SUPPRTING INFORMATION

Vibrational spectra of solid *cis*- and *trans*-2-thioxohexahydroquinazolin-4(1*H*)-one and theoretical calculations towards the interpretation of its thermal reactivity.

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Abstract

FT-Raman and FT-IR spectra of *cis* and *trans* 2-thioxohexahydroquinazolin-4(1*H*)-one are reported from 4000 to 200 cm^{-1}. The molecular geometry, Wiberg Index, NBO analysis and vibrational wavenumbers in the ground state have been calculated using a density functional method (B3LYP) with 6-31+G** and 6-311+G** basis set. Both compounds are stable as dimers in the solid phase, possessing C_2 symmetry. The scaled theoretical wavenumbers showed very good agreement with the experimental values. This work contributes to the knowledge of important data which are rather scarce for quinazolinones.

Computational data

z-matrix in Cartesian coordinates.

***cis* NH**			
atom	**x**	**y**	**z**
C	-2.68401	0.56738	1.28581
C	-2.36159	0.93217	-0.17815
C	-1.99664	-0.29742	-1.01736
C	-3.0793	-1.38822	-0.97029
C	-3.76535	-1.49625	0.36721
C	-3.59432	-0.63211	1.3742
H	-1.74963	0.37413	1.83203
H	-2.61982	-2.34788	-1.22989
H	-4.43832	-2.34146	0.49719
H	-4.11733	-0.78926	2.31508
C	0.05367	1.55225	-0.22061
H	-3.82987	-1.18581	-1.74709
H	-3.14226	1.43372	1.77893
N	-1.25998	1.8835	-0.29105
H	-1.43867	2.87419	-0.19991
C	-0.61938	-0.81578	-0.60575
O	-0.31618	-1.99399	-0.61985
S	1.24262	2.71955	-0.09574
C	1.68415	-0.2871	-0.0158
C	2.09005	-0.54066	1.29295
C	2.54686	-0.50885	-1.08785
C	3.38282	-1.00946	1.53304
H	1.40218	-0.36506	2.11381

C	3.83736	-0.9802	-0.84392
H	2.2114	-0.30694	-2.09986
C	4.25758	-1.22907	0.46578
H	3.70432	-1.20344	2.55189
H	4.51399	-1.15024	-1.67595
H	5.26296	-1.59429	0.65363
H	-1.87074	0.03896	-2.05667
H	-3.24258	1.40574	-0.62406
N	0.33006	0.17318	-0.26524

***trans* NH**			
atom	**x**	**y**	**z**
C	3.66396	1.04252	0.05302
C	2.23745	0.59049	0.38194
C	1.87678	-0.681	-0.38485
C	2.79734	-1.84457	0.01062
C	4.23648	-1.40103	0.0976
C	4.62655	-0.11991	0.10718
H	3.97888	1.82407	0.75734
H	2.47299	-2.27055	0.97006
H	4.98725	-2.1865	0.15651
H	5.686	0.12118	0.15648
H	3.67882	1.50313	-0.94607
H	2.69103	-2.65857	-0.71359
C	0.40629	-1.02266	-0.20508
O	-0.00872	-2.16726	-0.21047
N	1.26727	1.62075	0.03156
H	1.52698	2.59538	0.10986
C	-0.07193	1.41742	-0.05489
S	-1.14313	2.69505	-0.15397
N	-0.47656	0.07073	-0.06341
H	2.17915	0.37636	1.46249
H	2.01206	-0.4652	-1.45647
C	-1.89152	-0.24553	0.01173
C	-2.61773	-0.4527	-1.15981
C	-2.49561	-0.3763	1.2607
C	-3.97041	-0.78552	-1.07813
H	-2.12893	-0.34663	-2.12277
C	-3.84956	-0.70723	1.33791
H	-1.91151	-0.21312	2.16079
C	-4.58815	-0.91136	0.16943
H	-4.54109	-0.94361	-1.98826
H	-4.325	-0.80559	2.30917
H	-5.64137	-1.16917	0.23041

***cis* SH**			
atom	**x**	**y**	**z**
C	-3.7034	0.52488	-1.03509
C	-2.19167	0.25849	-1.03027
C	-1.85297	-1.09559	-0.38565
C	-2.40541	-1.20018	1.0584
C	-3.82484	-0.70292	1.15209

C	-4.39884	0.06819	0.22163
C	-0.26775	1.11003	-0.02145
N	-1.47558	1.34485	-0.3485
C	-0.3506	-1.30398	-0.39268
O	0.18815	-2.38896	-0.52239
S	0.72998	2.38373	0.75181
N	0.40066	-0.12763	-0.19638
H	-2.27992	-1.90784	-0.98195
H	-1.84295	0.24709	-2.07557
H	-2.34166	-2.24457	1.38505
H	-4.38715	-0.98758	2.03944
H	-1.77512	-0.62643	1.75319
H	-5.43102	0.38723	0.35453
H	-3.85791	1.60028	-1.1841
H	-4.15913	0.02674	-1.9036
C	1.83889	-0.22491	-0.11243
C	2.43789	-0.76406	1.02863
C	2.6197	0.21353	-1.18467
C	3.82861	-0.85564	1.09834
H	1.81683	-1.11044	1.84803
C	4.01081	0.12584	-1.10729
H	2.13678	0.62137	-2.06714
C	4.61608	-0.40895	0.03309
H	4.29594	-1.27563	1.98382
H	4.6189	0.47077	-1.93806
H	5.6982	-0.4798	0.09089
H	-0.29125	3.26204	0.72384

***trans* SH**			
atom	**x**	**y**	**z**
C	3.63247	1.11327	0.10574
C	2.21463	0.61854	0.41564
C	1.90721	-0.66394	-0.37184
C	2.8758	-1.80001	-0.00838
C	4.29875	-1.30652	0.07671
C	4.63773	-0.01127	0.11688
H	3.91093	1.88669	0.83207
H	2.57393	-2.25433	0.94586
H	5.07811	-2.06583	0.10629
H	5.68951	0.26558	0.15995
H	3.62716	1.61422	-0.87331
H	2.79412	-2.60543	-0.74628
C	0.4556	-1.07418	-0.19147
O	0.06651	-2.22869	-0.19737
N	1.24354	1.67826	0.14597
C	0.03309	1.3298	-0.03631
S	-1.23339	2.56687	-0.32385
N	-0.44573	-0.00266	-0.04687
H	2.16272	0.38082	1.49215
H	2.02416	-0.42556	-1.44213
C	-1.85794	-0.2972	0.03675
C	-2.57252	-0.61448	-1.12081
C	-2.49309	-0.27492	1.28059
C	-3.93535	-0.90184	-1.0318
H	-2.06085	-0.63811	-2.07747

C	-3.85741	-0.55849	1.36372
H	-1.91987	-0.03545	2.1707
C	-4.57903	-0.87182	0.20866
H	-4.49273	-1.14919	-1.93015
H	-4.35364	-0.53808	2.32925
H	-5.63978	-1.0949	0.27519
H	-0.33589	3.5682	-0.23975

Figures

Figure S1.

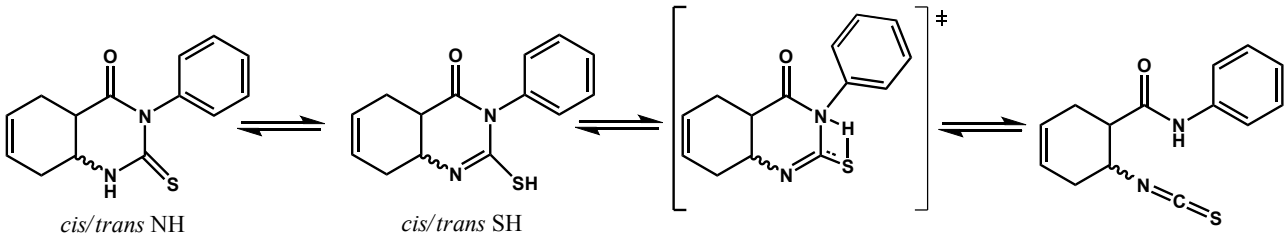
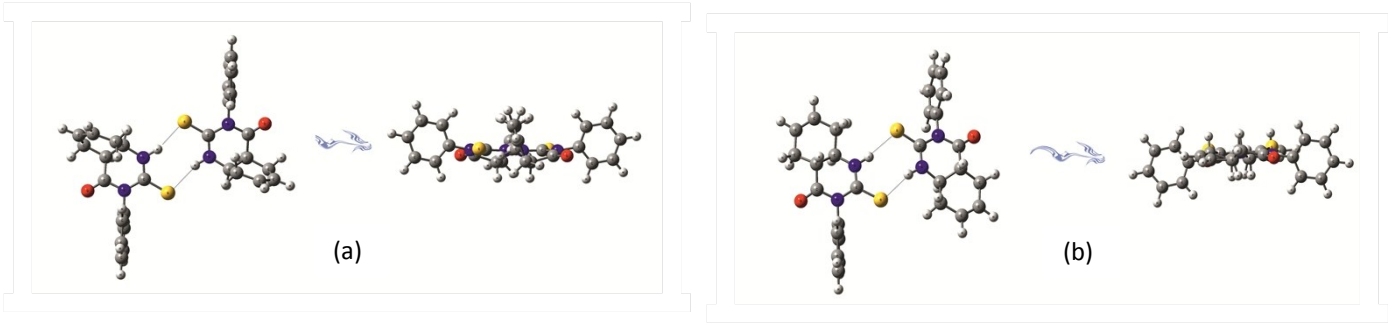


Figure S2. Molecular modeling of the conformers *cis* (a) and *trans* (b) NH viewed from two different perspectives.



