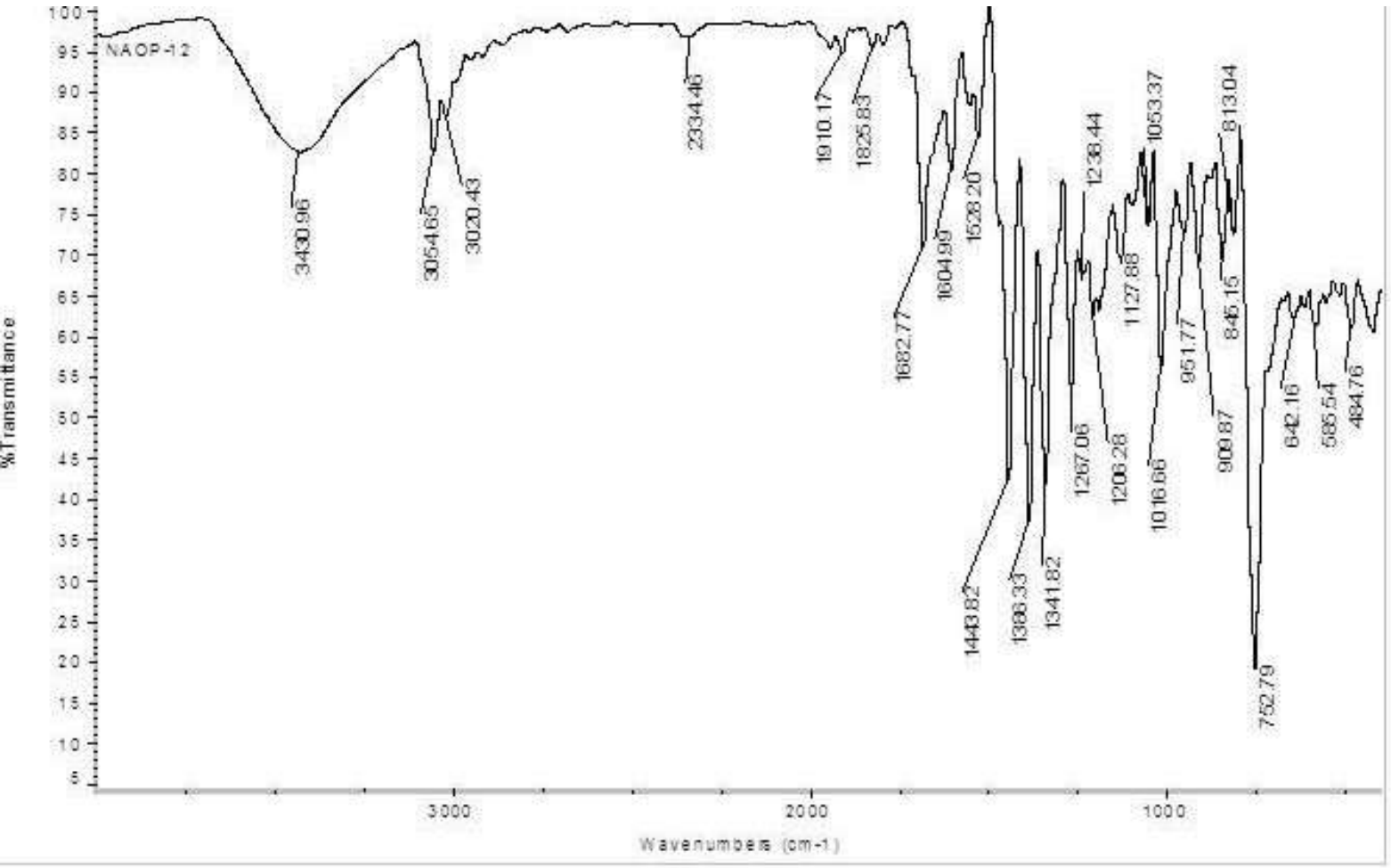

Fig. F1: FTIR spectra of NAOP-12

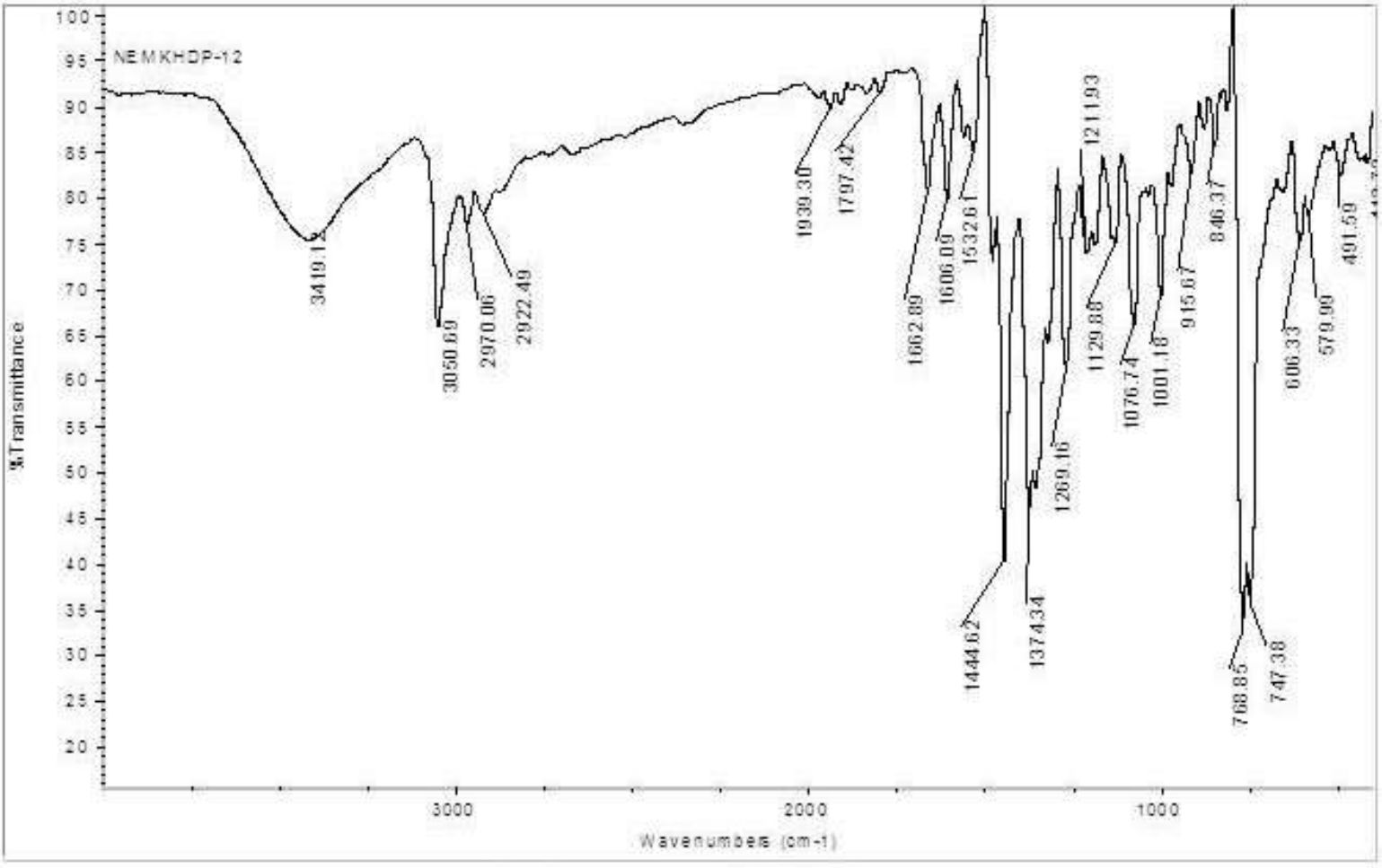

Fig. F2: FTIR spectra of NEMKH-12

Table: T1a Optimized ground state geometry parameters of NAOP-12 at B3LYP method

S.NO.	Parameter	Method		S.No.	Parameter	Method	
	Stretching	X-ray	DFT		*Bending*	X-ray	DFT
	Å		B3LYP		Deg		B3LYP
1	N1-C7	1.3219	1.314	42	C17-N3-C16	126	129
2	N1-C8	1.3215	1.3635	43	C2-C1-C6	119	117
3	N2-C14	1.318	1.3046	44	C2-C1-C23	117	109
4	N2-C13	1.3638	1.3675	45	C6-C1-C23	123	134
5	N3-C23	1.3823	1.411	46	C3-C2-H2A	119	119
6	N3-C16	1.0433	1.4092	47	C1-C2-H2A	119	117
7	N4-C23	1.3068	1.3139	48	C2-C3-C4	120	120
8	N4-C22	1.3965	1.379	49	H3A-C3-C4	120	121
9	C1-C6	1.4051	1.441	50	C3-C4-C5	120	119
10	C1-C23	1.4755	1.5127	51	C3-C4-H4A	120	121
11	C2-C3	1.3817	1.3843	52	C4-C5-C6	121	124
12	C3-C4	1.3632	1.3875	53	H5A-C5-C4	119	119
13	C3-H3A	0.93	1.084	54	H5A-C5-C6	119	117
14	C4-C5	1.3846	1.3844	55	C5-C6-C7	117	110
15	C4-H4A	0.93	1.0809	56	C1-C6-C7	125	117
16	C5-C6	1.398	1.4117	57	N1-C7-C14	121	120
17	C6-C7	1.4923	1.5181	58	N1-C7-C6	115	117
18	C7-C14	1.4367	1.4543	59	C14-C7-C6	123	123
19	C8-C13	1.4118	1.4232	60	N1-C8-C13	121	121
20	C9-C10	1.3657	1.3764	61	N1-C8-C9	120	120
21	C9-H9A	0.93	1.0836	62	C10-C9-C8	120	120
22	C10-C11	1.404	1.4147	63	C10-C9-H9A	120	122
23	C11-C12	1.3675	1.377	64	C8-C9-H9A	120	120
24	C11-H11A	0.93	1.084	65	C9-C10-H10A	120	120
25	C12-C13	1.4124	1.4132	66	C11-C10-H10A	120	119
26	C14-C15	1.4818	1.4707	67	C12-C11-C10	121	121
27	C15-C16	1.3255	1.3416	68	C10-C11-H11A	120	119
28	C15-H15A	0.93	1.0848	69	C11-C12-C13	120	120
29	C17-C18	1.3975	1.395	70	C11-C12-H12A	120	122
30	C17-C22	1.4028	1.4078	71	N2-C13-C8	120	120
31	C18-C19	1.3762	1.3909	72	N2-C13-C12	120	120
32	C19-C20	1.403	1.4081	73	C8-C13-C12	120	120
33	C19-H19A	0.93	1.0839	74	N2-C14-C15	115	126
34	C20-C21	1.3815	1.3885	75	C7-C14-C15	123	110
35	C21-C22	1.3943	1.3991	76	C16-C15-C14	128	126
36	C21-H21A	0.93	1.0833	77	C14-C15-H15A	116	127
37	C24-H24A	0.96	1.0888	78	N3-C16-C15	120	115
38	C24-H24B	0.96	1.0928	79	C15-C16-C24	125	126
39	C24-H24C	0.96	1.0956	80	N3-C17-C18	132	133
	Angle Bending(Deg)			81	N3-C17-C22	105	105
40	C23-N3-C17	106	107	82	C18-C17-C22	123	122
41	C23-N3-C16	126	121		*Dihedral Angles(Deg)*		
84	C17-C18-H18A	122	122	83	C19-C18-H18A	122	121
85	C18-C19-C20	122	122	130	C9-C8-C13-C12	-0.27	1.72
86	C20-C19-H19A	119	119	131	C11-C12-C13-N2	-178	177

87	C21-C20-C19	122	121
