

Supporting Information

Determining Binding Energies of Key Fluorinated Refrigerants 1,1,1,2-Tetrafluoroethane, 2,3,3,3-Tetrafluoropropene and 3,3,3-Trifluoropropene

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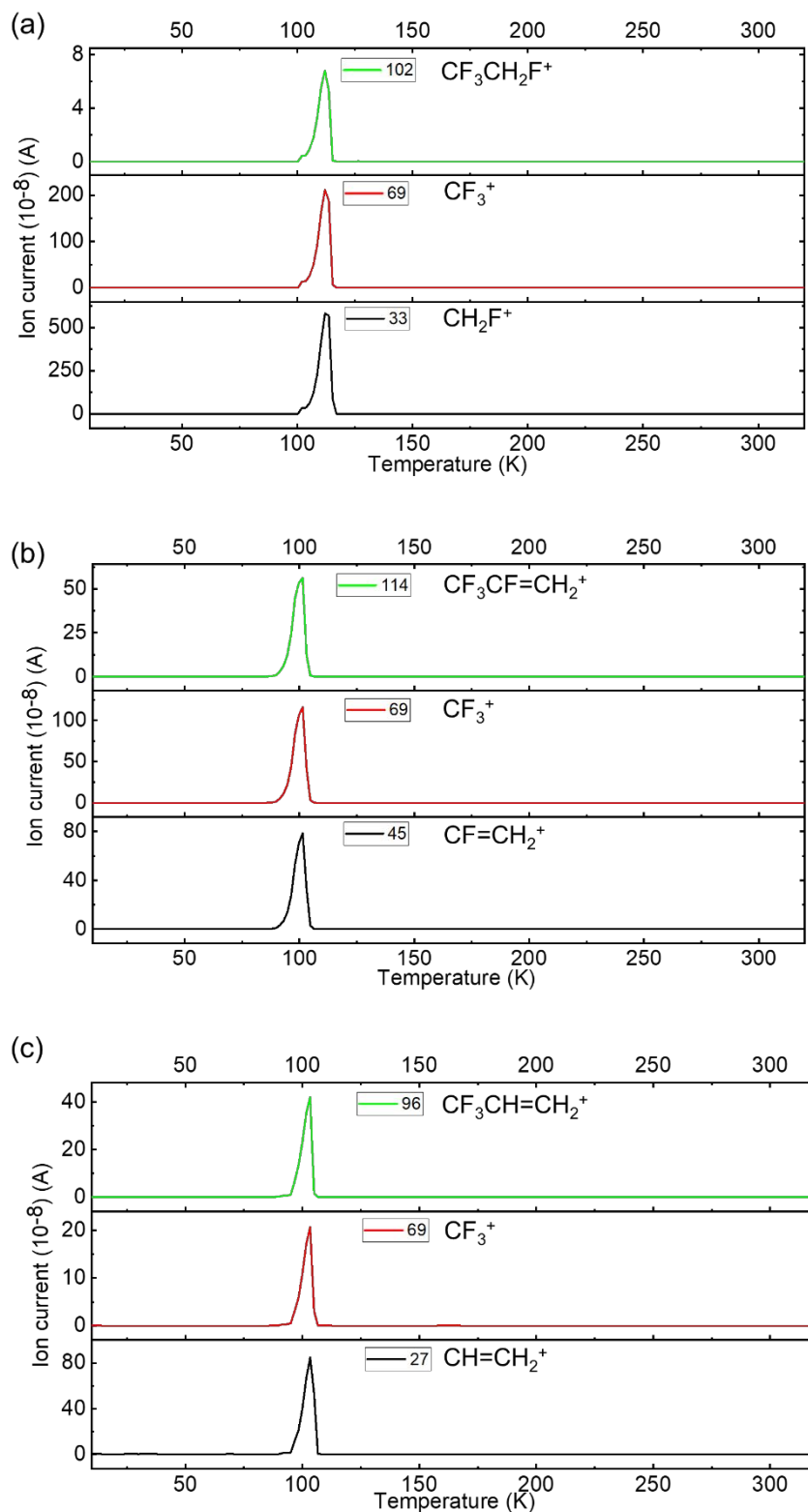


Figure S1: Raw temperature-programmed desorption (TPD) profiles of pure refrigerants recorded as ion current traces corresponding to their major mass fragments. (a) R-I, (b) R-II, and (c) R-III. These data represent the primary experimental signals prior to kinetic analysis.

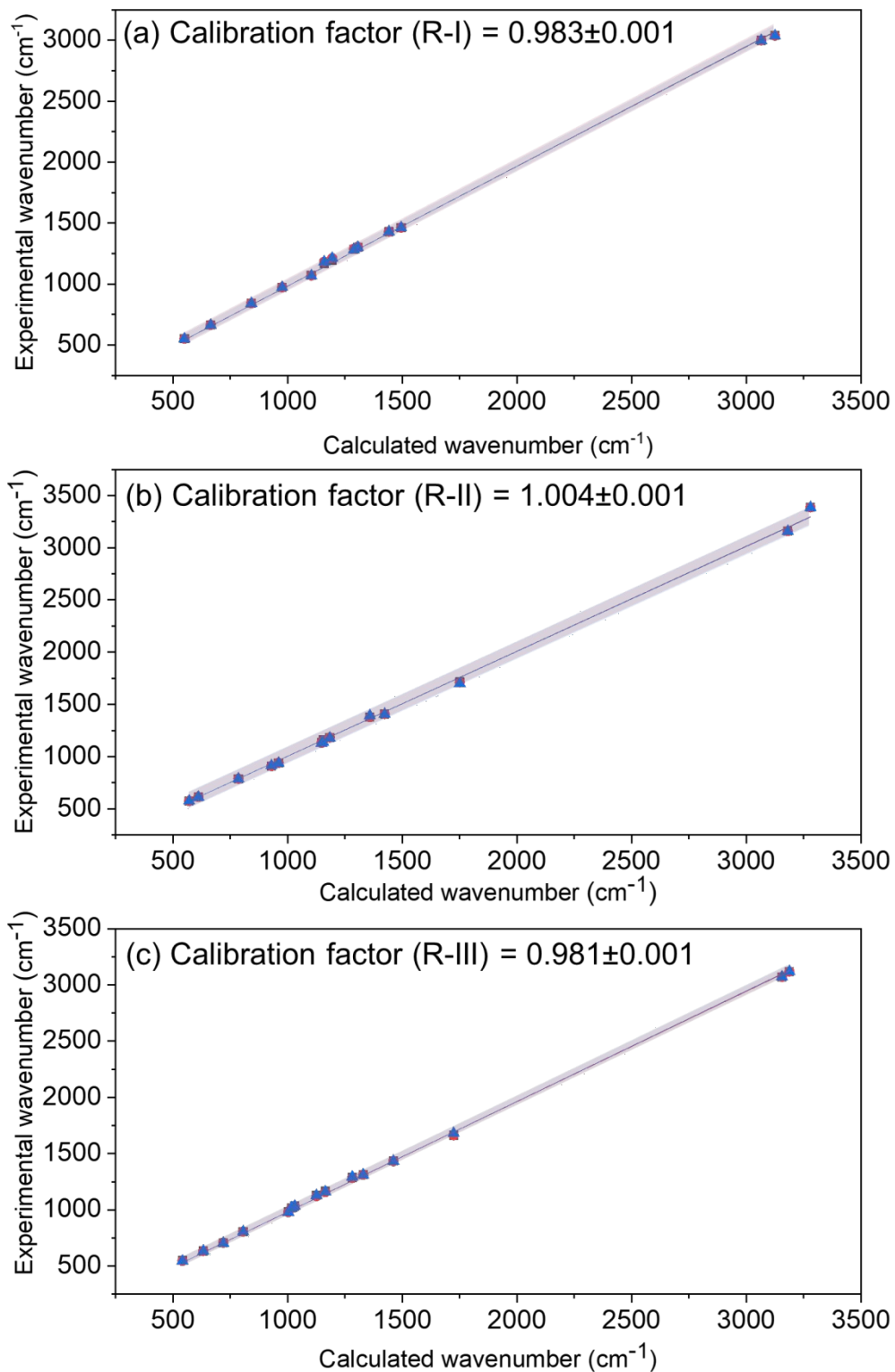


Figure S2: Calibration of calculated frequency with experimental ones; (a) R-I, (b) R-II and (c) R-III.