Tables

Table S1. Calculated and experimental wavenumbers (cm^{-1}), relative intensities and tentative assignments of *cis* and *trans* NH. [a] vs, very strong; s, strong; m, medium; w, weak; vw, very weak. [b] Raman intensities taken directly from the calculation. [c] Potential energy distribution (PED). ν, stretching; δ, in plane deformation; ρ, out of plane deformation; ω, wagging; γ, twisting; τ, torsion; i.ph., in phase; o.o.ph., out of phase. [d] I and II, monomers (See Figure 3). In brackets are defined the modes belonging to each monomer. [e] The pattern of the mode corresponding to the numbers in bold are illustrated in Fig. S3.

cis NH								Vibrational Assignment[c,d,e] PED %
	Calculated wavenumbers (cm^{-1}) B3LYP/6-311+G**			Observed Wavenumbers (cm^{-1})				
Block	Freq.	IR Int.	Raman Int.	FT-IR	(int) [a]	Raman	(int)[b]	
B	3245	2779	0.4	3165	m	3165	15	S1(99)=νNH (I,II)
A	3220	<1	2449					S2(97)=νNH (I,II)
A	3111	1	510					S3(94)=ph-**1** (I,II)
B	3111	6	111					S4(89)=ph-**1** (I,II)
A	3107	26	28					S5(91)=ph-**2** (I,II)
B	3107	2	6					S6(88)=ph-**2** (I,II)
A	3099	1	165	3067	w	3067	100	S7(93)=ph-**3** (I,II)
B	3099	58	8					S8(91)=ph-**3** (I,II)
B	3091	7	111					S9(97)=ph-**4** (I,II)
B	3091	5	158					S10(97)=ph-**4** (I,II)
A	3081	<1	82	3050	w	3050	74	S11(92)=ph-**5** (I,II)
B	3081	<1	9					S12(95)=ph-**5** (I,II)
A	3078	16	540	3025	w	3030	86	S13(99)=ν=C-$H_{i.ph.}$ (I,II)
B	3078	66	87					S14(99)=ν=C-$H_{i.ph.}$ (I,II)
A	3057	6	121					S15(99)=ν=C-$H_{o.o.ph.}$ (I,II)
B	3057	4	62					S16(99)=ν=C-$H_{o.o.ph.}$ (I,II)
A	2988	2	79	2979	w	2972	31	S17(92)=ν_aC-H (I,II)
B	2988	5	62					S18(92)=ν_aC-H (I,II)
B	2984	37	4	2954	w	2955	57	S19(93)=νC-H (I,II) + ν_aC9H_2+ ν_aC23H_2
A	2984	2	245					S20(93)=νC-H (I,II) + ν_aC9H_2+ ν_aC23H_2
B	3968	7	43			2945	51	S21(85)=ν_aC9H_2 + νC10H + ν_aC23H_2 + νC24H + ν_aC20H_2
B	2968	10	79					S22(91)= ν_aC9H_2 + νC-H + ν_aC23H_2 + νC24H
A	2934	40	364	2928	w	2917	53	S23(93)=[ν_aC-H_2 + νC-H] (I,II)
B	2934	3	56					S24(93)=[ν_aC-H_2 + νC-H] (I,II)
A	2925	18	101	2912	w	2907	87	S25(93)=[ν_sC-H_2 + νC-H] (I,II)
B	2925	33	5					S26(82)=[ν_sC-H_2 + νC-H] (I,II)
A	2921	<1	51					S27(81)=ν_sC-H_2 (I,II)+ νC5H + νC19H
A	2921	19	59					S28(81)=ν_sC-H_2 (I,II)+ νC5H + νC19H
A	1723	2	93	1742	vs	1732	57	S29(87)=[νC=O + ν_sNCN + νC=C] (I,II)
B	1722	601	2					S30(87)=[νC=O + ν_sNCN + νC=C] (I,II)
A	1668	2	51	1654	w	1653	23	S31(81)=νC=C (I,II) + νC6C7 + νC8C9 + + νC20C21 + νC22C23
B	1668	10	2					S32(81)=[νC=C + ν=CH] (I,II) + νC6C7 + νC8C9 + νC20C21 + νC22C23
A	1596	<1	75	1596	w	1596	11	S33(81)+ S77(20)=ρC9H_2 + ρC20H_2 + ν_sC4N3C14 + ν_sC18N17C28 + [ph-**17** + ph-**30** + δ=C-H + aryl**1**](I,II)
B	1596	14	7					S34(62)+ S78(16)=ρC9H_2 + ρC20H_2 + ν_sC4N3C14 + ν_sC18N17C28 + [ph-**17** + ph-**30** + δ=C-H + aryl**1**](I,II)
B	1589	1	15					S35(68)+ S80(10)=[ph-**18** + ph-**31**](I,II)
B	1589	3	5					S36(73)= ph-**6** (I,II)+ νN3H14+ νN17H28
B	1548	573	<1	1541	vs	-		S37(42)=τC10N1H11S26 + τC24N15H25S12
A	1523	<1	21			1520	7	S38(54)=τC10N1H11S26 + τC24N15H25S12
A	1483	2	1	1496	w	1497	3	S39(54)+S91(27)=δC2N3C4 + δC16N17C18 ν_aC10C9C8 + ν_aC10C5C6 + νC4C5 + νC6C7+

								ν_aC24C23C22 + νC20C21+ ν_aC24C19C20 + νC18C19 + ν_sN1C2N3 + ν_sN15C16N17 + ν_sC4N3C14 + ν_sC18N17C28 + νC18C19 + νC20C22 + [δNH + ph-**19** + ph-**32** + νC=S + νC=O + ph-**25**](I,II)
B	1483	45	<1					S40(60)+S92(29)=[δNH + ph-**19** + ph-**32**] (I,II) + δC2N3C4 + δC16N17C18 + ν_aC10C9C8 + ν_aC10C5C6 + νC4C5 + νC6C7+ ν_aC24C23C22 + νC20C21+ ν_aC24C19C20 + νC18C19 + ν_sN1C2N3 + ν_sN15C16N17 + ν_sC4N3C14 + ν_sC18N17C28 + νC18C19 + νC20C22 + [νC=S + νC=O + ph-**25**](I,II)
A	1441	8	4	1433	w	1446	12	S41(87)=[δNH + ph-**20**+ ph-**33**](I,II) + ρC9H_2 + δC8C9C10 + ρC23H_2 + δC22C23C24
B	1441	5	13					S42(86)=[δNH + ph-**20**+ ph-**33**](I,II) + ρC9H_2 + δC8C9C10 + ρC23H_2 + δC22C23C24
A	1440	4	<1					S43(33)+S85(34)+S62(14)=ρC9H_2 + ph-**32** + ρC23H_2+[ph-**33** + ρC-H + ph-**36**](I,II)
B	1440	<1	5					S44(56)+S86(23)=[ph-**10**](I,II) + ρC9H_2 + ρC23H_2 + ph-**32**
A	1428	12	12			1425	28	S45(94)=[δCH_2 + δNH] (I,II) + δC5C6C7 + δC19C20C21
B	1428	27	15					S46(92)=[δCH_2 + δNH] (I,II) + δC5C6C7 + δC19C20C21
A	1415	<1	27	1392	vw	1392	13	S38(27)+S47(39)= [δCH_2 + δ=C-H + δNHS + δNH + δNC(O)N + δNC(O) + ph-**34**] (I,II) + ρC10H + ν_aC14N3C4 + ν_aN1C2N3 + ρC24H + ν_aC28N17C18 + ν_aN15C16N17
B	1398	201	<1					S37(30)+S48(43)= [δCH_2 + δ=C-H + δNHS + δNH + δNC(O)N + δNC(O) + ph-**34**] (I,II) + ρC10H + ν_aC14N3C4 + ν_aN1C2N3 + ρC24H + ν_aC28N17C18 + ν_aN15C16N17
A	1372	<1	5	1371	vw	1369	12	S49(75)=[ρ=C-H + aryl**1**](I,II)
B	1372	2	2					S50(75)+ S108(11)=ν_sC8N9C10 + ν_sC22C23C24 + ν_sC10C5C6 + ν_sC24C19C20 + νC4C5 + νC18C19 + ν_aC6C7C8 + ν_aC20C21C22 + ν_sC10N1C2 + ν_sC24N15C16 + ν_sC2N3C4 + ν_sC16N17C18 [ρ=C-H + aryl**1**](I,II)
A	1359	283	2	1343	w	1343	14	S51(51)= γC9H_2 + δC6H_2 + γC23H_2 + δC20H_2 + [δ=C-H + ρC-H + aryl**2**](I,II)
B	1354	1	17					S52(53)=γC9H_2 + δC6H_2 + γC23H_2 + δC20H_2 + [δ=C-H + ρC-H + aryl**2**](I,II)
A	1340	9	15					S53(71)=γC9H_2 + δC6H_2 + γC23H_2 + δC20H_2 + [ρN-H + ρC-H + aryl**3**](I,II)
B	1339	34	1	1318	w	1313	20	S54(61)=γC9H_2 + δC6H_2 + γC23H_2 + δC20H_2 + [ρN-H + ρC-H + aryl**3**](I,II)
B	1329	11	1					S55(60)=δC9H_2 + C20H_2 + [ρN-H + ρC-H + ρ=C-H + aryl**4**](I,II)
A	1329	<1	6					S56(54)=δC9H_2 + C20H_2 + [ρN-H + ρC-H + ρ=C-H + aryl**4**](I,II)
B	1312	2	<1					S57(54)+S61(28)+S79(10) =aryl**26** + ρC-H + ph-**7** + ph-**36**](I,II)
B	1312	3	<1	-		1297	29	S58(58)+ S62(29)=aryl**5**
B	1298	1	8	-				S59(58)=δC9H_2 + C20H_2 + [ρN-H + ρC-H + ρ=C-H + aryl**5** + ph-**34**](I,II)
A	1297	10	4	-				S60(59)=δC9H_2 + C20H_2 + [ρN-H + ρC-H + ρ=C-H + aryl**5** + ph-**34**](I,II)
A	1293	1	1	-				S57(28)+S61(48)
B	1293	<1	1	-				S58(23)+S61(48)
B	1283	130	<1	-				S63(51)=ωC6H_2 + ωC20H_2 + [γC-H + δ=C-H + aryl**6**](I,II)
A	1280	1	26	-				S64(52)+S83(10)=ωC6H_2 + ωC20H_2 + [γC-H + νC=S + δ=C-H + aryl**6**](I,II) + ν_aC10C9C8 +

