Supplementary Information

Mechanistic Understanding on Difluoromethane Absorption on Novel Deep Eutectic Solvents by COSMO Simulation

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Table S1: Chemicals studied with abbreviations and identifiers.

A1	N44Br	tetrabutylammonium Bromide
A2	BTACl	benzyltriethylammonium
A3	N8Br	tetraoctylammonium Bromide
A4	N81Br	methyltrioctylammonium bromide
A5	DDDACl	Didodecyldimethylammonium chloride
A6	BTPPB	benzyltriphenylphosphonium bromide
A7	N10,111Cl	decyltrimethylammonium chloride
A8	[OMIM]Cl	1-octyl-3-methylimidazolium chloride
A9	[DMIM]Cl	1-decyl-3-methylimidazolium chloride
A10	P14,666Cl	trihexyl (tetradecyl)phosphonium tetrafluoroborate
A11	[TETA]Cl	triethylenetetramine chloride
A12	ChCl	choline chloride
A13	Lid	Lidocaine
A14	TOPO	trioctylphosphine oxide
A15	Atr	atropine
A16	Cam	camphor
A17	DDTP	diethyldithiophosphoric acid
A18	Car	Carvacrol
A19	PChCl	phosphocholine choline chloride
A20	Lim	limonene
A21	Thy	thymol
A22	Men	Menthol
D1	AceA	acetic
D2	ASA	acetylsalicylic
D3	ButA	butyric
D4	DecA	decanoic
D5	DodA	dodecanoic
D6	ForA	formic
D7	Glu	glutamic
D8	HexA	hexanoic
D9	LacA	lactic
D10	Lev	Levulinic
D11	PalA	palmitic
D12	PheA	phenylacetic
D13	ProA	propionic
D14	PyrA	pyruvic
D15	Ric	ricinoleic acid
D16	SA	stearic
D17	SalA	salicylic
D18	ValA	valeric
D19	Tfa	Trifluoroacetic acid

D20	M4H	Methyl 4-hydroxybenzoate
D21	E4H	ethyl 4-hydroxybenzoate
D22	Bor	borneol
D23	1-But	1-butanol
D24	Cate	catechol
D25	4-Cya	4-cyanophenol
D26	Cyc	cyclohexanol
D27	Dol	1-decanol
D28	3,5-DTBC	3,5-di-tertbutylcatechol
D29	1-Dod	1-dodecanol
D30	Eth	ethylene glycol
D31	Euc	eucalyptol
D32	Gly	glycerol
D33	Hex	hexanol
D34	Ole	oleyl
D35	Pen	PentaneDiol
D36	Peri	perillyl
D37	Phe	phenol
D38	4-ppl	4-phenylphenol
D39	PEG	polyethylene glycol
D40	1-Pro	1-propanol
D41	Res	resorcinol
D42	Sorb	sorbitol
D43	HFIP	hexafluoroisopropanol
D44	Atr	atropine
D45	Cam	camphor
D46	Lim	limonene
D47	Thy	thymol
D48	Men	Menthol
D49	Lid	Lidocaine
D50	Car	Carvacrol
D51	Hyd	hydroquinone
D52	Ibu	ibuprofen
D53	Ket	ketoprofen
D54	Nap	naproxen
D55	PEs	dimethylphthalate
D56	DTBC	Ditertbutylcatechol
D57	DHTU	N,N’-dihenylthiourea
D58	Pne	proline
D59	Ane	arginine

Table S2: Charged surface area distributions per molecule in percent.