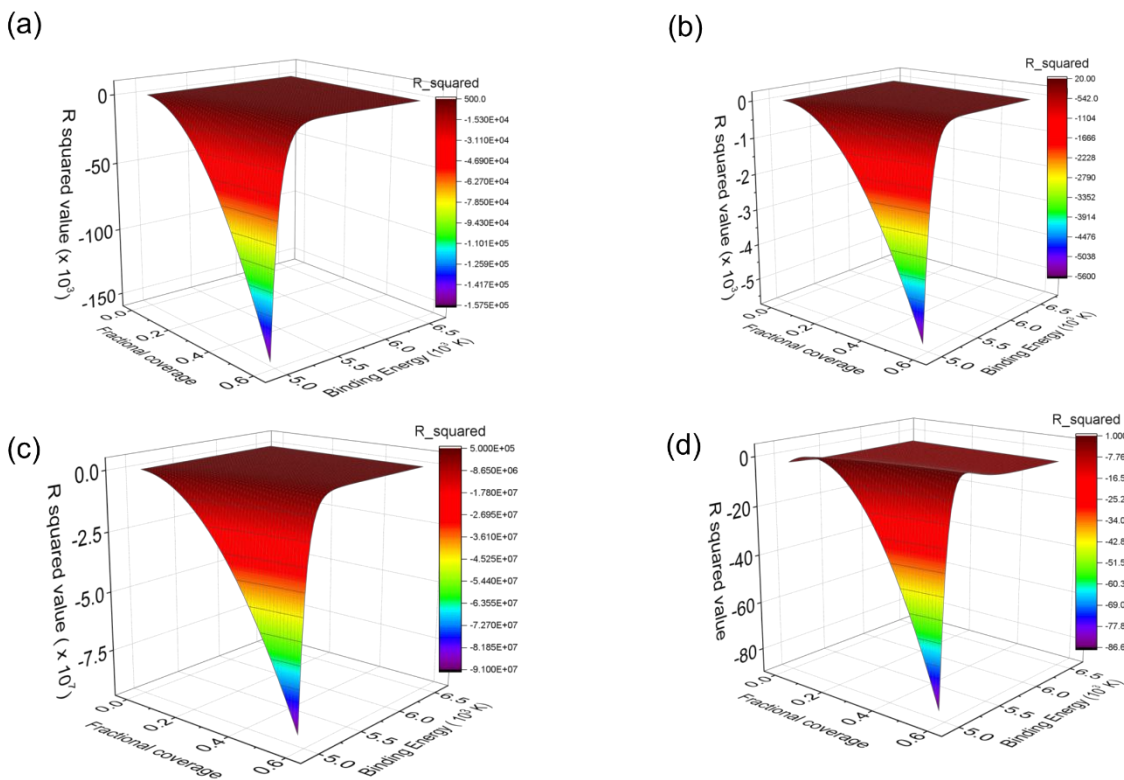


Figure S3: Correlation between fractional surface coverage (θ) and binding energy (E_b) obtained from nonlinear least-squares fitting (SciPy) of TPD data for R-I adsorbed on ASW. Panels correspond to (a) S_2 (layered), (b) S_3 (layered), (c) S_2 (co-deposition), and (d) S_3 (co-deposition). Color gradients represent the distribution of acceptable solutions, with associated R^2 values indicating goodness of fit.

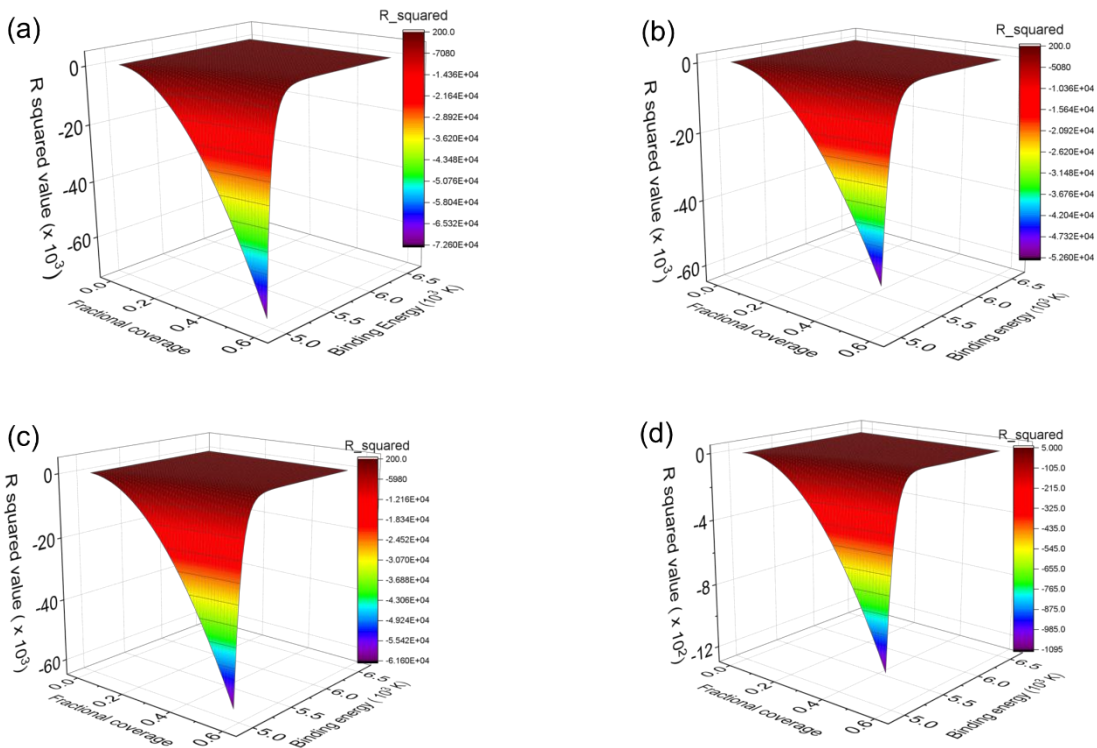


Figure S4: Correlation between fractional surface coverage (θ) and binding energy (E_b) obtained from nonlinear least-squares fitting (SciPy) of TPD data for R-II adsorbed on ASW. Panels correspond to (a) S_2 (layered), (b) S_3 (layered), (c) S_2 (co-deposition), and (d) S_3 (co-deposition). Color gradients represent the distribution of acceptable solutions, with associated R^2 values indicating goodness of fit.

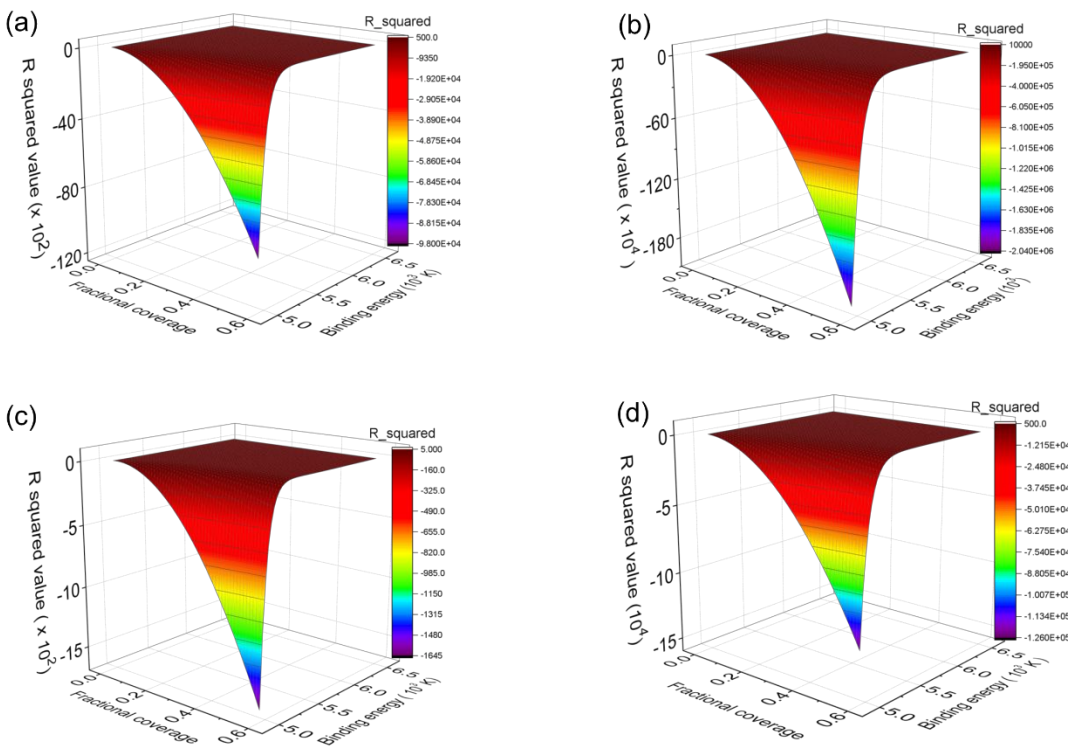


Figure S5: Correlation between fractional surface coverage (θ) and binding energy (E_b) obtained from nonlinear least-squares fitting (SciPy) of TPD data for R-III adsorbed on ASW. Panels correspond to (a) S_2 (layered), (b) S_3 (layered), (c) S_2 (co-deposition), and (d) S_3 (co-deposition). Color gradients represent the distribution of acceptable solutions, with associated R^2 values indicating goodness of fit.