								ν_aC10C5C6 + νC4C5 + ν_sC6C7C8 + ν_aC24C23C22 + ν_aC24C19C20 + νC18C19 + νC2N3 + νC16N17 + ν_sC20C21C22
B	1261	<1	11			1267	23	S65(61)=ωC6H_2 + ωC20H_2 + [ρC-H + δ=C-H + + ph-**37** + aryl**7**](I,II)
A	1260	1	24	-				S66(59)=ωC6H_2 + ωC20H_2 + [ρC-H + δ=C-H + + ph-**37** + aryl**7**](I,II)
A	1236	5	27	1237	s	1242	22	S66(10)+S67(44)=ν_aC5N6C7 + ν_aC19N20C21 + νC4C5 + ph-**6** + ν_sC2N3C4 + ν_sC16N17C18
B	1235	43	1					S68(42)=[τHCC(O)N + τNHSC](I,II) + τC10N1H11S26
A	1203	11	2	1188	vs	1209	6	S69(50)+S139(18)=δC9H_2 + δC20H_2 + [ρC-H + ω=C-H + aryl**28** + ρCH_2 + ρ=C-H + ph-**46** + aryl**28**] (I,II)
B	1203	<1	16					S70(50)+ S111(17)=δC9H_2 + δC20H_2 + δC5H + δC19H + [ρCH_2 + ρCH + ρ=C-H + ph-**46** + δ=C-H + δNH + aryl**9**] (I,II)
A	1190	3	41			1191	22	S71(22)+S73(17)=δC9H_2 + δC20H_2 + δC5H + δC19H + δC10H + δC24H + [δ=C-H + δNH + δNH + aryl**9** + aryl**10** + aryl**11**] (I,II)
B	1188	329	2					S72(45)=δC9H_2 + δC20H_2 + δC10H + δC24H + [δ=C-H + δNH + aryl**10** + aryl**11**](I,II)
A	1182	2	25					S71(10)+S73(54)
B	1179	610	5			1177	17	S72(19)+S131(12)=[δNH + ω=C-H + ph-**39** + δC=O + aryl**10**](I,II) + ν_aC4N3C14 + ν_aC18N17C28
A	1162	3	3			1167	9	S75(52)+S81(12)=δC9H_2 + δC20H_2 + ν_aC4N3C14 + ν_aC18N17C28 + νC5C6 + νC9C10 + νC19C20 + νC23C24 + νC4C5 + νC18C19 + [δ=C-H + δNH + ρCH + aryl**12** + ph-**22**](I,II)
B	1161	201	4					S76(43)+S82(15)=ρC9H_2 + ρC20H_2 + ν_aC4N3C14 + ν_aC18N17C28 + νC5C6 + νC9C10 + νC19C20 + νC23C24 + νC4C5 + νC18C19 + [δ=C-H + δNH + ρCH + ph-**17** + ph-**26** + ph-**30** + aryl**12**](I,II)
A	1158	<1	9			1154	11	S33(19)+S77(75)
B	1158	10	1					S34(19)+S78(69)
A	1146	<1	1	1144	w	1144	2	S79(77)
B	1146	<1	5					S80(79)
A	1121	6	11	1128	vw	-		S75(13)+S81(26)
B	1120	150	1			-		S82(28)
A	1093	1	9	1099	w	1099	13	S69(11)+S83(36)
B	1093	17	5					S72(12)+S84(41)=ν_aC10C9C8 + ν_aC10C5C6 + νC4C5 + ν_sC6C7C8 + ν_aC24C23C22 + ν_aC24C19C20 + νC18C19 + νC2N3 + νC16N17 + ν_sC20C21C22 + [νC=S](I,II)
A	1067	14	<1	1072	w	1072	9	S43(32)+S85(47)
B	1067	1	<1					S44(25)+S86(53)
B	1058	23	<1	1044	vw	1044	14	S87(53)=ν_aC9C10C5 + ν_aC23C24C19 + νC4C5 + ν_sC10N1C2 + ν_sC24N15C16 + ν_aC2C3C4 + ν_aC16C17C18 + νC18C19 + [νC=S + ph-**23** + νC=C](I,II)
A	1052	<1	12					S137(41)=ν_aC9C10C5 + ν_aC23C24C19 + νC4C5 + ν_sC10N1C2 + ν_sC24N15C16 + ν_aC2C3C4 + ν_aC16C17C18 + νC18C19 + [νC=S + ph-**23** + νC=C](I,II)
B	1044	1	<1					S89(41)=ν_aC10C9C8 + ν_sC10C5C6 + νC4C5 + ν_sC6C7C8 + ν_sC24C23C22 + ν_sC24C19C20 + νC18C19 + ν_sC2N3C4 + ν_sC16N17C18 + ν_sC20C21C22 + ν_sC10N1C2 + $_s$C24N15C16 + [νC=S, ph-**24**](I,II)
A	1044	<1	12			1033	15	S90(43)=ν_aC10C9C8 + ν_sC10C5C6 + νC4C5 +

								ν_sC6C7C8 + ν_sC24C23C22 + ν_sC24C19C20 + νC18C19 + ν_sC2N3C4 + ν_sC16N17C18 + ν_sC20C21C22 + ν_sC10N1C2 + $_s$C24N15C16 + [νC=S + ph-**24**](I,II)
A	1017	<1	15	1004	vw	1004	74	S39(17)+S91(48)
B	1017	11	1					S40(16)+S92(49)
A	1008	2	3					S94(11)=[ρCH_2 + ρCH+ ph-**38** + aryl**13**](I,II)
B	1008	<1	24					S74(10)+S154(12)=[ρCH_2 + ρCH+ ph-**38** + aryl**13** +ρ=C-H + aryl**40**](I,II)
A	986	<1	84	981	vw	983	15	S74(43)+S95(48)=[aryl**14** + ph-**8**](I,II)
B	986	6	1					S93(39)+S96(49)=[aryl**14** + ph-**8**](I,II)
B	974	25	<1			971	18	S101(13)=[ρCH_2 + ρ=C-H + ρC=O + ph-**44** + aryl**26**](I,II)
A	973	1	13					S102(12)=[ρCH_2 + ρ=C-H + ρC=O + ph-**44** + aryl**26**](I,II)
B	969	<1	<1					S99(85)=[ω=C-H + ph-**45** + aryl**27**](I,II)
A	969	<1	<1					S100(83)=[ω=C-H + ph-**45** + aryl**27**](I,II)
A	965	1	4	956	vw	956	11	S101(51)
B	965	1	1					S102(56)
A	956	26	<1					S101(21)+S159(10)=[ρ=C-H + ρCH + aryl**18**](I,II) + ν_aC4N3C14 + ν_aC18N17C28
B	956	3	4					S102(12)+S112(13)=[ρ=C-H + ρCH + aryl**15**](I,II) + ν_aC4N3C14 + ν_aC18N17C28
A	946	<1	<1	931	vw	931	19	S105(91)=[ph-**47]**(I,II)
B	946	<1	<1					S106(82)= [ph-**47]**(I,II)
A	921	8	14	913	vw			S107(39)=ν_sC8N9C10 + ν_sC22C23C24 + ν_sC10C5C6 + ν_sC24C19C20 + νC4C5 + νC18C19 + ν_aC6C7C8 + ν_aC20C21C22 + ν_sC10N1C2 + ν_sC24N15C16 + ν_sC2N3C4 + ν_sC16N17C18
B	921	7	<1					S108(38)
B	902	24	<1	902	vw	906	9	S109(38)=[γ=C-H + ωCH_2 + γC=O + ph-**44** + aryl**29**](I,II)
A	902	<1	28					S110(37)=[γ=C-H + ωCH_2 + γC=O + ph-**44** + aryl**29**](I,II)
B	894	8	<1	897	vw	897	8	S109(24)=[γ=C-H + ωCH_2 + γC=O + ph-**44** + aryl**29**](I,II)
A	894	4	1					S110(21)=[γ=C-H + ωCH_2 + γC=O + ph-**44** + aryl**29**](I,II)
B	878	4	1	874	vw	874	19	S109(24)+S113(38)=ν_sC9C10C5 + ν_sC23C24C19 + ν_sC7C8C9 + ν_sC21C22C23 + νC4C5 + νC18C19 + ν_sC6C7C8 + νC10N1 + ν_sC24N15 + νN3C4 + νC18O27 + ν_sN17C18 + [ph-**22** + νC=S](I,II)
A	878	<1	26					S110(11)+S114(52)=ν_sC9C10C5 + ν_sC23C24C19 + ν_sC7C8C9 + ν_sC21C22C23 + νC4C5 + νC18C19 + ν_sC6C7C8 + νC10N1 + ν_sC24N15 + νN3C4 + νC18O27 + ν_sN17C18 + [ph-**22** + νC=S](I,II)
B	841	16	2	844	vw	847	3	S115(30)=ν_aC9C10C5 + ν_aC23C24C19 + ν_aC10N5C6 + ν_aC24C19C20 + ν_sC21C22C23 + νC4C5 + νC18C19 + ν_sC6C7C8 + νC10N1 + νC24N15 + ν_aC2N3C14 +ν_aC16N17C28 + νC4O13 + [ph-**26**](I,II)
A	841	8	10					S116(20)=ν_aC9C10C5 + ν_aC23C24C19 + ν_aC10N5C6 + ν_aC24C19C20 + ν_sC21C22C23 + νC4C5 + νC18C19 + ν_sC6C7C8 + νC10N1 + νC24N15 + ν_aC2N3C14 +ν_aC16N17C28 + [ph-**26** + νC=O](I,II)
A	818	<1	<1	810	vw	809	8	S117(96)=[ph-**48** + aryl**30**](I,II)
B	818	<1	<1					S118(99)=[ph-**48** + aryl**30**](I,II)
A	772	5	<1	779	vw	775	7	S119(23)=ν_sC8N9C10 + ν_sC22C23C24 + νC4C5 + νC18C19 + ν_sC10N5C6 + ν_sC24C19C20 +

