## Paracyclophanes as Model Compounds for Strongly Interacting $\pi$ -Systems

Part 1: Pseudo-ortho-dihydroxy[2.2]paracyclophane

### Supplementary information

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In the following sections mass spectra as well as tables containing the observed and computed wavenumbers are collected. Note that *Pseudo–ortho–*dihydroxy[2.2]paracyclophane is abbreviated throughout as o-DHCP

# Figure 1:Mass spectra recorded on the $S_1 \leftarrow S_0$ origin of o-DHCP (upper trace) and the o-<br/>DHCP·H<sub>2</sub>O cluster (lower trace). As visible, fragmentation is negligible.



Table 1:	Observed bands of the $S_1 \leftarrow S_0$ transition of o-DHCP (s=strong, m=medium, w=
	weak).

position / cm <sup>-1</sup> position / cm <sup>-1</sup>	Intensity
31483 0	S
31494 11	m
31537 54	S
31578 95	W
31587 104	W
31596 113	s
31610 127	111
31632 149	w
31644 161	w
31650 167	m
31658 175	w
31673 190	S
31679 196	W
31000 203	m
31715 232	s
31726 243	s
31728 245	S
31733 250	m
31735 252	m
31736 253	m
31758 275	m
31759 276	s
31768 285	m
31774 291	m
31786 303	s
31800 317	m
31805 322	w
31813 330	m
31821 338	m
31828 345	s m
31837 354	m
31839 356	m
31840 357	S
31847 364	m
31849 366	m
31852 369	m
31861 378	S
31881 308	(1) e
31886 403	m
31898 415	s
31901 418	s
31906 423	s
31912 429	m
31915 432	m
31919 430	m
31932 449	m
31938 455	s
31948 465	m
31952 469	s
31954 471	m
31957 474	S
31961 478	m
31907 404	s m
31975 492	m
31983 500	m
31989 506	m
31994 511	m
32001 518	m
32010 527	s 
32014 531 32020 527	m
32020 557	m
32051 568	m
32060 577	m

32084	601	S
32092	609	S
32136	653	S
32196	713	S
32206	723	S

#### **Table 2:** Observed bands of the $S_1 \leftarrow S_0$ transition of o-DHPC·H<sub>2</sub>O.

Absolute band position / cm <sup>-1</sup>	Relative band position / cm <sup>-1</sup>	Intensity
31263	0	S
31313	50	m
31340	77	w
31360	97	m
31382	119	m
31388	125	w
31400	137	m
31409	146	w
31428	165	w
31432	169	w
31435	172	w
31453	190	S
31465	202	w
31485	222	m
31502	239	m
31514	251	m
31528	265	m
31533	270	m
31537	274	m
31544	281	m
31547	284	m
31550	287	s
31571	308	S
31587	324	m
31598	335	w
31604	341	w
31621	358	S
31639	376	S
31651	388	W
31654	391	w
31670	407	S
31690	427	m
31702	439	W
31715	452	m
31726	463	m
31734	471	W
31741	478	w
31745	482	m
31755	492	m
31759	496	S
31766	503	S
31770	507	m
31782	519	m
31784	521	S
31788	525	m
31800	537	m
31806	543	m
31807	544	m
31825	562	S
31831	568	S
31850	587	S
31853	590	S
31877	614	m
31884	621	m
31891	628	m
31893	630	m
31900	037	m
31904	041	m ~~
31906	043	m
31940	003 700	m
31972	109	S
32130	00/	S
JZ140	003	5

### **Table 3:**Computed SCS-CC2/SV(P) S1-wavenumbers of o-DHCP in cm<sup>-1</sup>. All values

are scaled by 0.95.

75	1074
101	1109
118	1119
154	1121
179.	1132
185	1137
232	1166
236	1171
251	1180
270	1183
285	1208
291	1233
325	1248
340	1256
353	1261
357	1201
205	1219
400	1209
400	1290
404	1009
419	1000
420	1413
450	1418
468	1425
502	1430
509	1438
518	1443
555	1495
579	1519
610	1524
652	1537
677	1563
682	1608
689	2842
696	2875
714	2877
724	2893
756	2925
762	2941
795	2941
799	2956
874	2993
883	2999
922	3001
929	3013
940	3016
954	3025
1029	3442
1037	3459