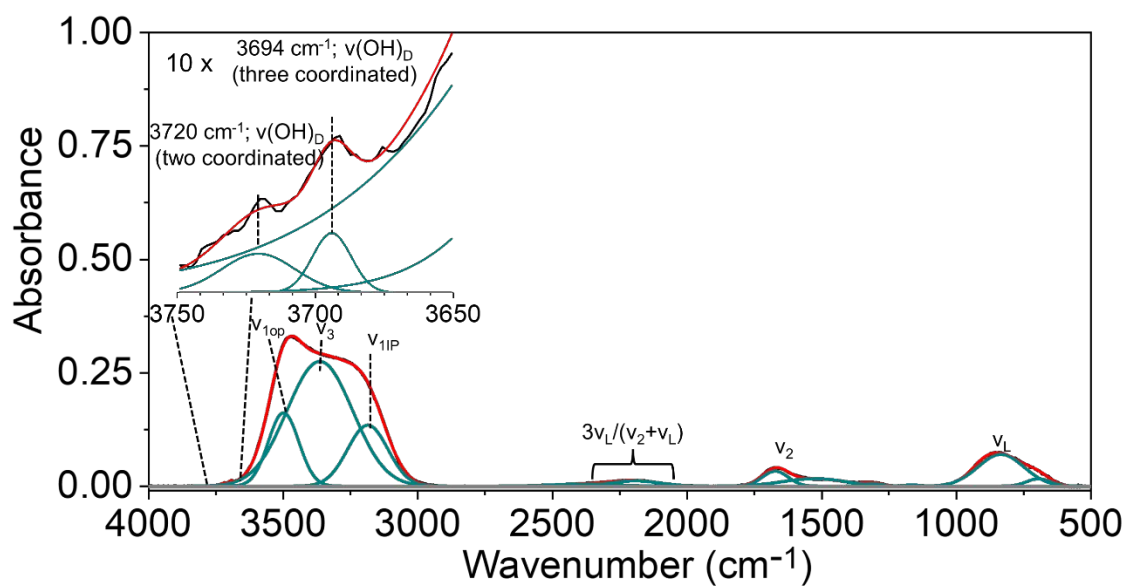


Figure S6: Infrared spectrum of amorphous solid water (ASW) deposited at 10 K, highlighting characteristic vibrational features of the hydrogen-bond network. The dangling OH stretching modes associated with under-coordinated surface water molecules are shown in the inset: $\sim 3720 \text{ cm}^{-1}$ (two-coordinated) and $\sim 3694 \text{ cm}^{-1}$ (three-coordinated).

Table S1: Characteristic vibrational frequencies (cm^{-1}) of amorphous solid water (ASW) and pure refrigerant ices (R-I, R-II, and R-III) with corresponding vibrational assignments. Mode notations follow standard spectroscopic conventions: ν : frequency; σ : Stretching; β : bending; ρ : rocking; δ : deformation; ω : wagging; τ : twisting, s: symmetric; as: asymmetric and OP/IP denote out-of-phase and in-phase motions, respectively.

<i>Pristine ice absorption of water and refrigerants (cm^{-1})</i>	
H₂O; Water	Assignments
3720	$\nu(\text{OH})_{\text{D}}$; Water dangling two coordinated
3694	$\nu(\text{OH})_{\text{D}}$; Water dangling three coordinated
3494	$\nu_{1\text{OP}}(\text{OH})$; $\sigma_{\text{s}}(\text{O-H})$ out of phase (OP)
3351	$\nu_3(\text{OH})$; $\sigma_{\text{as}}(\text{O-H})$ stretching
3110	$\nu_{1\text{IP}}(\text{OH})$; $\sigma_{\text{s}}(\text{O-H})$ in phase (IP)
2070-2400	$(\nu_{\text{L}} + \nu_2)(\text{OH})$; Combination band of libration (ν_{L}) and $\beta(\text{OH})$ (ν_2)
1550-1700	$\nu_2(\text{OH})$; $\beta(\text{OH})$
650-1000	ν_{L} ; Libration
CF₃CH₂F; R-I	Assignments
3002	ν_1 ; $\sigma_{\text{s}}(\text{CH}_2)$
1462	ν_2 ; $\beta(\text{CH}_2)$ scissoring
1429	ν_3 ; $\omega(\text{CH}_2)$ / $\sigma(\text{CC})$
1389	$\nu_7 + \nu_{16}$
1301	ν_{13} ; $\beta(\text{CC})/\tau(\text{CH}_2 \text{ out of plane})$
1283	ν_4 ; $\omega(\text{CH}_2)/\delta_{\text{s}}(\text{CF}_3)$ / $\sigma(\text{CC})$
1250	$\nu_{15} + \nu_{17}$
1190	ν_{14} ; $\nu_{\text{as}}(\text{CF})/\tau(\text{CH}_2 \text{ in plane})$
1162	ν_5 ; $\sigma_{\text{s}}(\text{CF}) + \omega(\text{CH}_2)$
971	ν_{15} ; $\rho(\text{CH}_2)/\beta(\text{CF of CH}_2\text{F})$
841	ν_7 ; $\sigma_{\text{s}}(\text{CF}_3)/\sigma(\text{CC})$
664	ν_8 ; $\delta_{\text{s}}(\text{CF}_3)/\delta(\text{CH}_2\text{F})$
551	ν_9 ; $\delta_{\text{s}}(\text{CF}_3)$
CF₃CF=CH₂; R-II	Assignments
3159	ν_1 ; $\sigma_{\text{as}}(\text{CH}_2)$
3052	ν_2 ; $\sigma_{\text{s}}(\text{CH}_2)$
1700	ν_3 ; $\sigma(\text{C=C})$
1395	ν_4 ; $\rho(\text{CH}_2)/\sigma_{\text{as}}(\text{CF}_3)$
1365	ν_5 ; $\sigma(\text{CF of alkene})/\beta(\text{C—C})$
1224	$\nu_{12} + \nu_{16}$
1208	ν_6 ; $\sigma_{\text{as}}(\text{CF}_3)/\beta(\text{CH}_2)$ scissoring/ $\beta(\text{CF of alkene})$
1172	ν_{15} ; $\delta_{\text{s}}(\text{CF}_3)/\sigma(\text{CF of alkene})/\rho(\text{CH}_2)$
1155	ν_7 ; $\sigma_{\text{s}}(\text{CF}_3)/\tau(\text{CH}_2)$
939	ν_8 ; $\rho(\text{CH}_2)/\sigma(\text{CF of alkene})$
911	ν_{16} ; $\omega(\text{CH}_2)/\beta(\text{C=C})$
787	ν_9 ; $\sigma(\text{C—C})/\rho(\text{CH}_2)/\delta_{\text{s}}(\text{CF}_3)$

617	$\nu_{10}; \delta(\text{CCF})$ in plane/ $\rho(\text{CH}_2)$
576	$\nu_{11}; \delta_s(\text{CF}_3)/\rho(\text{CH}_2)$
CF₃CF=CH₂; R-III	
1661	Assignments $\nu_4; \sigma(\text{C}=\text{C})$
1436	$\nu_5; \beta(\text{CH}_2)$ scissoring/ $\beta(\text{C}=\text{CH})/\beta(\text{C}-\text{C})$
1351	$\nu_{10} + \nu_{20}$
1313	$\nu_6; \rho(\text{HC}=\text{CH})/\delta_s(\text{CF}_3)$
1290	$\nu_7; \sigma_{\text{as}}(\text{CF}_3)/\rho(\text{HC}=\text{CH})/\beta(\text{C}-\text{C})$
1173	$\nu_8; \sigma_{\text{as}}(\text{CF}_3)/\rho(\text{HCH})/\delta(\text{C}=\text{C}-\text{C})$ in plane
1134	$\nu_{15}; \sigma_{\text{as}}(\text{CF}_3)/\tau(\text{HCH})$ in plane/ $\delta(\text{C}=\text{C}-\text{C})$ out of plane
1015	$\nu_9; \rho(\text{CH}_2)/\delta(\text{C}=\text{C}-\text{C})$ in plane
978	$\nu_{16}; \tau(\text{HCH})$ out of plane/ $\tau(\text{HC}=\text{CH})$ out of plane
635	$\nu_{11}; \delta(\text{CCF})$ in plane/ $\rho(\text{CH}_2)$
541	$\nu_{12}; \delta_{\text{as}}(\text{CF}_3)/\tau(\text{HCH})$ out of plane/ $\sigma(\text{C}-\text{C})/\delta(\text{C}=\text{C}-\text{C})$ in plane