								νC10N1 + νC24N15 + νN3C4 +νN17C18 + νC18O27 + [ph-**23** + νC=S](I,II)
B	772	<1	9					S120(20)=ν_sC8N9C10 + ν_sC22C23C24 + νC4C5 + νC18C19 + ν_sC10N5C6 + ν_sC24C19C20 + νC10N1 + νC24N15 + νN3C4 +νN17C18 + νC18O27 + [ph-**23** + νC=S](I,II)
A	752	43	2	753	vw	753	11	S121(20)=[γ NH + aryl**31**] (I,II)
A	740	29	<1	723	w	732	6	S122(58)=[ρ=C-H + δNH + δC-H + ph-**49** + aryl**32**](I,II)
B	739	1	16					S123(57)=[ρ=C-H + δNH + δC-H + ph-**49** + aryl**32**](I,II)
B	737	4	2					S124(57)+S144(41)=[ρC10H +ρC24H + δNH + δC-H + ph-**49** + aryl**33** +ρNH + aryl**34**](I,II)
A	735	5	6					S112(10)+S125(26)+S143(12)=[ρNH + δCH + ph-**44** + aryl**35** + aryl**36**](I,II)
B	720	14	2			712	13	S125(87)=[ρNH](I,II)
A	682	81	<1	692	m	693	5	S122(17)+S127(70)=[ωCH + aryl**37**](I,II)
B	682	8	2					S128(79)=[ωCH + aryl**37**](I,II)
B	669	70	<1	650	vw	666	27	S129(56)=[ω=C-H + aryl**35**](I,II)
A	669	11	6					S130(56)=[ω=C-H + aryl**35**](I,II)
B	657	15	<1			659	29	S131(10)
A	657	1	19					S132(42)=[δNH + ω=C-H + ph-**39** + δC=O + aryl**10**](I,II) + ν_aC4N3C14 + ν_aC18N17C28
B	627	6	2			638	15	S133(61)+S136(11)=[aryl**16** + aryl**38** + δNH + δCH + ph-**9**+ ph-**40**](I,II)
A	626	3	7					S134(64)+S135(10)=[aryl**16** + aryl**38** + δNH + δCH+ ph-**9**+ ph-**40**](I,II)
A	609	<1	3	615	m	615	18	S134(14)+S135(10)
B	609	5	1					S135(15)+S136(65)
B	606	12	<1					S88(27)+S130(11)+S160(12)=[ρCH_2 + ω=C-H + δNH + ν_sC4N3C14 + ν_sC18N17C28 + aryl**17**](I,II)
A	606	49	<1					S97(13)+S129(14)+S144(10)+S138(14)=[ω=C-H + δC=O + ν_sC4N3C14 + ν_sC18N17C28 + aryl**18+** ρCH_2 + δNH + aryl**17**](I,II)
A	573	3	14	559	vw	587	3	S98(34)=[ω=C-H + ρNH + ν_sC4N3C14 + ν_sC18N17C28 + aryl**12**](I,II)
B	572	5	<1					S124(10)+S140(30)=[ω=C-H + ρNH + ν_sC4N3C14 + ν_sC18N17C28 + aryl**12**](I,II)
B	531	<1	2	534	vw	558	19	S148(24)=[ph-**46**+ aryl**39**](I,II)
A	530	63	1			516	57	S140(10)+ S142(24)=[ph-**46** + aryl**39**](I,II)
A	504	3	5	515	vw	501	12	S125(14)+S143(34)
B	503	1	<1					S144(32)=[ρNH + δCH + ph-**44** + aryl**35** + aryl**36**](I,II)
A	500	28	1					S145(47)+S168(11)=[δ=C-H + δC-H + δNH + δC=O+ γCH + ν_aC4N3C14 + ν_aC18N17C28 + ph-**32** + aryl**19** + aryl**40**](I,II)
B	497	1	11	495	vw	491	3	S146(39)=[δ=C-H + δC-H + δNH + δC=O+ γCH + ν_aC4N3C14 + ν_aC18N17C28 + ph-**32** + aryl**19** + aryl**40**](I,II)
B	479	4	<1	459	vw	459	18	S142(28)+S147(30)=[ρNH + ph-**50** + aryl**41**](I,II)
A	478	<1	21					S141(3)+S148(35)=[ph-**46** + aryl**39** + ρNH + ph-**50** + aryl**23**](I,II)
A	409	1	<1			416	15	S149(34)+S151(22)==[ρNH + ρC=O + ph-**50** + aryl**28**](I,II)
B	409	<1	1					S150(31)+S152(30)=[ρNH + ρC=O + ph-**50** + aryl**28**](I,II)
B	407	<1	<1					S106(11)+S149(16)+S151(53)
A	407	<1	<1					S150(18)+S152(53)
B	378	1	2	-		387	14	S111(23)+S153(43)=[ρCH_2 + ρ=C-H + aryl**25**](I,II)
A	378	<1	3	-				S139(23)+S154(50)=[ρCH_2 + ρ=C-H + aryl**25**](I,II)

B	374	6	<1	-				S155(42)=[ρ=C-H + aryl**29** + aryl**32**] (I,II)
A	372	3	3	-				S156(53)=[ρ=C-H + aryl**29** + aryl**32**] (I,II)
B	343	9	<1	-		-		S157(45)=[ν_aC9C10C5 + ν_aC23C24C19 + ν_aC6C5C4 + ν_aC20C19C18 + ν_aC10N1C2 + ν_aC24N15C16 + νC2S12 + νC16S26 + νS12H25 + νS26H11](I,II)
A	338	1	7	-		322	12	S158(47)=[ν_aC9C10C5 + ν_aC23C24C19 + ν_aC6C5C4 + ν_aC20C19C18 + ν_aC10N1C2 + ν_aC24N15C16 + νC2S12 + νC16S26 + νS12H25 + νS26H11](I,II)
B	321	19	<1	-				S103(46)=[ρ=C-H + ρC=O + aryl**6** + ph-**39**] (I,II)
A	321	<1	11	-				S160(35)=[ρ=C-H + ρC=O + aryl**6** + ph-**39**] (I,II)
B	284	13	<1	-		279	20	S161(57)=[γ=C-H + aryl**29** + aryl**32**](I,II)
A	284	<1	2	-				S162(55)=[γ=C-H + aryl**29** + aryl**32**](I,II)
B	249	<1	6	-		263	36	S163(32)=[ρC=O + aryl**29** + aryl**32**](I,II) S171(28)=[νS12H25 + νS26H11](I,II)
A	249	6	<1	-				S164(41)=[ρC=O + aryl**29** + aryl**32**](I,II) S174(18)=[νS12H25 + νS26H11](I,II)
B	215	<1	<1	-		218	11	S166(41)=[ν_aC10C5C4 + ν_aC24C19C18 + ν_aC2N3C4 + ν_aC16N17C18 + νC10N1 + νC24N15 + νN3C14 + νN17C28 + νC2S12 + νC16S26 + νS12H25 + νS26H11 + ph-**23**](I,II)
A	213	<1	2	-				S167(45)= [ν_aC10C5C4 + ν_aC24C19C18 + ν_aC2N3C4 + ν_aC16N17C18 + νC10N1 + νC24N15 + νN3C14 + νN17C28 + νC2S12 + νC16S26 + νS12H25 + νS26H11 + ph-**23**](I,II)

	trans NH							
	Calculated wavenumbers (cm^{-1}) B3LYP/631+G**			Observed Wavenumbers (cm^{-1})				Tentative Assignment[c,d,e] PED %
	Freq.	IR int.	Raman Int.	FT-IR	(int) [a]	Raman	(int) [b]	
B	3257	2235	0.1	3182	s	3178	14	S1(99)=νNH (I,II)
A	3235	<1	1949					S2(98)=νNH (I,II)
A	3111	1	588	3056	m	3080	sh	S14(12)+S17(78)= ph-**1** (I,II)
B	3111	7	27					S4(78)=ph-**1** (I,II)
A	3106	28	54					S5(81)+S9(13)= ph-**10** (I,II)
B	3106	1	4					S5(14)+S9(84)= ph-**10** (I,II)
A	3098	<1	167			3065	100	S8(90)=ph-**11** (I,II)
B	3098	55	3					S10(91)=ph-**11** (I,II)
A	3091	11	32					S3(84)+S7(11)=ph-**12** (I,II)
B	3091	1	236					S3(12)+S7(81)=ph-**12** (I,II)
A	3081	<1	71			3057	sh	S6(86)=ph-**13** (I,II)
B	3081	<1	7					S14(75)+S17(12)=ph-**13** (I,II)
A	3081	<1	633					S16(98)=ν=C-$H_{i.ph.}$ (I,II)
B	3081	80	2					S13(98)=ν=C-$H_{i.ph.}$ (I,II)
A	3059	3	162	3035	m	3036	78	S15(98)=ν=C-$H_{o.o.ph.}$ (I,II)
B	3059	8	57					S12(98)=ν=C-$H_{o.o.ph.}$ (I,II)
A	2989	9	124	2976	m	2976	32	S28(90)=[ν_aC9H_2+ ν_aC23H_2](I,II)
B	2989	12	77					S22(90)=[ν_aC9H_2+ ν_aC23H_2](I,II)
B	2974	14	52			2954	30	S11(87)+S18(12)=[ν_aC6H_2+ ν_aC20H_2](I,II)
A	2973	9	186					S23(87)+S24(12)=[ν_aC6H_2+ ν_aC20H_2](I,II)
A	2938	19	119	2931	m	2933	28	S27(82)=[ν_sC9H_2+ ν_sC23H_2](I,II)
B	2938	23	26					S21(82)=[ν_sC9H_2+ ν_sC23H_2](I,II)
B	2926	26	20	2923	m	2923	37	S11(87)+S18(12)=[ν_sC6H_2+ ν_sC20H_2](I,II)
A	2926	12	271					S23(12)+S24(83)=[ν_sC6H_2+ ν_sC20H_2](I,II)
B	2913	7	18	2872	m	2898	51	S20(75)+S26(13)=[νC5H + νC19H](I,II)
A	2913	8	36					S20(13)+S26(75)=[νC5H + νC19H](I,II)
A	2884	20	231	2852	m	2853	76	S25(91)=[νC10H + νC24H](I,II)

