP2

ω	H-C	C≡N	N···H	H-C	C≡N	ΔE_{CP}	μ
0.00	1.0652	1.1643	2.1966	1.0713	1.1663	-4.56	6.83
0.04	1.0642	1.1633	2.1937	1.0703	1.1653	-4.58	6.83
0.08	1.0610	1.1605	2.1879	1.0672	1.1624	-4.62	6.81
0.12	1.0561	1.1561	2.1788	1.0624	1.1579	-4.68	6.78
0.16	1.0498	1.1505	2.1677	1.0561	1.1522	-4.73	6.74
0.20	1.0425	1.1440	2.1554	1.0489	1.1454	-4.75	6.70
0.24	1.0344	1.1367	2.1425	1.0409	1.1380	-4.74	6.65
0.28	1.0259	1.1289	2.1297	1.0324	1.1301	-4.69	6.59
0.32	1.0172	1.1207	2.1168	1.0237	1.1218	-4.58	6.52
0.36	1.0084	1.1124	2.1040	1.0150	1.1135	-4.41	6.43
0.40	0.9996	1.1041	2.0911	1.0064	1.1052	-4.19	6.34
0.44	0.9911	1.0958	2.0782	0.9979	1.0970	-3.93	6.25
0.48	0.9827	1.0877	2.0654	0.9898	1.0890	-3.62	6.15
0.52	0.9747	1.0798	2.0529	0.9819	1.0811	-3.28	6.06
0.56	0.9670	1.0720	2.0408	0.9744	1.0735	-2.92	5.97
0.60	0.9595	1.0645	2.0294	0.9671	1.0661	-2.52	5.89
0.70	0.9422	1.0468	2.0045	0.9502	1.0486	-1.47	5.75
0.80	0.9264	1.0305	1.9848	0.9344	1.0323	-0.33	5.66

M06-2X

ω	H-C	C≡N	N···H	H-C	C≡N	ΔE_{CP}	μ
0.00	1.0667	1.1403	2.2240	1.0726	1.1424	-4.46	6.93
0.04	1.0660	1.1396	2.2210	1.0717	1.1417	-4.48	6.93
0.08	1.0629	1.1368	2.2157	1.0687	1.1389	-4.53	6.91
0.12	1.0582	1.1326	2.2074	1.0640	1.1345	-4.60	6.89
0.16	1.0520	1.1272	2.1970	1.0579	1.1290	-4.67	6.85
0.20	1.0449	1.1208	2.1853	1.0508	1.1225	-4.71	6.81
0.24	1.0370	1.1138	2.1731	1.0429	1.1154	-4.72	6.76
0.28	1.0286	1.1063	2.1605	1.0346	1.1078	-4.67	6.70
0.32	1.0201	1.0985	2.1479	1.0260	1.0999	-4.58	6.62
0.36	1.0115	1.0906	2.1347	1.0175	1.0920	-4.43	6.53
0.40	1.0029	1.0827	2.1211	1.0090	1.0840	-4.23	6.43
0.44	0.9946	1.0748	2.1070	1.0008	1.0762	-3.98	6.33
0.48	0.9864	1.0670	2.0926	0.9928	1.0685	-3.69	6.22
0.52	0.9786	1.0594	2.0783	0.9852	1.0610	-3.37	6.13
0.56	0.9710	1.0521	2.0645	0.9779	1.0537	-3.02	6.04
0.60	0.9638	1.0449	2.0517	0.9709	1.0467	-2.65	5.96
0.70	0.9469	1.0280	2.0243	0.9544	1.0300	-1.65	5.82
0.80	0.9315	1.0123	2.0030	0.9389	1.0145	-0.59	5.74