	HBD	VdW	HBA
BTACl	5	82	13
N4Br	6	79	15
N8Br	5	82	13
PEG	4	87	9
Camphor	0	87	13
MTOA	0	91	9
Lidocaine	0	95	5
Eucalyptol	0	93	6
[TETA]Cl	95	5	0
TOPO	83	15	3
R32	18	82	0

	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	A16	A17	A18	A19	A20	A21	A22
D39	-1.39	-1.28	-1.11	-1.04	-0.94	-0.89	-0.95	-0.96	-0.93	-0.55	-0.99	-0.70	-0.62	-0.75	-0.38	0.09	0.15	-0.12	-0.12	-0.05	0.26	0.01
D45	-1.34	-1.20	-1.07	-1.01	-0.90	-0.85	-0.90	-0.90	-0.88	-0.50	-0.91	-0.62	-0.52	-0.69	-0.31	-0.44	0.01	0.00	-0.14	0.09	0.32	0.04
D31	-1.27	-1.11	-1.02	-0.94	-0.83	-0.78	-0.81	-0.81	-0.79	-0.42	-0.79	-0.49	-0.38	-0.62	-0.13	-0.06	0.29	0.23	-0.05	0.35	0.66	0.42
D49	-1.27	-1.16	-1.06	-1.00	-0.92	-0.87	-0.93	-0.91	-0.89	-0.58	-0.90	-0.68	-0.58	-0.70	-0.38	0.11	0.00	-0.19	-0.27	-0.14	0.19	-0.06
D58	-1.20	-0.89	-0.92	-0.82	-0.70	-0.63	-0.55	-0.55	-0.56	-0.62	-0.47	-0.51	-0.50	-0.57	-0.23	-0.27	0.81	-0.14	0.29	-0.08	0.34	0.15
D55	-1.14	-1.07	-0.96	-0.90	-0.84	-0.78	-0.84	-0.82	-0.81	-0.56	-0.79	-0.62	-0.51	-0.58	-0.40	-0.04	-0.03	-0.15	-0.17	-0.09	0.01	-0.10
D46	-1.14	-0.99	-0.91	-0.83	-0.73	-0.66	-0.70	-0.68	-0.67	-0.32	-0.61	-0.41	-0.14	-0.44	0.01	-0.31	0.01	0.57	-0.03	0.78	0.54	0.66
D50	-1.09	-0.97	-0.89	-0.81	-0.73	-0.67	-0.71	-0.69	-0.67	-0.36	-0.61	-0.46	-0.19	-0.42	-0.06	-0.52	0.17	0.4	-0.09	0.57	0.40	0.48
D26	-1.04	-0.86	-0.84	-0.76	-0.62	-0.60	-0.55	-0.55	-0.54	-0.36	-0.36	-0.22	-0.17	-0.24	-0.01	0.12	0.28	0.40	0.23	0.59	0.69	0.65
D40	-1.03	-0.85	-0.82	-0.74	-0.60	-0.56	-0.52	-0.51	-0.51	-0.36	-0.33	-0.20	-0.15	-0.20	0.00	-0.57	0.26	0.42	0.36	0.62	0.70	0.69
D23	-1.01	-0.83	-0.81	-0.73	-0.59	-0.56	-0.51	-0.50	-0.50	-0.35	-0.30	-0.18	-0.13	-0.18	0.01	0.13	0.27	0.44	0.30	0.64	0.71	0.70
D44	-0.99	-0.89	-0.84	-0.80	-0.70	-0.72	-0.69	-0.67	-0.66	-0.51	-0.48	-0.51	-0.38	-0.34	-0.29	0.36	0.23	-0.06	-0.22	0.01	0.14	0.04
D10	-0.99	-0.89	-0.81	-0.76	-0.65	-0.65	-0.62	-0.61	-0.60	-0.52	-0.44	-0.44	-0.38	-0.25	-0.31	0.00	0.06	-0.13	0.11	-0.06	0.07	0.04
D36	-0.98	-0.83	-0.80	-0.73	-0.61	-0.60	-0.57	-0.55	-0.54	-0.36	-0.34	-0.31	-0.14	-0.19	-0.05	-0.02	0.20	0.33	0.05	0.48	0.52	0.51