88	C21-C20-H20A	119	120
89	C20-C21-C22	117	118
90	C20-C21-H21A	121	120
91	C22-C21-H21A	121	122
92	C21-C22-C17	120	120
93	N4-C22-C17	110	110
94	N4-C23-N3	113	111
95	N3-C23-C1	123	129
96	C16-C24-H24A	110	111
97	C16-C24-H24B	110	111
98	C16-C24-H24C	110	111
99	H24A-C24-H24C	110	108
100	H24B-C24-H24C	110	110
	Dihedral Angles(Deg)		
101	C6-C1-C2-C3	-0.18	0.85
102	C23-C1-C2-C3	-175	-175
103	C1-C2-C3-C4	1.91	0.65
104	C2-C3-C4-C5	-1.61	-1.04
105	C3-C4-C5-C6	-0.4	-0.087
106	C4-C5-C6-C1	2.1	1.59
107	C4-C5-C6-C7	179	-176
108	C2-C1-C6-C5	-1.79	-1.88
109	C23-C1-C6-C5	173	174
110	C2-C1-C6-C7	-179	175
111	C23-C1-C6-C7	-4.44	-9.1
112	C8-N1-C7-C14	1.58	-3.41
113	C8-N1-C7-C6	173	169
114	C5-C6-C7-N1	-49	-41
115	C1-C6-C7-N1	129	141
116	C5-C6-C7-C14	123	130
117	C1-C6-C7-C14	-59	-46
118	C7-N1-C8-C13	-1.95	-1.5
119	C7-N1-C8-C9	179.81	179.71
120	N1-C8-C9-C10	178.53	177.5
121	C13-C8-C9-C10	0.3	-1.4
122	C8-C9-C10-C11	0.2	0.19
123	C9-C10-C11-C12	-0.6	0.72
124	C10-C11-C12-C13	0.6	-0.39
125	C14-N2-C13-C8	3.18	-2.9
126	C14-N2-C13-C12	-178.72	179
127	N1-C8-C13-N2	-0.42	4.9
128	C9-C8-C13-N2	177.84	-176
129	N1-C8-C13-C12	-178.52	-177
132	C11-C12-C13-C8	-0.2	-0.83
133	C13-N2-C14-C7	-3.58	-2.18
134	C13-N2-C14-C15	-177	168
135	N1-C7-C14-N2	1.25	5.65
136	C6-C7-C14-N2	-170.25	-166.26
137	N1-C7-C14-C15	174	-166
138	C6-C7-C14-C15	2.59	22
139	N2-C14-C15-C16	-124.4	-92
140	C7-C14-C15-C16	62.36	79
141	C14-C15-C16-N3	-1.4	-129.6
142	C14-C15-C16-C24	179.8	34
143	C23-N3-C16-C15	-70.61	55.14
144	C17-N3-C16-C15	122.7	-148.54
145	C23-N3-C16-C24	108.3	-110.2
146	C17-N3-C16-C24	-58.41	46
147	C23-N3-C17-C18	176.8	-178.56
148	C16-N3-C17-C18	-14.36	-22.6
149	C23-N3-C17-C22	0.4	-1.11
150	C16-N3-C17-C22	169.3	-160
151	N3-C17-C18-C19	-176.4	178.12
152	C 22-C17-C18-C19	-0.58	1.03
153	C 17-C18-C19-C20	-0.521	-0.466
154	C 18-C19-C20-C21	1.14	-0.25
155	C19-C20-C21-C22	-0.61	0.41
156	C20-C21-C22-N4	177.8	-179.41
157	C20-C21-C22-C17	-0.45	0.14
158	C23-N4-C22-C21	-177.7	179.2
159	C23-N4-C22-C17	0.73	-0.39
160	N3-C17-C22-C21	177.9	-178.68
161	C18-C17-C22-C21	1.08	-0.9
162	N3-C17-C22-N4	-0.71	0.96
163	C18-C17-C22-N4	-177.5	178.71
164	C22-N4-C23-N3	-0.48	-0.34
165	C22-N4-C23-C1	-179	-176.31
166	C17-N3-C23-N4	0.05	0.94
167	C16-N3-C23-N4	-168.5	161.96
168	C17-N3-C23-N1	178.6	176.47
169	C16-N3-C23-C1	9.73	-22.5
170	C2-C1-C23-N4	54.8	25.26
171	C6-C1-C23-N4	-120	-150.6
172	C2-C1-C23-N3	-123.6	-149.99
173	C6-C1-C23-N3	61.46	34.21