B3LYP

ω	H-C	C≡N	N···H	H-C	C≡N	ΔE_{CP}	μ
0.00	1.0663	1.1444	2.2348	1.0728	1.1466	-4.20	6.93
0.04	1.0654	1.1435	2.2257	1.0717	1.1457	-4.23	6.92
0.08	1.0624	1.1408	2.2179	1.0688	1.1429	-4.30	6.91
0.12	1.0577	1.1365	2.2064	1.0643	1.1385	-4.39	6.88
0.16	1.0517	1.1310	2.1924	1.0584	1.1329	-4.49	6.85
0.20	1.0447	1.1247	2.1770	1.0515	1.1264	-4.56	6.81
0.24	1.0369	1.1176	2.1610	1.0439	1.1193	-4.60	6.76
0.28	1.0287	1.1101	2.1452	1.0358	1.1117	-4.60	6.70
0.32	1.0202	1.1023	2.1295	1.0275	1.1038	-4.54	6.63
0.36	1.0116	1.0943	2.1143	1.0190	1.0958	-4.43	6.55
0.40	1.0031	1.0863	2.0994	1.0107	1.0878	-4.27	6.46
0.44	0.9947	1.0784	2.0851	1.0025	1.0799	-4.06	6.36
0.48	0.9866	1.0706	2.0713	0.9946	1.0722	-3.81	6.26
0.52	0.9787	1.0630	2.0582	0.9869	1.0647	-3.52	6.17
0.56	0.9711	1.0556	2.0458	0.9795	1.0574	-3.20	6.08
0.60	0.9639	1.0484	2.0344	0.9725	1.0503	-2.85	6.00
0.70	0.9469	1.0314	2.0099	0.9559	1.0335	-1.91	5.86
0.80	0.9314	1.0157	1.9912	0.9404	1.0180	-0.87	5.77

Table 9 The values of bond lengths [Å] for the HCN$\cdots$HCCH complex in the presence of the confining potential of cylindrical symmetry. All calculations have been performed using 6-311++G(2df,2pd) basis set. The results are based on the geometry optimized for each ω value.

MP2

ω	H-C	C≡N	N$\cdots$H	H-C	C=C	C-H	ΔE_{CP}	μ
0.00	1.0648	1.1650	2.3472	1.0659	1.2119	1.0614	-2.41	3.59
0.04	1.0638	1.1641	2.3472	1.0649	1.2106	1.0604	-2.39	3.59
0.08	1.0606	1.1617	2.3467	1.0616	1.2067	1.0572	-2.36	3.54
0.12	1.0558	1.1570	2.3446	1.0568	1.2011	1.0524	-2.28	3.55
0.16	1.0494	1.1514	2.3411	1.0505	1.1941	1.0462	-2.19	3.52
0.20	1.0421	1.1447	2.3377	1.0432	1.1860	1.0390	-2.07	3.49
0.24	1.0341	1.1374	2.3339	1.0352	1.1771	1.0311	-1.91	3.46
0.28	1.0256	1.1296	2.3298	1.0268	1.1679	1.0227	-1.70	3.42
0.32	1.0169	1.1215	2.3239	1.0181	1.1586	1.0142	-1.46	3.38
0.36	1.0081	1.1132	2.3150	1.0094	1.1494	1.0058	-1.19	3.34
0.40	0.9993	1.1049	2.3039	1.0011	1.1405	0.9974	-0.90	3.29
0.44	0.9908	1.0966	2.2895	0.9928	1.1320	0.9893	-0.57	3.25
0.48	0.9825	1.0885	2.2733	0.9850	1.1238	0.9815	-0.22	3.21
0.52	0.9744	1.0805	2.2561	0.9774	1.1160	0.9740	0.15	3.18
0.56	0.9667	1.0728	2.2390	0.9701	1.1085	0.9667	0.55	3.14
0.60	0.9593	1.0653	2.2214	0.9630	1.1013	0.9597	0.97	3.12
0.70	0.9420	1.0475	2.1821	0.9461	1.0841	0.9428	2.13	3.07
0.80	0.9262	1.0310	2.1499	0.9300	1.0679	0.9267	3.44	3.05