B	2884	12	18					S19(91)=[νC10H + νC24H](I,II)
A	1720	4	113	1719	vs	1723	sh	S31(87)=νC=O (I,II)
B	1718	632	<1			1716	61	S30(87)=νC=O (I,II)
B	1662	14	<1	1641	s	1652	24	S51(80)=νC=C (I,II)
A	1662	<1	56					S33(80)=νC=C (I,II)
A	1596	<1	75	1617	s	1594	44	S45(67)+S75(19)=[ph-**17** + ph-**30]** (I,II)
B	1596	14	7					S39(55)+S79(15)+S112(12)=[ph-**17** + ph-**30]** (I,II)
A	1589	<1	16					S36(63)+S111(10)=[ph-**18** + ph-**31]** (I,II)
B	1589	4	3					S42(64)=[ph-**18** + ph-**31]** (I,II)
B	1542	645	<1	1545	vs	-		S34(20)+S122(49)=ν_aN1C2N3 + ν_aN15C16N1 + [δNH](I,II)
A	1520	1	15			-		S34(20)+S122(49)=ν_aN1C2N3 + ν_aN15C16N17 + [aryl**20**](I,II)
A	1483	1	1	1494	m	-		S74(74)+S108(20)=[ph-**27** + ph-**41]** (I,II)
B	1483	43	<1			-		S78(62)+S105(12)=[ph-**27** + ph-**41]** (I,II)
B	1442	11	4	1431	sh	1442	29	S94(87)=δC9H$_2$ + δC23H$_2$
A	1442	<1	46					S88(88)=δC9H$_2$ + δC23H$_2$
A	1440	7	1					S37(23)+S80(47)=[ph-**28** + ph-**35]** (I,II)
B	1440	<1	3					S41(33)+S87(48)=[ph-**28** + ph-**35]** (I,II)
B	1436	19	3			1428	18	S98(83)=δC6H$_2$ + δC20H$_2$
A	1436	3	16					S91(84)=δC6H$_2$ + δC20H$_2$
A	1413	1	12	1421	m	-		S38(55)=ν_aN1C2N3 + ν_aN15C16N17
B	1403	288	<1	1383	m	-		S34(45)+S122(29)=ν_aN1C2N3 + ν_aN15C16N17 + [δNH](I,II)
A	1369	<1	8	1364	s	1361	23	S53(12)+S83(78)=ν_sC8C9N10 + ν_sC22C23N24 + νC6C7 + νC20C21 + νN3C4 + νN17C18 + [νC=S + δ=C-H](I,II)
B	1369	40	<1					S86(79)=δ=C-H
A	1353	2	6					S89(36)+S149(13)=[ωCH$_2$ + ρC-H](I,II)
B	1352	140	4					S96(37)+S143(12)=[ωCH$_2$ + ρC-H](I,II)
B	1349	183	3	1341	m	1338	16	S96(37)+S143(12)=[ωCH$_2$ + ρC-H](I,II)
A	1347	<1	12					S144(11)+S151(37)=[ωCH$_2$ + ρC-H](I,II)
A	1325	<1	23	1336	m			S89(10)+S151(16)=[ωCH$_2$ + ρC-H](I,II)
B	1325	5	<1					S95(20)+S150(16)=[ωCH$_2$ + ρC-H](I,II)
A	1312	4	<1	1306	m	1308	12	S43(50)+S73(17)+S70(10)=[ph-**19** + ph-**29** + ph-**32**] (I,II)
B	1312	<1	1					S35(49)+S77(14)= [ph-**19** + ph-**29** + ph-**32**] (I,II)
A	1293	<1	<1	1289	sh	1292	sh	S43(24)+S73(21)=ph-**29** (I,II)
B	1293	2	<1					S35(18)+S77(20)+S84(24)=[ph-**19** + ph-**29** + ph-**32**] + ph-**29** + ph-**42**] (I,II)
B	1291	49	6					S93(61)=ωC9H$_2$ + ωC23H$_2$ + [δNH](I,II)
A	1290	1	2					S81(68)=ωC9H$_2$ + ωC23H$_2$ + [δNH](I,II)
A	1279	<1	15	1281	m	1281	17	S92(45)+S153(13)=ωC9H$_2$ + ωC23H$_2$ + [δCH](I,II)
B	1279	32	2					S90(42)+S153(15)=ωC9H$_2$ + ωC23H$_2$ + [δCH](I,II)
A	1264	2	11	1253	sh	1264	22	S144(28)+S151(10)=ρNH (I,II)
B	1264	53	2					S145(28)=ρNH (I,II)
A	1235	4	35	1225	vs	1225	30	S47(37)= ν_sC2N3C4 + ν_sC16N17C28 + ν_aN1C2N3 + ν_aN15C16N17
B	1235	44	1					S46(42)=ν_sC2N3C4 + ν_sC16N17C28 + ν_aN1C2N3 + ν_aN15C16N17
B	1210	572	4	1209	vs	1209	26	S52(15)+S85(13)=ν_aC2N3C14 + ν_aC16N17C28
A	1210	2	91					S55(15)+S82(11)=ν_aC2N3C14 + ν_aC16N17C28
A	1194	1	24	1193	s	1198	18	S149(10)=[ρCH2 + δCH](I,II)
B	1193	255	<1			-		S143(13)+S147(12)=[ρCH2 + δCH](I,II)
B	1180	180	3	1176	s	1174	19	S85(45)=δ=C-H (I,II)
A	1180	1	5			-		S82(46)=δ=C-H (I,II)
A	1160	2	4	1167	vs	1153	17	S45(13)+S75(31)=ρC6H$_2$ + ρC20H$_2$ + ρC5H + ρC19H + [ph-**17** + ph-**30**](I,II)
B	1159	150	3					S39(15)+S79(44)=ρC6H$_2$ + ρC20H$_2$ + ρC5H + ρC19H + [ph-**17** + ph-**30**](I,II)
A	1157	3	6					S75(38)=ρC6H$_2$ + ρC20H$_2$ + ρC5H + ρC19H +