D48	-0.96	-0.80	-0.78	-0.70	-0.58	-0.57	-0.52	-0.51	-0.51	-0.32	-0.27	-0.25	-0.06	-0.16	0.04	0.32	0.25	0.48	0.08	0.66	0.69	0.68
D10	-0.96	-0.82	-0.76	-0.69	-0.57	-0.54	-0.50	-0.49	-0.48	-0.39	-0.29	-0.29	-0.16	-0.10	-0.11	-0.44	0.17	0.24	0.42	0.39	0.46	0.46
D33	-0.96	-0.78	-0.78	-0.70	-0.57	-0.55	-0.49	-0.48	-0.48	-0.32	-0.25	-0.17	-0.07	-0.14	0.05	-0.01	0.32	0.49	0.21	0.68	0.73	0.72
D13	-0.95	-0.80	-0.75	-0.68	-0.55	-0.53	-0.49	-0.48	-0.47	-0.37	-0.26	-0.22	-0.12	-0.07	-0.07	-0.02	0.18	0.29	0.35	0.45	0.48	0.51
D22	-0.94	-0.77	-0.76	-0.68	-0.55	-0.55	-0.50	-0.48	-0.48	-0.31	-0.23	-0.22	-0.03	-0.10	0.05	0.07	0.25	0.49	0.12	0.68	0.67	0.71
D3	-0.93	-0.78	-0.75	-0.67	-0.55	-0.53	-0.49	-0.47	-0.47	-0.36	-0.24	-0.19	-0.09	-0.05	-0.06	-0.12	0.19	0.31	0.29	0.47	0.49	0.52
D18	-0.92	-0.77	-0.74	-0.67	-0.54	-0.53	-0.49	-0.47	-0.47	-0.35	-0.22	-0.19	-0.08	-0.04	-0.04	0.18	0.20	0.33	0.22	0.49	0.51	0.53
D8	-0.90	-0.75	-0.73	-0.65	-0.54	-0.53	-0.48	-0.47	-0.46	-0.34	-0.20	-0.19	-0.05	-0.03	-0.03	0.16	0.22	0.35	0.18	0.51	0.52	0.55
D27	-0.90	-0.74	-0.74	-0.66	-0.54	-0.53	-0.48	-0.47	-0.46	-0.29	-0.18	-0.21	0.00	-0.10	0.10	-0.03	0.39	0.53	0.09	0.71	0.74	0.72
D57	-0.89	-0.75	-0.75	-0.71	-0.61	-0.58	-0.59	-0.55	-0.55	-0.51	-0.50	-0.37	-0.33	-0.26	-0.30	0.52	0.76	-0.10	-0.03	-0.04	0.03	-0.01
D30	-0.88	-0.72	-0.72	-0.65	-0.50	-0.50	-0.39	-0.38	-0.39	-0.39	-0.17	-0.22	-0.15	-0.07	-0.04	0.23	0.34	0.28	0.49	0.44	0.58	0.57
D14	-0.87	-0.77	-0.71	-0.65	-0.55	-0.52	-0.50	-0.48	-0.48	-0.43	-0.25	-0.32	-0.22	-0.08	-0.20	-0.06	-0.13	0.00	0.29	0.10	0.12	0.21
D35	-0.87	-0.70	-0.72	-0.65	-0.51	-0.52	-0.42	-0.41	-0.42	-0.38	-0.19	-0.13	-0.14	-0.08	-0.02	0.24	0.41	0.31	0.33	0.46	0.61	0.55
D29	-0.86	-0.71	-0.71	-0.63	-0.52	-0.52	-0.46	-0.45	-0.44	-0.26	-0.14	-0.21	0.04	-0.06	0.13	0.39	0.42	0.56	0.06	0.74	0.75	0.74
D12	-0.83	-0.70	-0.68	-0.62	-0.52	-0.50	-0.47	-0.44	-0.44	-0.37	-0.23	-0.20	-0.09	-0.02	-0.09	0.25	0.13	0.19	0.22	0.31	0.31	0.37
D4	-0.83	-0.69	-0.68	-0.61	-0.50	-0.51	-0.46	-0.44	-0.43	-0.30	-0.13	-0.22	0.03	0.02	0.04	-0.03	0.29	0.42	0.05	0.57	0.55	0.59