M06-2X

ω	H-C	C≡N	N$\cdots$H	H-C	C=C	C-H	ΔE_{CP}	μ
0.00	1.0665	1.1410	2.3855	1.0671	1.1946	1.0627	-2.17	3.64
0.04	1.0655	1.1402	2.3857	1.0661	1.1933	1.0618	-2.15	3.64
0.08	1.0625	1.1374	2.3860	1.0631	1.1894	1.0588	-2.11	3.62
0.12	1.0577	1.1332	2.3849	1.0584	1.1836	1.0541	-2.06	3.60
0.16	1.0516	1.1278	2.3828	1.0524	1.1763	1.0482	-1.97	3.57
0.20	1.0444	1.1214	2.3805	1.0453	1.1681	1.0412	-1.86	3.54
0.24	1.0366	1.1144	2.3778	1.0375	1.1591	1.0335	-1.71	3.51
0.28	1.0283	1.1069	2.3739	1.0292	1.1498	1.0254	-1.52	3.47
0.32	1.0197	1.0991	2.3675	1.0207	1.1405	1.0171	-1.29	3.43
0.36	1.0111	1.0911	2.3580	1.0123	1.1313	1.0089	-1.04	3.38
0.40	1.0026	1.0832	2.3435	1.0041	1.1224	1.0008	-0.77	3.34
0.44	0.9943	1.0753	2.3282	0.9961	1.1139	0.9929	-0.47	3.29
0.48	0.9862	1.0675	2.3092	0.9884	1.1057	0.9853	-0.15	3.25
0.52	0.9783	1.0600	2.2906	0.9810	1.0979	0.9780	0.20	3.21
0.56	0.9708	1.0526	2.2713	0.9739	1.0904	0.9709	0.57	3.18
0.60	0.9636	1.0455	2.2532	0.9670	1.0831	0.9641	0.97	3.15
0.70	0.9467	1.0285	2.2119	0.9503	1.0657	0.9476	2.06	3.10
0.80	0.9313	1.0127	2.1779	0.9344	1.0491	0.9318	3.30	3.09

B3LYP

ω	H-C	C≡N	N$\cdots$H	H-C	C=C	C-H	ΔE_{CP}	μ
0.00	1.0659	1.1451	2.4150	1.0659	1.1972	1.0615	-1.89	3.63
0.04	1.0650	1.1442	2.4170	1.0650	1.1959	1.0606	-1.88	3.62
0.08	1.0620	1.1414	2.4134	1.0620	1.1919	1.0577	-1.86	3.61
0.12	1.0573	1.1371	2.4096	1.0575	1.1861	1.0531	-1.81	3.58
0.16	1.0513	1.1317	2.4038	1.0516	1.1788	1.0473	-1.75	3.56
0.20	1.0443	1.1253	2.3970	1.0447	1.1706	1.0405	-1.66	3.53
0.24	1.0365	1.1182	2.3893	1.0371	1.1617	1.0329	-1.53	3.50
0.28	1.0283	1.1107	2.3799	1.0290	1.1525	1.0249	-1.36	3.47
0.32	1.0199	1.1028	2.3679	1.0208	1.1433	1.0167	-1.17	3.43
0.36	1.0113	1.0949	2.3528	1.0125	1.1341	1.0086	-0.94	3.39
0.40	1.0028	1.0869	2.3356	1.0043	1.1253	1.0005	-0.68	3.35
0.44	0.9944	1.0789	2.3154	0.9964	1.1168	0.9926	-0.39	3.31
0.48	0.9863	1.0711	2.2948	0.9888	1.1086	0.9850	-0.08	3.27
0.52	0.9784	1.0635	2.2729	0.9815	1.1009	0.9777	0.25	3.24
0.56	0.9708	1.0561	2.2528	0.9743	1.0934	0.9706	0.62	3.21
0.60	0.9636	1.0489	2.2335	0.9676	1.0862	0.9637	1.00	3.18
0.70	0.9467	1.0319	2.1918	0.9511	1.0690	0.9473	2.07	3.14
0.80	0.9312	1.0161	2.1583	0.9353	1.0527	0.9316	3.31	3.13

Table 10 Leading intermolecular interaction energy components for the HF$\cdots$HF, HCN$\cdots$HCN, HCN$\cdots$HCCH complexes in the presence of spatial confinement computed using the variational–perturbational scheme for the geometry optimized in vacuum (model 'u'). All interaction energy components are given in [kcal/mol].