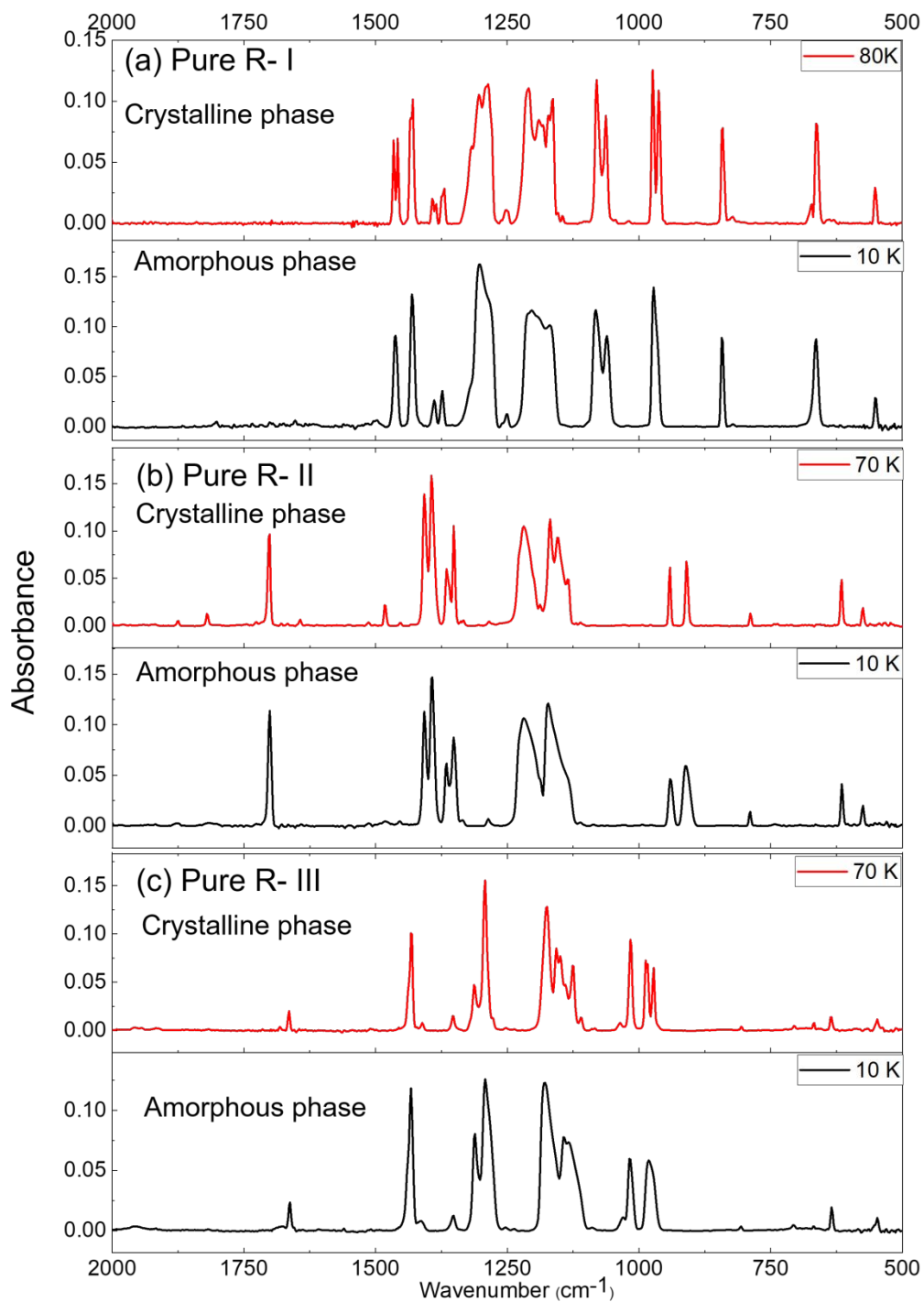


Figure S7: Comparison of the infrared spectra of the pure refrigerants. (a) R-I, (b) R-II, and (c) R-III at 10 K and near the S_1 sublimation event.

Table S2: Coordinates of optimized refrigerants on ice surfaces and encapsulated within the ice matrix. Distances in Angstrom.

R-I Encapsulated:

O	-2.89513045	-2.11547904	-2.61255735
O	-1.90847046	-3.97521731	0.18068697
O	-3.91378306	-1.13510140	-0.20306670
O	-2.77012315	-2.40255025	4.13599111
O	4.64764545	2.36611552	-3.45941923
O	1.07188503	0.02339514	-3.43510557
O	5.33129973	-2.12292646	-3.16755481
O	-2.40947719	1.88342367	-3.13829292
O	-5.51053326	2.65527301	-0.27727518
O	-0.93552804	3.31835447	-0.02607187
O	4.96887301	2.21594776	4.56762061
O	1.26646990	-0.28059781	4.24652555
O	5.41254219	-2.26419478	2.57390580
O	-2.46913171	2.23240422	3.80825028
O	5.80280304	0.80639168	0.36620737
O	1.13044478	-4.41770962	-2.51776388
O	-6.57878397	0.19707207	-3.02697049
O	1.30644267	4.63928718	-2.77035641
O	1.03873142	-4.72067185	2.85733425
O	-6.48730616	0.05351301	2.62166425
O	1.64837005	4.38189331	2.46785904
O	0.81138358	-3.92667712	0.22808540
O	-6.46477736	0.12935945	-0.24434811
O	1.70269801	3.81654587	-0.16090255

O	-1.38025937	-0.31168431	3.42469514
O	-1.52354206	-0.55397715	-4.31082182
O	2.32354075	2.33980733	4.24795293
O	2.64471739	-2.38696363	3.37880837
O	6.16490980	0.30648523	3.15164471
O	-1.17933884	4.40905637	2.47722655
O	-4.81766765	2.28996853	2.44412133
O	4.07388486	2.53314866	-0.65552039
O	5.75926486	-1.88457172	-0.20062467
O	2.11305072	2.45493745	-4.46013850
O	2.63141622	-2.14294293	-2.93238717
O	6.01170552	0.22470745	-4.36442880
O	-1.49338640	4.42456386	-2.42440378
O	-5.08414125	2.36235041	-2.96538918
O	-1.62382751	-4.68392807	2.82156749
O	-4.90144977	-2.16036199	2.48117705
O	-1.72986069	-4.53905748	-2.64390577
O	-5.29737726	-2.07039118	-3.88434380
H	-3.06314306	-1.74020016	-1.71781484
H	-0.95927607	-3.72564981	0.10367691
H	-3.98777219	-1.71612181	0.57440423
H	-2.83787812	-2.45957899	5.10068250
H	4.41766406	2.30608964	-2.51173167
H	0.87042385	0.24027609	-2.51081446
H	5.72386546	-2.08183346	-2.27971301
H	-2.22514068	1.38159376	-2.32415725
H	-4.73227577	2.58710276	0.30432069

H	-1.15404292	3.83539548	0.78989671
H	5.12056838	2.35263270	5.51461401
H	1.33558212	-0.47166809	5.19455798
H	5.70672781	-2.85734610	3.27909983
H	-2.65544582	2.48538776	4.72411803
H	5.83537000	0.70924833	1.33971647
H	1.06604014	-4.42982556	-1.53686170
H	-6.75052915	-0.01418222	-2.08840929
H	1.58224665	4.45084141	-1.83918717
H	1.33020329	-5.57809486	3.20983536
H	-7.03127523	0.03814456	3.42795811
H	2.09356200	5.21066345	2.70679331
H	-2.33160747	-1.47840351	-3.13686213
H	-2.07019230	-4.49485913	-0.63204608
H	-4.80438443	-0.72225609	-0.29032411
H	-2.20694124	-1.58787477	3.92902435
H	3.77161055	2.40652234	-3.92159002
H	1.69545657	-0.74636005	-3.38063949
H	5.62888649	-1.29621638	-3.63285334
H	-3.38685678	2.02778205	-3.14759589
H	-5.19979662	2.72712175	-1.21104994
H	-1.24689199	3.83595295	-0.81935281
H	3.97651814	2.26390192	4.43215439
H	1.78884180	-1.01048783	3.80738423
H	5.65076540	-1.35209245	2.87421643
H	-3.33903494	2.27068558	3.32817904
H	5.80719042	-0.11738996	0.01223550