Table T1b: Optimized ground state geometry parameters of NEMKH at B3LYP method

S.No.	Parameter	Method		S.No.	Parameter	Method	
	Stretching	X-ray	DFT		*Stretching*	X-ray	DFT
	Angstrom		B3LYP		*Angstrom*		B3LYP
1	C1-C2	1.47	1.51	41	N33-C35	1.40	1.39
2	C1-N33	1.39	1.40	42	C35-C42	1.40	1.39
3	C1=N34	1.31	1.32	43	C36-H37	0.93	1.08
4	C2-C17	1.40	1.44	44	C36-C38	1.39	1.39
5	C2-C18	1.40	1.42	45	C38-H39	0.93	1.08
6	C3-C6	1.44	1.45	46	C38-C40	1.41	1.41
7	C3=N7	1.32	1.32	47	C40-H41	0.93	1.08
8	C3-C17	1.49	1.53	48	C40-C42	1.38	1.39
9	C4-C5	1.42	1.42	49	C42-H43	0.93	1.08
10	C4-N8	1.37	1.37	50	C44-H45	0.96	1.10
11	C4-C11	1.42	1.41	51	C44-H46	0.96	1.09
12	C5-N7	1.36	1.36	52	C44-H47	0.96	1.09
13	C5-C15	1.42	1.42		***Angle Bending(deg)***		
14	C6=N8	1.32	1.31	53	C2-C1-N33	122.50	128.05
15	C6-C26	1.50	1.48	54	C2-C1=N34	123.98	120.94
16	C9-H10	0.93	1.08	55	N33-C1=N34	113.51	110.98
17	C9-C11	1.37	1.38	56	C1-C2-C17	120.63	134.02
18	C9-C13	1.41	1.42	57	C1-C2-C18	119.19	109.13
19	C11-H12	0.93	1.08	58	C17-C2-C18	119.98	116.78
20	C13-H14	0.93	1.08	59	C6-C3-N7	121.79	119.06
21	C13-C15	1.36	1.38	60	C6-C3-C17	122.18	124.00
22	C15-H16	0.93	1.08	61	N7=C3-C17	115.92	116.27
23	C17-C24	1.40	1.41	62	C5-C4-N8	121.00	120.13
24	C18-H19	0.93	1.08	63	C5-C4-C11	119.60	119.69
25	C18-C20	1.39	1.38	64	N8-C4-C11	119.40	120.12
26	C20-H21	0.93	1.08	65	C4-C5-N7	120.90	120.98
27	C20-C22	1.38	1.39	66	C4-C5-C15	119.43	119.31
28	C22-H23	0.93	1.08	67	N7-C5-C15	119.65	119.69
29	C22-C24	1.39	1.38	68	C3-C6=N8	121.38	123.22
30	C24-H25	0.93	1.08	69	C3-C6-C26	122.59	111.08
31	C26=C27	1.34	1.35	70	N8=C6-C26	115.93	125.38
32	C26-C44	1.52	1.50	71	C3=N7-C5	117.23	118.68
33	C27-C28	1.50	1.51	72	C4-N8-C6	117.00	117.20
34	C27-N33	1.44	1.41	73	H10-C9-C11	119.40	119.96
35	C28-H29	0.96	1.09	74	H10-C9-C13	119.40	119.44
36	C28-H30	0.96	1.09	75	C11-C9-C13	121.17	120.60
37	C28-H31	0.96	1.10	76	C4-C11-C9	119.24	119.80
38	C32-N34	1.39	1.38	77	C4-C11-H12	120.40	118.27
39	C32-C35	1.40	1.41	78	C9-C11-H12	120.40	121.92
40	C32-C36	1.40	1.40	79	C9-C13-H14	119.70	119.41