	HF$\cdots$HF				HCN$\cdots$HCN				HCN$\cdots$HCCH			
ω [au]	$\epsilon_{el}^{(10)}$	$\epsilon_{ex}^{(10)}$	$\epsilon_{disp}^{(20)}$	$\Delta E_{del}^{HF}+\Delta_F+\Delta_W$	$\epsilon_{el}^{(10)}$	$\epsilon_{ex}^{(10)}$	$\epsilon_{disp}^{(20)}$	$\Delta E_{del}^{HF}+\Delta_F+\Delta_W$	$\epsilon_{el}^{(10)}$	$\epsilon_{ex}^{(10)}$	$\epsilon_{disp}^{(20)}$	$\Delta E_{del}^{HF}+\Delta_F+\Delta_W$
0.00	-4.6559	2.5862	-1.0393	-1.2500	-6.5347	4.1853	-1.8463	-1.6548	-3.4230	2.5780	-1.4762	-0.8057
0.04	-4.6742	2.5851	-1.0384	-1.2478	-6.5707	4.1857	-1.8448	-1.6519	-3.4209	2.5799	-1.4746	-0.8033
0.08	-4.7264	2.5817	-1.0357	-1.2416	-6.6655	4.1843	-1.8406	-1.6443	-3.4116	2.5826	-1.4704	-0.7982
0.12	-4.8052	2.5753	-1.0316	-1.2318	-6.7915	4.1773	-1.8346	-1.6349	-3.3919	2.5811	-1.4644	-0.7935
0.16	-4.9008	2.5655	-1.0262	-1.2197	-6.9225	4.1627	-1.8276	-1.6256	-3.3522	2.5732	-1.4576	-0.7909
0.20	-5.0043	2.5522	-1.0200	-1.2061	-7.0386	4.1409	-1.8199	-1.6170	-3.2825	2.5594	-1.4505	-0.7904
0.24	-5.1084	2.5355	-1.0132	-1.1917	-7.1248	4.1137	-1.8120	-1.6095	-3.1764	2.5409	-1.4431	-0.7917
0.28	-5.2084	2.5163	-1.0061	-1.1770	-7.1708	4.0829	-1.8040	-1.6028	-3.0326	2.5188	-1.4353	-0.7949
0.32	-5.3015	2.4954	-0.9987	-1.1624	-7.1706	4.0499	-1.7960	-1.5966	-2.8546	2.4937	-1.4270	-0.7998
0.36	-5.3864	2.4736	-0.9914	-1.1481	-7.1228	4.0155	-1.7877	-1.5908	-2.6485	2.4657	-1.4178	-0.8062
0.40	-5.4627	2.4515	-0.9840	-1.1340	-7.0298	3.9802	-1.7791	-1.5854	-2.4214	2.4351	-1.4076	-0.8139
0.44	-5.5304	2.4295	-0.9766	-1.1203	-6.8975	3.9444	-1.7701	-1.5806	-2.1802	2.4022	-1.3962	-0.8225
0.48	-5.5896	2.4077	-0.9690	-1.1070	-6.7330	3.9081	-1.7603	-1.5766	-1.9301	2.3675	-1.3837	-0.8321
0.52	-5.6405	2.3858	-0.9613	-1.0939	-6.5443	3.8717	-1.7496	-1.5739	-1.6751	2.3316	-1.3701	-0.8424
0.56	-5.6834	2.3634	-0.9533	-1.0808	-6.3389	3.8353	-1.7381	-1.5725	-1.4176	2.2954	-1.3555	-0.8534
0.60	-5.7185	2.3403	-0.9448	-1.0679	-6.1233	3.7992	-1.7256	-1.5729	-1.1589	2.2594	-1.3402	-0.8649
0.70	-5.7737	2.2753	-0.9212	-1.0350	-5.5721	3.7122	-1.6903	-1.5808	-0.5084	2.1750	-1.2998	-0.8957
0.80	-5.7864	2.1949	-0.8931	-1.0008	-5.0369	3.6331	-1.6503	-1.5978	0.15070	2.1043	-1.2581	-0.9288

Table 11 Leading intermolecular interaction energy components for the HF$\cdots$HF, HCN$\cdots$HCN, HCN$\cdots$HCCH complexes in the presence of spatial confinement computed using the variational–perturbational scheme for the geometry optimized for each ω value (model 'r'). All interaction energy components are given in [kcal/mol].