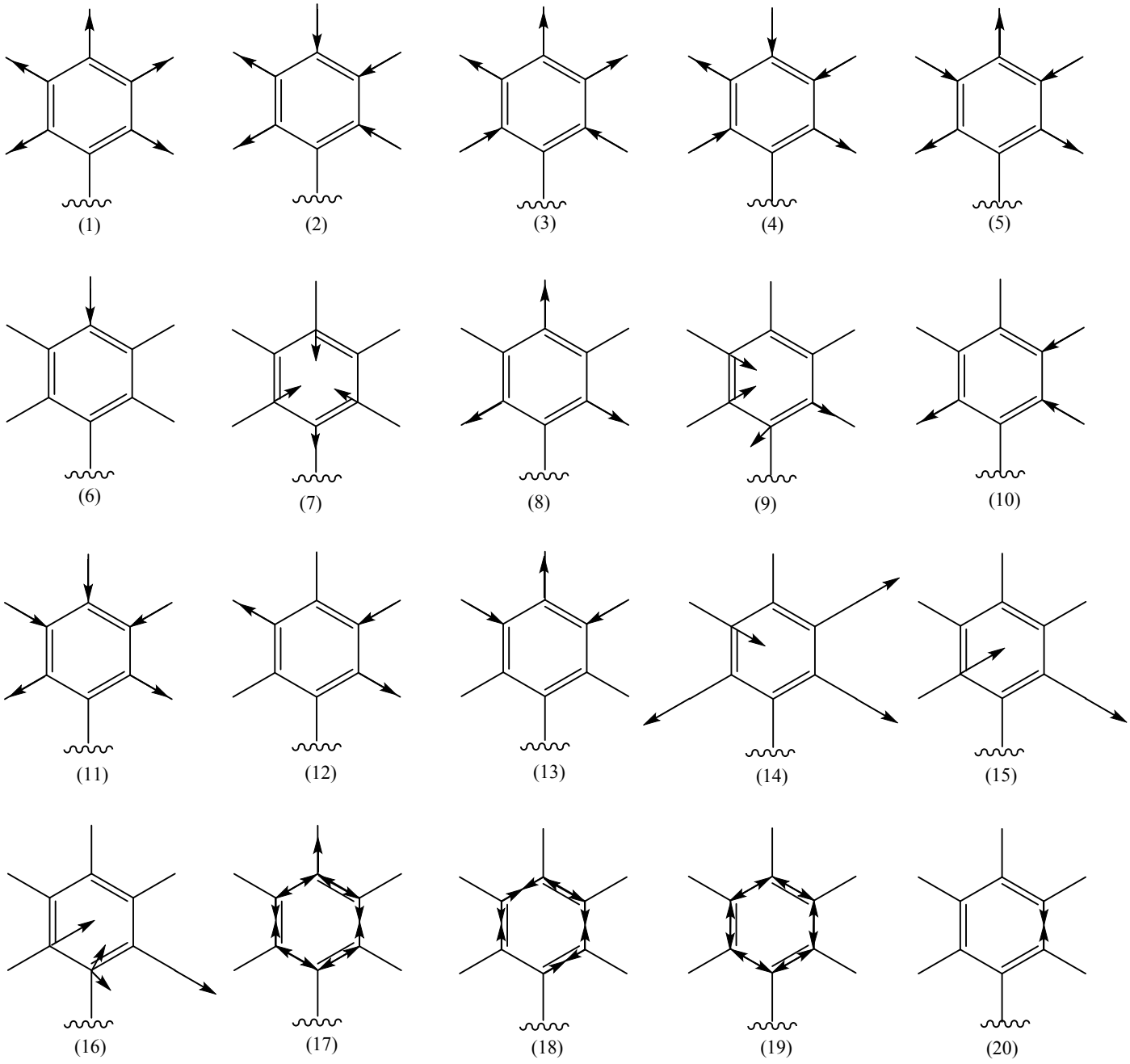
								[ph-**30**](I,II)
B	1157	98	3					S79(30)=ρC6H$_2$ + ρC20H$_2$ + ρC5H + ρC19H + [ph-**30**](I,II)
B	1146	<1	<1	1143	sh	1146	12	S76(72)=ph-**39** (I,II)
A	1146	<1	5			-		S84(62)=ph-**39** (I,II)
A	1129	1	10	1117	s	1119	19	S94(30)=ρC6H$_2$ + ρC20H$_2$ + [ρCH](I,II)
B	1129	19	1					S96(10)+S97(10)=ρC6H$_2$ + ρC20H$_2$ + [ρCH](I,II)
A	1098	<1	11	1097	m	1098	11	S59(21)+S82(13)=ν$_a$C5C10N1 + ν$_a$C19C24N15 + [ρ=C-H](I,II)
B	1097	71	1			-		S57(22)+S85(13)=ν$_a$C5C10N1 + ν$_a$C19C24N15 + [ρ=C-H](I,II)
B	1073	3	1	1074	m	1074	11	S60(26)=νC5C10 + νC19C24
A	1072	5	6					S61(21)=νC5C10 + νC19C24
B	1070	1	1					S57(25)+S119(141)=ν$_a$C5C10N1 + ν$_a$C19C24N15
A	1069	<1	2					S58(32)=ν$_s$C5C10N1 + ν$_s$C19C24N15
A	1065	15	<1					S37(13)+S73(12)+S77(17)+S80(12)+S112(10)=[ph-**17** + ph-**43** + ph-**32** + ph-**42** + ph-**27]**(I,II)
B	1065	1	<1					S41(21)+S73(18)+S77(13)+S87(15)+S110(11)=[ph-**17** + ph-**43** + ph-**32** + ph-**42** + ph-**27]**(I,II)
A	1024	2	9	1029	m	1029	19	S97(10)+S170(36)=ρC6H$_2$ + ρC20H$_2$ + [δCH + aryl**42**](I,II)
B	1024	1	1					S167(27)=ρC6H$_2$ + ρC20H$_2$ + [δCH + aryl**42**](I,II)
A	1016	<1	29	1006	m	1004	86	S74(14)+S108(41)+S110(17)=[ph-**32** + ph-**27**](I,II)
B	1016	8	<1					S40(10)+S78(20)+S112(36)=[ph-**32** + ph-**27**](I,II)
B	987	14	<1	984	m	988	20	S50(37)+S65(13)+S105(13)+S112(13)=νC8C9 + νC22C23 + νC6C7 + νC20C21 + νN3C4 + νN1718 + [νC=S + δNH + δNCS + ph-**26** + aryl**21**](I,II)
A	987	<1	74					S44(37)+S108(19)+S110(31)=νC8C9 + νC22C23 + νC6C7 + νC20C21 + νN3C4 + νN1718 + [νC=S + δNH + δNCS + ph-**26** + aryl**21**](I,II)
B	984	36	<1					S40(19)+S65(40)=ph-**32** (I,II)
A	983	<1	20					S53(12)+S110(13)=ν$_s$C8C9N10 + ν$_s$C22C23N24 + νC6C7 + νC20C21 + νN3C4 + νN17C18 + [νC=S + ph-**27**](I,II)
B	974	6	2					S62(21)+S140(10)=νN3C4 + νN17C18 + [δ=C-H](I,II)
A	973	<1	24					S59(10)+S137(12)=νN3C4 + νN17C18 + [δ=C-H](I,II)
A	969	<1	<1					S139(56)+S160(23)=ph-**44** (I,II)
B	969	<1	<1					S135(70)=ph-**44** (I,II)
B	963	<1	2					S140(68)=δ=C-H (I,II)
A	963	<1	8					S137(63)=δ=C-H (I,II)
B	946	<1	<1	947	m	947	12	S131(77)=ph-**51** (I,II)
A	946	<1	<1					S133(75)=ph-**51** (I,II)
A	930	3	<1	931	m	931	16	S40(12)+S60(11)=νC5C10 + νC19C24 + [ph-**32]**(I,II)
A	929	7	14					S53(12)+S61(11)+S63(11)=ν$_s$C8C9N10 + ν$_s$C22C23N24 + νC6C7 + νC20C21 + νN3C4 + νN17C18 + νC5C10 + νC19C24 + [νC=S](I,II)
B	915	4	12	917	m	917	23	S148(11)=ρCH$_2$ (I,II)
B	915	12	<1					S136(11)=[ρCH + ρCH$_2$](I,II)
A	897	<1	29			907	sh	S54(47)+S142(13)=ν$_s$C7C8N9 + ν$_s$C21C22N23 + νC5C10 + νC19C24 + νC6C7 + νC20C21 + [ph-**46**](I,II)
A	897	1	<1					S32(47)+S129(12)=ν$_s$C7C8N9 + ν$_s$C21C22N23 + νC5C10 + νC19C24 + νC6C7 + νC20C21 + [ph-**46**](I,II)
B	894	7	<1	849	m	862	6	S32(15)+S129(59)=ν$_s$C7C8N9 + ν$_s$C21C22N23 + νC5C10 + νC19C24 + νC6C7 + νC20C21 + [ph-**46**](I,II)
B	894	<1	4					S54(15)+S142(58)=ν$_s$C7C8N9 + ν$_s$C21C22N23 + νC5C10 + νC19C24 + νC6C7 + νC20C21 + [ph-**46**](I,II)
A	818	<1	<1	824	m	824	14	S128(92)=ph-**44** (I,II)
A	818	<1	<1					S134(92)=ph-**44** (I,II)
B	809	<1	17					S66(15)+S117(10)=δC7C8C9 + δC21C22C23 + δC8C9C10 + δC22C23C24