contd…

80	C9-C13-C15	120.57	120.68	111	H30-C28-H31	109.50	106.82
81	H14-C13-C15	119.70	119.91	112	N34-C32-C35	110.28	110.12
82	C5-C15-C13	119.91	119.89	113	N34-C32-C36	129.17	129.95
83	C5-C15-H16	120.00	118.19	114	C35-C32-C36	120.47	119.93
84	C13-C15-H16	120.00	121.92	115	C1-N33-C27	125.80	118.71
85	C2-C17-C3	121.53	134.26	116	C1-N33-C35	105.90	107.28
86	C2-C17-C24	119.59	116.95	117	C27-N33-C35	126.59	130.90
87	C3-C17-C24	118.78	108.73	118	C1=N34-C32	105.00	106.73
88	C2-C18-H19	120.00	116.76	119	C32-C35-N33	105.26	104.86
89	C2-C18-C20	119.96	124.20	120	C32-C35-C42	122.42	122.61
90	H19-C18-C20	120.00	119.04	121	N33-C35-C42	132.28	132.50
91	C18-C20-H21	119.90	119.69	122	C32-C36-H37	121.20	120.41
92	C18-C20-C22	120.16	119.06	123	C32-C36-C38	117.61	117.87
93	H21-C20-C22	119.90	121.26	124	H37-C36-C38	121.20	121.72
94	C20-C22-H23	119.90	121.41	125	C36-C38-H39	119.50	119.56
95	C20-C22-C24	120.29	118.65	126	C36-C38-C40	121.05	121.45
96	H23-C22-C24	119.90	119.94	127	H39-C38-C40	119.50	118.99
97	C17-C24-C22	120.00	124.35	128	C38-C40-H41	118.90	119.22
98	C17-C24-H25	120.00	117.14	129	C38-C40-C42	122.20	121.52
99	C22-C24-H25	120.00	118.51	130	H41-C40-C42	118.90	119.26
100	C6-C26=C27	121.93	111.55	131	C35-C42-C40	116.24	116.62
101	C6-C26-C44	113.59	119.28	132	C35-C42-H43	121.90	122.03
102	C27=C26-C44	124.45	126.24	133	C40-C42-H43	121.90	121.35
103	C26=C27-C28	126.15	126.14	134	C26-C44-H45	109.50	108.52
104	C26=C27-N33	119.80	116.71	135	C26-C44-H46	109.50	112.26
105	C28-C27-N33	114.02	115.01	136	C26-C44-H47	109.50	111.70
106	C27-C28-H29	109.50	111.63	137	H45-C44-H46	109.50	106.88
107	C27-C28-H30	109.50	109.67	138	H45-C44-H47	109.50	108.59
108	C27-C28-H31	109.50	111.47	139	H46-C44-H47	109.50	108.72
109	H29-C28-H30	109.50	107.85				
110	H29-C28-H31	109.50	109.22				

Table T2a:Frequency assignments for NAOP-12 at B3LYP/6-311G(d,p) in cm–1, with PED[%]

	Calc Freq		Exp freq	Assignment Modes [PED %]
S.No.	Unscaled	Scaled	FTIR	
1	3228	3092	3431(w)	ν(C18-H19)[97]
2	3212	3077		ν(C24-H25)[93]
3	3198	3063		ν(C-H)R3[74] + ν(C-H)R5[20]
4	3193	3058		ν(C-H)R5[69]
5	3187	3053	3055(w)	ν(C-H)R1[94]
6	3181	3047		ν(C-H)R3[58] + ν(C-H)R5[37]
7	3171	3038		ν(C-H)R1[98]
8	3169	3036		ν(C-H)R5[87]
9	3161	3028	*3020(w)*	ν(C26-H27)[100]
10	3139	3007	2985(w)	ν(C29-H30)[86]
11	3087	2957		ν(C29-H31)[76]
12	3028	2900		ν(C29-H32)[72]
13	1680	1651	1683(m)	ν(C26=C28)[73]
14	1651	1623		ν(C9=C11)[22] + ν(C13-C5)[21]
15	1634	1606		ν(C-C)R1[65]
16	1622	1594		ν(C-C)R5[37] + φ(C-C-C)R5[27]
17	1608	1581	1605(w)	ν(C6=N8)[50]
18	1585	1558	1557(w)	ν(C9-C13)[21]
19	1516	1490	1526(w)	R3-ROCK[38]
20	1510	1484		R5-ROCK[42]
21	1496	1471	1477(w)	φ(H-C-C)R3[18] +φ(H-C-C)R5[10]
22	1486	1461		φ(H30-C29-H31)[45]
23	1474	1449	1444(s)	φ(H30-C29-H32)[47]
24	1466	1441		ν(C1-N35)[29]
25	1449	1424		φ(H21-C20-C22)R1[21]
26	1422	1398		φ(H25-C24-C22)[20] + φ(H27-C26-C28)[12]
27	1413	1389	1386(s)	ν(C5-C15)[12]
28	1398	1375	1379(w)	ν(N34-C36)[15]+ν(N34-C28)[28]
29	1381	1357		ν(C33-C37)[11]
30	1376	1352	1342(s)	ν(C13-C15)[13]
31	1356	1333		φ(H27-C26-C28)[23]
32	1339	1316		ν(N8-C4)[10] + ν(N7-C5)[16]
33	1325	1302		R5-Rock[11]
34	1316	1294		R1-Breath[11]
35	1306	1284		ν(N8-C4)[16] + ν(N7-C5)[13]
36	1297	1275		ν(N35-C33)[10] + ν(C24-C17)[12] +φ(H25-C24-C22)[11]
37	1286	1264	1267(m)	ν(N34-C1)[11] + ν(C18-C20)[12]
38	1267	1245	1238(wsh)	ν(C5-C15)[10]+ν(N8-C4)[10]+ φ(H16-C15-C13)[13]
39	1232	1211	1206(m)	R2-Breath[10]
40	1204	1183	1182(w)	φ(H23-C22-C24)[24] + φ(H21-C20-C22)[12]
41	1180	1160		φ(H10-C9-C13)[11] + φ(H12-C11-C9)[12]
42	1174	1154	1150(w)	R5-Boat[57]
43	1155	1135	1128(m)	φ(H14-C13-C15)[20] + φ(H16-C13-C15)[22]
44	1132	1113		φ(H40-C39-C41)[10]
45	1114	1095		τ(H-C-C-C)R1[15] +φ(C6-C3-N7][10]
46	1085	1066		τ(H30-C29-C28-N34][15]