D2	-0.81	-0.70	-0.68	-0.63	-0.54	-0.52	-0.50	-0.47	-0.47	-0.41	-0.27	-0.24	-0.16	-0.08	-0.16	-0.12	0.10	0.07	0.12	0.17	0.20	0.23
D53	-0.81	-0.72	-0.69	-0.65	-0.57	-0.55	-0.55	-0.51	-0.51	-0.43	-0.31	-0.33	-0.19	-0.14	-0.19	0.10	0.07	0.06	-0.04	0.15	0.20	0.17
D52	-0.81	-0.69	-0.66	-0.60	-0.50	-0.51	-0.47	-0.44	-0.44	-0.32	-0.16	-0.26	0.00	0.03	-0.01	0.38	0.18	0.30	0.01	0.44	0.39	0.47
D34	-0.80	-0.68	-0.68	-0.61	-0.51	-0.52	-0.48	-0.45	-0.45	-0.25	-0.12	-0.28	0.06	-0.04	0.12	0.09	0.39	0.51	-0.05	0.66	0.65	0.65
D5	-0.80	-0.67	-0.66	-0.59	-0.48	-0.50	-0.45	-0.42	-0.42	-0.28	-0.09	-0.23	0.06	0.04	0.06	0.15	0.31	0.44	0.01	0.59	0.56	0.60
D54	-0.79	-0.68	-0.66	-0.61	-0.52	-0.53	-0.50	-0.47	-0.46	-0.38	-0.25	-0.29	-0.11	-0.05	-0.13	-0.14	0.03	0.12	0.00	0.22	0.21	0.26
D19	-0.78	-0.64	-0.61	-0.54	-0.43	-0.43	-0.37	-0.34	-0.34	-0.25	0.02	-0.01	0.20	0.24	0.09	0.00	-0.20	0.27	0.37	0.37	0.27	0.68
D59	-0.78	-0.50	-0.68	-0.58	-0.45	-0.40	-0.27	-0.24	-0.27	-0.44	-0.11	0.01	-0.10	-0.18	-0.10	-0.39	0.11	0.26	0.51	0.38	0.63	0.54
D21	-0.77	-0.63	-0.64	-0.57	-0.48	-0.46	-0.43	-0.39	-0.39	-0.34	-0.15	-0.14	-0.02	0.03	-0.03	0.05	0.25	0.30	0.19	0.43	0.43	0.46
D15	-0.76	-0.65	-0.65	-0.61	-0.50	-0.56	-0.47	-0.46	-0.45	-0.36	-0.17	-0.34	-0.11	-0.04	-0.08	-0.23	0.31	0.22	-0.14	0.32	0.38	0.33
D20	-0.76	-0.62	-0.63	-0.57	-0.47	-0.45	-0.42	-0.38	-0.38	-0.34	-0.15	-0.11	-0.03	0.03	-0.04	0.32	0.23	0.27	0.25	0.40	0.40	0.44
D37	-0.75	-0.60	-0.61	-0.54	-0.42	-0.40	-0.35	-0.31	-0.31	-0.27	-0.07	-0.02	0.13	0.15	0.08	-0.01	0.03	0.36	0.44	0.49	0.40	0.65
D11	-0.74	-0.63	-0.62	-0.56	-0.46	-0.48	-0.43	-0.40	-0.40	-0.25	-0.04	-0.24	0.11	0.07	0.10	-0.38	0.35	0.47	-0.04	0.62	0.57	0.62
D6	-0.74	-0.56	-0.61	-0.53	-0.40	-0.36	-0.28	-0.25	-0.27	-0.32	-0.02	-0.03	0.02	0.12	0.00	0.19	0.11	0.33	0.78	0.49	0.49	0.60
D47	-0.73	-0.59	-0.60	-0.52	-0.41	-0.41	-0.36	-0.32	-0.32	-0.24	-0.01	-0.11	0.19	0.18	0.14	0.09	0.30	0.40	0.17	0.54	0.41	0.69
D17	-0.73	-0.59	-0.59	-0.52	-0.42	-0.40	-0.37	-0.32	-0.33	-0.28	-0.06	-0.07	0.10	0.16	0.03	0.28	0.02	0.33	0.27	0.47	0.38	0.57
D9	-0.73	-0.57	-0.60	-0.54	-0.40	-0.41	-0.31	-0.29	-0.30	-0.35	-0.08	-0.06	-0.05	0.09	-0.05	0.03	0.18	0.25	0.50	0.40	0.43	0.49