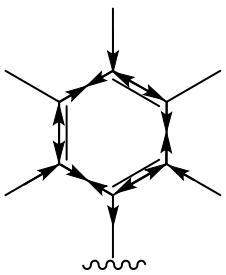
A	809	43	<1					S102(16)=δC7C8C9 + δC21C22C23 + δC8C9C10 + δC22C23C24 + δC9C10N1 + δC23C24N15 + [δC=S](I,II)
B	803	4	<1			787	7	S147(11)=ρCH_2 (I,II)
B	802	3	3					S169(12)=ρCH_2 (I,II)
A	745	1	21	756	m	758	16	S132(40)+S185(11)=[ωCH_2 + ph-**51]** (I,II)
A	745	9	1					S130(37)+S157(10)=ph-**51** (I,II)
B	737	40	2	739	m	739	13	S126(36)+S158(11)+S166(13)=[ρNH + δC=S] (I,II)
A	729	45	<1					S130(13)+S178(15)=[ρC=O + ωCH_2 + ph-**51]** (I,II)
B	726	8	4			-		S132(17)+S177(12)=[ρC=O + ωCH_2 + ph-**51]** (I,II)
A	712	9	2	718	m	-		S126(50)+S158(12)+S166(12)=[ρNH + δC=S**]** (I,II)
B	681	88	<1	694	s			S130(25)+S139(20)+S160(35)=[ωCH_2 + ph-**44 +** ph-**51]** (I,II)
B	681	<1	1					S132(24)+S164(48)+S185(11)=[ωCH_2 + ph-**44 +** ph-**51]** (I,II)
A	668	13	1	679	s	679	27	S138(20)=[ω=C-H + ρCH_2**]** (I,II)
A	667	17	16	664	s	665	15	S64(11)+S141(21)=[ω=C-H + ρCH_2**]** (I,II)
B	651	65	3	632	s	646	13	S141(42)=[ω=C-H + ρCH_2**]** (I,II)
A	651	9	3					S138(43)=[ω=C-H + ρCH_2**]** (I,II)
B	626	20	3			632	22	S111(10)+S183(50)=[ρC=S + ph-**15**][(I,II)
B	625	<1	2					S106(13)+S179(51)=[ph-**14** + ρC=S] (I,II)
A	615	3	15	613	s	615	21	S177(18)+S181(11)=γC=O (I,II)
A	614	22	<1					S178(19)+S180(11)=γC=O (I,II)
A	605	15	6	598	sh	597	7	S111(54)=ph-**15** [(I,II)
B	605	2	3					S106(51)+S179(10)=[ρC=S + ph-**14**][(I,II)
A	570	4	<1	582	m	578	11	S102(25)=δC7C8C9 + δC21C22C23 + δC8C9C10 + δC22C23C24 + δC9C10N1 + δC23C24N15 + [δC=S](I,II)
B	569	<1	2	578	sh			S63(10)+S66(23)=δC7C8C9 + δC21C22C23 + δC8C9C10 + δC22C23C24 + [δC=S](I,II)
A	521	1	5	531	s	531	17	S55(14)+S116(27)=ν_sC2N3C4 + ν_sC16N17C18 + δC2N3C4 + δC16N17C18
A	250	81	<1					S52(20)+S115(28)=ν_sC2N3C4 + ν_sC16N17C18 + δC2N3C4 + δC16N17C18
A	498	8	<1	512	m	511	25	S67(51)=aryl**22** (I,II)
B	498	<1	12					S103(51)=aryl**22** (I,II)
B	489	<1	1	-		463	13	S100(22)+S157(25)=[ph-**17** + ωCH_2 + ph-**51]** (I,II)
B	489	<1	26	-		-		S101(18)+S185(35)=[ph-**17** + ωCH_2 + ph-**51]** (I,II)
B	453	<1	<1	465	m	433	10	S60(10)=νC5C10 + νC19C24
A	451	2	1					S61(10)=νC5C10 + νC19C24
A	419	3	<1	410	m	418	10	S118(40)=δC9C10C5 + δC23C24C19 + δC9C10N1 + δC23C24N15 + [δC=S](I,II)
B	419	<1	1					S109(38)=δC9C10C5 + δC23C24C19 + δC9C10N1 + δC23C24N15 + [δC=S](I,II)
B	407	<1	<1			-		S162(80)=ph-**52** (I,II)
A	407	<1	<1			-		S133(12)+S163(76)=[ph-**51** + ph-**52**](I,II)
B	384	3	3	-		392	18	S140(14)+S147(20)+S167(23)=[δ=C-H + δCH_2 + aryl**42**](I,II)
A	384	<1	1	-				S137(17)+S152(24)+S169(17)=[δ=C-H + δCH_2 + aryl**42**](I,II)
B	353	22	<1	-		363	41	S49(22)=νN3C4 + νN17C18
A	351	<1	16	-				S63(20)=δC=S (I,II)
B	324	21	<1	-		336	27	S100(13)+S180(19)=[ph-**17 +** δC=S + δC=O + δNH + aryl**24]** (I,II)
A	324	1	10	-				S101(13)+S185(19)=[ph-**17 +** δC=S + δC=O + δNH + aryl**24]** (I,II)
A	300	5	<1	-		305	9	S182(11)=τC7C8C9C10 + τC21C22C23C24 + τC5C4N3C2 + τC19C18N17C16
A	300	4	<1	-		262	52	S184(11)= τC7C8C9C10 + τC21C22C23C24 + τC5C4N3C2 + τC19C18N17C16
B	253	<1	12	-				S125(11)+S157(12)=[δNH + δC=S + ω=C-H + ph-**51**](I,II)
B	251	<1	4	-		252	sh	S125(13)+S159(17)=[δNH + δC=S + ω=C-H +

							ph-**51**](I,II)
A	243	6	<1	-			S124(31)+S159(12)=δC9C10N1 + δC23C24N15 + δC2N3C14 + δC16N17C28
A	241	16	<1	-	217	23	S123(30)=δC9C10N1 + δC23C24N15 + δC2N3C14 + δC16N17C28
B	205	<1	3	-			S70(15)+S123(11)=δC9C10N1 + δC23C24N15 + δC2N3C14 + δC16N17C28 + [δC=S + ph-**16]**(I,II)
B	203	1	2	-			S70(18)+S124(12)+S125(11)=δC9C10N1 + δC23C24N15 + δC2N3C14 + δC16N17C28 [δC=S + ph-**16]**(I,II)

Figure S3. Representation of the mode patterns for selected calculated modes. The numbering in brackets refers to the corresponding mode in the table.

ph- structures

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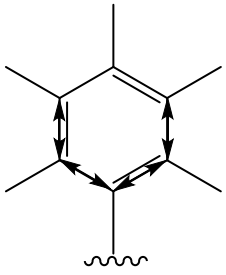
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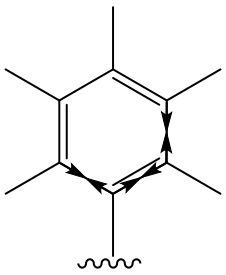
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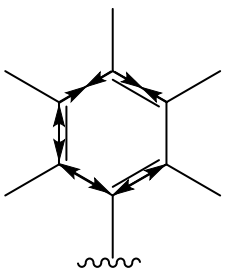
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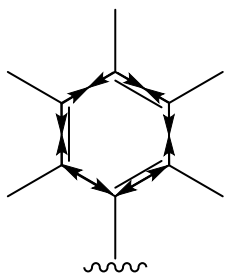
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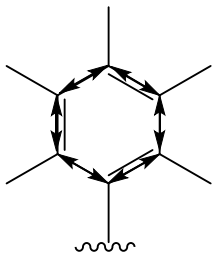
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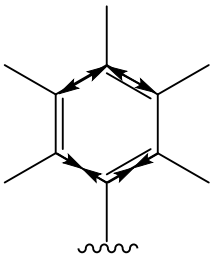
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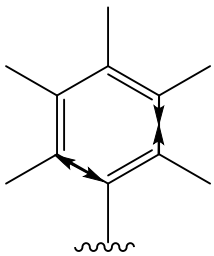
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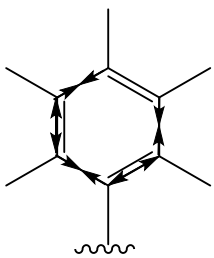
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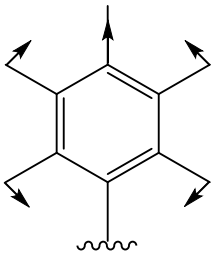
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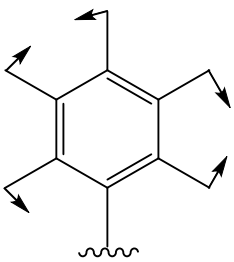
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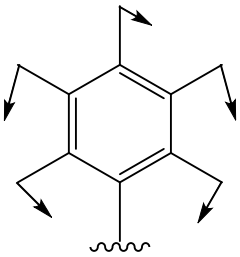
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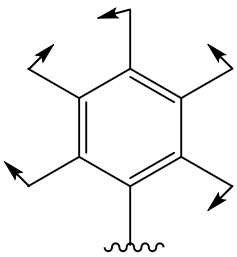
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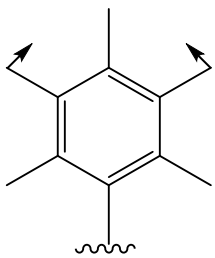
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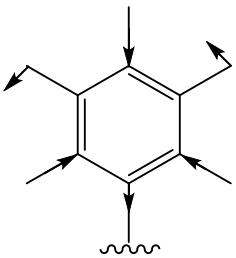
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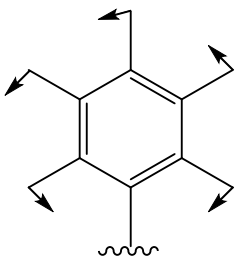
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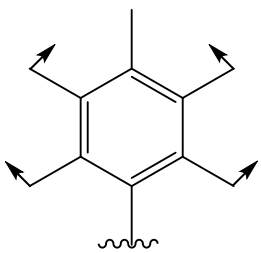
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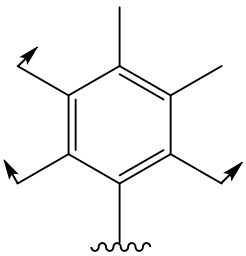
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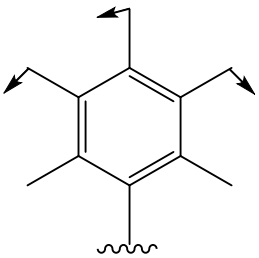
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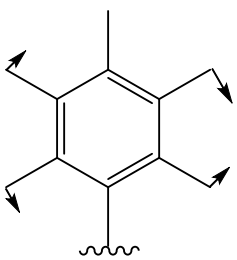
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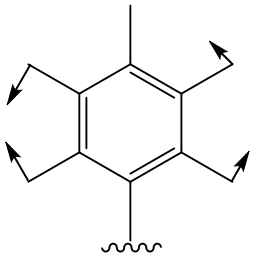
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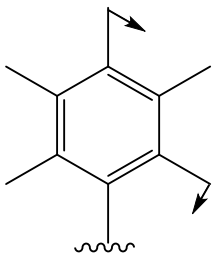
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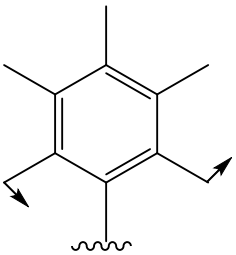
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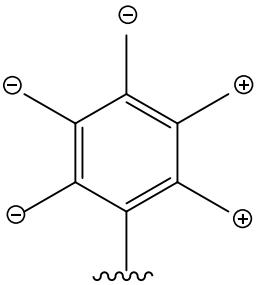
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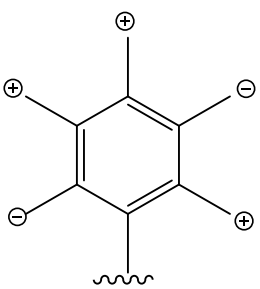
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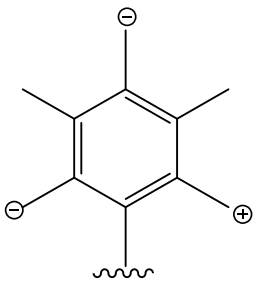
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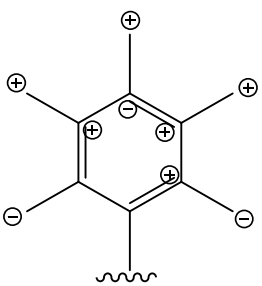
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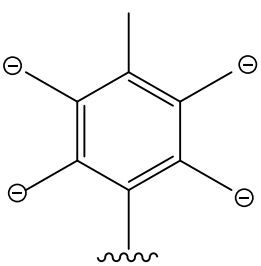
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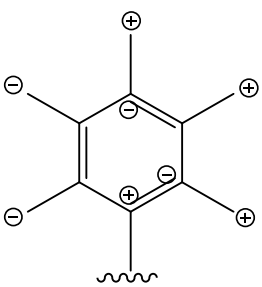
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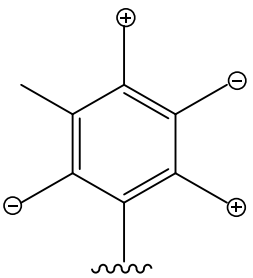
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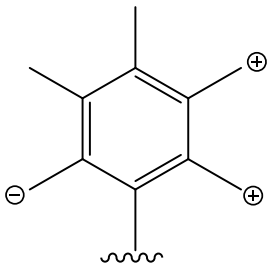