47	1064	1046	1053(wsh)	τ(H31-C29-C28-N34)[28] +φ(H31-C29-H30][16]+τ(H30-C29-C28-N34)[23]
48	1042	1024		R4-Def[12]
49	1035	1017	*1017(s)*	R1- Breath[23]+ν(C9-C13)[34]+ν(C13-C15)[10]
50	1028	1011		R5- Breath[43]
51	1021	1004		R2- Breath[12]+ φ(C3-C2-C1)[14]
52	1008	991		τ(H21-C20-C22-C24)[34] +τ(H19-C18-C2-C17)[26]+τ(H23-C22-C24-C17)[20]
53	1002	985		τ(H14-C13-C15-C5)[47] +τ(H10-C9-C13-C15)[31]+τ(H12-C11-C9-C13)[22]
54	988	972		τ(H19-C18-C2-C17)[20] +τ(H23-C22-C24-C17)[20]
55	979	962	*952(m)*	τ(H-C-C-C)R3[83]
56	946	930		ω(H-C-C-C)R5[90]
57	928	913	910(m)	R5-Def[18] + φ(C39-C37-C33)[18]
58	901	886		τ(H-C-C-C)R1[68]
59	890	875		τ(H27-C26-C28-C29)[40]
60	861	846	*845(m)*	R5-Def[71]
61	840	826		τ(C6-N8-C4-C5)[26] +ω(N8-C5-C11-C4)[12]
62	822	808	813(wsh)	R1-R5-Breath[46]
63	784	771		ω(H-C-C-C)R1[66]
64	778	764		ω(H-C-C-C)R3[61]
65	761	748	*753(vs)*	τ(H19-C18-C2-C17)[10] + ω(C3-C24-C2-C17)[10]
66	754	741		ω(H-C-C-C)R5[61]
67	747	735		R1-R5-Breath[66]
68	727	715		ω(H-C-C-C)R1[10]+ω(C-N-C-C)R2R6[11]
69	716	704		τ(C36-C33-N35-C1)[10]
70	711	698		φ(C24-C22-C20][12]
71	670	658		φ(C28-N34-C36][13]
72	661	650	642(w)	φ(C20-C18-C2)[11]
73	634	623		R4-Rock[12]
74	618	608		φ(C4-C11-C9)[25] +φ(C11-C9-C13)[10]
75	601	591		φ(N7-C3-C17)[10]+R2-Rock[11]
76	593	583	586(m)	ω(H-C-C-C)R5[61]
77	571	561		ω(H-C-C-C)R3[20]+φ(C11-C9-C13)[20]+φ(N8-C4-C11)[11]
78	537	528		ω(H-C-C-C)R1[10]
79	531	522		τ(C24-C22-C20-C18)[10]
80	520	511		τ(C15-C13-C9-C11)[11]
81	498	490		ω(N8-C5-C11-C4)[17]+τ(C15-C13-C9-C11)[11]
82	489	481	*485(m)*	ω(N8-C5-C11-C4)[19]
83	451	443		τ(C22-C20-C18-C2)[10] + τ(C17-C24-C22-C20)[11]
84	440	432	428(m)	τ(C39-C37-C33-C36)[14] + τ(C41-C43-C36-C33)[20]
85	390	384		τ(C4-C11-C9-C13)[11] +ϕ(C15-C5-N7)[12]
86	356	350		ϕ(C29-C28-C26)[13]
87	326	320		τ(C11-C9-C13-C15)[10]
88	318	312		τ(C17-C24-C22-C20)[11]
89	283	278		τ(C11-C9-C13-C15)[11]
90	234	230		τ(C37-C33-C36-C43)[24]
91	130	128		ω(C28-C1-C36-N34)[13]
92	47	46		ω(C2-N34-N35-C1)[10]
93	28	28		ω(C17-N7-C6-C5)[11]

Table T2b : Frequency assignments for NEMKH at B3LYP/6-311G(d,p) level in cm^{-1}, with PED % in square brackets

S.No.	Calc Freq		Exp freq	Assignment Modes[PED]
	Unscaled	Scaled	FTIR	
1	3225	3089		ν(C18-H19)s[96]
2	3214	3079		ν(C24-H25)s[93]
3	3198	3063		ν(C-H)sR3[97]
4	3196	3061	3051(m)	ν(C-H)sR5[97]
5	3193	3059		ν(C-H)aR3[94]
6	3189	3055		ν(C-H)aR5[98]
7	3186	3053		ν(C-H)aR6[96]
8	3181	3048		ν(C-H)aR3[96]
9	3178	3045		ν(C-H)aR5[95]
10	3170	3037		ν(C-H)aR6[96]
11	3169	3036		ν(C-H)aR3[91]
12	3167	3034		ν(C-H)aR5[88]
13	3135	3003		ν(C28-H30)s[82]+ ν(C28-H29)ss[14]+ν(C28-H31)s[4]
14	3119	2988	2970(w)	ν(C44-H45)s[87]+ ν(C44-H46)s[11]+ν(C44-H47)s[2]
15	3074	2945		ν(C28-H30)s[79]+ ν(C28-H29)s[13]+ν(C28-H31)s[8]
16	3063	2935	2922(w)	ν(C44-H45)s[89]+ ν(C44-H46)s[10]+ν(C44-H47)s[1]
17	3018	2891		ν(C44-H45)s[86]+ ν(C36-H37)s[12]
18	3017	2891		ν(C28-H29,30,31)s[13]+ ν(C44-H45,46,47)s[85]
19	1691	1662	1663(m)	ν(C26=C27)s[65]
20	1651	1623		ν(C6=N8)s[29]+ν(C3=N7)s[49] *{char}*
21	1647	1619		ν(C1=N34)s[39] + R5-def[66]
22	1635	1607	1606(m)	R6-def[38]+φ(C20-C22-H23)[35]
23	1619	1591		R5-def[56]
24	1604	1577		R2-def[49]
25	1594	1567		R6-def[48]
26	1582	1555	1533(msh)	R3-def[24]+R2-def[26]
27	1514	1489		ν(C-C)R3[13]+φ(H-C-C)R3[59]
28	1511	1485		ν(C-C)R5[23]+φ(H-C-C)R5[59]
29	1507	1482		ν(C-C)R6[28]+φ(H-C-C)R6[41]
30	1495	1470		ν(C-C)R3[32]+φ(H-C-C)R3[40]
31	1490	1465		(C28H29H30H31)-boat[47]+φ(H45-C44-H46,47)[49]
32	1487	1462		ν(C-C)R3,R5,R6[53]+φ(H-C-C)R3,R5,R6[40]
33	1485	1460		(C28H29H30H31)-boat[10]+(C44H45H46H47)-boat[34]
34	1477	1452		(C44H45H46H47)-boat[73]
35	1475	1450	1445(vs)	(C28H29H30H31)-boat[32]+(C44H45H46H47)-boat[40]
36	1464	1439		ν(C-C)R5,R6[72]
37	1446	1422		ν(C-C)R5,R6[62]
38	1419	1394		(C28H29H30H31)-boat[15]+(C44H45H46H47)-boat[24]
39	1412	1388		ν(C-C)R2,R3[23]
40	1409	1385		ν(C4-C11)a[17]
41	1402	1378	1374(vs)	(C28H29H30H31)-boat[28]+(C44H45H46H47)-boat[35]
42	1379	1356		R3,R2-def[23]
43	1374	1351		R4,R5-def[17]
44	1345	1322		ν(C-C)R3[25]+ν(C-N)R2[19]
45	1337	1315		ν(C-N)R4[34]+ rock-R5[34]