D32	-0.72	-0.55	-0.61	-0.54	-0.39	-0.44	-0.28	-0.26	-0.28	-0.38	-0.05	-0.06	-0.10	0.05	-0.05	-0.25	0.29	0.22	0.50	0.36	0.49	0.50
D16	-0.72	-0.61	-0.60	-0.54	-0.44	-0.47	-0.41	-0.39	-0.38	-0.23	-0.01	-0.24	0.14	0.09	0.13	-0.01	0.37	0.49	-0.05	0.63	0.59	0.63
D38	-0.72	-0.57	-0.60	-0.54	-0.43	-0.42	-0.38	-0.34	-0.34	-0.33	-0.08	-0.14	0.02	0.11	-0.01	0.24	0.01	0.26	0.13	0.38	0.29	0.44
D43	-0.69	-0.53	-0.55	-0.48	-0.33	-0.42	-0.27	-0.24	-0.24	-0.25	0.11	-0.01	0.19	0.37	0.09	-0.06	0.07	0.24	0.27	0.37	0.24	0.67
D25	-0.67	-0.51	-0.58	-0.51	-0.41	-0.35	-0.32	-0.26	-0.28	-0.34	-0.10	0.03	0.03	0.08	0.00	0.36	0.32	0.29	0.47	0.41	0.42	0.48
D42	-0.61	-0.47	-0.51	-0.47	-0.33	-0.43	-0.26	-0.25	-0.26	-0.38	-0.07	-0.04	-0.12	0.09	-0.12	0.42	0.10	0.10	0.28	0.21	0.28	0.32
D28	-0.52	-0.37	-0.42	-0.36	-0.23	-0.29	-0.17	-0.13	-0.14	-0.19	0.19	0.06	0.28	0.43	0.17	0.18	0.01	0.38	0.27	0.50	0.40	0.68
D24	-0.51	-0.34	-0.42	-0.35	-0.22	-0.25	-0.13	-0.08	-0.10	-0.21	0.19	0.20	0.27	0.43	0.15	0.01	0.06	0.34	0.55	0.46	0.38	0.67
D7	-0.47	-0.17	-0.53	-0.44	-0.32	-0.18	-0.04	0.00	-0.07	-0.38	0.10	0.56	-0.01	-0.08	0.08	0.08	0.78	0.33	0.90	0.44	0.66	0.57
D56	-0.43	-0.34	-0.39	-0.32	-0.20	-0.27	-0.15	-0.10	-0.11	-0.13	0.29	0.01	0.39	0.49	0.26	-0.45	0.05	0.41	0.15	0.53	0.39	0.74
D51	-0.41	-0.24	-0.35	-0.28	-0.15	-0.19	-0.05	0.00	-0.02	-0.21	0.25	0.32	0.28	0.46	0.17	0.00	0.14	0.38	0.70	0.50	0.46	0.68
D41	-0.38	-0.21	-0.32	-0.26	-0.13	-0.16	-0.03	0.03	0.00	-0.19	0.29	0.36	0.32	0.51	0.19	-0.03	0.11	0.37	0.71	0.48	0.43	0.68

Figure S1: Activity coefficients for each HBA and HBD combination computed for R32. This figure depicts a heat map containing a gradient from yellow to red. This map represents the activity coefficient (lnγ) values of difluoromethane in DES component mixtures. Yellow represents the lower values of lnγ while red is for higher values of lnγ. The component mixtures are referenced as Axx for HBA and Dxx for HBD along the x and y axes, respectively. The reference key for these numbers-solvents can be found in table S1.