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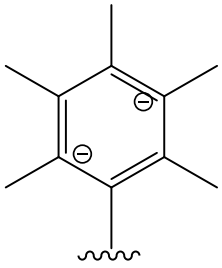

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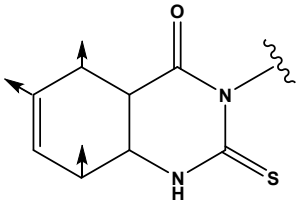

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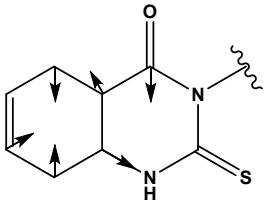

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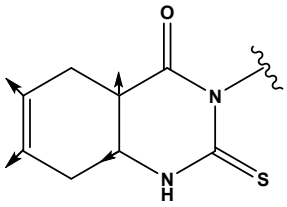

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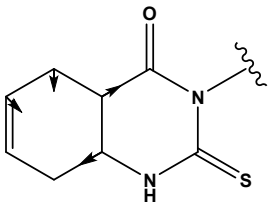

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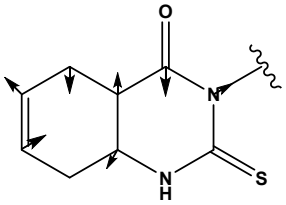

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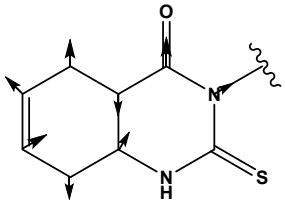

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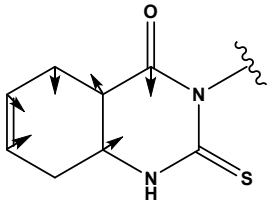

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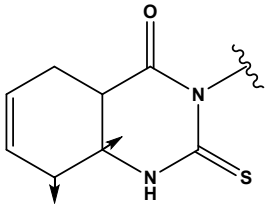

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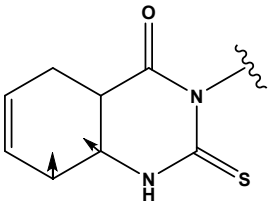

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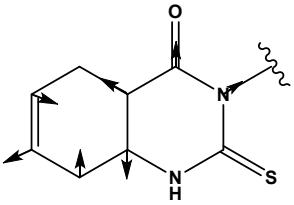

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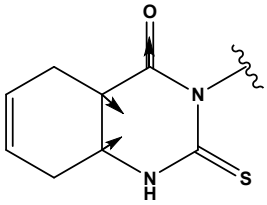

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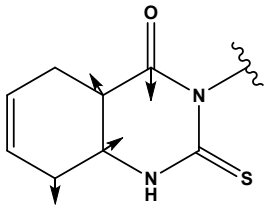

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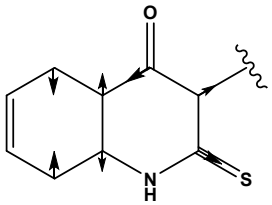

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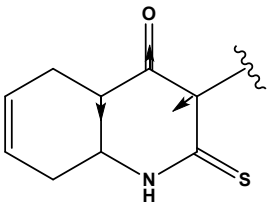

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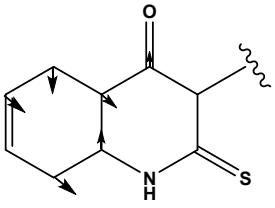

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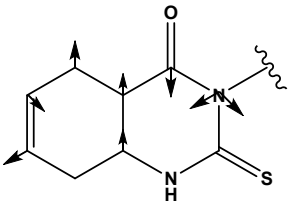

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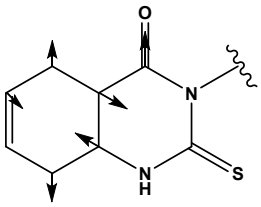

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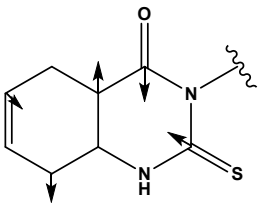

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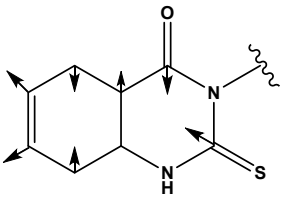

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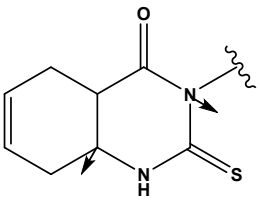

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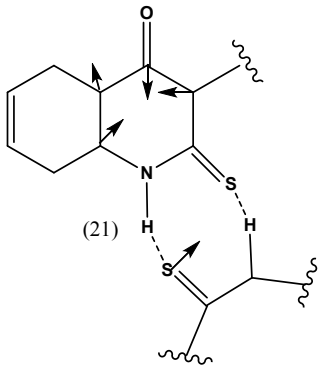

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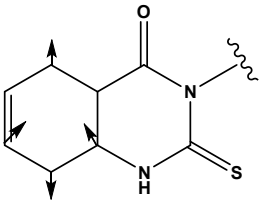

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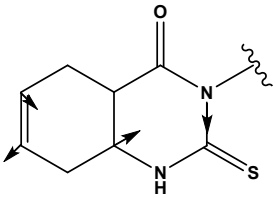

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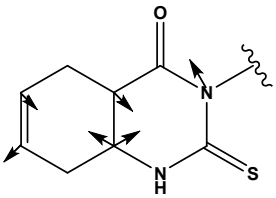

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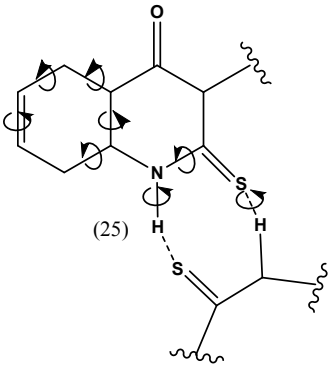

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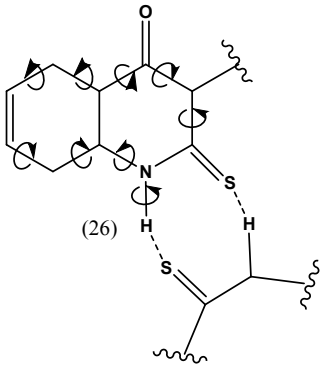

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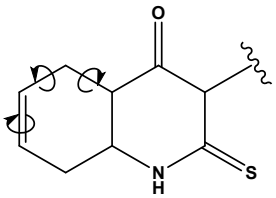

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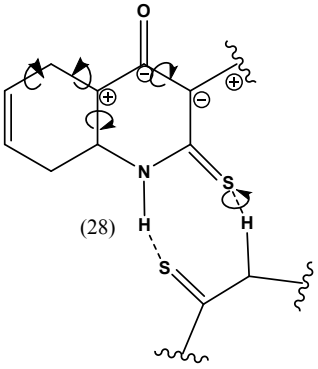

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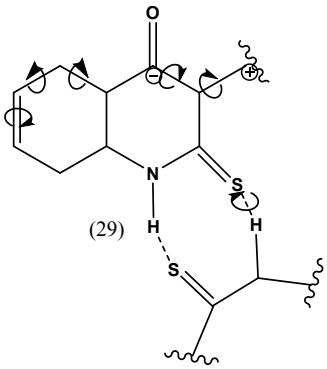

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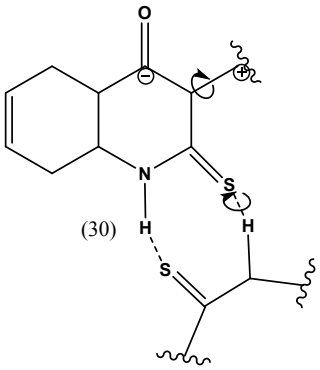

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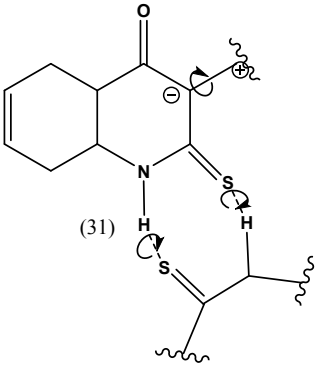

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