46	1323	1300		ν(C-N)R2,R4[20] + ν(C-C)R3[17]
47	1314	1292		ν(C-N)R2,R4[24] + ν(C-C)R5[20]
48	1298	1276		ν(C-C)R6[19] + φ(H-C-C)R6[11]
49	1294	1272	1269(s)	ν(C-N)R4[24] + ν(C-C)R5[10] + ν(C-C)R1[100]
50	1278	1257		ν(C-N)R2[14] + ν(C-C)R3[10]
51	1261	1239		ν(C-N)R2[14] + ν(C-C)R3,R6[10]+ φ(C-C-C)R1[11]
52	1257	1236		ν(C-C)R1[10]+ φ(C-C-C)R1[11]+φ(C-C-N)R2[11]
53	1227	1206	1212(w)	R2,R3-breath[10]
54	1205	1185		φ(H-C-C)R6[11] + φ(H-C-C)R5[11]
55	1203	1183		φ(H-C-C)R5a[32] + φ(C-C-C)R5[28]
56	1173	1153		φ(H-C-C)R5a[21] + φ(C-C-N)R4[27]
57	1167	1147		φ(H-C-C)R3[35] + φ(C-C-H)R6[12] +τ(H-C-C-H)R3,R6[27]
58	1150	1130	1130(m)	φ(C-C-H)R3[13] +τ(H-C-C-H)R3,R6[26]
59	1143	1124		φ(C-C-C)R3[13] +τ(H-C-C-H)R6[11]
60	1134	1115		φ(C-C-C)R6[12] +τ(H-C-C-H)R5[10]
61	1122	1103		φ(C-C-C)R6[22] +R3-breath[10]
62	1111	1092		(C44-H45-H46-H47)-boat[10]+(C28-H29-H30-H31)-boat[10]
63	1084	1065	1077(s)	R1,R6-breath[54]
64	1074	1056		R6-def[47]
65	1065	1047		(C28-H29-H30-H31)-boat[64] + ω(C26-C44-H45-H46)[15]
66	1045	1027		ω(C26-C44-H45-H46)[11]+ω(C27-C28-H29-H31)[15]+ω(C27-C28-H29-H31)[11]
67	1033	1016		R3-breath[26]
68	1029	1012		ω(C27-C28-H29-H31)[15]+R6-breath[12]
69	1025	1008	1001(s)	R5-breath[42]
70	1011	994		τ(H-C-C-H)R6[10] + ω(H-C-C-H)R6[29]
71	1005	987		τ(H-C-C-H)R6[20] + ω(H-C-C-H)R6[10]
72	1002	985		τ(H-C-C-H)R3[11] + ω(H-C-C-H)R3[12]
73	990	973		τ(H-C-C-H)R6[13] + ω(H-C-C-H)R6[12]
74	980	963		τ(H-C-C-H)R5[10] + ω(H-C-C-H)R5[11]
75	979	962		τ(H-C-C-H)R3[10] + ω(H-C-C-H)R3[12]
76	946	930		τ(H-C-C-H)R5[15] + ω(H-C-C-H)R5[13]
77	944	928		ω(C26-C44-H45-H46)[32]+ω(C27-C28-H29-H31)[28]
78	928	912	916(m)	R4,R5-def[83]
79	905	889		τ(H-C-C-H)R6[10] + ω(H-C-C-H)R6[50]
80	898	883		φ(C-C-C)R3[12] + φ(C-C-N)R2[22]
81	888	872		τ(H-C-C-H)R3[-] + ω(H-C-C-H)R6[-]
82	860	845	846(m)	τ(H-C-C-H)R5[-] + ω(H-C-C-H)R5[-]
83	856	841		Mol-breath[-]
84	839	825		τ(C-C-N-C)R2[22] +τ(N-C-C-N)R3[20]
85	812	798		Mol-breath[10]
86	785	772		τ(H-C-C-H)R6[-] + ω(H-C-C-H)R6[-]
87	779	766	769(vs)	τ(H-C-C-H)R3[11] + ω(H-C-C-H)R6[33]
88	777	764		τ(H-C-C-H)R3,R5[-] + ω(H-C-C-H)R3,R5[-]
89	774	761		τ(H-C-C-H)R3[-] + ω(H-C-C-H)R3[-]
90	755	742	747(vs)	τ(H-C-C-H)R5,R6[10] + ω(H-C-C-H)R5,R6[5]
91	753	740		τ(C27=C26-C44-H)[-] + τ(C26=C27-C20-H)[-]
92	749	736		τ(H-C-C-H)R5,R6[-] + ω(H-C-C-H)R5,R6[-]
93	720	708		τ(H-C-C-H)R6[20] + ω(H-C-C-H)R6[25]
94	718	706		τ(H-C-C-H)R3,R5,R6[36] + ω(H-C-C-H)R3,R5,R6[30]
95	681	670		φ(C5-N7-C3)[18] + φ(C=N34-C32)[23]

96	668	657		R1-breath[45]
97	659	648		R2-rock[12] + R6-breath[11] + φ(N8=C6-C26)[14]
98	625	614		R4-rock[10] + R6-breath[4] + R1-breath[6]
99	621	610	606(m)	φ(C-C-C)R3[10] + φ(C-C-N)R2[12]
100	610	600		φ(C-C-C)R5,R6[23] + R2-rock[20]
101	593	583		τ(H-C-C-H)R3,R5[-] + ω(H-C-C-C)R3,R5[-]
102	588	578	580(m)	τ(H-C-C-H)R3,R5[10] + ω(H-C-C-C)R3,R5[5]
103	577	568		τ(H-C-C-H)R5[-] + φ(C-C-C)R3[-]
104	569	559		τ(H-C-C-H)R3,R6[-] + ω(H-C-C-C)R3,R6[-]
105	556	547		τ(H-C-C-H)R5,R6[-] + ω(H-C-C-C)R5,R6[-]
106	542	533		τ(H-C-C-H)R3,R6[-] + ω(H-C-C-C)R3,R6[-]
107	528	519		τ(H-C-C-H)R6[27] + ω(H-C-C-C)R3[20] +φ(C-C-C)R5[20]
108	512	503		R1-breath[27]
109	497	488	492(m)	τ(H-C-C-H)R3[22] + ω(H-C-C-C)R3[11]
110	445	438	448(wsh)	τ(C-N-C-C)R2[8] + τ(N-C-C-N)R2[5]
111	440	433		τ(H-C-C-H)R4[10] + ω(H-C-C-C)R4[5]
112	420	413		τ(N33-C27-C28-H)[-] + φ(C-C-C)R3[-]
113	416	409		τ(C6-C26=C27-C28)[-] + τ(C6-C26=C27-N33)[-]
114	401	394		τ(H-C-C-H)R3[20] + φ(C-C-C)R6[15]
115	363	357		τ(C-C-C-C)R3,R5[8] + τ(C-N-C-C)R2,R4[3]
116	336	330		τ(C-C-C-C)R3,R5[51] + τ(C-N-C-C)R2,R4[40]
117	320	315		τ(C-C-C-C)R5,R6[32] + τ(H-C-C-H)R5,R6[25]
118	287	282		τ(C-C-C-C)R3,R5[28] + τ(C-N-C-C)R2,R4[14]
119	272	268		Mol-breath[20]
120	260	255		Mol-breath[14]
121	255	251		Mol-breath[18]
122	213	209		φ(C26-C44-H45,46,47)[47]
123	199	196		φ(C27-C28-H29,30,31)[10] + τ(C-C-C-C)R3[18]
124	193	189		φ(C26-C44-H45,46,47)[26] + φ(C27-C28-H29,30,31)[10]
125	190	186		φ(C26-C44-H45,46,47)[-] + φ(C27-C28-H29,30,31)[-]
126	179	176		φ(C44-H46-H45,46,47)[-]
127	165	162		φ(H29-C28-H29,30,31)[42]
128	148	145		φ(H29-C28-H29,30,31)[23]
129	122	120		R4,R5-rock[52]
130	97	95		R2,R3,R4,R5,R6-rock[48]
131	83	82		CH3-rock[-]
132	74	72		CH3-rock[-]
133	57	56		CH3-rock[41]
134	52	51		τ(H-C-C-H)R1,R2,R3,R4,R5,R6[-]
135	29	29		τ(H-C-C-H)R1,R2,R3,R4,R5,R6[-]