H	0.18670523	-4.44352792	-2.78910351
H	-6.14410725	-0.60693494	-3.40783561
H	1.84612166	5.38120472	-3.08149741
H	0.03625079	-4.70147754	2.96501522
H	-5.94385303	-0.77754555	2.63363413
H	1.77911891	4.25103580	1.48400149
H	1.52950078	-3.26045516	0.18043032
H	2.36062212	3.09287319	-0.28909729
H	-1.73446982	0.59408406	3.56779427
H	-0.42518832	-0.28170411	3.66808821
H	-6.20257773	1.08834161	-0.24263663
H	0.77465218	3.43708573	-0.15033790
H	-1.88927072	0.35312311	-4.24700075
H	-0.56612647	-0.43314766	-4.11642097
H	1.92149401	1.46374200	4.05253284
H	3.45830273	-2.35415086	2.84052848
H	5.70118006	0.98296660	3.72832204
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H	4.63366374	1.80662090	-0.24971281
H	4.79641646	-2.09192050	-0.21828210
H	1.70919093	1.60006523	-4.19290559
H	3.58822352	-2.21700263	-3.20510587
H	5.51397925	1.02721052	-4.03780907
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H	-5.46904920	3.04927549	-3.53399364
H	-4.16511514	-2.25032343	3.14034692

H	-1.99416565	-3.91269106	3.29909682
H	-4.41432155	-2.13019871	-3.42968028
H	-2.12911043	-3.62399222	-2.66983082
H	4.62323114	3.32506701	-0.55802360
H	6.01806133	-2.18428856	0.69307854
H	-5.41845942	1.50755995	2.48796332
H	-0.21039611	4.44207721	2.62534219
H	2.13002702	-3.18835403	3.13081893
H	2.05278831	2.96917310	3.54309923
H	7.11673880	0.46131055	3.26185649
H	-5.65759416	1.53339660	-3.05986232
H	-0.57880432	4.60905773	-2.72929098
H	2.15870795	-3.00574898	-3.05806752
H	1.70000418	3.14842706	-3.90773616
H	6.92180400	0.52322281	-4.50104448
H	0.96119578	-4.40873602	1.07045354
H	-6.88819224	-0.01974804	0.61907326
H	-1.82340969	-4.52523006	1.86228725
H	-5.25995330	-3.05141594	2.35979048
H	-2.08978003	-5.00204451	-3.41717330
H	-5.74331000	-2.91428731	-3.73697749
O	3.19443524	-2.75711673	-0.41696488
H	3.47709602	-3.65641143	-0.66157079
H	2.92462249	-2.36153832	-1.30108308
C	-1.14953144	0.28963741	0.19244439
C	0.34980343	0.22418375	0.42882240
F	-1.36199106	-0.01302220	-1.16320008

H	-1.66493565	-0.44445661	0.81230476
H	-1.49384951	1.31120625	0.37486832
F	0.81593118	-1.04492143	0.43200655
F	1.04262618	0.88707289	-0.53986312
F	0.67750022	0.78824174	1.60994289

R-I Surface:

C	-1.10455171	0.97469325	-4.07441213
C	0.20224392	0.58298259	-4.74388809
F	-2.04377128	1.26487001	-5.06251169
H	-1.45543493	0.13394665	-3.47186166
H	-0.94203826	1.86289977	-3.45773953
F	0.06884424	-0.52070053	-5.51998183
F	0.68158208	1.57098084	-5.53987977
F	1.13613681	0.31979003	-3.80554299
H	1.60687727	5.40925859	2.35534812
H	-3.16747418	-5.66289944	0.14935955
H	0.73922663	0.89237295	0.20693536
H	4.62578175	3.18243176	0.16133311
H	0.59965853	-3.43852827	0.23160384
H	-3.26017948	3.47145220	0.34729176
H	-3.13236938	-1.25678812	0.37572134
H	4.46337251	-1.24941043	0.36763268
H	0.61178079	5.45999803	0.15439153
O	-3.20814269	3.46053524	-0.64098256
O	0.62128636	-3.49751406	-0.74740832
O	-4.54371182	-3.32498263	-1.41905252

H	-2.21444834	3.17027752	2.34215783
H	-3.57142275	-0.40802239	2.33285692
O	-0.68645425	-5.67602663	-1.72760533
H	3.29497016	5.58615974	-2.42959780
H	-0.08720514	-6.43280890	-1.66159536
H	-2.36575649	-5.70582787	-1.19015744
H	1.62588568	0.95714817	-1.09961838
H	4.19825020	3.94156739	-1.11570044
H	0.15536904	-2.67389352	-1.10098600
H	-3.63189585	4.26729606	-0.96800282
H	-3.63080035	-1.93727550	-0.94843115
H	4.06213356	-1.98293133	-0.94970385
H	0.18691024	4.67831397	-1.12428253
O	0.63367922	5.51365455	-0.81720974
O	4.71058871	3.15431159	-0.80671029
O	-3.28009513	-5.65314221	-0.81930249
O	-0.58929079	-1.35062106	-1.67105736
H	0.19157030	1.77290678	2.33210461
O	0.66845364	0.90973954	-0.76595226
O	-0.56552207	-5.54742573	3.01038955
H	-3.62474896	-4.81592414	2.36302358
H	-3.87861607	0.24380493	-1.18893876
H	3.68513035	0.19049111	-1.21481961
H	-0.10676511	-0.53583010	-1.38870549
H	-4.80501484	-3.31642968	-2.35148054
H	2.27375475	-3.41007345	-1.23473670
H	-1.50851925	3.19895276	-1.21182479

H	-0.18511531	-4.89044282	-1.38588602
H	-3.96080491	1.80627529	-1.31638572
H	3.73034509	1.76947273	-1.33016055
H	-4.08255636	-4.19341943	-1.26248904
H	3.22658977	-3.35818916	-2.46726299
H	-0.14271906	2.36962873	-1.21902631
H	-1.49686220	-1.27679636	-1.29003779
H	2.26049091	5.38933627	-1.27061413
H	-3.55108595	2.36065764	2.30359495
O	4.45104323	3.21567311	2.07373322
O	-3.10403877	-1.17010089	-0.59714178
H	-3.57258977	-6.41043589	2.42568122
O	3.16073723	0.98079711	-1.49774778
O	4.49952723	-1.17010089	-0.59714178
O	3.22987223	-3.36920789	-1.49774778
O	-4.44282877	0.98079711	-1.49774778
O	3.22987223	5.33080311	-1.49774778
O	-0.57191077	3.21567311	-1.49774778
H	3.99732323	2.38883611	2.42568122
O	-3.08338777	-5.60408389	2.07373322
H	5.39396523	-1.23359289	2.42568122
O	-0.62039477	-1.17010089	2.97433922
O	-0.62039477	3.13169611	2.97433922
O	-3.15252277	-1.25407789	2.07373322
H	0.22919323	0.17444611	2.42568122
H	1.59218223	-3.38969389	2.42568122
H	-0.57586777	-5.60408389	3.97985422

H	-4.37765077	0.98079711	3.97985422
H	3.22591523	0.98079711	3.97985422
H	3.19728323	5.38724911	3.97985422
H	-0.60449977	-1.19763289	3.97985422
H	-4.40628277	-3.42565389	3.97985422
H	3.19728323	-3.42565389	3.97985422
H	-0.60449977	3.15922811	3.97985422
O	3.25770523	0.98079711	2.97433922
H	-2.20960077	-1.23359289	2.42568122
H	3.99732323	-0.42724089	2.42568122
O	3.18138823	-3.45318489	2.97433922
H	0.19554023	6.15764011	2.42568122
O	0.64926023	-3.36920789	2.07373322
O	0.64926023	5.33080311	2.07373322
O	-4.42217777	-3.45318489	2.97433922
H	-1.49988377	-5.60408389	2.65282022
H	-5.30166677	0.98079711	2.65282022
H	2.30189923	0.98079711	2.65282022
H	3.65929123	4.58702811	2.65282022
H	-0.14249177	-1.99785389	2.65282022
H	-3.94427477	-2.62543289	2.65282022
H	3.65929123	-2.62543289	2.65282022
H	-0.14249177	3.95944911	2.65282022
H	5.39396523	3.19518811	2.42568122
O	3.18138823	5.41478011	2.97433922
O	4.45104323	-1.25407789	2.07373322
O	0.71839523	0.98079711	2.07373322

O	-4.34586077	0.98079711	2.97433922
H	0.19554023	-4.19604489	2.42568122
O	-3.15252277	3.21567311	2.07373322

R-II Encapsulated:

