

	[NH3+] CC (I) I	NCC (I) I	CCC (I) I	CC1CC (I) I
<i>nbd</i>	SCORE = 0.979 N1 H2 H3 H4 C5 C6 I7 I8 H9 H10 H11	SCORE = 0.980 N1 H2 H3 C4 C5 I6 I7 H8 H9 H10	SCORE = 0.995 C1 H2 H3 H4 C5 C6 I7 I8 H9 H10 H11	SCORE = 0.748 C1 C12 H3 H4 C5 C6 I7 I8 H9 H10 H11
<i>ele</i>	SCORE = 0.980 N1 H2 H3 H4 C5 C6 I7 I8 H9 H10 H11	SCORE = 0.981 N1 H2 H3 C4 C5 I6 I7 H8 H9 H10	SCORE = 0.979 C1 H2 H3 H4 C5 C6 I7 I8 H9 H10 H11	SCORE = 0.381 C1 C12 H3 H4 C5 C6 I7 I8 H9 H10 H11
<i>vdw</i>	SCORE = 0.849 N1 H2 H3 H4 C5 C6 I7 I8 H9 H10 H11	SCORE = 0.493 N1 H2 H3 C4 C5 I6 I7 H8 H9 H10	SCORE = 0.989 C1 H2 H3 H4 C5 C6 I7 I8 H9 H10 H11	SCORE = 0.968 C1 C12 H3 H4 C5 C6 I7 I8 H9 H10 H11