Abbreviations:- *R-> Ring, rock->rocking, boat-> boating, breath-> Ring breathing, def-> Ring doformation, Mol-> Molecule, ν->stretchin mode, φ-> in-plane bending mode, τ-> torsional mode, ω-> out of plane wagging, s->symmetric stretch, a->asymmetric stretch, char->characteristic mode*

Table T3(a) -Condensed Fukui Functions, dual descriptors and Local softness of NAOP-12

Atom	Mulliken Atomic Charges			Fukui function			dual descriptor	Local softness		
	q(N)	q(N+1)	q(N-1)	f_k^+	f_k^-	f_k^0	Δf_k	Sf_k^+	Sf_k^-	Sf_k^0
1 C	-0.52753	0.049714	-0.000061	0.577246	-0.52747	0.02483	1.104717	0.151104	-0.138074	0.0064987
2 C	0.53084	0.205191	0.176911	-0.325649	0.353929	0.19105	-0.679578	-0.085244	0.0926467	0.0500107
3 C	-0.29082	-0.055355	-0.056207	0.235466	-0.23461	-0.0558	0.47008	0.061637	-0.061414	-0.014602
4 C	-0.05727	0.036609	0.032902	0.09388	-0.09017	0.03476	0.184053	0.024575	-0.023604	0.0090978
5 C	-0.02424	0.035794	0.035105	0.060035	-0.05935	0.03545	0.119381	0.015715	-0.015535	0.0092795
6 C	-0.33578	0.020291	0.03105	0.356067	-0.36683	0.02567	0.722893	0.093206	-0.096023	0.0067197
7 N	0.263642	0.003234	-0.137524	-0.260408	0.401166	-0.0671	-0.661574	-0.068166	0.1050118	-0.017576
8 N	0.156233	0.018041	-0.136063	-0.138192	0.292296	-0.059	-0.430488	-0.036174	0.0765133	-0.015447
9 C	-0.20018	-0.188075	-0.240734	0.012102	0.040557	-0.2144	-0.028455	0.003168	0.0106165	-0.056124
10 H	0.175651	0.250982	0.186656	0.075331	-0.01101	0.21882	0.086336	0.019719	-0.002881	0.0572795
11 C	-0.1532	-0.308104	-0.383842	-0.154908	0.230646	-0.346	-0.385554	-0.04055	0.0603754	-0.090564
12 H	0.188636	0.271213	0.219723	0.082577	-0.03109	0.24547	0.113664	0.021616	-0.008138	0.0642553
13 C	-0.27702	-0.190934	-0.242746	0.086081	-0.03427	-0.2168	0.12035	0.022533	-0.00897	-0.056761
14 H	0.174185	0.251081	0.187209	0.076896	-0.01302	0.21915	0.08992	0.020129	-0.003409	0.0573648
15 C	-0.06648	-0.310832	-0.387919	-0.244352	0.321439	-0.3494	-0.565791	-0.063963	0.0841419	-0.091455
16 H	0.186507	0.271716	0.223923	0.085209	-0.03742	0.24782	0.122625	0.022305	-0.009794	0.0648708
17 C	0.641361	0.301026	0.266931	-0.340335	0.37443	0.28398	-0.714765	-0.089088	0.0980132	0.074336
18 C	-0.28652	-0.322643	-0.392757	-0.036126	0.10624	-0.3577	-0.142366	-0.009457	0.0278101	-0.093634
19 H	0.215469	0.281771	0.240393	0.066302	-0.02492	0.26108	0.091226	0.017356	-0.006524	0.0683425
20 C	-0.5374	-0.217909	-0.255597	0.31949	-0.2818	-0.2368	0.601292	0.083632	-0.073766	-0.061974
21 H	0.173648	0.26111	0.201916	0.087462	-0.02827	0.23151	0.11573	0.022895	-0.0074	0.0606023
22 C	-0.45416	-0.19023	-0.243971	0.263932	-0.21019	-0.2171	0.474123	0.069089	-0.055021	-0.05683
23 H	0.171887	0.258001	0.200817	0.086114	-0.02893	0.22941	0.115044	0.022542	-0.007573	0.0600516
24 C	-0.43142	-0.337691	-0.378164	0.093725	-0.05325	-0.3579	0.146977	0.024534	-0.01394	-0.093693
25 H	0.197438	0.270982	0.25846	0.073544	-0.06102	0.26472	0.134566	0.019251	-0.015974	0.0692951
26 C	0.290684	-0.393288	-0.415501	-0.683972	0.706185	-0.4044	-1.390157	-0.179041	0.1848555	-0.105857
27 H	0.223635	0.264937	0.211123	0.041302	0.012512	0.23803	0.02879	0.010811	0.0032752	0.0623083
28 C	-0.61535	0.239603	0.398072	0.854952	-1.01342	0.31884	1.868373	0.223798	-0.26528	0.0834609
29 C	-0.41269	-0.731089	-0.781787	-0.318399	0.369097	-0.7564	-0.687496	-0.083346	0.0966172	-0.19801
30 H	0.169682	0.247784	0.213943	0.078102	-0.04426	0.23086	0.122363	0.020444	-0.011586	0.0604323
31 H	0.159291	0.23685	0.217848	0.077559	-0.05856	0.22735	0.136116	0.020302	-0.015328	0.0595123
32 H	0.215147	0.238195	0.214303	0.023048	0.000844	0.22625	0.022204	0.006033	0.0002209	0.0592244
33 C	0.235523	0.005542	0.004183	-0.229981	0.23134	0.00486	-0.461321	-0.060201	0.060557	0.0012728
34 N	0.37445	-0.332083	-0.314614	-0.706533	0.689064	-0.3233	-1.395597	-0.184947	0.1803738	-0.084642
35 N	0.098517	-0.025842	-0.088325	-0.124359	0.186842	-0.0571	-0.311201	-0.032553	0.048909	-0.014943
36 C	0.302284	0.298189	0.237123	-0.004095	0.065161	0.26766	-0.069256	-0.001072	0.017057	0.0700633
37 C	-0.39875	-0.267288	-0.348861	0.131459	-0.04989	-0.3081	0.181345	0.034412	-0.013058	-0.080644
38 H	0.175372	0.282744	0.229657	0.107372	-0.05429	0.2562	0.161657	0.028106	-0.01421	0.0670647
39 C	-0.24251	-0.193327	-0.227821	0.04918	-0.01469	-0.2106	0.063866	0.012874	-0.003844	-0.055121
40 H	0.16094	0.264418	0.200582	0.103478	-0.03964	0.2325	0.14312	0.027087	-0.010377	0.0608607
41 C	-0.20467	-0.160555	-0.231645	0.044114	0.026976	-0.1961	0.017138	0.011548	0.0070614	-0.051332
42 H	0.172106	0.258595	0.201424	0.086489	-0.02932	0.23001	0.115807	0.02264	-0.007674	0.0602088
43 C	-0.28442	-0.336855	-0.361861	-0.052439	0.077445	-0.3494	-0.129884	-0.013727	0.0202725	-0.09145
44 H	0.147254	0.278484	0.235746	0.13123	-0.08849	0.25712	0.219722	0.034352	-0.023164	0.0673041