O	-2.80289441	-2.45065457	-2.11993171
O	-1.58854360	-4.28461547	-0.54292397
O	-5.01502273	-2.26429058	-0.30446866
O	-2.65343142	-2.24796104	3.78653407
O	4.19756110	2.22544534	-3.80510580
O	0.48006390	1.14582693	-2.20208641
O	4.82210626	-1.37763836	-2.54595028
O	-3.22180487	2.36611747	-3.31087641
O	-3.58555151	1.68134686	-0.60178325
O	-0.32172194	3.23727363	-0.61580702
O	4.95043805	2.34102344	4.90891522
O	1.71169418	-0.16013019	4.24997557
O	5.40083826	-2.20490439	3.10794102
O	-1.96232859	2.34530290	3.72461542
O	4.24459151	0.57625873	0.92552667
O	1.04741072	-2.99436321	-3.06883235
O	-6.58301339	-0.15387870	-3.40186940
O	1.21458990	5.14272509	-3.24210852
O	0.97135153	-4.60394717	2.50201168
O	-6.08652402	0.64806146	2.14924802
O	2.11693488	4.50051264	1.97622798
O	1.14746867	-4.84515826	-0.33884700
O	-5.94656384	0.31570516	-0.68392813

O	2.11463202	4.31547621	-0.71567153
O	-1.06739553	-0.21244181	4.33455078
O	-2.02424766	0.13826412	-2.19906763
O	2.46253402	2.53041388	3.97116865
O	2.63445951	-2.59509185	3.68684724
O	5.90248732	0.48628239	3.27164383
O	-0.67810595	4.09510542	1.94280118
O	-4.10082960	2.47736863	2.07475315
O	4.17925017	2.48718610	-0.96120609
O	5.34681008	-1.85607470	0.31529509
O	1.54695665	2.55139850	-4.38507828
O	2.22193643	-0.88477256	-1.82917332
O	5.67393214	0.13445532	-4.61611113
O	-1.53300303	4.46768429	-2.65099973
O	-5.47717763	1.90985073	-4.75707587
O	-1.77967861	-4.39972349	2.35785654
O	-5.03404196	-1.73749262	2.36136711
O	-1.33489735	-2.92451489	-4.43559578
O	-5.42037481	-2.71802235	-3.23375231
H	-2.25854565	-3.04874701	-1.53919701
H	-1.75168491	-4.18437211	0.41510015
H	-4.17566690	-2.34103475	-0.80661076
H	-2.95494172	-2.45330260	4.68534720
H	4.13841395	2.17457628	-2.83103590
H	0.30030004	1.77078708	-1.46559043
H	5.45238154	-1.28727313	-1.81152941
H	-3.59600007	2.46734834	-2.41329313

H	-3.43859300	1.92901818	0.33136946
H	-0.64136618	3.50962236	0.27924461
H	4.91049289	2.29699838	5.87486223
H	1.90149138	-0.18659788	5.20136397
H	5.98134477	-2.72925398	3.67906722
H	-2.19430263	2.77053967	4.56449072
H	4.74933952	0.72061713	1.75216784
H	0.80872579	-3.60613611	-2.35262942
H	-6.55212074	0.06906127	-2.44834390
H	1.64861442	5.00582827	-2.36574983
H	1.17145471	-5.42480461	2.97935495
H	-6.85865317	0.68623711	2.73313401
H	2.50101088	5.32744713	2.30600321
H	-2.43859000	-1.52805512	-2.07546991
H	-0.62439658	-4.47472902	-0.60750544
H	-5.36147242	-1.36642872	-0.53078037
H	-2.00318159	-1.48538719	3.89696437
H	3.25684876	2.30764605	-4.11355174
H	1.18564288	0.50718021	-1.92608733
H	5.21183905	-0.90453540	-3.32892822
H	-4.00138331	2.27197212	-3.91887906
H	-2.85255886	1.08185814	-0.88399124
H	-0.87130791	3.71097189	-1.30437709
H	4.01247135	2.47555056	4.58558138
H	2.05296052	-1.03946869	3.91204883
H	5.58786926	-1.25376146	3.30962043
H	-2.78749951	2.35550228	3.17189104

H	4.56829495	-0.30410267	0.60112167
H	0.24957202	-2.95604648	-3.65236105
H	-6.16563068	-1.04390388	-3.46667170
H	1.65136615	5.90134818	-3.65575264
H	-0.01371635	-4.50808951	2.53852451
H	-5.66417680	-0.26616101	2.29035088
H	2.21374255	4.51836804	0.97933910
H	1.96596015	-4.35473705	-0.58596479
H	2.79477052	3.61583494	-0.87414370
H	-1.37518914	0.67454804	4.04301563
H	-0.08994632	-0.21954051	4.21581167
H	-5.10214173	0.83680895	-0.71480466
H	1.22141785	3.86086829	-0.70315627
H	-2.44208805	0.73481078	-2.86569495
H	-1.06159591	0.37544674	-2.23628598
H	2.15627962	1.61725172	3.78277916
H	3.54291535	-2.58495005	3.32202127
H	5.58457671	1.13035297	3.97029896
H	-0.97959302	3.47879728	2.64180104
H	-4.45531724	3.36050174	1.88684790
H	4.21013436	1.76603001	-0.26991668
H	4.64879458	-2.47049286	-0.01430977
H	1.08620448	2.01998312	-3.69678696
H	3.12737387	-0.81132902	-2.21831196
H	5.12659233	0.94555217	-4.41163808
H	-2.03740517	3.79790853	-3.16679359
H	-5.47045958	1.71913578	-5.70579114

H	-4.15809678	-1.84134950	2.78971453
H	-2.11581880	-3.61556103	2.86695629
H	-4.46756055	-2.64786094	-3.01895806
H	-1.98279565	-2.80602014	-3.70179773
H	5.02662801	2.95436118	-0.89346210
H	5.54270375	-2.14880598	1.22736311
H	-4.87931126	1.86078267	2.16123339
H	0.24652233	4.34526973	2.14673942
H	2.08890183	-3.21997614	3.16178694
H	2.36325733	3.07522597	3.16213096
H	6.79646324	0.77234967	3.03032910
H	-5.90852438	1.12492050	-4.31601680
H	-0.74830311	4.74087454	-3.16263878
H	1.72562674	-1.51739931	-2.41512888
H	1.40093493	3.48210836	-4.12220363
H	5.41532562	-0.15041609	-5.50514937
H	1.15004326	-4.82226843	0.64178009
H	-6.30667185	0.49596441	0.20685644
H	-2.39408417	-5.13028392	2.53070670
H	-4.94507857	-2.05790575	1.42435142
H	-1.64502601	-3.67727959	-4.95874224
H	-5.80792529	-3.00525184	-2.38848249
O	3.29706317	-3.20214123	-0.88315713
H	3.71360514	-3.28042074	-1.76218559
H	2.79668627	-2.34961001	-0.97036104
C	0.03521840	0.20330290	1.04956898
C	0.12001363	-1.27325185	0.77709705

F	-0.26698681	-1.57391198	-0.48125735
F	1.37214819	-1.74127449	0.95493081
C	1.05371274	1.02522083	1.22995395
F	-0.69572337	-1.96749843	1.61564449
F	-1.25866292	0.61367575	1.06429359
H	2.07589166	0.66004207	1.19290409
H	0.86262577	2.07875029	1.39549034

R-II Surface:

C	0.14378591	-0.57606571	-4.05528255
C	0.94130580	-1.81737294	-4.34543057
F	2.26634725	-1.62082165	-4.13044949
F	0.55967055	-2.86011303	-3.57012876
C	0.61742318	0.59084990	-3.64970892
F	0.79572547	-2.21650157	-5.63421021
F	-1.17605750	-0.80515247	-4.26740307
H	1.67695443	0.72165091	-3.45766510
H	-0.05432095	1.42079298	-3.45552729
H	-3.16864480	-5.49865354	0.08526092
H	0.76308483	1.19198096	0.24861425
H	4.61037812	3.36569592	0.09971511
H	0.71420779	-3.57988067	0.25812520
H	-3.26827541	3.65165344	0.29005255
H	-3.21732384	-1.10971948	0.31335969
H	4.45736253	-1.06447896	0.31506341