	HF$\cdots$HF				HCN$\cdots$HCN				HCN$\cdots$HCCH			
ω [au]	$\epsilon_{el}^{(10)}$	$\epsilon_{ex}^{(10)}$	$\epsilon_{disp}^{(20)}$	$\Delta E_{del}^{HF}+\Delta_F+\Delta_W$	$\epsilon_{el}^{(10)}$	$\epsilon_{ex}^{(10)}$	$\epsilon_{disp}^{(20)}$	$\Delta E_{del}^{HF}+\Delta_F+\Delta_W$	$\epsilon_{el}^{(10)}$	$\epsilon_{ex}^{(10)}$	$\epsilon_{disp}^{(20)}$	$\Delta E_{del}^{HF}+\Delta_F+\Delta_W$
0.00	-4.6559	2.5862	-1.0393	-1.2500	-6.5347	4.1853	-1.8463	-1.6548	-3.4238	2.5780	-1.4762	-0.8057
0.04	-4.6901	2.6228	-1.0475	-1.2603	-6.5971	4.2358	-1.8558	-1.6625	-3.4204	2.5855	-1.4748	-0.8026
0.08	-4.7698	2.6909	-1.0617	-1.2753	-6.7444	4.3374	-1.8725	-1.6724	-3.4051	2.6006	-1.4696	-0.7937
0.12	-4.9036	2.8154	-1.0880	-1.3044	-6.9562	4.4973	-1.9000	-1.6913	-3.3863	2.6318	-1.4659	-0.7878
0.16	-5.0806	2.9850	-1.1232	-1.3441	-7.1978	4.6974	-1.9349	-1.7168	-3.3477	2.6722	-1.4644	-0.7850
0.20	-5.2948	3.1977	-1.1666	-1.3935	-7.4419	4.9256	-1.9747	-1.7466	-3.2735	2.7094	-1.4615	-0.7836
0.24	-5.5387	3.4480	-1.2166	-1.4508	-7.6671	5.1738	-2.0174	-1.7792	-3.1593	2.7469	-1.4586	-0.7845
0.28	-5.8097	3.7373	-1.2728	-1.5162	-7.8576	5.4361	-2.0614	-1.8130	-3.0052	2.7853	-1.4559	-0.7880
0.32	-6.1084	4.0702	-1.3356	-1.5902	-8.0053	5.7115	-2.1067	-1.8481	-2.8243	2.8407	-1.4583	-0.7977
0.36	-6.4309	4.4407	-1.4031	-1.6708	-8.1087	6.0009	-2.1532	-1.8852	-2.6300	2.9262	-1.4695	-0.8162
0.40	-6.7953	4.8814	-1.4812	-1.7668	-8.1710	6.3062	-2.2015	-1.9254	-2.4264	3.0381	-1.4881	-0.8428
0.44	-7.2115	5.4084	-1.5718	-1.8820	-8.1975	6.6275	-2.2513	-1.9694	-2.2241	3.1915	-1.5180	-0.8798
0.48	-7.6967	6.0495	-1.6787	-2.0222	-8.1932	6.9624	-2.3021	-2.0174	-2.0192	3.3744	-1.5551	-0.9249
0.52	-8.2814	6.8557	-1.8090	-2.2005	-8.1620	7.3060	-2.3528	-2.0687	-1.8101	3.5830	-1.5979	-0.9770
0.56	-9.3004	8.4898	-2.0661	-2.5530	-8.1062	7.6517	-2.4021	-2.1224	-1.5898	3.8034	-1.6421	-1.0331
0.60	-9.8455	9.1267	-2.1561	-2.7025	-8.0273	7.9930	-2.4485	-2.1773	-1.3611	4.0458	-1.6902	-1.0951
0.70	-12.6742	13.4353	-2.7525	-3.6282	-7.6564	8.9364	-2.5626	-2.3304	-0.7055	4.6556	-1.8033	-1.2552
0.80	-16.2881	19.0502	-3.4418	-4.7595	-7.3116	9.4912	-2.6191	-2.4402	0.0908	5.2426	-1.9007	-1.4151