Table-3(b) Condensed Fukui Functions, dual descriptors and Local softness of NEMKH-12

Atom	Mulliken Atomic Charges			Fukui function			dual descriptor	Local softness		
	q(N)	q(N+1)	q(N-1)	f_k^+	f_k^-	f_k^0	Δf_k	Sf_k^+	Sf_k^-	Sf_k^0
1 C	0.2736	0.0628	0.0069	-0.2108	0.2666	0.0279	-0.4774	-0.0571	0.0723	0.0076
2 C	0.3172	0.1841	0.0873	-0.133	0.2299	0.0484	-0.3629	-0.0361	0.0623	0.0131
3 C	0.3468	0.0243	0.1043	-0.3225	0.2425	-0.04	-0.565	-0.0874	0.0657	-0.0108
4 C	0.155	0.0594	0.0287	-0.0956	0.1263	0.0153	-0.2219	-0.0259	0.0342	0.0042
5 C	0.2481	0.0227	-0.071	-0.2253	0.319	0.0469	-0.5443	-0.0611	0.0865	0.0127
6 C	0.1546	-0.1084	-0.0556	-0.263	0.2103	-0.0264	-0.4733	-0.0713	0.057	-0.0071
7 N	-0.2873	-0.0461	0.2928	0.2413	-0.5801	-0.1694	0.8214	0.0654	-0.1572	-0.0459
8 N	-0.3105	0.0782	0.1747	0.3887	-0.4851	-0.0482	0.8738	0.1053	-0.1315	-0.0131
9 C	0.0255	-0.189	0.1011	-0.2145	-0.0756	-0.145	-0.1389	-0.0581	-0.0205	-0.0393
10 H	0.1163	0.2509	-0.0073	0.1346	0.1236	0.1291	0.011	0.0365	0.0335	0.035
11 C	-0.3149	-0.3168	0.0357	-0.0019	-0.3506	-0.1763	0.3487	-0.0005	-0.095	-0.0478
12 H	0.1164	0.2727	-0.003	0.1562	0.1194	0.1378	0.0368	0.0423	0.0324	0.0374
13 C	0.0126	-0.1925	-0.0301	-0.2051	0.0427	-0.0812	-0.2478	-0.0556	0.0116	-0.022
14 H	0.1162	0.2504	0.0009	0.1341	0.1154	0.1247	0.0187	0.0364	0.0313	0.0338
15 C	-0.2842	-0.3094	0.1426	-0.0252	-0.4268	-0.226	0.4016	-0.0068	-0.1157	-0.0612
16 H	0.117	0.2684	-0.0092	0.1514	0.1262	0.1388	0.0252	0.041	0.0342	0.0376
17 C	0.3944	0.2464	0.0391	-0.148	0.3553	0.1036	-0.5033	-0.0401	0.0963	0.0281
18 C	-0.2972	-0.291	-0.0394	0.0062	-0.2578	-0.1258	0.264	0.0017	-0.0699	-0.0341
19 H	0.1365	0.3162	0.0017	0.1796	0.1348	0.1572	0.0448	0.0487	0.0365	0.0426
20 C	-0.296	-0.2399	0.076	0.0562	-0.3721	-0.158	0.4283	0.0152	-0.1008	-0.0428
21 H	0.1128	0.2623	-0.0052	0.1495	0.1181	0.1338	0.0314	0.0405	0.032	0.0363
22 C	-0.3874	-0.2113	-0.0029	0.1761	-0.3845	-0.1042	0.5606	0.0477	-0.1042	-0.0282
23 H	0.1132	0.2607	-0.0002	0.1476	0.1134	0.1305	0.0342	0.04	0.0307	0.0354
24 C	-0.1822	-0.3033	0.0322	-0.1211	-0.2144	-0.1677	0.0933	-0.0328	-0.0581	-0.0455
25 H	0.1288	0.2949	-0.0035	0.1661	0.1323	0.1492	0.0338	0.045	0.0359	0.0404
26 C	0.3185	0.1601	0.0359	-0.1585	0.2827	0.0621	-0.4412	-0.043	0.0766	0.0168
27 C	-0.3788	0.1163	-0.0151	0.4951	-0.3637	0.0657	0.8588	0.1342	-0.0986	0.0178
28 C	-0.6716	-0.7113	0.0017	-0.0397	-0.6733	-0.3565	0.6336	-0.0108	-0.1825	-0.0966
29 H	0.1676	0.2566	-0.0003	0.089	0.1679	0.1285	-0.0789	0.0241	0.0455	0.0348
30 H	0.1703	0.2351	0.0008	0.0648	0.1696	0.1172	-0.1048	0.0176	0.046	0.0318
31 H	0.1737	0.2371	-0.0008	0.0634	0.1745	0.119	-0.1111	0.0172	0.0473	0.0322
32 C	0.1972	-0.0137	-0.0138	-0.2108	0.211	0	-0.4218	-0.0571	0.0572	0
33 N	0.0464	-0.2673	0.0102	-0.3138	0.0362	-0.1388	-0.35	-0.085	0.0098	-0.0376
34 N	-0.4557	-0.0583	0.0408	0.3974	-0.4965	-0.0495	0.8939	0.1077	-0.1346	-0.0134
35 C	0.6877	0.2932	0.0054	-0.3945	0.6823	0.1439	-1.0768	-0.1069	0.1849	0.039
36 C	-0.267	-0.2755	0.0286	-0.0085	-0.2956	-0.152	0.2871	-0.0023	-0.0801	-0.0412
37 H	0.1104	0.2793	-0.0019	0.1689	0.1123	0.1406	0.0566	0.0458	0.0304	0.0381
38 C	-0.14	-0.1924	-0.0106	-0.0524	-0.1294	-0.0909	0.077	-0.0142	-0.0351	-0.0246
39 H	0.1061	0.263	0.0005	0.1569	0.1056	0.1312	0.0513	0.0425	0.0286	0.0356
40 C	-0.1356	-0.1538	0.0219	-0.0182	-0.1575	-0.0878	0.1393	-0.0049	-0.0427	-0.0238
41 H	0.1071	0.2582	-0.0015	0.1511	0.1086	0.1299	0.0425	0.041	0.0294	0.0352
42 C	-0.4738	-0.3386	0.0022	0.1352	-0.476	-0.1704	0.6112	0.0366	-0.129	-0.0462
43 H	0.1271	0.2757	-0.0003	0.1486	0.1274	0.138	0.0212	0.0403	0.0345	0.0374
44 C	-0.6998	-0.7276	-0.0024	-0.0278	-0.6973	-0.3626	0.6695	-0.0075	-0.189	-0.0983
45 H	0.1656	0.2602	0.0006	0.0946	0.165	0.1298	-0.0704	0.0256	0.0447	0.0352
46 H	0.1682	0.2342	0.0012	0.066	0.1669	0.1165	-0.1009	0.0179	0.0452	0.0316
47 H	0.1509	0.2226	0.0004	0.0717	0.1505	0.1111	-0.0788	0.0194	0.0408	0.0301