H	0.62608501	5.62907276	0.10638231
O	-3.22326687	3.64876089	-0.69849595
O	0.68259674	-3.56844822	-0.72364149
O	-4.30678196	-3.17224865	-1.77260697
H	-2.22045512	3.34354638	2.28271497
H	-3.57534869	-0.22948132	2.27712976
O	-0.70902176	-5.60622676	-1.85030149
H	3.29658019	5.83467550	-2.45997350
H	-0.10845559	-6.36076967	-1.92506237
H	-2.35892304	-5.63948021	-1.24499603
H	1.66388166	1.20364991	-1.05210673
H	4.18238368	4.11699301	-1.18395342
H	0.23407513	-2.68463967	-0.88223791
H	-3.66195433	4.45138360	-1.01515532
H	-3.54889937	-1.77502277	-1.08049573
H	4.04312408	-1.80673169	-0.99182923
H	0.17841701	4.84114950	-1.16545830
O	0.63815640	5.67504781	-0.86603269
O	4.68776805	3.32658157	-0.86904994
O	-3.27288860	-5.53847741	-0.88343279
O	-0.44429308	-1.23092822	-0.58756864
H	0.18802432	1.94808901	2.29343874
O	0.70767705	1.19429034	-0.72664853
O	-0.57150366	-5.38165078	2.95564627
H	-3.63014220	-4.63797320	2.31025488
H	-3.88362968	0.41194625	-1.26794552
H	3.67025640	0.36166817	-1.25942448

H	-0.01507782	-0.37719985	-0.83069509
H	-4.24723354	-3.16111903	-2.73943153
H	2.28773778	-3.33518063	-1.24828565
H	-1.52272272	3.37780664	-1.29193159
H	-0.17778951	-4.86020225	-1.46570477
H	-3.95373143	1.97593326	-1.37289004
H	3.73159286	1.94299323	-1.37887739
H	-3.93641049	-4.04859817	-1.48260833
H	3.15619798	-3.09530695	-2.51439005
H	-0.15139320	2.55652242	-1.24421062
H	-1.41205540	-1.12874071	-0.75982380
H	2.25134330	5.55971412	-1.32296884
H	-3.55687642	2.53548475	2.24281788
O	4.44397124	3.39324529	2.01982427
O	-3.11111076	-0.99252871	-0.65105073
H	-3.57966176	-6.23286371	2.37177227
O	3.15366524	1.15836929	-1.55165673
O	4.49245524	-0.99252871	-0.65105073
O	3.22280024	-3.19163571	-1.55165673
O	-4.44990076	1.15836929	-1.55165673
O	3.22280024	5.50837529	-1.55165673
O	-0.57898276	3.39324529	-1.55165673
H	3.99025124	2.56640829	2.37177227
O	-3.09045976	-5.42651171	2.01982427
H	5.38689324	-1.05602071	2.37177227
O	-0.62746676	-0.99252871	2.92043027
O	-0.62746676	3.30926829	2.92043027

O	-3.15959476	-1.07650571	2.01982427
H	0.22212124	0.35201829	2.37177227
H	1.58511024	-3.21212171	2.37177227
H	-0.58293976	-5.42651171	3.92594527
H	-4.38472276	1.15836929	3.92594527
H	3.21884324	1.15836929	3.92594527
H	3.19021124	5.56482129	3.92594527
H	-0.61157176	-1.02006071	3.92594527
H	-4.41335476	-3.24808171	3.92594527
H	3.19021124	-3.24808171	3.92594527
H	-0.61157176	3.33680029	3.92594527
O	3.25063324	1.15836929	2.92043027
H	-2.21667276	-1.05602071	2.37177227
H	3.99025124	-0.24966871	2.37177227
O	3.17431624	-3.27561271	2.92043027
H	0.18846824	6.33521229	2.37177227
O	0.64218824	-3.19163571	2.01982427
O	0.64218824	5.50837529	2.01982427
O	-4.42924976	-3.27561271	2.92043027
H	-1.50695576	-5.42651171	2.59891127
H	-5.30873876	1.15836929	2.59891127
H	2.29482724	1.15836929	2.59891127
H	3.65221924	4.76460029	2.59891127
H	-0.14956376	-1.82028171	2.59891127
H	-3.95134676	-2.44786071	2.59891127
H	3.65221924	-2.44786071	2.59891127
H	-0.14956376	4.13702129	2.59891127

H	5.38689324	3.37276029	2.37177227
O	3.17431624	5.59235229	2.92043027
O	4.44397124	-1.07650571	2.01982427
O	0.71132324	1.15836929	2.01982427
O	-4.35293276	1.15836929	2.92043027
H	0.18846824	-4.01847271	2.37177227
O	-3.15959476	3.39324529	2.01982427
H	1.58511024	5.52886129	2.37177227

R-III Encapsulated:

O	-2.19136612	-2.49428537	-3.25348141
O	-1.33003608	-3.22321277	-0.65435392
O	-4.05317877	-2.88593645	0.05997154
O	-2.47307338	-2.00890295	4.29453798
O	4.40447523	2.47781953	-3.52847155
O	0.71624405	0.69866166	-2.25524791
O	4.70416118	-1.57808736	-2.77573800
O	-2.32213810	2.35474753	-3.43103009
O	-3.76434911	2.31354412	-0.28278690
O	-1.20109758	3.41863221	-0.63458683
O	5.22765843	2.34463839	4.32157374
O	1.68227872	-0.23112396	4.13246873
O	5.21590162	-2.38987363	2.81966319
O	-2.23029768	2.58290092	3.77083641
O	4.22568744	0.22082377	0.72959895
O	1.24588771	-4.04720759	-3.19201657

O	-6.02789553	-0.10356230	-2.57090346
O	1.25433827	5.12814198	-3.05898588
O	0.91121804	-4.73392111	2.50584090
O	-5.95477411	-0.08368510	2.34158454
O	1.73399653	4.31887966	2.01766656
O	0.72710154	-5.00124971	-0.29472858
O	-4.76722106	-0.24543431	-0.14411980
O	1.55035434	3.82433730	-0.63672244
O	-1.05365305	0.17957472	4.63929452
O	-1.21824929	-0.15303052	-4.13654249
O	2.59939708	2.42215360	3.92366148
O	2.34250251	-2.25690099	2.47403627
O	6.02375397	0.22069072	2.95388532
O	-1.07386882	4.32388884	1.91705126
O	-4.50462339	2.33595459	2.44801454
O	3.87486346	2.40099279	-0.73347777
O	5.21958932	-2.24469433	0.00503697
O	1.73696297	2.52772373	-4.16936625
O	2.07984222	-1.62538664	-2.22022024
O	5.91915749	0.36398064	-4.24184632
O	-1.55109352	4.96816310	-2.79921373
O	-4.99069490	2.29231343	-2.81112992
O	-1.58955902	-3.86754627	2.50234517
O	-4.76718800	-2.40817536	2.72713644
O	-0.80930150	-4.10198801	-4.96447318
O	-4.95581833	-2.64063178	-2.97132940
H	-1.79906662	-2.65932685	-2.36792177

H	-1.05417218	-2.55826311	0.00034785
H	-3.14461578	-3.13091487	-0.21481466
H	-2.64778015	-2.28631284	5.20645025
H	4.27403865	2.36794634	-2.56427362
H	0.22185784	0.77061609	-1.42480119
H	5.22474956	-1.63456068	-1.95407427
H	-1.97909519	2.13969275	-2.54713446
H	-2.86340610	2.68586034	-0.43063152
H	-1.23296765	3.85947785	0.25806940
H	5.37977821	2.48572846	5.26742923
H	2.03606629	-0.51407984	4.98934031
H	5.62706751	-3.00144888	3.44727752
H	-2.47164321	3.10529414	4.55113675
H	4.80151012	0.32679959	1.51398480
H	0.80680901	-4.54595273	-2.48267551
H	-5.73582956	-0.19478222	-1.63413652
H	1.50663851	4.81859067	-2.15535368
H	1.04432330	-5.44976207	3.14525715
H	-6.91322775	-0.13460818	2.48613777
H	2.17289211	5.16486313	2.19074517
H	-1.88620927	-1.59153453	-3.54718706
H	-0.63768493	-3.92757877	-0.58100575
H	-4.14472133	-1.92017522	-0.12384341
H	-1.94236193	-1.15292644	4.35926542
H	3.48231341	2.46673206	-3.89027310
H	1.24959747	-0.14122447	-2.19243299
H	5.16378295	-0.92087160	-3.35996771

H	-3.30623265	2.32993071	-3.33030545
H	-4.29400018	2.52714339	-1.08336240
H	-1.37197393	4.12547186	-1.32223908
H	4.23836180	2.42059951	4.17672964
H	1.88568977	-0.97852427	3.50190831
H	5.53439986	-1.48174844	3.04457159
H	-3.10136770	2.40946646	3.29141886
H	4.50818634	-0.63811863	0.32867358
H	0.62313685	-4.12250594	-3.96142011
H	-5.70193419	-0.94685053	-2.96940878
H	1.93662562	5.75082798	-3.35357614
H	-0.04221777	-4.45438202	2.58669380
H	-5.57053203	-0.98316932	2.58015628
H	1.75025532	4.18914893	1.02777563
H	1.60612094	-4.57056660	-0.43177690
H	2.22732067	3.11926112	-0.78305506
H	-1.41338536	1.02680004	4.28953422
H	-0.11263927	0.10812867	4.36744799
H	-4.18473949	0.54693626	-0.18640014
H	0.64411396	3.43498072	-0.71316623
H	-1.75263656	0.66361225	-4.20066304
H	-0.45917159	0.12049656	-3.57967619
H	2.21026292	1.52654721	3.82337887
H	3.30883308	-2.40173547	2.51474950
H	5.77140757	0.98393631	3.55402137
H	-1.47929500	3.75103883	2.60742709
H	-4.32957122	2.44707541	1.48726989

H	4.03232653	1.54607455	-0.23283320
H	4.48308598	-2.86527685	-0.21619376
H	1.32176256	1.93941399	-3.50823852
H	3.00521109	-1.49522732	-2.56978591
H	5.37369501	1.17931435	-4.05537758
H	-1.81840368	4.19406163	-3.34153680
H	-5.64256246	2.89026788	-3.20434996
H	-3.95892973	-2.19427690	3.23922535
H	-1.89559626	-3.21444922	3.17567250
H	-3.98547183	-2.59772432	-3.14705295
H	-1.42096743	-3.53977387	-4.42052202
H	4.52211104	3.03169573	-0.38276733
H	5.46578596	-2.46438679	0.92638102
H	-5.01795478	1.50417433	2.53268353
H	-0.12727884	4.41699792	2.14941862
H	1.91063458	-3.13936677	2.51523195
H	2.24809549	2.99918719	3.21384048
H	6.90338211	0.42584026	2.60498575
H	-5.38484596	1.35931705	-2.85665278
H	-0.64225475	5.19907801	-3.08093562
H	1.66459049	-2.33662389	-2.77180535
H	1.46432816	3.43541509	-3.93173351
H	5.95361000	0.27062666	-5.20451878
H	0.71701867	-5.16640871	0.67128349
H	-5.29683138	-0.13733367	0.67962180
H	-2.37269585	-4.19509100	2.03249639
H	-4.47439134	-2.67533577	1.82145190

H	-1.30355193	-4.89640220	-5.21092149
H	-5.01420743	-2.98473607	-2.06334196
O	3.08578191	-3.70646055	-0.85022543
H	3.37367861	-4.15413502	-1.66496102
H	2.64553414	-2.88089915	-1.19319659
C	-0.09402241	1.00786345	1.25830646
C	-1.18491438	0.00279627	1.09830912
F	-0.81642889	-1.25343011	1.47521101
F	-2.29789905	0.31422078	1.79142086
C	1.19306925	0.66510392	1.19547277
F	-1.57006876	-0.10754072	-0.21546537
H	-0.43599542	2.02999348	1.37406149
H	1.53149336	-0.36163444	1.09087020
H	1.97329620	1.41458231	1.25919846

R-III Surface:

C	1.21515856	-1.41467067	-4.12008114
C	0.97664811	-2.62218996	-4.96383230
F	1.98081919	-2.90287453	-5.83109618
F	0.82395763	-3.74215232	-4.17848810
C	2.33130874	-0.68641703	-4.18535668
F	-0.16501677	-2.52424476	-5.69365820
H	0.40345614	-1.19715506	-3.42861462
H	3.12941529	-0.92750279	-4.88358048
H	2.47869420	0.16843986	-3.52907192
H	-3.29900518	-5.20706655	0.07840252
H	0.51421502	1.33883124	0.19557025

H	4.41666479	3.63024202	0.12834338
H	0.43124747	-3.08087223	0.25088772
H	-3.45897967	3.91355328	0.31071053
H	-3.31470144	-0.80624773	0.35081750
H	4.27294548	-0.81568767	0.34180338
H	0.43678367	5.88770432	0.13576740
O	-3.42522439	3.91139813	-0.67780289
O	0.44279267	-3.11065961	-0.72984145
O	-4.82834535	-2.86117642	-1.32674367
H	-2.41132586	3.60780836	2.31155330
H	-3.76902655	0.03221037	2.30593241
O	-0.89746648	-5.16809342	-1.93749923
H	3.10535370	6.09588037	-2.43283627
H	-0.74668393	-5.02808796	-2.88484766
H	-2.54568206	-5.16785720	-1.30244152
H	1.42107991	1.39013537	-1.09311702
H	3.99014945	4.38351385	-1.15493921
H	-0.02558263	-2.27813042	-1.04105752
H	-3.84247499	4.72828309	-0.98687618
H	-3.86309484	-1.48259545	-0.95041541
H	3.85800837	-1.54253156	-0.97606805
H	-0.00294362	5.09657304	-1.13579263
O	0.45007356	5.93322825	-0.83644978
O	4.49178822	3.59032268	-0.84045894
O	-3.44269440	-5.13767935	-0.88337951
O	-0.76890232	-0.94532222	-1.63162099
H	-0.00711715	2.21261492	2.30679543

O	0.46371619	1.32898575	-0.77909550
O	-0.76429852	-5.09763512	2.98529642
H	-3.82475752	-4.37613725	2.33065388
H	-4.06162123	0.69040450	-1.22617197
H	3.48940278	0.64011019	-1.20935006
H	-0.32732677	-0.10439439	-1.35541776
H	-5.20118434	-2.86280279	-2.22020263
H	2.08972474	-3.01332629	-1.22540240
H	-1.71869873	3.62975847	-1.28840427
H	-0.37315445	-4.45707315	-1.48965016
H	-4.16216779	2.25139507	-1.35451540
H	3.52079018	2.22018767	-1.35285863
H	-4.32409042	-3.71518408	-1.22519228
H	2.97351079	-2.88363621	-2.49072143
H	-0.36902764	2.78107646	-1.30997608
H	-1.70753401	-0.86985304	-1.33105885
H	2.06057606	5.82061927	-1.29521025
H	-3.74856828	2.79980959	2.27389717
O	4.25338947	3.65583375	2.04763837
O	-3.30169253	-0.72994025	-0.62323663
H	-3.77024353	-5.97027525	2.39958637
O	2.96308347	1.42095775	-1.52384263
O	4.30187347	-0.72994025	-0.62323663
O	3.03221847	-2.92904725	-1.52384263
O	-4.64048253	1.42095775	-1.52384263
O	3.03221847	5.77096375	-1.52384263
O	-0.76956453	3.65583375	-1.52384263

H	3.79966947	2.82899675	2.39958637
O	-3.28104153	-5.16392325	2.04763837
H	5.19631147	-0.79343225	2.39958637
O	-0.81804853	-0.72994025	2.94824437
O	-0.81804853	3.57185675	2.94824437
O	-3.35017653	-0.81391725	2.04763837
H	0.03153947	0.61460675	2.39958637
H	1.39452847	-2.94953325	2.39958637
H	-0.77352153	-5.16392325	3.95375937
H	-4.57530453	1.42095775	3.95375937
H	3.02826147	1.42095775	3.95375937
H	2.99962947	5.82740975	3.95375937
H	-0.80215353	-0.75747225	3.95375937
H	-4.60393653	-2.98549325	3.95375937
H	2.99962947	-2.98549325	3.95375937
H	-0.80215353	3.59938875	3.95375937
O	3.06005147	1.42095775	2.94824437
H	-2.40725453	-0.79343225	2.39958637
H	3.79966947	0.01291975	2.39958637
O	2.98373447	-3.01302425	2.94824437
H	-0.00211353	6.59780075	2.39958637
O	0.45160647	-2.92904725	2.04763837
O	0.45160647	5.77096375	2.04763837
O	-4.61983153	-3.01302425	2.94824437
H	-1.69753753	-5.16392325	2.62672537
H	-5.49932053	1.42095775	2.62672537
H	2.10424547	1.42095775	2.62672537

H	3.46163747	5.02718875	2.62672537
H	-0.34014553	-1.55769325	2.62672537
H	-4.14192853	-2.18527225	2.62672537
H	3.46163747	-2.18527225	2.62672537
H	-0.34014553	4.39960975	2.62672537
H	5.19631147	3.63534875	2.39958637
O	2.98373447	5.85494075	2.94824437
O	4.25338947	-0.81391725	2.04763837
O	0.52074147	1.42095775	2.04763837
O	-4.54351453	1.42095775	2.94824437
H	-0.00211353	-3.75588425	2.39958637
O	-3.35017653	3.65583375	2.04763837
H	1.39452847	5.79144975	2.39958637